

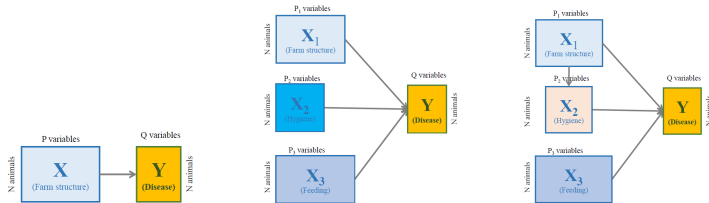
1. Introduction
2. Supervised two-block analyses
3. Supervised (K+1)-block analyses
4. Supervised (K+K')-block analyses
5. Conclusion & perspectives

# Supervised multiblock analyses

## Cases of two-blocks, (K+1)-blocks, (K+K')-blocks

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Journée Analyses Factorielles  
 March 30 2023, INRAe Jouy-en-Josas

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2. Supervised two-block analyses
3. Supervised (K+1)-block analyses
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# Outline

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- 2 Supervised two-block analyses
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## From factorial analyses to **multiblock** factorial analyses



PCA / MCA  
Active &  
supplementary  
variables

### Data features

#### 1 Blocks of variables

- Of known structure,
- Links between blocks are known.

#### 2 Block features

- Large dimension (nb var. > nb obs.),
- Quantitative and quasi-collinear variables,
- No distributional assumptions.

→ Ill-conditioned (multidimensional) blocks.

#### 3 Observations (same for all the variables)

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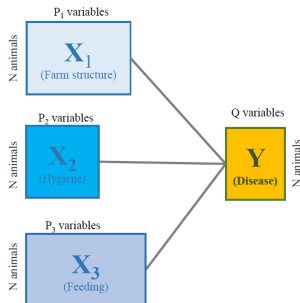
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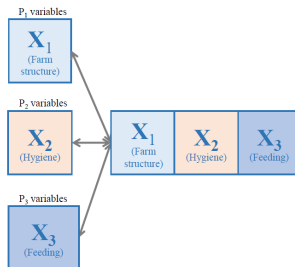
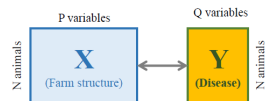
## From unsupervised to supervised analyses

### Unsupervised or supervised (two-block case)

- Unsup.: Study the relationships between  $\mathbf{X}$  and  $\mathbf{Y}$  or between  $(\mathbf{X}_1, \dots, \mathbf{X}_K)$
- Supervised: Explain  $\mathbf{Y}$  with  $\mathbf{X}$

### Supervised cases

- Two-block case:  $\mathbf{X} \rightarrow \mathbf{Y}$
- K+1 case:  $(\mathbf{X}_1, \dots, \mathbf{X}_K) \rightarrow \mathbf{Y}$
- K+K' case: e.g.,  $\mathbf{X}_1 \rightarrow \mathbf{X}_2$  and  $(\mathbf{X}_1, \dots, \mathbf{X}_K) \rightarrow \mathbf{Y}$



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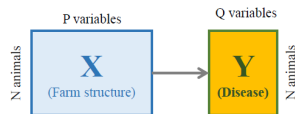
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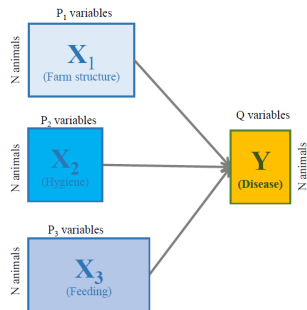
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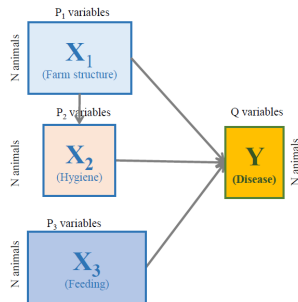
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## 1 Introduction

## 2 Supervised two-block analyses

- Methods
- Application
- Doing my own supervised two-block analyses

## 3 Supervised (K+1)-block analyses

## 4 Supervised (K+K')-block analyses

## 5 Conclusion & perspectives

## Relate two-block data sets with a criterion

### Aim

Explore/Explain **Y** with **X**

### How blocks are linked?

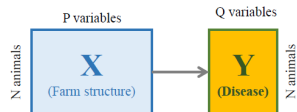
- Raw data sets ...
- Are summarized with components ...
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### Two-block case criterion (first-order solution)

Maximize  $\text{cov}^2(\mathbf{t}, \mathbf{u})$

with  $\mathbf{t} = \mathbf{X}\mathbf{w}$  and  $\mathbf{u} = \mathbf{Y}\mathbf{v}$

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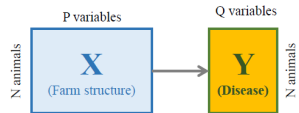
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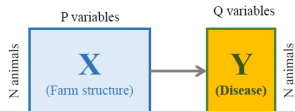
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## How to be a supervised two-block method? Constraints and deflation

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### Constraints and deflation

Method	Constraints	$\mathbf{w}$ eigenvector of	Deflation
Canonical an. [Hotelling, 36]	$\ \mathbf{t}\  = \ \mathbf{u}\  = 1$	$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}(\mathbf{Y}'\mathbf{Y})^{-1}\mathbf{Y}'\mathbf{X}$	No deflation (DVS)
Redundancy an. [Rao, 64]	$\ \mathbf{t}\  = \ \mathbf{v}\  = 1$	$(\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X})$	No deflation (DVS) Or deflation on $\mathbf{t}$
PLS regression* [Wold, 66]	$\ \mathbf{w}\  = \ \mathbf{v}\  = 1$	$\mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X}$	Deflation on $\mathbf{t}$

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- RA: supervised constraint-based method
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## Supervised two-block analyses: advices for application

### Choice according to your aim (and knowledge)

- My first two-block analysis: PCA( $\mathbf{X}$ ) with  $\mathbf{Y}$  as supplementary variables
- Unsupervised: Canonical analysis, co-inertia analysis, concordance analysis
- Supervised: RA or PLS
  - Explain: RA better explains the inertia of  $\mathbf{Y}$ ,
  - Predict: PLS leads to more stable results thus best predictions.

