Factor model in multiblock component-based GLM

Julien GIBAUD¹, Xavier BRY¹ and Catherine TROTTIER^{1,2}

IMAG, CNRS, Univ. Montpellier, France.
 AMIS, UPV Montpellier 3, Montpellier, France.





RJS 2022

Outline

- Motivations
- Searching for supervised components
- Random latent factors
- SCGLR with latent factors
- Experimental study

Outline

- Motivations
- 2 Searching for supervised components
- Random latent factors
- SCGLR with latent factors
- Experimental study



Motivations

Ecological motivations

In a context of global warming, we aim at:

- Finding the main determinants of species observations, among a thematic partitioning of the explanatory variables
- Identifying groups of species sharing mutual dependencies

Motivations

Ecological motivations

In a context of global warming, we aim at:

- Finding the main determinants of species observations, among a thematic partitioning of the explanatory variables
- Identifying groups of species sharing mutual dependencies

Statistical counterparts

- Finding strong dimensions allowing to explain the responses as best as possible
 - → Supervised components
- Identifying blocks in the responses' conditional variance-covariance matrix
 - → Random latent variables: factors

Outline

- Motivations
- Searching for supervised components
- 3 Random latent factors
- SCGLR with latent factors
- Experimental study

What is a supervised component?

Notations

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

4□▶
4□▶
4□▶
4□▶
4□▶
4□▶
4□▶
4□▶
4□▶
4□▶
4□▶

What is a supervised component?

Notations

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

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, ..., H
- $f^h \perp f^g$, for all $h \neq g$

What is a supervised component?

Notations

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

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, ..., H
- $f^h \perp f^g$, for all $h \neq g$

Demands

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

F-SCGLR RJS 2022 6 / 28

SCGLR (Bry et al., 2020)

Structural Relevance (SR)

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

SCGLR (Bry et al., 2020)

Structural Relevance (SR)

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

Goodness-of-Fit (GoF)

The criterion $\psi(u,\theta)$ is the likelihood of the component model

SCGLR (Bry et al., 2020)

Structural Relevance (SR)

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

Goodness-of-Fit (GoF)

The criterion $\psi(u,\theta)$ is the likelihood of the component model



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

THEME-SCGLR (Bry et al., 2020)

Notations

- Let $X = [X_1, \dots, X_R] \in \mathbb{R}^{n \times p}$ be the matrix of R thematic subsets
- Let $f_r^h = X_r u_r^h$ be the hth component of theme X_r

< ロト < 個 ト < 重 ト < 重 ト 三 重 ・ の Q @

THEME-SCGLR (Bry et al., 2020)

Notations

- Let $X = [X_1, \dots, X_R] \in \mathbb{R}^{n \times p}$ be the matrix of R thematic subsets
- Let $f_r^h = X_r u_r^h$ be the *h*th component of theme X_r

New demands

- Components must be explicitly identified in the themes
- Components must be orthogonal to the other components within the theme
- Components must again predict responses Y

THEME-SCGLR (Bry et al., 2020)

Notations

- Let $X = [X_1, \dots, X_R] \in \mathbb{R}^{n \times p}$ be the matrix of R thematic subsets
- Let $f_r^h = X_r u_r^h$ be the *h*th component of theme X_r

New demands

- Components must be explicitly identified in the themes
- Components must be orthogonal to the other components within the theme
- Components must again predict responses Y

The THEME-SCGLR combined criterion

$$\underset{\forall r, \|u_r\|^2=1}{\operatorname{argmax}} \ s \sum_{r=1}^R \ln \left(\phi(u_r)\right) + (1-s) \ln \left(\psi(u_1, \dots, u_R, \theta)\right)$$

Julien GIBAUD (IMAG) F-SCGLR RJS 2022 8/28

Estimation steps

Iterate:

Estimation steps

Iterate:

Estimation of u_r given θ

The PING algorithm allows to solve a program of the form

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

where D is the constraint matrix of components' orthogonality

Estimation steps

Iterate:

Estimation of u_r given θ

The PING algorithm allows to solve a program of the form

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

where D is the constraint matrix of components' orthogonality

Estimation of θ given all u_r

Maximize the likelihood on θ , e.g. solve

$$\nabla_{\theta} \psi(u_1,\ldots,u_R,\theta) = 0$$

Outline

- Motivations
- 2 Searching for supervised components
- Random latent factors
- SCGLR with latent factors
- Experimental study

