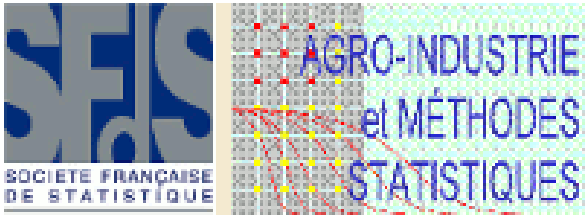
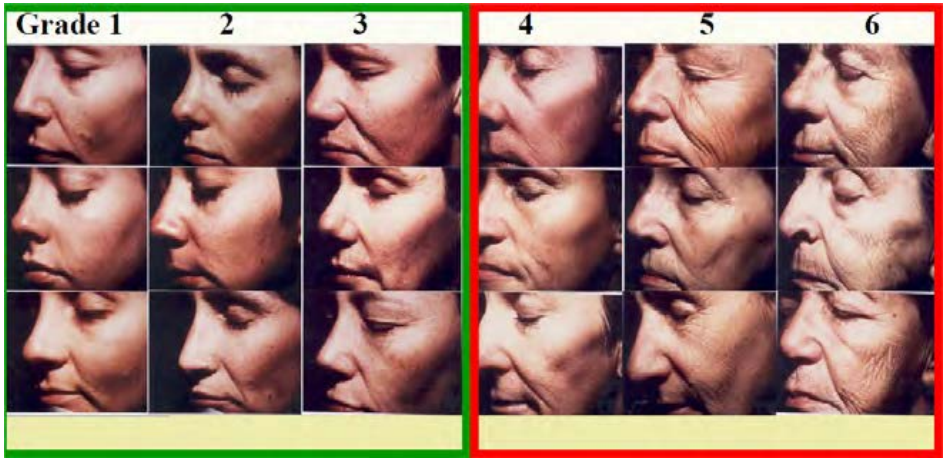



# From Sparse Regression to Sparse Multiple Correspondence Analysis

Anne Bernard
QFAB, Brisbane
a.bernard@qfab.org

Gilbert Saporta
CEDRIC, CNAM, Paris
gilbert.saporta@cnam.fr

- Joint work with Anne Bernard, Ph.D student funded by the R&D department of Chanel cosmetic company
- Industrial context and motivation:
  - Relate gene expression data to skin aging measures




  - n=500, p= 800 000 SNP's, 15 000 genes

# Outline

1. Introduction
2. Sparse regression
3. Sparse PCA
4. Sparse MCA
5. Conclusion and perspectives

# 1.Introduction

- High dimensional data: p>>n
  - Gene expression data
  - Chemometrics
  - etc.
- Several solutions for regression problems with **all** variables; but interpretation is difficult
- Sparse methods: provide combinations of **few** variables

- This talk:
  - a survey of sparse methods for supervised (regression) and unsupervised (PCA) problems
  - New propositions in the unsupervised case when variables belong to disjoint groups or blocks:
    - Group sparse PCA
    - Sparse multiple correspondence analysis

# 2. Sparse regression

- Ridge, PCR, PLS regression: solutions with all predictors
  - However: keeping all predictors is a drawback for high dimensional data: combinations of too many variables cannot be interpreted
- Sparse methods simultaneously shrink coefficients and select variables, hence better predictions

# 2.1 Lasso and elastic-net

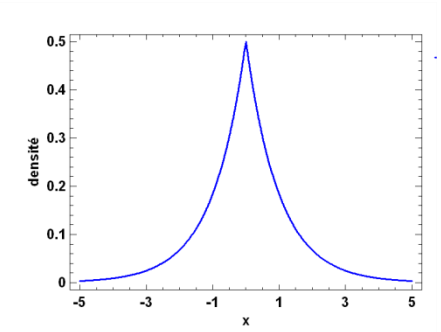
- **Lasso** (Tibshirani, 1996) imposes a $L_1$ constraint on the coefficients $\sum_{j=1}^{p} \left| b_j \right| < c$

$$\hat{\boldsymbol{\beta}}_{lasso} = \arg\min_{\boldsymbol{\beta}} \left( \left\| \mathbf{y} - \mathbf{X}\boldsymbol{\beta} \right\|^2 + \lambda \sum_{j=1}^{p} \left| \beta_j \right| \right)$$

- Lasso continuously shrinks the coefficients towards zero
- Convex optimisation; no explicit solution

- Constraints and log-priors
  - Like ridge regression, the Lasso is a bayesian regression but with an exponential prior

$$f(\beta_j) = \frac{\lambda}{2}\exp\left(-\lambda\left|\beta_j\right|\right)$$




  - $\left|\beta_j\right|$ is proportional to the log-prior

- Finding the optimal parameter
  - Cross validation if optimal prediction is needed
  - BIC  when the sparsity is the main concern

$$\lambda_{opt} = \arg\min_{\lambda} \left( \frac{\left\| y - X\hat{\beta}(\lambda) \right\|^2}{n\sigma^2} + \frac{\log(n)}{n} \hat{df}(\lambda) \right)$$

a good unbiased estimate of df is the number of nonzero coefficients .  (Zou et al., 2007)