### Choice according to the data features

- Limited within-correlation in  $\mathbf{X} \rightarrow$  RA
- High within-correlation in  $\mathbf{X} \rightarrow$  PLS

### Not able to choose

- Trade-off with regularization on the norm-constraint:  $\gamma\|\mathbf{w}\|^2 + (1 - \gamma)\|\mathbf{t}\|^2 = 1$
- Solution: DVS of  $[\gamma\mathbf{I} + (1 - \gamma)(\mathbf{X}'\mathbf{X})]^{-1}(\mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X})$
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## (Some) extensions for supervised two-block analyses

### Extensions according to data features

- **Y** is a single nominal variable: discriminant PLS (PLS-DA) [Barker, 2003]
- **X** contains a very large number of variables: sparse PLS (sPLS) [Lê Cao, 2008]

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- Known group-structure of observations: multigroup PLS [Eslami, 2014]
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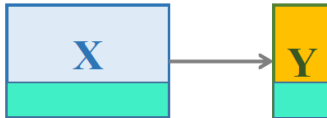
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## Extensions for supervised two-block analyses: multigroup PLS

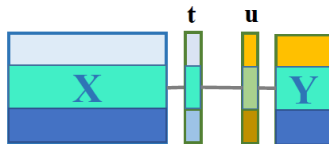
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Explore the links between **X** and **Y** while taking into account their multigroup structure, i.e.:

- Observations with a structure in known groups (which they should be freed).

### Sub-aims

- 1 Summarize each block of variables by components adjusted to the data features (i.e., ill-conditioned multidimensional blocks),
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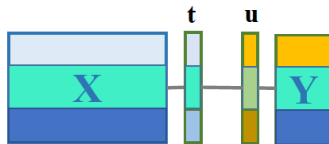
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### Criterion to maximize (first-order solution)

$$\sum_{m=1}^M N_m \text{cov}(\mathbf{t}_m, \mathbf{u}_m)$$

s.t.  $\mathbf{t}_m = \mathbf{X}_m \mathbf{a}$ ,  $\mathbf{u}_m = \mathbf{Y}_m \mathbf{b}$ ,  $\|\mathbf{a}\| = \|\mathbf{b}\| = 1$

### Main features

- Solved by a monotonous convergent algorithm,
- Robust to within-block multicollinearity,
- Group-components specific to each group,
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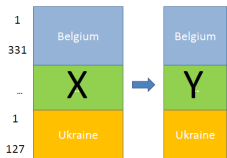
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# Mg-PLS: 'European School Survey Project on Alcohol and other Drugs' data



## X dataset: use and context

### P=9 questions

Cannabis consumption in the last year or month (c25b, c25c), age they first take cannabis (c26), number of smoked cigarettes in the last month (c09), number of times they were drunk in their life or in the last year (c19a, c19b), facility to get cannabis (c24), number of friends who take cannabis (c34d) and perceived risk of taking cannabis (c36h)

## Individuals

N=5204 teenagers from M=13 countries

Belgium (331), Cyprus (177), Czech Republic (1013), France (723), Germany (365), Italy (617), Kosovo (55), Latvia (292), Lichtenstein (52), Poland (1113), Romania (93), Slovak Republic (246) and Ukraine (127).

## Y dataset: drug consumption (CAST)

### Q=6 questions

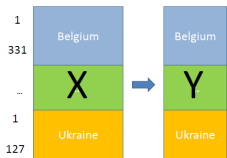
Non-recreational use (rcast1, rcast2), memory disorder (rcast3), reproaches from family or friends (rcast4), unsuccessful quit attempts (rcast5) and problems associated with cannabis consumption (rcast6)

## Aims

- Investigate the relationships between the cannabis consumption variables (Y),
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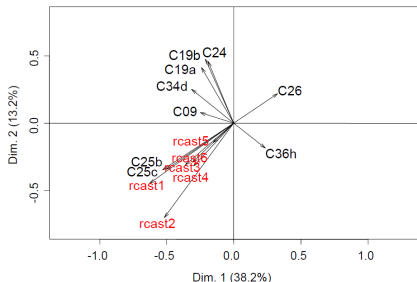
## Aims

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# Mg-PLS: Common relationships between consumption, use and context

## Pre-processing

- Variables are centred and scaled globally → Variables have the same weights,
- Variables are centred and scaled by group → Groups have the same weights,
- Group effect=11% of inertia (discarded) → Focus on the within-group analysis.