More notations

- Let J be the number of factors
- Let $g_i \sim \mathcal{N}(0, I_J), i = 1, \dots n$, be the random vector of factors
- ullet Let $B \in \mathbb{R}^{L \times q}$ be the loading matrix of factors
- Let ε_i be the error vector

More notations

- Let J be the number of factors
- Let $g_i \sim \mathcal{N}(0, I_J), i = 1, \dots n$, be the random vector of factors
- ullet Let $B \in \mathbb{R}^{L imes q}$ be the loading matrix of factors
- Let ε_i be the error vector

Classic linear factor model

The model expressed row-wise is given by $y_i = B^T g_i + \varepsilon_i$ of likelihood $L(Y; B) = \prod_{i=1}^n L(y_i; B)$

More notations

- Let J be the number of factors
- Let $g_i \sim \mathcal{N}(0, I_J), i = 1, \dots n$, be the random vector of factors
- Let $B \in \mathbb{R}^{L \times q}$ be the loading matrix of factors
- Let ε_i be the error vector

Classic linear factor model

The model expressed row-wise is given by $y_i = B^T g_i + \varepsilon_i$ of likelihood $L(Y; B) = \prod_{i=1}^n L(y_i; B)$

Problem 1: The model is not unique

More notations

- Let J be the number of factors
- Let $g_i \sim \mathcal{N}(0, I_J), i = 1, \dots n$, be the random vector of factors
- ullet Let $B \in \mathbb{R}^{L imes q}$ be the loading matrix of factors
- Let ε_i be the error vector

Classic linear factor model

The model expressed row-wise is given by $y_i = B^T g_i + \varepsilon_i$ of likelihood $L(Y; B) = \prod_{i=1}^n L(y_i; B)$

Problem 1: The model is not unique

Problem 2: Likelihood difficult to maximize

Problem 1: The model is not unique

Identification problem

Let Ω be an orthogonal matrix $(\Omega^T \Omega = I)$. The model also writes

$$y_i = B^T g_i + \varepsilon_i = B^T \Omega^T \Omega g_i + \varepsilon_i$$

with
$$\mathbb{E}\left[\Omega g_i\right] = \Omega \mathbb{E}\left[g_i\right] = 0$$

and $\mathbb{V}\left[\Omega g_i\right] = \Omega \mathbb{V}\left[g_i\right] \Omega^T = I_J$

◆ロト ◆個ト ◆差ト ◆差ト を めんぐ

Problem 1: The model is not unique

Identification problem

Let Ω be an orthogonal matrix $(\Omega^T \Omega = I)$. The model also writes

$$y_i = B^T g_i + \varepsilon_i = B^T \Omega^T \Omega g_i + \varepsilon_i$$

with
$$\mathbb{E}\left[\Omega g_i\right] = \Omega \mathbb{E}\left[g_i\right] = 0$$

and $\mathbb{V}\left[\Omega g_i\right] = \Omega \mathbb{V}\left[g_i\right] \Omega^T = I_J$

 \rightarrow We get the same distribution !!!

Julien GIBAUD (IMAG)

Problem 1: The model is not unique

Identification problem

Let Ω be an orthogonal matrix $(\Omega^T \Omega = I)$. The model also writes

$$y_i = B^T g_i + \varepsilon_i = B^T \Omega^T \Omega g_i + \varepsilon_i$$

with
$$\mathbb{E}\left[\Omega g_i\right] = \Omega \mathbb{E}\left[g_i\right] = 0$$

and $\mathbb{V}\left[\Omega g_i\right] = \Omega \mathbb{V}\left[g_i\right] \Omega^T = I_J$

 \rightarrow We get the same distribution !!!

Geweke and Zhou (1996) assure the uniqueness of the solution by imposing a upper triangle constraint on the matrix *B*:

$$B = \begin{pmatrix} b_{11} & \dots & b_{1J} & b_{1,J+1} & \dots & b_{1q} \\ & \ddots & \vdots & \vdots & \ddots & \vdots \\ & & b_{JJ} & b_{J,J+1} & \dots & b_{Jq} \end{pmatrix}.$$

◆ロト ◆個ト ◆差ト ◆差ト 差 めなぐ

Problem 2: Likelihood difficult to maximize

We perform the Expectation-Maximization (EM) algorithm.