- A more general form:

$$\hat{\boldsymbol{\beta}}_{lasso} = \arg\min_{\boldsymbol{\beta}} \left( \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q \right)$$

  - q=2 ridge; q=1 Lasso; q=0 subset selection (counts the number of variables)
  - q>1 do not provide null coefficients (derivability)

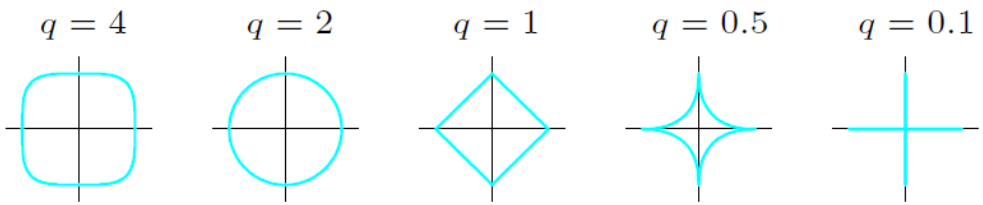



**FIGURE 3.12.** *Contours of constant value of* $\sum_j |\beta_j|^q$ *for given values of* $q$.

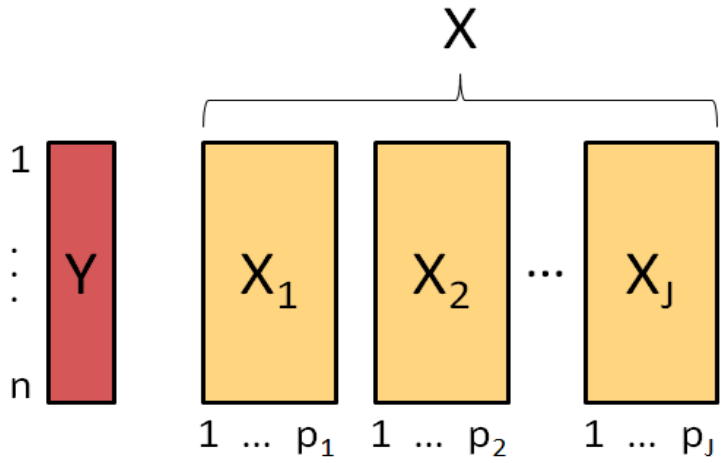
Elements of Statistical Learning (2nd Ed.) ©Hastie, Tibshirani & Friedman 2009 Chap 3

- Lasso produces a sparse model but the number of selected variables cannot exceed the number of units
- **Elastic net:** combine ridge penalty and lasso penalty to select more predictors than the number of observations (Zou & Hastie, 2005)

$$\hat{\boldsymbol{\beta}}_{en} = \arg\min_{\boldsymbol{\beta}} \left( \left\| \mathbf{y} - \mathbf{X}\boldsymbol{\beta} \right\|^2 + \lambda_2 \left\| \boldsymbol{\beta} \right\|^2 + \lambda_1 \left\| \boldsymbol{\beta} \right\|_1 \right)$$

# 2.2 Group-lasso

- X matrix divided into J sub-matrices $X_j$ of $p_j$ variables
- **Group Lasso**: extension of Lasso for selecting groups of variables (Yuan & Lin, 2007):




$$\hat{\boldsymbol{\beta}}_{GL} = \arg\min_{\beta} \left\| \mathbf{y} - \sum_{j=1}^{J} \mathbf{X}_j \boldsymbol{\beta}_j \right\|^2 + \lambda \sum_{j=1}^{J} \sqrt{p_j} \left\| \boldsymbol{\beta}_j \right\|$$

If $p_j$=1 for all j, group Lasso = Lasso

- Drawback: no sparsity within groups
- A solution: **sparse group lasso** (Simon et al. , 2012)

$$\min_{\boldsymbol{\beta}} \left( \left\| \mathbf{y} - \sum_{j=1}^{J} \mathbf{X}_j \boldsymbol{\beta}_j \right\|^2 + \lambda_1 \sum_{j=1}^{J} \left\| \boldsymbol{\beta}_j \right\| + \lambda_2 \sum_{j=1}^{J} \sum_{i=1}^{p_j} \left| \beta_{ij} \right| \right)$$

  - Two tuning parameters: grid search

# 3.Sparse PCA

- In PCA, each PC is a linear combination of **all** the original variables : difficult to interpret the results
- **Challenge of SPCA:** obtain components easily interpretable (lot of zero loadings in principal factors)
- **Principle of SPCA:** modify PCA imposing lasso/elastic-net constraints to construct modified PCs with sparse loadings
- **Warning:** Sparse PCA does not provide a global selection of variables but a selection **dimension by dimension** : different from the regression context (Lasso, Elastic Net, …)