**Y:** Non-recreational use (rcast1, rcast2), memory disorder (rcast3), reproaches from family or friends (rcast4), unsuccessful quit attempts (rcast5) and problems associated with cannabis consumption (rcast6) - **X:** Cannabis consumption in the last year or month (c25b, c25c), age they first take cannabis (c26), number of smoked cigarettes in the last month (c09), number of times they were drunk in their life or in the last year (c19a, c19b), facility to get cannabis (c24), number of friends who take cannabis (c34d) and perceived risk of taking cannabis (c36h)

## Interpretation

- All the CAST variables (**Y**) are linked and explained with the cannabis consumption in the last year or month (c25b, c25c) and the age they first take cannabis (c26)
- The non-recreational use (rcast1, rcast2) are the variables which are more linked to c25b, c25c and c26.

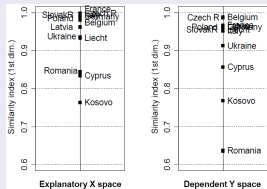


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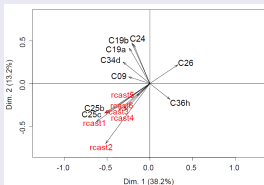
## Mg-PLS: Group specificities in comparison with the common structure

### Similarities between groups



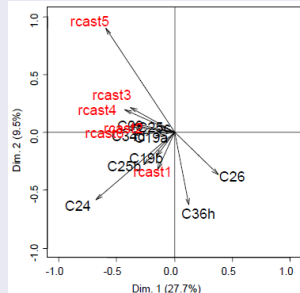
Most of the countries are similar to the common structure, except Kosovo, Cyprus and Romania.

### Common loadings



**Y:** Non-recreational use (rcast1, rcast2), memory disorder (rcast3), reproaches from family or friends (rcast4), unsuccessful quit attempts (rcast5) and problems associated with cannabis consumption (rcast6) - **X:** Cannabis consumption in the last year or month (c25b, c25c), age they first take cannabis (c26), number of smoked cigarettes in the last month (c09), number of times they were drunk in their life or in the last year (c19a, c19b), facility to get cannabis (c24), number of friends who take cannabis (c34d) and perceived risk of taking cannabis (c36h)

### Group loadings: Kosovo



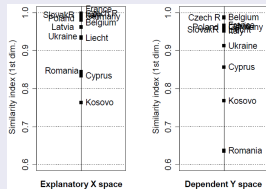
The relationships between the variables from Kosovo are really different than those from the common structure.

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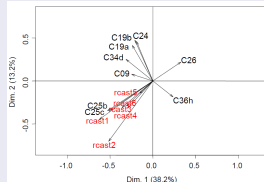
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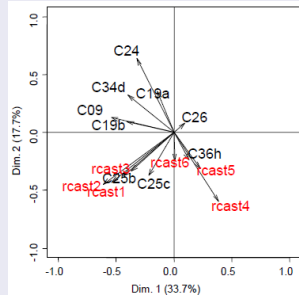
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### Group loadings: Romania



The variables rcast1, rcast2 and rcast3 are linked and explained with different explanatory variables than rcast4 and rcast5.

## Supervised two-block analyses with R

### Standard supervised two-block analyses

- RA: `pcaiv` function in the `ade4` package, `rda` function in the `vegan` package
- PLS regression: e.g., `pls` function in the `pls` package, `pls` function in the `MixOmics` package
- Regularized-RA: `cw.multiblock` function with 'mbregular' option, a single-block **X** and a single-cluster ('G=1') in the `mbclusterwise` package
- Regularized-CCA: `rcca` function in the `MixOmics` package

### Extensions of supervised two-block analyses

- Discriminant PLS: e.g., `plsda` function in the `mdatools` or `MixOmics` package
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- 1 Introduction
- 2 Supervised two-block analyses
- 3 Supervised (K+1)-block analyses**
  - Methods
  - Applications
  - Doing my own supervised (K+1)-block analyses
- 4 Supervised (K+K')-block analyses
- 5 Conclusion & perspectives



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### 3.1. Methods

#### 3.2. Applications

#### 3.3. Doing my own supervised (K+1)-block analyses

## Relate (K+1) blocks with a criterion

### Aim

Explore/Explain  $\mathbf{Y}$  with  $(\mathbf{X}_1, \dots, \mathbf{X}_K)$

### How blocks are linked?

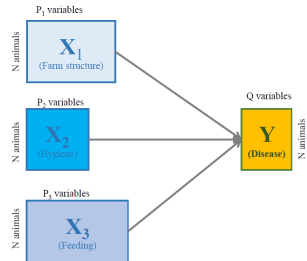
- Raw data sets ...
- Are summarized with block-components ...
- Which are linked by a criterion\*

### (K+1)-block case criterion (first-order solution)

Maximize  $\sum_{k=1}^K \text{cov}^2(\mathbf{t}_k, \mathbf{u})$

with  $\mathbf{t}_k = \mathbf{X}_k \mathbf{w}$  and  $\mathbf{u} = \mathbf{Y} \mathbf{v}$

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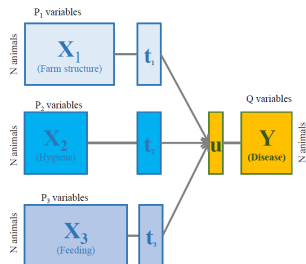
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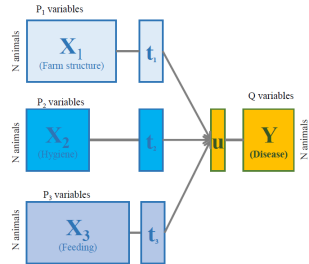
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## Pre-processing: an important step

### Variable-centering

- Centering = All the variable-means are equal to 0
- Variables are supposed to be centered (without loss of generality)