It allows to:

Problem 2: Likelihood difficult to maximize

We perform the Expectation-Maximization (EM) algorithm.

It allows to:

- Maximize a likelihood in presence of random latent variables
 - \rightarrow Here: the factors

Julien GIBAUD (IMAG)

Problem 2: Likelihood difficult to maximize

We perform the Expectation-Maximization (EM) algorithm.

It allows to:

- Maximize a likelihood in presence of random latent variables
 - \rightarrow Here: the factors
- Estimate the model's parameters
 - \rightarrow Here: the matrix B

Outline

- Motivations
- 2 Searching for supervised components
- Random latent factors
- SCGLR with latent factors
- Experimental study

Factors SCGLR

Component-based model with factors

$$\eta = \underbrace{(X_1 u_1) \gamma_1 + \dots + (X_R u_R) \gamma_R}_{\text{deterministic}} + \underbrace{GB}_{\text{stochastic}}$$

where the $X_r u_r$'s are the components, $\Gamma = [\gamma_1, \dots, \gamma_R]$ the regression parameters and G the realizations of the factors.

The likelihood writes $L(Y; u_1, ..., u_R, \Gamma, B)$

Factors SCGLR

Component-based model with factors

$$\eta = \underbrace{(X_1 u_1) \gamma_1 + \dots + (X_R u_R) \gamma_R}_{\text{deterministic}} + \underbrace{GB}_{\text{stochastic}}$$

where the $X_r u_r$'s are the components, $\Gamma = [\gamma_1, \dots, \gamma_R]$ the regression parameters and G the realizations of the factors.

The likelihood writes $L(Y; u_1, \ldots, u_R, \Gamma, B)$

Combined criterion

$$\underset{\forall r, \|u_r\|^2=1}{\operatorname{argmax}} s \sum_{r=1}^R \ln \left(\phi(u_r) \right) + (1-s) \ln \left(L(Y; u_1, \dots, u_R, \Gamma, B) \right)$$

Factors SCGLR

Component-based model with factors

$$\eta = \underbrace{(X_1 u_1) \gamma_1 + \dots + (X_R u_R) \gamma_R}_{\text{deterministic}} + \underbrace{GB}_{\text{stochastic}}$$

where the $X_r u_r$'s are the components, $\Gamma = [\gamma_1, \dots, \gamma_R]$ the regression parameters and G the realizations of the factors.

The likelihood writes $L(Y; u_1, \ldots, u_R, \Gamma, B)$

Combined criterion

$$\underset{\forall r, \|u_r\|^2=1}{\operatorname{argmax}} s \sum_{r=1}^R \ln \left(\phi(u_r)\right) + (1-s) \ln \left(\frac{L(Y; u_1, \dots, u_R, \Gamma, B)}{L(Y; u_1, \dots, u_R, \Gamma, B)}\right)$$

Estimation steps

The overall algorithm consists in alternating the following steps:

- We find $\{\Gamma, B\}$ through the EM algorithm
- We find all u_r through the PING algorithm

Outline

- Motivations
- 2 Searching for supervised components
- Random latent factors
- SCGLR with latent factors
- Experimental study

Deterministic simulation

Response variables

 $Y = [y_1, \dots, y_{50}]$ is composed by 20 Gaussian responses, 20 Poisson responses and 10 Bernoulli responses

Deterministic simulation

Response variables

 $Y = [y_1, \dots, y_{50}]$ is composed by 20 Gaussian responses, 20 Poisson responses and 10 Bernoulli responses

Explanatory variables

$$X_1 = [\underbrace{x_1, \dots, x_{60}}_{:=\mathcal{X}_1} | \underbrace{x_{61}, \dots, x_{100}}_{:=\mathcal{X}_2}] \text{ and } X_2 = [\underbrace{x_{101}, \dots, x_{160}}_{:=\mathcal{X}_3} | \underbrace{x_{161}, \dots, x_{200}}_{:=\mathcal{X}_4}]$$

- Theme X_1 is composed by two explanatory bundles
- Theme X_2 is composed by two explanatory bundles
- Bundles are sets of correlated variables