# 3.1 First attempts:

- **Simple PCA**
  - by Vines (2000) : integer loadings
  - Rousson, V. and Gasser, T. (2004) : loadings (+ , 0, -)
- **SCoTLASS** (Simplified Component Technique – Lasso) by Jolliffe & al. (2003) : extra $L_1$ constraints

$$\max \mathbf{u'Vu} \quad \text{with } \|\mathbf{u}\|^2 = \mathbf{u'u} = 1 \text{ and } \sum_{j=1}^{p} |u_j| \leq t$$

SCotLass properties:

$t \geq \sqrt{p}$ usual PCA

$t < 1$ no solution

$t = 1$ only one nonzero coefficient

$1 < t < \sqrt{p}$

- Non convex problem

# 3.2 S-PCA by Zou et al (2006)

Let the SVD of X be $\mathbf{X} = \mathbf{UDV}'$ with $\mathbf{Z} = \mathbf{UD}$ the principal components

Ridge regression:

$$\hat{\boldsymbol{\beta}}_{ridge} = \arg\min_{\beta} \left\| \mathbf{Z} - \mathbf{X}\boldsymbol{\beta} \right\|^2 + \lambda \left\| \boldsymbol{\beta} \right\|^2$$

$$\mathbf{X}'\mathbf{X} = \mathbf{V}\mathbf{D}^2\mathbf{V}' \; with \; \mathbf{V}'\mathbf{V} = \mathbf{I}$$

$$\hat{\boldsymbol{\beta}}_{\mathbf{i,ridge}} = \left(\mathbf{X}'\mathbf{X} + \boldsymbol{\lambda}\,\mathbf{I}\right)^{-1} \mathbf{X}' \left(\mathbf{X}\mathbf{v}_{\mathbf{i}}\right) = \mathbf{v}_{\mathbf{i}} \frac{d_{ii}^2}{d_{ii}^2 + \lambda} \quad \Longrightarrow \quad \tilde{\mathbf{v}} = \mathbf{v}_i$$

**Loadings can be recovered by regressing (ridge regression) PCs on the p variables**

→PCA can be written as a **regression-type optimization problem**

Sparse PCA add a new penalty to produce sparse loadings:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\beta} \left\| \mathbf{Z} - \mathbf{X}\boldsymbol{\beta} \right\|^2 + \lambda \left\| \boldsymbol{\beta} \right\|^2 + \lambda_1 \left\| \boldsymbol{\beta} \right\|_1$$

Lasso penalty

$\hat{\mathbf{v}}_i = \dfrac{\hat{\boldsymbol{\beta}}}{\left\| \hat{\boldsymbol{\beta}} \right\|}$ is an approximation to $\mathbf{v}_i$, and $\mathbf{X}\hat{\mathbf{v}}_i$ the i$^{th}$ approximated component

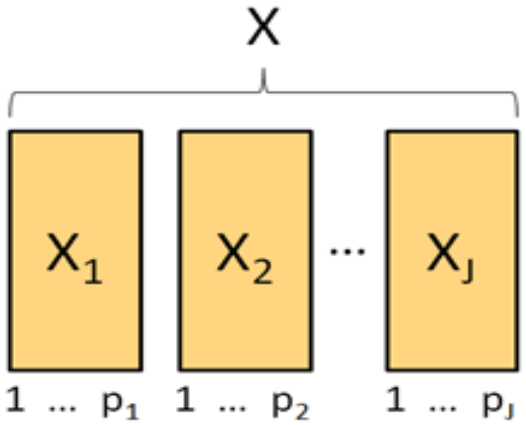
→Produces sparse loadings with zero coefficients to facilitate interpretation

Alternated algorithm between elastic net and SVD

- Loss of orthogonality
  - SCotLass: orthogonal loadings but correlated components
  - S-PCA: neither loadings, nor components are orthogonal
  - Necessity of  adjusting the % of explained variance

# 3.4 Group Sparse PCA

Data matrix X divided into J groups $X_j$ of $p_j$ variables




**Group Sparse PCA**: compromise between SPCA and group Lasso

**Goal**: select groups of continuous variables (zero coefficients to entire blocks of variables)

**Principle:** replace the penalty function in the SPCA algorithm

$$\hat{\boldsymbol{\beta}} = \arg\min_{\beta} \left\| \mathbf{Z} - \mathbf{X}\boldsymbol{\beta} \right\|^2 + \lambda \left\| \boldsymbol{\beta} \right\|^2 + \lambda_1 \left\| \boldsymbol{\beta} \right\|_1$$

by that defined in the group Lasso

$$\hat{\boldsymbol{\beta}}_{GL} = \arg\min_{\beta} \left\| \mathbf{Z} - \sum_{j=1}^{J} \mathbf{X}_j \boldsymbol{\beta}_j \right\|^2 + \lambda \sum_{j=1}^{J} \sqrt{p_j} \left\| \boldsymbol{\beta}_j \right\|$$

# 4. Sparse MCA

Original table

| $X_J$ |
|---|
| 1 |
| $p_J$ |
| . |
| . |
| . |
| 3 |

**In MCA:**

Selection of ***1 column*** in the original table (categorical variable $X_j$ )