### Variable-reduction

- Reduction = All the variable-standard deviations are equal to 1  
→ All the variable have the same importance in the analysis
- No reduction → The variables with the largest variances are the most important

### Block-scaling (variables are supposed to be standardized)

- Scaling /  $\lambda_k^{(1)}$  = Variable-sd are equal to  $1/\lambda_k^{(1)}$  → Block-inertia are equal to  $P_k/\lambda_k^{(1)}$   
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### (K+1)-prediction model

- Aim: Explain  $\mathbf{Y}$  with  $\mathbf{X} = [\mathbf{X}_1 | \dots | \mathbf{X}_K]$  (regression coefficients)
- Method:
  - Build a global-component  $\mathbf{t} = \mathbf{X}\mathbf{w}$
  - Deflation on  $\mathbf{t}$  (orthogonal)
  - NB:  $\mathbf{t}$  is also a summary of the block-components:  $\mathbf{t} = \sum_k \mathbf{a}_k \mathbf{t}_k$
- Solution:  $\mathbf{Y} = \sum_h \mathbf{t}^{(h)} (\mathbf{c}^{(h)})' = \mathbf{X} \left[ \sum_h (\mathbf{w}^{(h)})' * (\mathbf{c}^{(h)})' \right]$

### Limits of the (K+1)-prediction model

- Deflation of  $(\mathbf{X}_1, \dots, \mathbf{X}_K)$  on  $\mathbf{t}$  'mix' the block-information
- Consideration of the same number of dimensions for all blocks
- The criterion maximize symmetrical links  $(\sum_k \text{cov}^2(\mathbf{t}_k, \mathbf{u}))$  whereas the prediction model is based on asymmetrical ones  $(\mathbf{u} = f(\mathbf{t}_1, \dots, \mathbf{t}_K))$

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## Supervised (K+1)-block analyses: interpretation tools

### Optimal dimension

- Select the optimal number of dimension  $H$  to be taken into account
- E.g., minimization of the cross-validated prediction error

### Block-importance [Vivien, 2005; Bougeard, 2011]

- Obtained from the  $\mathbf{a}_k$  coefficients which reflect the links between the block-components  $\mathbf{t}_k$  and  $\mathbf{u}$
- Can be computed for each and several dimensions

### Variable-importance [Wold, 1994; Gosselin, 2010; Bougeard, 2011]

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## Extensions for supervised (K+1)-block analyses: clusterwise (r-)multiblock RA

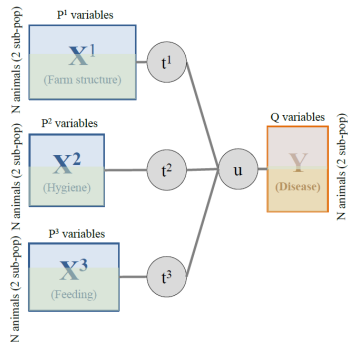
### Main aim

Explore the links between the blocks while taking into account their complex structure, i.e.:

- Known block-structure and block-links,
- **Unknown sub-populations of observations.**

### Sub-aims

- 1 Summarize each block of variables by components adjusted to the data features (i.e., ill-conditioned multidimensional blocks),
- 2 Get the partition of the observations into clusters,
- 3 Get (multiblock) regression models for each cluster.



## Extensions for supervised (K+1)-block analyses: clusterwise (r-)multiblock RA

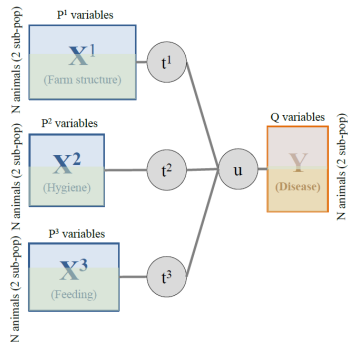
### Main aim

Explore the links between the blocks while taking into account their complex structure, i.e.:

- Known block-structure and block-links,
- **Unknown sub-populations of observations.**

### Sub-aims

- 1 Summarize each block of variables by components adjusted to the data features (i.e., ill-conditioned multidimensional blocks),
- 2 Get the **partition** of the observations into clusters,
- 3 Get **(multiblock) regression** models for each cluster.





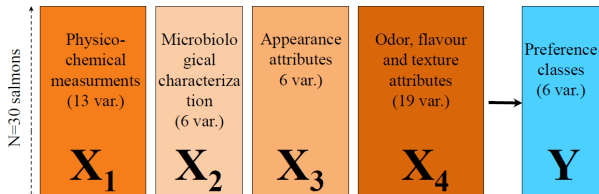
## Extensions for supervised (K+1)-block analyses: clusterwise (r-)multiblock RA

[Bougeard, 2017, 2018]

### Algorithm

- 1 Start from an initialization of the  $N$  observations into  $G$  clusters
- 2 For each observation  $n$ 
  - Compute R-MBRA where  $n$  belongs alternatively to each of the  $G$  clusters
  - For each of the  $G$  solutions, compute the criterion  $C = \sum_g \|\mathbf{Y}_g - \sum_h \mathbf{t}_g^{(h)} (\mathbf{c}_g^{(h)})'\|^2$
  - Update the assignment of  $n$  to the cluster which minimize  $C$
  - Update the regression coefficients
- 3 Repeat the procedure for several initializations and select the best one.

