Supervised Component-based Generalized Linear Regression with finite mixture models of responses

Julien GIBAUD[1], Xavier BRY[1] and Catherine TROTTIER[1,2]

[1] IMAG, CNRS, Univ. Montpellier, France.
[2] AMIS, Univ. Paul-Valéry Montpellier 3, Montpellier, France.

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Outline

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Motivations

Ecological motivations

In a context of global warming, we aim at

- Finding the main determinants of species observations, among a large number of explanatory variables
- Identifying species communities influenced by common determinants

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Statistical counterparts

- Finding strong dimensions allowing to explain the responses as best as possible
  - ↪ Searching for supervised components
- Identifying groups of responses with explanatory dimensions specific to each group
  - ↪ Clustering

Outline

What is a supervised component ?

Notations

- Let $Y = [y_1, \ldots, y_q] \in \mathbb{R}^{n \times q}$ be the matrix of responses (species)
- Let $X = [x_1, \ldots, x_p] \in \mathbb{R}^{n \times p}$ be the matrix of explanatory variables

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Definition

A component is a vector $f \in \mathbb{R}^n$ linearly combining the explanatory variables, such that

- $f_h = Xu_h$, for $h = 1, \ldots, H$, and $F = [f_1, \ldots, f_H]$
- $f_h \perp f_g$, for all $h \neq g$

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Demands

- Components must be close to some explanatory variables to be interpreted
- Components must predict responses Y $\Rightarrow$ supervised components

SCGLR (Bry et al., 2013)

Structural Relevance (SR)

The criterion $\phi(u)$ measures the "strength" of the component $f = Xu$ (overall closeness to explanatory variables) under the constraint $\|u\|^2 = 1$

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$$\Downarrow$$

The SCGLR combined criterion

$$\underset{u,\, \|u\|^2=1}{\operatorname{argmax}} \; s \ln\left(\phi(u)\right) + (1-s) \ln\left(\psi(u,\theta)\right)$$

The real $s \in [0, 1]$ allows to tune the trade-off between SR and GoF

Estimation steps

Iterate :

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Estimation of u given θ

The PING algorithm allows to solve a program of the form

$$\begin{cases} \max_{u} \quad c(u), \\ \text{s.t.} \quad \|u\|^2 = 1 \quad \text{and} \quad D^T u = 0, \end{cases}$$

where D is the constraint matrix of components' orthogonality

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Estimation of θ given u

Maximize the likelihood on θ, *e.g.* solve

$$\nabla_\theta \, \psi(u, \theta) = 0$$

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Mixture of responses (Dunstan et al., 2013)

More notations

- Let G be the number of groups
- Let z_{kg} be the latent dummy variable equal to 1 if the response y_k belongs to the group g
- Let p_g be the *a priori* probability of belonging to the group g

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Model

Conditionally to $z_{kg} = 1$, $y_k \sim \mathbb{P}(\theta_g)$ with pdf $d(y_k; \theta_g)$.
The model likelihood writes : $\psi(u_1, \ldots, u_G; \Theta) = \prod_{k=1}^{q} \sum_{g=1}^{G} p_g d(y_k; \theta_g)$,
with θ_g including :

- the loading vectors u_g specific to each group
- the parameters of within cluster regression model of responses on components

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Problem : this likelihood is hard to maximize

Estimation (Dempster et al., 1977)

We use the Expectation-Maximization (EM) algorithm.
It allows to :

- Maximize a likelihood in the presence of latent variables
  - $\rightarrow$ Here : the dummy variable z_{kg}
- Estimate the posterior distribution of each z_k conditional on the observations
  - $\rightarrow$ Here : the posterior group membership probabilities of each response

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A new enhanced criterion

The separation criterion

We introduce the criterion $\varphi(u_1, \ldots, u_G)$ in order to separate the explanatory spaces

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Maximized criterion

$$\underset{\forall g,\, \|u_g\|^2=1}{\operatorname{argmax}} \; s \sum_{g=1}^{G} \ln\left(\phi(u_g)\right) + t \ln\left(\varphi(u_1, \dots, u_G)\right) + (1 - s - t) \ln\left(\psi(u_1, \dots, u_G; \Theta)\right)$$

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Estimation

We alternate on the two maximization steps :

- Find Θ through the EM algorithm
- Find u_g through the PING algorithm, for all g

Outline

Simulation study

Random responses

$$Y = [\underbrace{y_1, \ldots, y_{20}}_{\text{G1 : Gaussian}} \mid \underbrace{y_{21}, \ldots, y_{50}}_{\text{G2 : Poisson}} \mid \underbrace{y_{51}, \ldots, y_{100}}_{\text{G3 : Bernoulli}}]$$