=

Selection of ***a block of $p_j$ indicator variables*** in the complete disjunctive table

Complete disjunctive table

| $X_{J1}$ | … | $X_{Jpj}$ |
|---|---|---|
| 1 | | 0 |
| 0 | | 1 |
| . | | . |
| . | | . |
| . | | . |
| 0 | | 0 |

**Sparse MCA :** select categorical variables, not categories

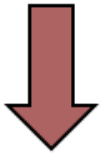
**Principle:** a straightforward extension of Group Sparse PCA for groups of indicator variables, with the chi-square metric . Uses s-PCA r-SVD algorithm (Shen & Huang, 2008).

| Properties | MCA | Sparse MCA |
|---|---|---|
| Uncorrelated Components | TRUE | FALSE |
| Orthogonal loadings | TRUE | FALSE |
| Barycentric property | TRUE | Partly TRUE |
| % of inertia | $\lambda_j / tot \times 100$ | $\left\| \tilde{\mathbf{z}}_{\mathbf{j.1,\ldots,j\text{-}1}} \right\|^2$ |
| Total inertia | $\frac{1}{p} \sum_{j=1}^{p} p_j - 1$ | $\sum_{j=1}^{k} \left\| \tilde{\mathbf{z}}_{\mathbf{j.1,\ldots,j\text{-}1}} \right\|^2$ |

$\tilde{\mathbf{z}}_{\mathbf{j.1,\ldots,j\text{-}1}}$ are the residuals after adjusting $\tilde{\mathbf{z}}_{\mathbf{j}}$ for $\tilde{\mathbf{z}}_{\mathbf{1,\ldots,j\text{-}1}}$(regression projection)

# Toy example: Dogs

| $X_1$ Size | ... | $X_6$ Aggressiveness |
|---|---|---|
| large (L) | | agressive (A) |
| medium (M) | | agressive (A) |
| . | . . . | . |
| . | | . |
| . | | . |
| small (S) | | nonagressive (N) |



| $K_1$ Size | | | ... | $K_6$ Aggressiveness | |
|---|---|---|---|---|---|
| S. | M. | L. | | A | N |
| 0 | 0 | 1 | | 1 | 0 |
| 0 | 1 | 0 | | 1 | 0 |
| . | . | . | . . . | . | . |
| . | . | . | | . | . |
| . | . | . | | . | . |
| 1 | 0 | 0 | | 0 | 1 |

**Data:**

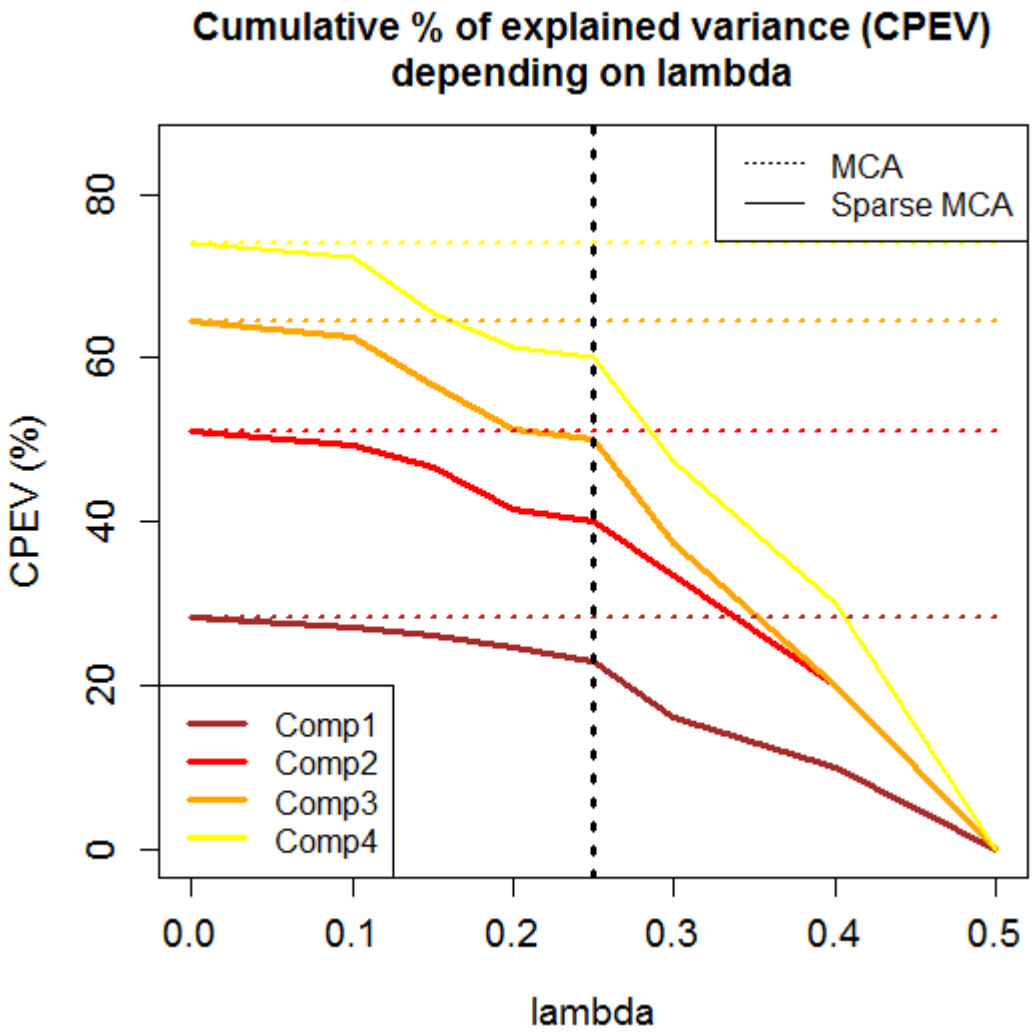
n=27 breeds of dogs
p=6 variables
q=16 (total number of columns)

