Variable selection with Multi-Layer Group Lasso

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Plan

Introduction

Context :

Regression analysis in high dimension ($n \ll p$)

Notations :

- $y \in \mathbb{R}^n$ response variable
- $X \in \mathcal{M}_{n,p}(\mathbb{R})$ matrix containing the values of p explanatory variables for n individuals
- $\beta \in \mathbb{R}^p$ containing k non-zero elements.

Use of penalized regression techniques to deal with high dimension.

$$\widehat{\beta}(\lambda) = \underset{\beta \in \mathbb{R}^p}{\arg\min}\{C(\beta) + \lambda \text{pen}(\beta)\}$$

with for example $C(\beta) = \|y - X\beta\|_2^2 = \sum_{i=1}^n (y_i - \sum_{j=1}^p x_{ij}\beta_j)^2$

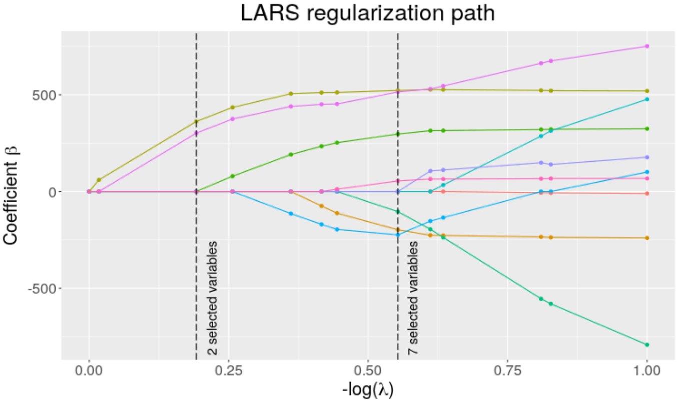
Focus on variable selection (not only prediction) to ease interpretability.

Lasso (Tibshirani, 1996 ; Efron et al., 2004)

Lasso example in the high dimension context :

$$\widehat{\beta}(\lambda) = \arg\min_{\beta \in \mathbb{R}^p} \{ C(\beta) + \lambda \mathrm{pen}(\beta) \}$$

with $\mathrm{pen}(\beta) = \|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$



Redundancy

High dimension induces linear dependence between vectors corresponding to variables, thus inducing problems associated to redundancy or correlation (e.g. instability).

The performance of classical Lasso-based approaches strongly deteriorates as the redundancy strengthens (when p grows for a given n).

Grouping variables in a first step and then selecting groups mitigates the instability default, but this usually requires either the calibration of additional parameters or knowledge of groups.

Objective of Multi-Layer Group-Lasso (MLGL) :
Select groups of correlated variables in high dimension, without knowing groups a priori.

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Multi-layer group lasso

MLGL procedure :

- building a hierarchy (HCA : hierarchical cluster analysis)
- computing the paths of groups selected by group-Lasso with respect to λ
- performing hierarchical multiple testing (HMT) to remove false positives for each λ
- tuning λ to select the final groups of influential variables.

Originality :

Exploitation of hierarchical structure of HCA and weighing in Group-lasso in order to reduce the complexity induced by the flexibility related to the possibility to choose groups from different levels of HCA.

Multi-Layer Group-Lasso

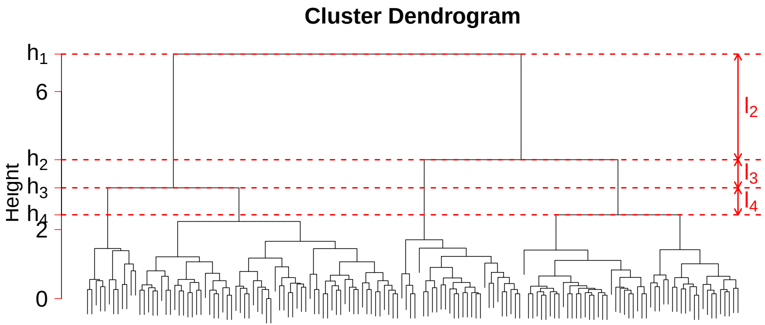
Given $\mathcal{G}_*$ the union of all the partitions at the different levels of the hierarchy $\mathcal{G}_s$ of p variables in s groups $(1 \leq s \leq p)$, we define $X^{\mathcal{G}_*} = [\underbrace{X, \ldots, X}_{p \text{ times}}]$. MLGL estimator is