Stochastic simulation

Factors

We generate 3 factors to model the covariance between the responses

Stochastic simulation

Factors

We generate 3 factors to model the covariance between the responses

Loading matrix

We generate the matrix B of the form

$$B = [\underbrace{b_1, \dots, b_5}_{\sim \mathcal{N}(\mu_1, 0.1 l_3)} \mid \underbrace{b_6, \dots, b_{10}}_{\sim \mathcal{N}(-\mu_1, 0.1 l_3)} \mid \underbrace{b_{11}, \dots, b_{20}}_{\sim \mathcal{N}(\mu_2, 0.1 l_3)} \mid \underbrace{b_{21}, \dots, b_{35}}_{\sim \mathcal{N}(-\mu_2, 0.1 l_3)} \mid \underbrace{b_{36}, \dots, b_{50}}_{\sim \mathcal{N}(\mu_3, 0.1 l_3)}],$$

where
$$\mu_1 = (2,0,0)^T$$
, $\mu_2 = (0,-1,0)^T$ and $\mu_3 = (0,0,1.5)^T$.

Simulation: variance-covariance matrix

The variance-covariance matrix of the responses B^TB becomes

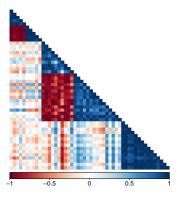


Figure 1: Conditional variance-covariance matrix

Simulation: variance-covariance matrix

The variance-covariance matrix of the responses B^TB becomes

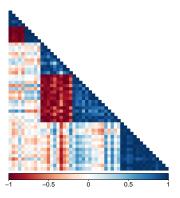


Figure 1: Conditional variance-covariance matrix

Question: How to identify the blocks?

We perform several a posteriori steps:

• We estimate the variance-covariance matrix B^TB

- We estimate the variance-covariance matrix B^TB
- We estimate the correlation matrix

- We estimate the variance-covariance matrix B^TB
- We estimate the correlation matrix
- We calculate a dissimilarity matrix from the correlations: $d(x, y) = 2(1 cor^2(x, y))$



- We estimate the variance-covariance matrix B^TB
- We estimate the correlation matrix
- We calculate a dissimilarity matrix from the correlations: $d(x, y) = 2(1 cor^2(x, y))$
- We perform the Multidimensional Scaling (MDS) on the dissimilarity matrix

- We estimate the variance-covariance matrix B^TB
- We estimate the correlation matrix
- We calculate a dissimilarity matrix from the correlations: $d(x, y) = 2(1 cor^2(x, y))$
- We perform the Multidimensional Scaling (MDS) on the dissimilarity matrix
- We perform the K-means on the output of the MDS

Results

Bundles recovery

Components	of theme 1
$\operatorname{cor}^2(\mathcal{X}_1, \mathit{f}_1^{1})$	0.984
$\operatorname{cor}^2(\mathcal{X}_2,f_1^2)$	0.979

Components of theme 2	
$\operatorname{cor}^2(\mathcal{X}_3, f_2^1)$	0.975
$\operatorname{cor}^2(\mathcal{X}_4, f_2^2)$	0.983

Results

Bundles recovery

Components of theme 1	
$\operatorname{cor}^2(\mathcal{X}_1, \mathit{f}_1^{1})$	0.984
$\operatorname{cor}^2(\mathcal{X}_2, f_1^2)$	0.979

Components of theme 2	
$\operatorname{cor}^2(\mathcal{X}_3, f_2^1)$	0.975
$\operatorname{cor}^2(\mathcal{X}_4, f_2^2)$	0.983

Correctness of classification steps

Rand Index: 0.948

Adjusted Rand Index: 0.904

Results

Bundles recovery

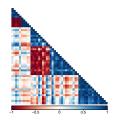
Components of theme 1	
$\operatorname{cor}^2(\mathcal{X}_1, \mathit{f}_1^{1})$	0.984
$\operatorname{cor}^2(\mathcal{X}_2, f_1^2)$	0.979

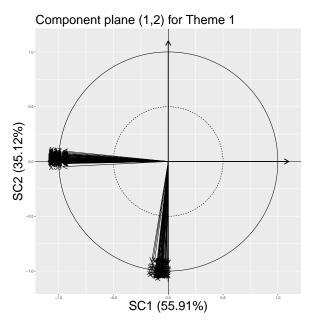
Components of theme 2	
$\operatorname{cor}^2(\mathcal{X}_3, f_2^1)$	0.975
$\operatorname{cor}^2(\mathcal{X}_4, f_2^2)$	0.983