X : 27 x 6 matrix of categorical variables

K : 27 x 16 complete disjunctive table → $K=(K_1, \ldots, K_6)$

**1 block**
**= 1 $K_j$ matrix**

# Toy example: Dogs




$\lambda$= 0:25 is a compromise between the number of variables selected and the % of variance lost.

# Toy example: Comparison of the loadings

| | MCA | | | | Sparse MCA | | | |
|---|---|---|---|---|---|---|---|---|
| Variable | Comp1 | Comp2 | Comp3 | Comp4 | Comp1 | Comp2 | Comp3 | Comp4 |
| large | -0.361 | 0.071 | -0.005 | 0.060 | -0.389 | 0.000 | 0.000 | 0.000 |
| medium | 0.280 | 0.287 | 0.300 | -0.055 | 0.226 | 0.000 | 0.000 | 0.000 |
| small | 0.291 | -0.400 | -0.293 | -0.041 | 0.390 | 0.000 | 0.000 | 0.000 |
| lightweight | 0.316 | -0.389 | -0.193 | -0.081 | 0.368 | -0.256 | 0.000 | 0.000 |
| heavy | -0.047 | 0.390 | -0.133 | 0.088 | -0.075 | 0.451 | 0.000 | 0.000 |
| very heavy | -0.294 | -0.215 | 0.458 | -0.055 | -0.305 | -0.479 | 0.000 | 0.000 |
| slow | 0.059 | -0.383 | 0.296 | 0.133 | 0.000 | -0.561 | 0.000 | 0.000 |
| fast | 0.224 | 0.256 | 0.057 | -0.299 | 0.000 | 0.282 | 0.000 | 0.000 |
| veryfast | -0.303 | 0.156 | -0.391 | 0.168 | 0.000 | 0.328 | 0.000 | 0.000 |
| unintelligent | 0.173 | 0.157 | 0.356 | 0.236 | 0.000 | 0.000 | 0.693 | -0.693 |
| avg intelligent | -0.145 | -0.309 | -0.168 | 0.125 | 0.000 | 0.000 | -0.327 | 0.327 |
| very intelligent | -0.086 | 0.125 | -0.330 | -0.491 | 0.000 | 0.000 | -0.642 | 0.642 |
| unloving | -0.366 | -0.084 | 0.030 | 0.087 | -0.462 | 0.000 | 0.000 | 0.000 |
| veryaffectionate | 0.353 | 0.081 | -0.029 | -0.084 | 0.445 | 0.000 | 0.000 | 0.000 |
| agressive | -0.170 | -0.096 | 0.162 | -0.515 | 0.000 | 0.000 | 0.000 | 0.000 |
| non agressive | 0.164 | 0.093 | -0.156 | 0.497 | 0.000 | 0.000 | 0.000 | 0.000 |
| **Nb non-zero loadings** | 16 | 16 | 16 | 16 | 8 | 6 | 3 | 3 |
| **Adjusted variance (%)** | 28.19 | 22.80 | 13.45 | 9.55 | 23.03 | 17.40 | 10.20 | 9.50 |

# Application on genetic data

## Single Nucleotide Polymorphisms

| SNP1=$X_1$ | … | SNP537=$X_{537}$ |
|---|---|---|
| AA | | AB |
| AB | | BB |
| . | . . . | . |
| . | | . |
| . | | . |
| AA | | AA |
| BB | | AA |

| SNP1=$D_{[1]}$ | | | … | SNP537=$D_{[537]}$ | | |
|---|---|---|---|---|---|---|
| AA | AB | BB | | AA | AB | BB |
| 1 | 0 | 0 | | 0 | 1 | 0 |
| 0 | 1 | 0 | | 0 | 0 | 1 |
| . | . | . | | . | . | . |
| . | . | . | . . . | . | . | . |
| . | . | . | | . | . | . |
| 1 | 0 | 0 | | 1 | 0 | 0 |
| 0 | 0 | 1 | | 1 | 0 | 0 |