## Standard mbRA: Eurosalmon data [Cardinal et al., 2004]



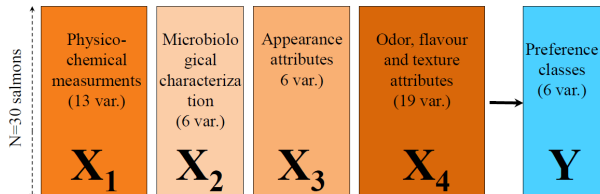
### Salmon data features

- **Y**: 6 preference classes from 1063 consumers [Semenou et al., 2007],
- **X**: 44 potential preference drivers organized into 4 blocks,

### Aims

- **Descriptive**: explain the consumer preferences with the explanatory variables and blocks in relation with the tasted salmon,
- **Predictive**: assess the key drivers of preference at the variable and block levels.

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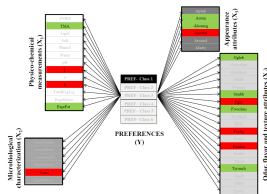
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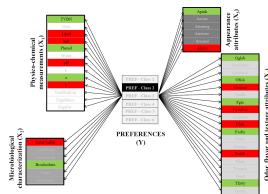
- 3.1. Methods
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## Key drivers of preference at the variable level (2)

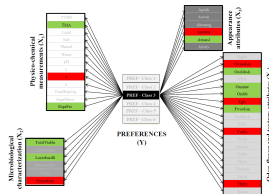
Regression coefficients and bootstrapped tolerance interval. Optimal model with 4 components.



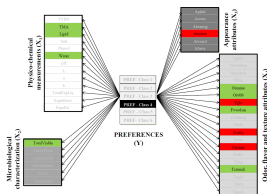
Pref 1 (N=121)



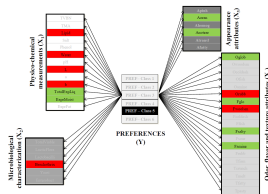
Pref 2 (N=74)



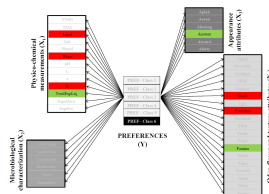
Pref 3 (N=349)



Pref 4 (N=78)



Pref 5 (N=404)

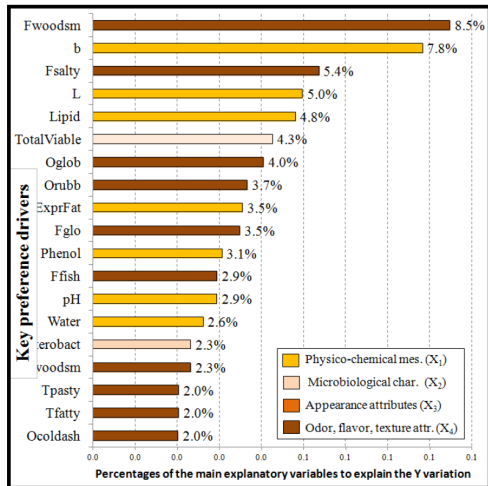


Pref 6 (N=37)

Results are difficult to sum up → Difficulties to get overall interpretation of key drivers.

## Standard mbRA: Key drivers of preference at the variable-level

Variable Importance expressed as percentage and bootstrapped tolerance interval. Optimal model with 4 components.



### Interpretation for overall preference

The model explains 82% of the variation in **Y** which is significantly explained by:

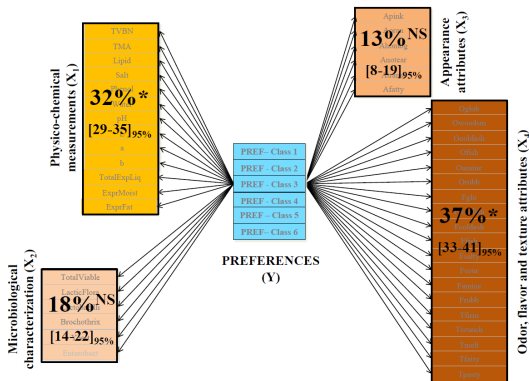
- The wood smoked flavor ("++" for classes 1, 3 and 4, "-" for classes 2, 5 and 6),
  - The hue parameter  $b^*$  (yellow) ("-" for classes 1, 2, 5 and 6),
- Both these variables explain 14.3% of the overall preference.

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## Standard mbRA: Key drivers of preference at the block-level

Block Importance expressed as percentage and bootstrapped tolerance interval. Optimal model with 4 components.



### Interpretation for overall preference

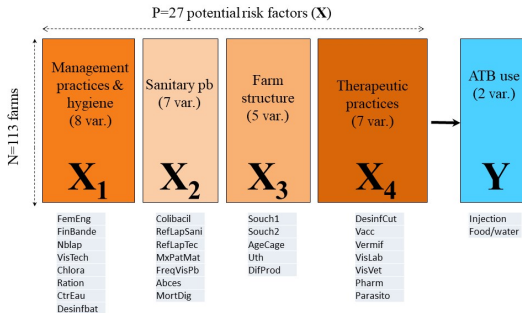
The model explains 82% of the variation in **Y**, which is significantly explained by:

- The odor, flavor and texture attributes (37%),
- The physico-chemical measurements (32%),

## Clusterwise mbRA: 'antibiotic consumption in rabbit farms' data

### Data & aim

- Data: Retrospective survey conducted in 2010 in 113 French rabbit farms
- Aim: Identify risk markers for antibiotic use in rabbit farming

