

Structured variable selection with continuous shrinkage priors

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1 Introduction

- Context
- Selection
- Structure

2 Group fused horseshoe prior

3 Horseshoe Gaussian Markov field prior

4 Conclusion/Perspectives

5 Bibliography

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Context

Dependence structures between variables may be induced by various factors in different applications:

- Between **observations** in the response variable:
 - Structure in space and/or time (Dynamic linear model, state-space model, spatio-temporal model,...)
 - Structure induced by grouping factors (Linear mixed model,...)
 - ...



Figure 1: Oil palm trees from different families

Context

Dependence structures between variables may be induced by various factors in different applications:

- Between **predictors**:

- Dependence structure between genes belonging to the same biological pathways or co-expressed (Gaussian graphical model,...),
- Dependence structure between covariates collected over years,
- ...

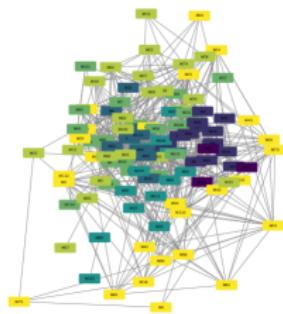


Figure 2: Gene network based on co-expressions.

Context

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- Between observations in the response variable:
 - Structure in space and/or time (Dynamic linear model, state-space model, spatio-temporal model,...)
 - Structure induced by grouping factors (Linear mixed model,...)
 - ...
- Between predictors:
 - Dependence structure between genes belonging to the same biological pathways or co-expressed (Gaussian graphical model,...),
 - Dependence structure between covariates collected over years,
 - ...

Such structures need to be taken into account into statistical models

Context

In many domains high-dimensional data are generated: the number of variables p may be greater than the number of observations n :

- Genetic/genomic studies: high-throughput technologies provide genetic/genomic information on the whole genome,
- Environmental studies: high-throughput technologies provide regular and intense monitoring of phenotypic traits over time,
- ..

Need to use statistical approaches preventing ill-posed problems (**non-invertible matrix, overfitting**) and leading to **parsimonious** models

Context

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- Between observations in the response variable:
 - Structure in space and/or time (Dynamic linear model, state-space model, spatio-temporal model,...)
 - Structure induced by grouping factors (Linear mixed model,...)
 - ...
- Between predictors:
 - Dependence structure between genes belonging to the same biological pathways or co-expressed (Gaussian graphical model,...),
 - Dependence structure between variables collected over years,
 - ...

Such structures need to be taken into account into statistical models

Linear model context

$$Y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}_n(0, \sigma^2 I_n)$$

with

- $Y = (y_1, \dots, y_n)'$ the n -vector of outcomes,,
- X the $n \times p$ matrix of predictors which may be structured and/or of high dimension,,
- $\beta = (\beta_1, \dots, \beta_p)'$ the p -vector of coefficients,
- $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)'$ the n -vector of residuals,
- σ^2 the residual variance.

↳ To estimate parameters β and σ^2

Classical regression technique

Ordinary Least Square (OLS) regression

To minimize the loss function $L^{OLS}(\beta) = \| Y - X\beta \|^2$:

$$\hat{\beta}^{OLS} = (X'X)^{-1}(X'Y)$$

But

- In presence of structures between predictors (as collinearity): $(X'X)^{-1}$ close to singularity and so, $\hat{\beta}^{OLS}$ not accurate
 - When the number of predictors is high: $\hat{\beta}^{OLS}$ does not perform well in unseen datasets (overfitting), does not provide parsimonious models (Hadamard, 1902) and in very high dimension $(X'X)^{-1}$ not invertible
- Need to use **regularization methods**

Regularization methods

Consist in introducing additional information into the problem:

- By imposing constraints as in ANOVA,
- By adding a penalty term to the minimization of the loss function as in **penalized regressions** (Ridge ([Hoerl and Kennard, 1970](#)), Lasso ([Tibshirani, 1996](#)),...),
- By specifying a dependence structure for effects of variables,
- ...