**Data:**

n=502 individuals

p=537 SNPs (among more than 800 000 of the original data base, 15000 genes)

q=1554 (total number of columns)

X : 502 x 537matrix of qualitative variables

K : 502 x 1554 complete disjunctive table → K=($K_1$, …, $K_{1554}$)

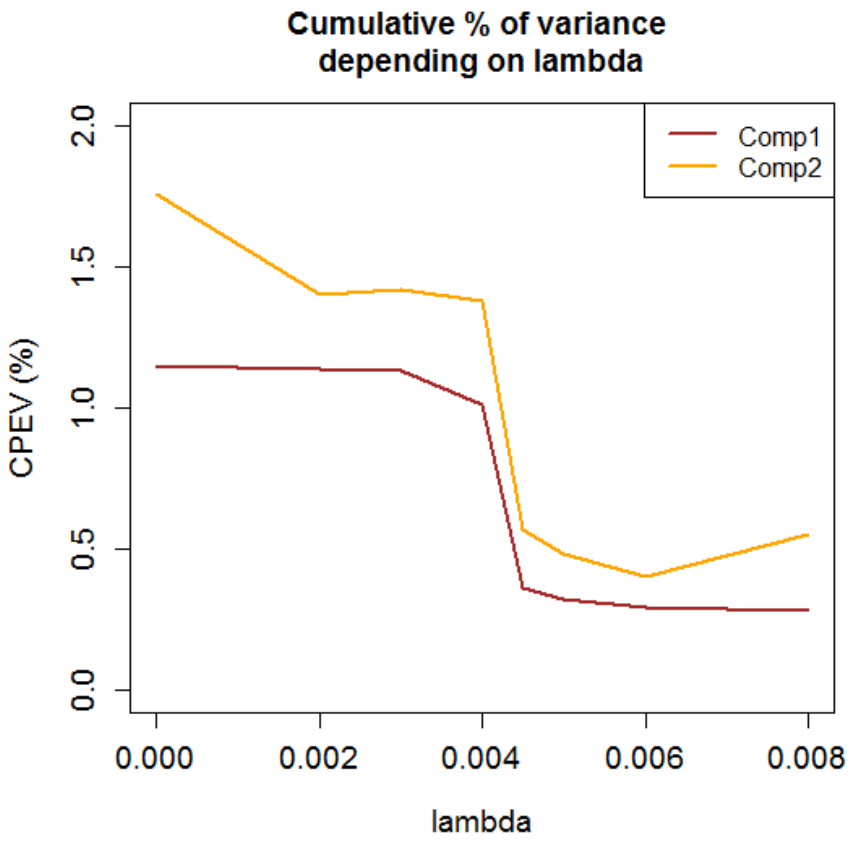
**1 block**

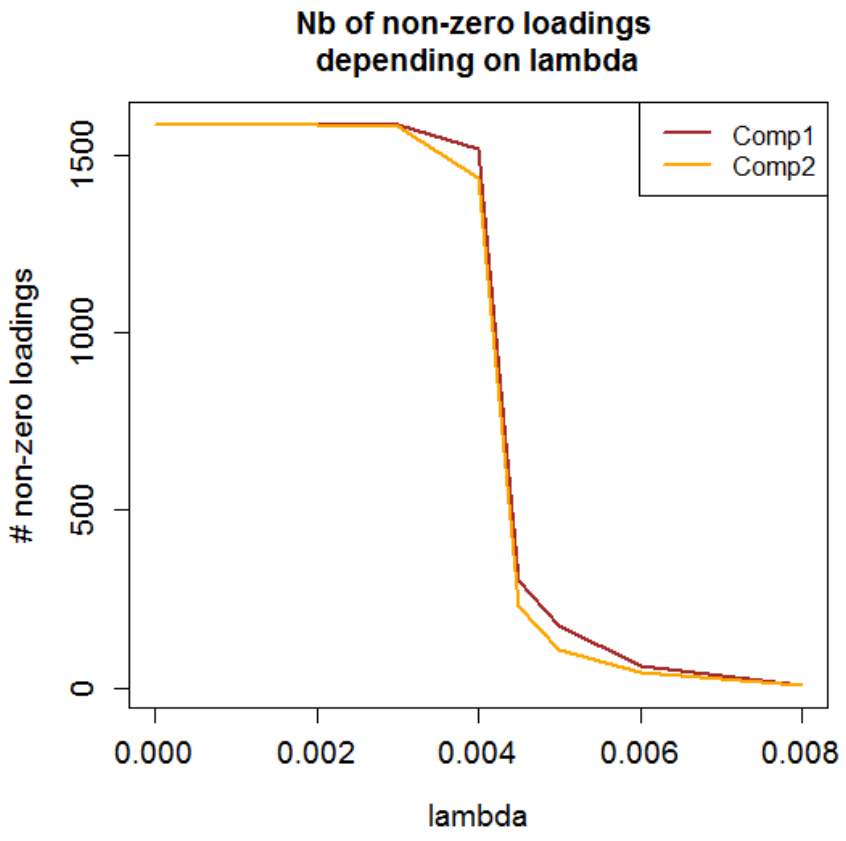
**=**

**1 SNP = 1 $K_j$ matrix**

# Application on genetic data

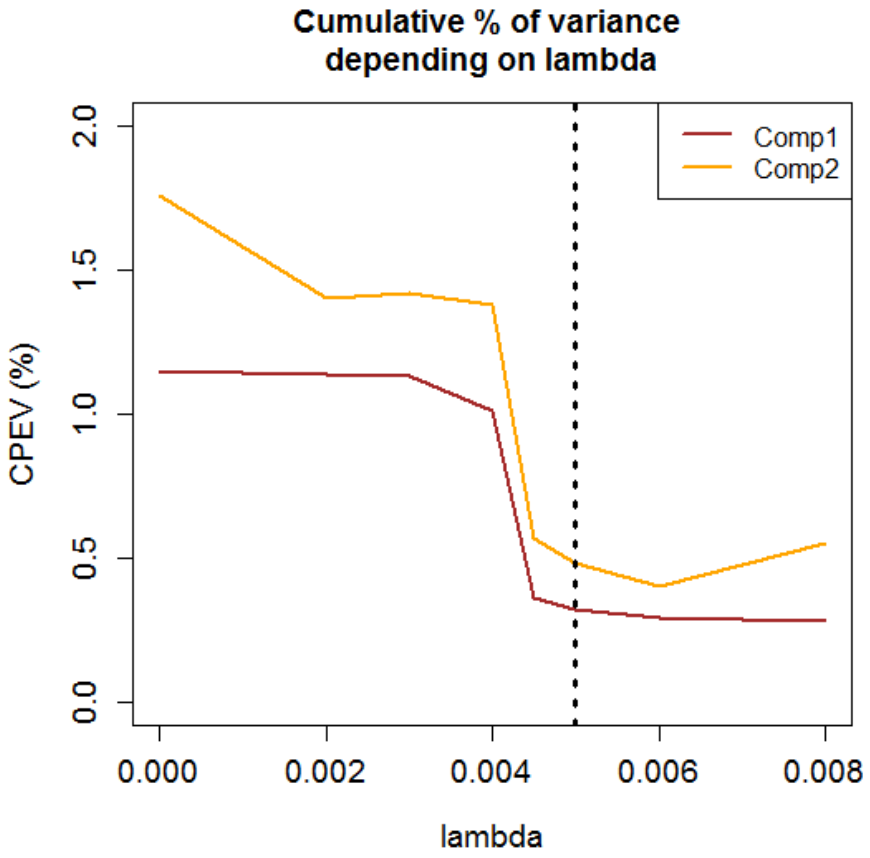
## Single Nucleotide Polymorphisms

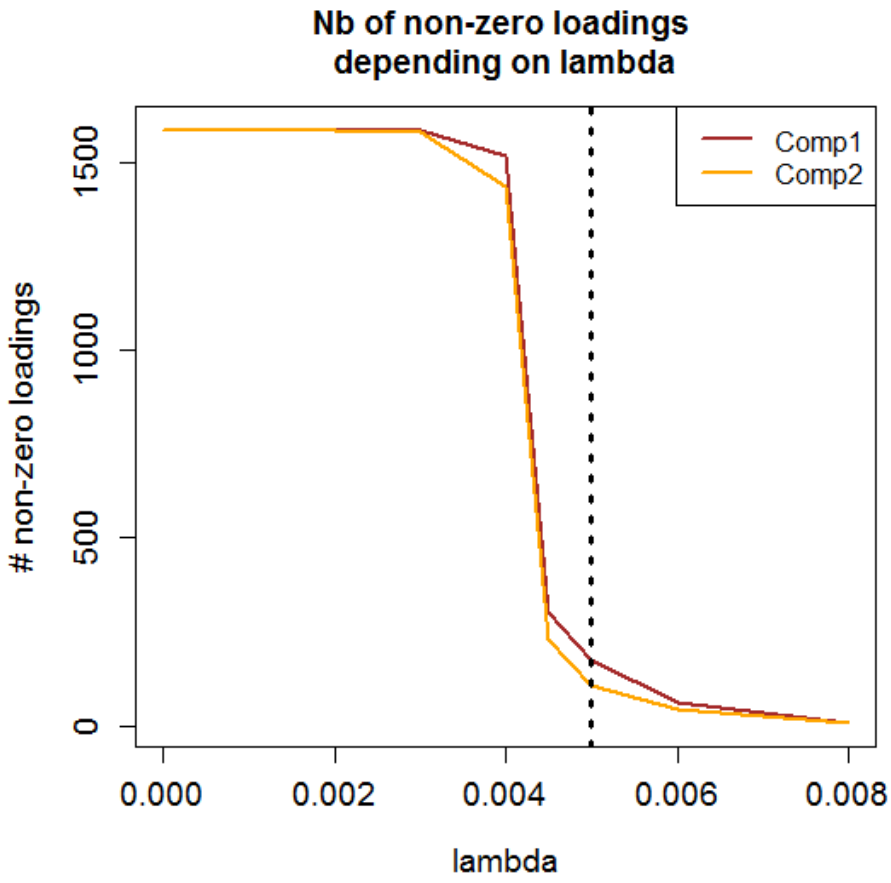


# Application on genetic data

## Single Nucleotide Polymorphisms




$\lambda$= 0:005: CPEV= 0:32% and 174 columns selected on Comp 1

# Application on genetic data

## Comparison of the loadings

| SNPs | MCA | | SMCA | |
|---|---|---|---|---|
| | Comp1 | Comp2 | Comp1 | Comp2 |
| SNP1.AA | -0.078 | 0.040 | -0.092 | 0.102 |
| SNP1.AG | -0.014 | -0.027 | -0.022 | -0.053 |
| SNP1.GG | 0.150 | -0.002 | 0.132 | -0.003 |
| SNP2.AA | -0.082 | 0.041 | -0.118 | 0.000 |
| SNP2.AG | -0.021 | -0.025 | -0.020 | 0.000 |
| SNP2.GG | -0.081 | 0.040 | -0.001 | 0.000 |
| SNP3.CC | -0.004 | 0.050 | 0.000 | 0.000 |
| SNP3.CG | 0.016 | 0.021 | 0.000 | 0.000 |
| SNP3.GG | -0.037 | -0.325 | 0.000 | 0.000 |
| SNP4.AA | 0.149 | -0.003 | 0.050 | 0.000 |
| SNP4.AG | -0.016 | -0.025 | -0.002 | 0.000 |
| SNP4.GG | -0.081 | 0.040 | -0.100 | 0.000 |
| ... | ... | ... | ... | ... |
| Nb non-zero loadings | 1554 | 1554 | 172 | 108 |
| Variance (%) | 1.14 | 0.63 | 0.32 | 0.16 |