Y is composed in 3 groups of responses

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Explanatory variables

$$X = [\underbrace{x_1, \ldots, x_{50}}_{\text{X1 : predict G1}} \mid \underbrace{x_{51}, \ldots, x_{90}}_{\text{X2 : predict G2}} \mid \underbrace{x_{91}, \ldots, x_{120}}_{\text{X3 : predict G3}} \mid \underbrace{x_{121}, \ldots, x_{140}}_{\text{X4 : predict G1}} \mid \underbrace{x_{141}, \ldots, x_{150}}_{\text{X5 : predict G2}} \mid \underbrace{x_{151}, \ldots, x_{200}}_{\text{X6 : noise}}]$$

- X is composed in 5 bundles plus 1 set of noise
- Bundles $X1$, $X3$ and $X5$ are weakly correlated ($\text{cor} = 0.5$)

Results obtained with the best classification index

Hyperparameters

The optimized parameters are $s = 0.1$ and $t = 0.6$

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Posterior group membership probabilities

- $\forall i = 1, \ldots, 20$, $\mathbb{P}(y_i$ belongs to the group 1$) > 0.9$
- $\forall i = 21, \ldots, 50$, $\mathbb{P}(y_i$ belongs to the group 2$) > 0.9$
- $\forall i = 51, \ldots, 100$, $\mathbb{P}(y_i$ belongs to the group 3$) > 0.9$

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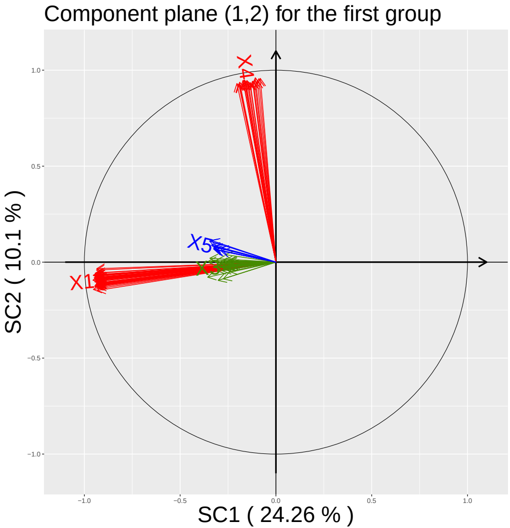
Correlations

group 1	
$\text{cor}^2(X_1, f_1)$	0.960
$\text{cor}^2(X_4, f_2)$	0.966

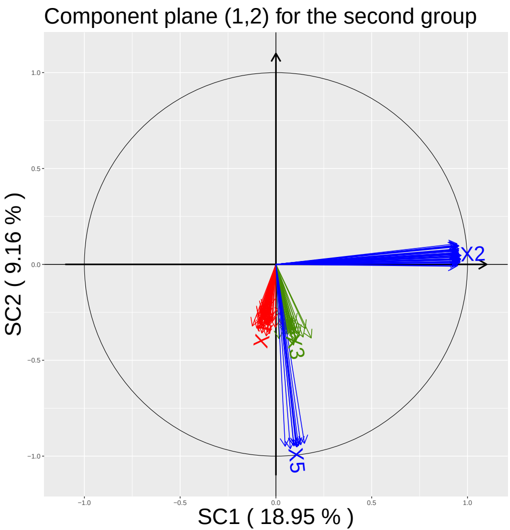
group 2	
$\text{cor}^2(X_2, f_1)$	0.993
$\text{cor}^2(X_5, f_2)$	0.911

group 3	
$\text{cor}^2(X_3, f_1)$	0.987

Correlation scatterplot for the first group



Correlation scatterplot for the second group



Real data

The *Genus* dataset

- 27 species abundances (Y matrix)
- 39 explanatory variables (X matrix)
  - ↬ subset of 13 rainfall variables ("pluvio")
  - ↬ subset of 23 photosynthesis variables ("evi")
  - ↬ subset of 3 location variables

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Results

Groups	Responses	Explanatory variables
1	Y_4	"pluvio1", "pluvio12"
2	Y_8, Y_{19}	"pluvio7", "pluvio6"
3	Y_1, Y_3, Y_5, Y_7, Y_{11}, Y_{12}, Y_{13}, Y_{14}, Y_{16} Y_{21}, Y_{24}, Y_{25}, Y_{26}, Y_{27}	"pluvio8", "pluvio1"
4	Y_9	"pluvio10", "evi13"
5	Y_6, Y_{15}, Y_{18}, Y_{22}, Y_{23}	"pluvio7", "pluvio8"
6	Y_2, Y_{10}, Y_{17}, Y_{20}	"pluvio7", "pluvio11"

Conclusion

We have :

- Extended SCGLR to response mixture
- Enhanced the combined criterion
- Developed an algorithm able to find groups of responses predicted by specific explanatory spaces

Acknowledgments and bibliography

Thank you for your attention

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