$$\hat{\beta}_{\lambda}^{\mathcal{G}_*} = \underset{\beta \in \mathbb{R}^{p^2}}{\operatorname{argmin}} \left\{ \frac{1}{2} \| y - X^{\mathcal{G}_*} \beta \|_2^2 + \lambda \sum_{s=1}^{p} \rho_s \sum_{g=1}^{s} w_g^s \| \beta_{G_g^s} \|_2 \right\} \tag{1}$$

with $\lambda \geq 0$ regularisation parameter, w_{g^s} the weight associated to group G_g^s and ρ_s the weight associated to the quality of partition $\mathcal{G}_s$.

Multi-Layer Group-Lasso

Weight associated to the quality defined by the highest jump rule :
$\rho_s = \frac{1}{\sqrt{l_s}}$



Multi-Layer Group-Lasso

- reformulation of the problem such that a given group only appears once, by keeping the smallest weight
- use of classical algorithms of Group-Lasso (e.g. Yang and Zou, 2015)
- multiple testing procedure to control both multiple testing and redundancy (including a hierarchical tests procedure)
- choice of the regularisation paramater which maximises the number of rejections

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Application on the *gasoline* dataset (package pls)

Near infrared (NIR) spectra measured using diffuse reflectance from intervals. Search of wavelengths which enable to predict octane number.

- 60 observations
- 401 wavelengths

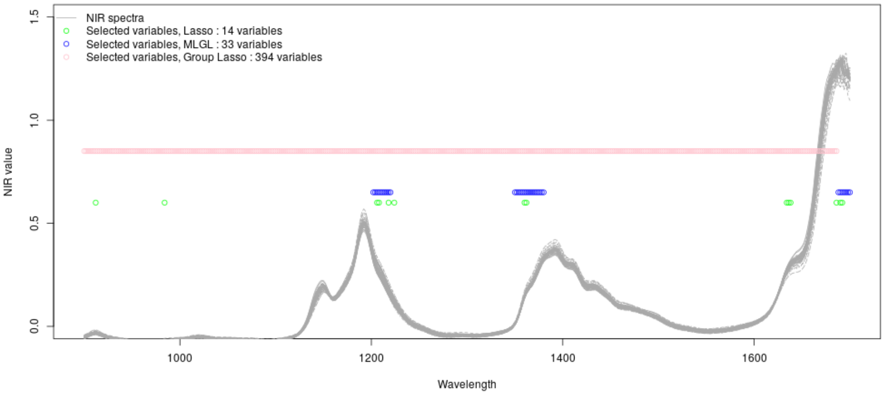
```
R> hc <- bootstrapHclust(scaleGasNIR, frac = 1, method =
"average", B = 50)
R> groupWeight <- computeGroupSizeWeight(hc, sizeMax = 100)
```

```
R> res <- fullProcess(scaleGasNIR, octane, hc = hc,
+ fractionSampleMLGL = 0.5, weightSizeGroup = groupWeight)
```

`summary` and `plot` give the main results and useful graphs to interpret the quality of the regularisation parameter choice.

Application on the *gasoline* dataset (package pls)

Comparison with Lasso and Group-Lasso



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Conclusions - Discussion

MLGL selects groups of correlated variables in high dimension, by combining hierarchical clustering and Group-Lasso.

MLGL allows different levels of the hierarchy to be selected.

The optimal value of regularisation is chosen with a hierarchical multiple testing procedure which gives a low number of rejections. Perspectives would be to improve this step.

MLGL R package is available on CRAN, and its vignette in post-processing stage for publication in Journal of Statistical Software.