| Cumulative variance (%) | 1.14 | 1.77 | 0.32 | 0.48 |

# 5. Conclusions and perspectives

- Sparse techniques provide elegant and efficient solutions to problems posed by high-dimensional data:
  - A new generation of data analysis methods with few restrictive hypothesis
- 2 new methods in a unsupervised multiblock data context: **Group Sparse PCA** for continuous variables, and **Sparse MCA** for categorical variables
  - Both methods produce sparse loadings structures that makes easier the interpretation and the comprehension of the results
  - Possibility of selecting superblocks (genes)

- **Research in progress**:
  - Extension of Sparse MCA to select groups and predictors within a group (sparsity within groups)
    - sparsity at both group and individual feature levels
    - compromise between Sparse MCA and sparse group lasso developed by Simon et al. (2012).
  - Sparse correspondence analysis for large contingency tables (textual data) as a special case of sparse PCA

# Thanks for your attention

# References


- Bernard, A. , Guinot, C. , Saporta, G. (2012) Sparse principal component analysis for multiblock data and its extension to sparse multiple correspondence analysis, *Compstat 2012*, pp.99-106, Limassol, Chypre,
- Bernard, A. (2013) *Développement de méthodes statistiques nécessaires à l'analyse de données génomiques*, Thèse de doctorat, CNAM
- Hastie T., Tibshirani R., Friedman J. (2009) *The elements of statistical learning*, 2nd edition, Springer, 2009