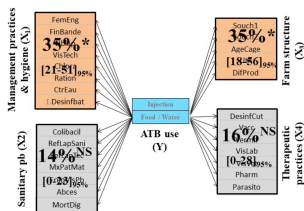


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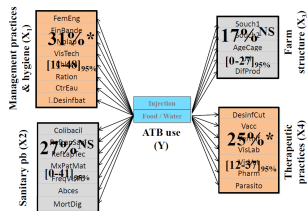
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## Clusterwise mbRA: Risk markers for each cluster [blocks]

Cluster 1  
 $N_1=52$  farms;  $R^2=0.56$



Cluster 2  
 $N_2=61$  farms;  $R^2=0.65$



### Interpretation

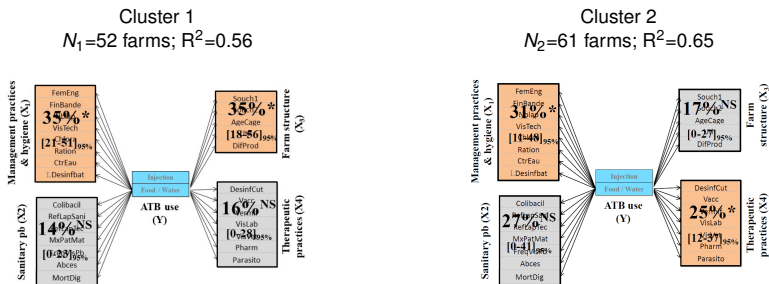
- Cluster 1: importance of management and hygiene practices ( $X_1$ ) and of the farm structure ( $X_3$ )
- Cluster 2: importance of management and hygiene practices ( $X_1$ ) and of therapeutic practices ( $X_4$ )
- NB: For all observations:  $R^2=0.25$ ; importance of  $X_2$  (32%) and  $X_4$  (25%).



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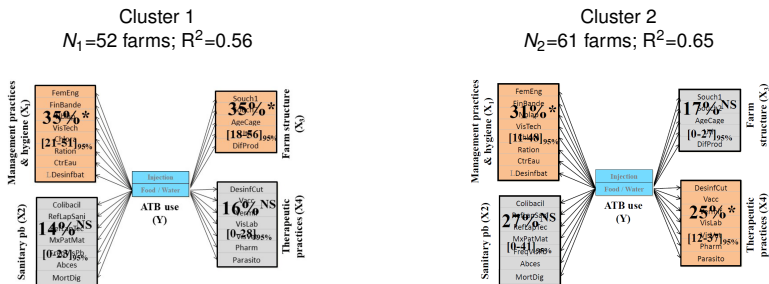
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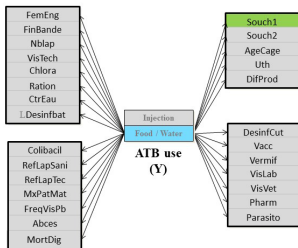


### Interpretation

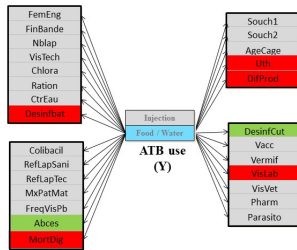
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## Clusterwise mbRA: Risk markers for each cluster [variables]

Cluster 1 ( $|\text{Reg.coef.}|>0.5$ )  
 $N_1=52$  farms;  $R^2=0.56$



Cluster 2 ( $|\text{Reg.coef.}|>0.5$ )  
 $N_2=61$  farms;  $R^2=0.65$



Grey : Not significant / Green : significant (positive link) & coef.  $>0.5$  / Red : significant (negative link) & coef.  $<-0.5$

### Interpretation

- Cluster 1: importance of the rabbit strain,
- Cluster 2: importance of disinfection of the building, abscesses, digestive pb, . . .
- NB: For all observations:  $R^2=0.25$ ; importance of the digestive pb.

## Supervised (K+1)-block analyses with R

### Standard supervised (K+1)-block analyses

- **mbRA**: `mbpcaiv` function in the `ade4` package (thus `mbrda` in in the `multiblock` package),
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### Extensions of supervised (K+1)-block analyses

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- 4 Supervised (K+K')-block analyses**
  - Methods
  - Application
  - Doing my own supervised (K+K')-block analyses
- 5 Conclusion & perspectives

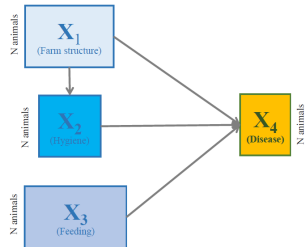
## Relate (K+K')-blocks with a criterion

### Aim

- Explore the relationships between blocks
- Blocks connected by the user (*a priori* information)

### How blocks are linked?

- Raw data sets ...
- Are summarized with block-components ...
- Which are linked by a criterion\*