Correctness of classification steps

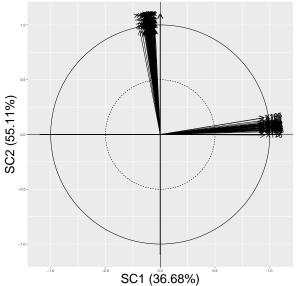
Rand Index: 0.948

Adjusted Rand Index: 0.904





Component plane (1,2) for Theme 2



Real data

The Genus dataset

- 27 species abundances (Y matrix)
- 36 explanatory variables (X matrix)
 - → subset of 23 photosynthesis variables "evi" (Theme 1)
 - → subset of 13 rainfall variables "pluvio" (Theme 2)

Real data

The Genus dataset

- 27 species abundances (Y matrix)
- 36 explanatory variables (X matrix)
 - → subset of 23 photosynthesis variables "evi" (Theme 1)
 - → subset of 13 rainfall variables "pluvio" (Theme 2)

Results

Clusters	Responses
1	Y ₁ , Y ₅ , Y ₇ , Y ₉ , Y ₁₂ , Y ₁₅ , Y ₂₆ , Y ₂₇
2	Y ₂ , Y ₈ , Y ₂₃ , Y ₂₄
3	Y ₃ , Y ₁₃
4	Y ₄ , Y ₁₉
5	Y ₆ , Y ₁₆ , Y ₂₂ , Y ₂₅
6	Y ₁₀ , Y ₁₈ , Y ₂₀
7	Y ₁₁ , Y ₁₄
8	Y ₁₇ , Y ₂₁

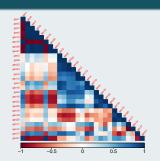
Real data

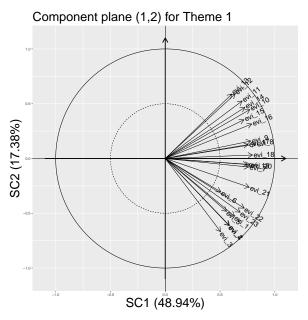
The Genus dataset

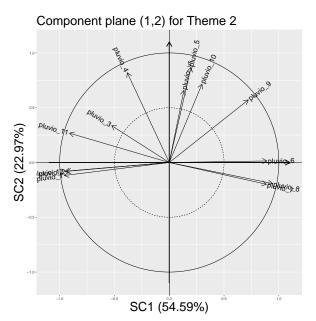
- 27 species abundances (Y matrix)
- 36 explanatory variables (X matrix)
 - → subset of 23 photosynthesis variables "evi" (Theme 1)
 - → subset of 13 rainfall variables "pluvio" (Theme 2)

Results

Clusters	Responses
1	Y ₁ , Y ₅ , Y ₇ , Y ₉ , Y ₁₂ , Y ₁₅ , Y ₂₆ , Y ₂₇
2	Y ₂ , Y ₈ , Y ₂₃ , Y ₂₄
3	Y_3, Y_{13}
4	Y ₄ , Y ₁₉
5	$Y_6, Y_{16}, Y_{22}, Y_{25}$
6	Y ₁₀ , Y ₁₈ , Y ₂₀
7	Y ₁₁ , Y ₁₄
8	Y ₁₇ , Y ₂₁







Conclusion

We have:

- Extended SCGLR to the factor model
- Developed an algorithm allowing to find relevant components and to model the variance-covariance matrix

Conclusion

We have:

- Extended SCGLR to the factor model
- Developed an algorithm allowing to find relevant components and to model the variance-covariance matrix

Perspectives

We want to:

- Add new distributions for the responses
- Better identify blocks in the variance-covariance matrix

Acknowledgments and references

Thank you for your attention

Bry, X., Trottier, C., Mortier, F., and Cornu, G. (2020). Component-based regularization of a multivariate GLM with a thematic partitioning of the explanatory variables. *Statistical Modelling*, 20(1):96–119.

Geweke, J. and Zhou, G. (1996). Measuring the pricing error of the arbitrage pricing theory. *The review of financial studies*, 9(2):557–587.