- Jolliffe, I.T. , Trendafilov, N.T. and Uddin, M. (2003) A modified principal component technique based on the LASSO*. Journal of Computational and Graphical Statistics,* **12,** 531–547,
- Rousson, V. , Gasser, T. (2004) Simple component analysis. *Journal of the Royal Statistical Society*: *Series C (Applied Statistics),* **53**,539-555
- Shen, H. and Huang, J. Z. (2008) Sparse principal component analysis via regularized low rank matrix approximation. *Journal of Multivariate Analysis*, 99:1015-1034.

- Simon, N., Friedman, J., Hastie, T., and Tibshirani, R. (2012) A Sparse-Group Lasso. *Journal of Computational and Graphical Statistics,*
- Tibshirani, R. (1996) Regression shrinkage and selection via the Lasso. *Journal of the Royal Statistical Society, Series B*, **58**, 267-288
- Vines, S.K., (2000) Simple principal components, *Journal of the Royal Statistical Society*: *Series C (Applied Statistics)*, **49**, 441-451
- Yuan, M., Lin, Y. (2007) Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society, Series B*, **68**, 49-67,
- Zou, H., Hastie , T. (2005*)* Regularization and variable selection via the elastic net. *Journal of Computational and Graphical Statistics*, **67**, 301-320,
- Zou, H., Hastie, T. and Tibshirani, R. (2006) Sparse Principal Component Analysis. *Journal of Computational and Graphical Statistics*, **15**, 265-286.
- H. Zou, T. Hastie, R. Tibshirani, (2007), On the “degrees of freedom” of the lasso, *The Annals of Statistics*, 35, 5, 2173–2192.