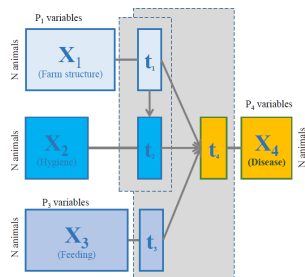
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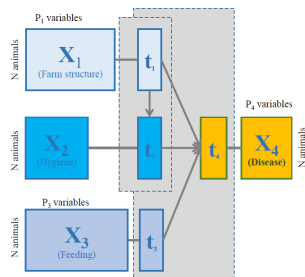
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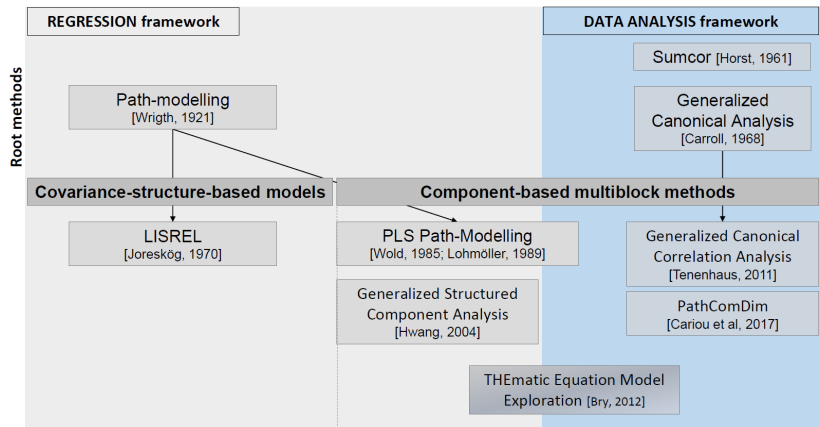
- Raw data sets ...
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\* Methods which are not based on a criterion are not given here.



## Supervised (K+K')-block analyses: methods

(K+K')-block analyses come from two different frameworks.



In the following, only component-based multiblock methods (with criterion) will be studied.

## (Three) supervised (K+K')-block analyses: criteria (in a nutshell)

### Regularized Generalized Canonical Correlation Analysis (rGCCA) [Tenenhaus, 2011]

$$\max \sum_{k,l=1,k \neq l}^K d_{kl} \text{cov}^2(\mathbf{X}_k \mathbf{w}_k, \mathbf{X}_l \mathbf{w}_l) \quad \text{s.t.} \quad \tau_k \|\mathbf{w}_k\|^2 + (1 - \tau_k) \text{var}(\mathbf{X}_k \mathbf{w}_k) = 1$$

- Symmetrical links
- Several components per block (block-dim. are supposed to be identical)

### Regularized Generalized Structured Component Analysis (rGSCA) [Hwang, 2004]

$$\min \|\mathbf{XW}_M - \mathbf{XWB}\|^2 + \|\mathbf{XI}_R - \mathbf{XWC}\|^2 + \lambda_1 \|\mathbf{B}\|^2 + \lambda_2 \|\mathbf{W}\|^2 + \lambda_3 \|\mathbf{C}\|^2 \quad \text{s.t.} \quad \text{diag}(\mathbf{W}^T \mathbf{X}^T \mathbf{XW}) = \mathbf{I}, \quad \lambda_1 \geq 0, \quad \lambda_2 \geq 0, \quad \lambda_3 \geq 0$$

- Asymmetrical links (regression)
- Blocks are supposed to be unidimensional

### (Simplified) THEmatic Equation Model Exploration (THEME) [Bry, 2015]

$$\max \prod_{m=1}^M \left( 1 - \frac{\|\mathbf{x}_{w_m} - \mathbf{x}_{w_b_m}\|^2}{\|\mathbf{x}_{w_m}\|^2} \right) \prod_{k=1}^K \left( \sum_{p_k=1}^{P_k} \text{cor}^2(\mathbf{X}_k \mathbf{w}_k, \mathbf{x}_{p_k}) \right) \quad \text{s.t.} \quad \|\mathbf{X}_k \mathbf{w}_k\|^2 = 1$$

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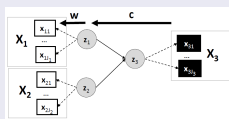
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## Supervised (K+K')-block analyses: prediction model

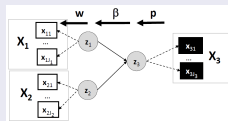
Work in progress with M. Hanafi - Application to PLS Path Modelling

Two proposed estimation of the regression coefficients  $\mathbf{B}$  such as  $\mathbf{X} = \mathbf{X}\mathbf{B} + \mathbf{R}$

$$\hat{\mathbf{B}}_{lk} = \begin{cases} \mathbf{w}_l \mathbf{c}_{lk}^T & \text{for the PLSR-like estimation} \\ \beta_{lk} \mathbf{w}_l \mathbf{p}_k^T & \text{for the PLSPM-like estimation (=PLSpredict) [Shmueli, 2016]} \end{cases}$$



(a) PLSR-like estimation.



(b) PLSPM-like estimation.

Property: These estimations are reformulations of the structural model.

### Deflation

- Explanatory blocks are deflated with respect to their measurement model ( $\mathbf{w}_k \mathbf{p}_k^T$ )
- Intermediate and blocks to be explained are deflated with respect to the prediction model ( $\mathbf{B}$ )

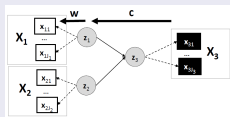
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## Supervised (K+K')-block analyses: prediction model

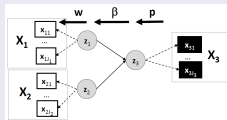
Work in progress with M. Hanafi - Application to PLS Path Modelling

Two proposed estimation of the regression coefficients  $\mathbf{B}$  such as  $\mathbf{X} = \mathbf{X}\mathbf{B} + \mathbf{R}$

$$\hat{\mathbf{B}}_{lk} = \begin{cases} \mathbf{w}_l \mathbf{c}_{lk}^T & \text{for the PLSR-like estimation} \\ \beta_{lk} \mathbf{w}_l \mathbf{p}_k^T & \text{for the PLSPM-like estimation (=PLSpredict) [Shmueli, 2016]} \end{cases}$$



(c) PLSR-like estimation.



(d) PLSPM-like estimation.

Property: These estimations are reformulations of the structural model.

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## Supervised $(K+K')$ -block analyses: Advices for application

### Explain or predict?

- First explain (rGCCA, Path-Comdim)
- If the explanation is good enough, model and predict (rGSCA, THEME)

### Uni or multidimensional blocks?

- In practice, multidimensional blocks

### Within-block multicollinearity?

- Data analysis framework: regularization of the block-norm constraints
- Regression framework: elastic-net (=lasso + ridge) regularization
- Both: Data summary with component(s)

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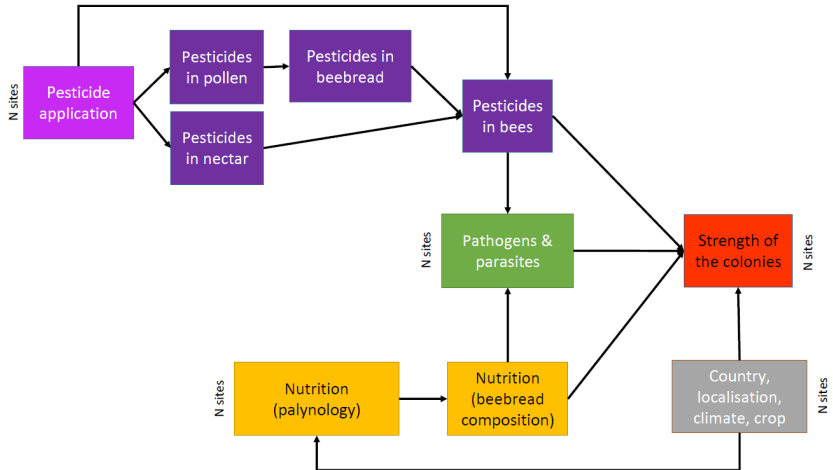
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4.1. Methods

4.2. Application

4.3. Doing my own supervised (K+K')-block analyses

## Explain the bee-mortality (In progress)



## Supervised (K+K')-block analyses with R

### Standard supervised (K+K')-block analyses

- PLS-PM: `SEMinR` package
- GSCA: `gsca` package or <https://www.gscapro.com/>
- GCCA: `rgcca` function in the `RGCCA` package or <https://github.com/rgcca-factory/RGCCA>
- THEME: `SCGLR` package
- PathComDim: `MBAanalysis` package (In progress)

### Extension of supervised (K+K')-block analyses

- Sparse: `sgcca` function in the `RGCCA` package
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# Outline

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- 2 Supervised two-block analyses
- 3 Supervised  $(K+1)$ -block analyses
- 4 Supervised  $(K+K')$ -block analyses
- 5 Conclusion & perspectives**

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## Conclusion related to multiblock **methods**

### From data ...

- Data that answer complex questions come from different sources → **Multiblock**
- Numerous blocks with complex links →  **$(K+K')$ -block methods**
- Blocks are multidimensional → Component-based methods with **several dimensions**
- Users usually seek to explain block(s) → **Supervised with models**

### ... To methods

- Multiblock methods are increasingly applied
- Development of multiblock methods from 2-block to  $(K+1)$ -blocks and  $(K+K')$ -blocks
- But many points remain to be clarified / developed (new methods)

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## Perspectives related to multiblock **methods**

### (Some) extensions related to the data features

- Structure of observations in known (covariables / multigroup) or unknown groups (clusterwise)
- Temporal structure of blocks
- Large number of variables (e.g., regularization, sparse)
- Mixed data (numeric, nominal ordinal)

### Other extensions

- Prediction model (write model, relevant deflation, component selection, elastic-net regularization)
- Link with IA / machine learning
  - Integrate IA in multiblock prediction models (e.g., neural networks)
  - Integrate multiblock methods in machine learning packages/software

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### Know and be able to (link between developers and users)

- Train and disseminate methods
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### Apply and publish

- Multi-source data come from all fields
- Apply to different fields (psychometry → chimiometry → biology (e.g., sensometry, epidemiology, omic) → all fields)
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## Working together

### A multiblock joined program

- Métaprogramme INRAe DIGIT-BIO 2022 « Biologie Numérique pour explorer et prédire le vivant » / Consortium inter-disciplinaire 'MIMS' (Regards Méthodologiques Croisés pour l'Intégration de données Multi-sources)

Contact : [mohamed.hanafi@oniris-nantes.fr](mailto:mohamed.hanafi@oniris-nantes.fr)



A part of the “French multiblock team”! Join us!



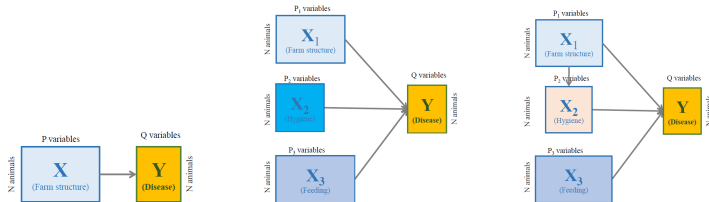
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# Supervised multiblock analyses

## Cases of two-blocks, (K+1)-blocks, (K+K')-blocks

Stéphanie Bougeard

*French Agency for Food, Environmental, Occupational Health & Safety (Anses), Ploufragan, France*



Journée Analyses Factorielles  
March 30 2023, INRAe Jouy-en-Josas