Bayesian approach: a natural framework

Bayesian approaches

In Bayesian framework additional information integrating into models via prior distributions

↪ Regularization is done by specifying **specific priors**

Selection

To shrink towards zero small coefficients while leaving large signals large: **Shrinkage** priors

Structure

Priors with a **variance-covariance matrix** related to structure information between variables

Objective:

To present **shrinkage** priors integrating **structure** information to select structured variables

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Shrinkage priors

Two classes of shrinkage priors:

- **Spike-and-slab priors:** Discrete mixture of two distributions ([Mitchell and Beauchamp, 1988; George and McCulloch, 1997](#))
- **Continuous shrinkage priors:** Unimodal continuous distributions (Bayesian Lasso prior, Horseshoe prior, Elastic-Net prior, ...) ([Kyung et al., 2010; Carvalho et al., 2008](#))

Spike-and-slab prior

- Introduction of γ :

$$\gamma_j = \begin{cases} 1 & \text{if variable } j \text{ is selected} \\ 0 & \text{otherwise} \end{cases}$$

$$\beta_j | (\gamma_j = 1) \sim p_{Slab}(\beta_j)$$

$$\beta_j | (\gamma_j = 0) \sim p_{Spike}(\beta_j)$$

- The estimation of $\mathbb{P}(\gamma_j = 1 | Y)$ gives access to the a posteriori probability of variable selection

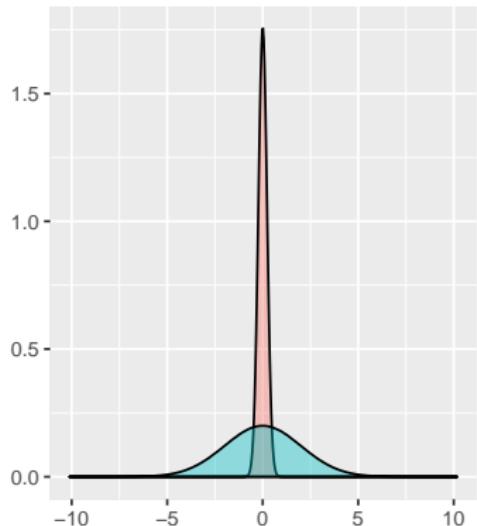


Figure 3: Spike-and-Slab prior distribution. Slab part in blue and spike part in red

Continuous shrinkage prior

Bayesian version of penalized approaches:

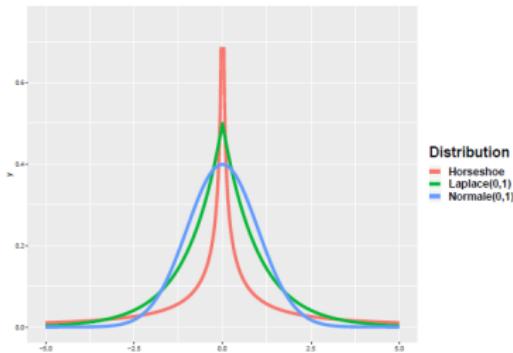
$$\beta_j | \tau^2, \omega_j \sim \mathcal{N}(0, \tau^2 \omega_j^2) \quad j = 1, \dots, p$$

$$\tau^2, \omega_j^2 \sim \mathcal{F}(\tau^2; \omega_j^2)$$

where

- \mathcal{F} is a distribution to specify
 - ↪ Bayesian Lasso prior,
 - Global-local priors**, ...

Figure 4: Continuous shrinkage prior distributions



Horseshoe prior (Carvalho et al., 2009)

A global-local prior with $\tau \sim \mathcal{C}^+(0, 1)$ and $\omega_j \sim \mathcal{C}^+(0, 1) \quad j = 1, \dots, p$

- τ controls the global shrinkage
- ω_j controls the individual shrinkage: allows large signals to escape from the overall shrinkage

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Structure

$$Y = X_1\beta_1 + \cdots + X_p\beta_p + \varepsilon, \quad \varepsilon \sim \mathcal{N}_n(0, \sigma^2)$$

- X the $n \times p$ matrix of predictors which may be structured and/or of high dimension,
- ↪ $\beta = (\beta_1, \dots, \beta_p)'$ $\sim \mathcal{N}_p(0, \Sigma)$ with Σ related to structure between variables

↪ **Context dependent**

Examples

- $X_{t-1} \not\perp \!\!\! \perp X_t$: $\Sigma = AR(\rho)$ with ρ autoregressive parameter
- X_i 's belong to a same group (pathways in genomic, genes in genetic, ...)

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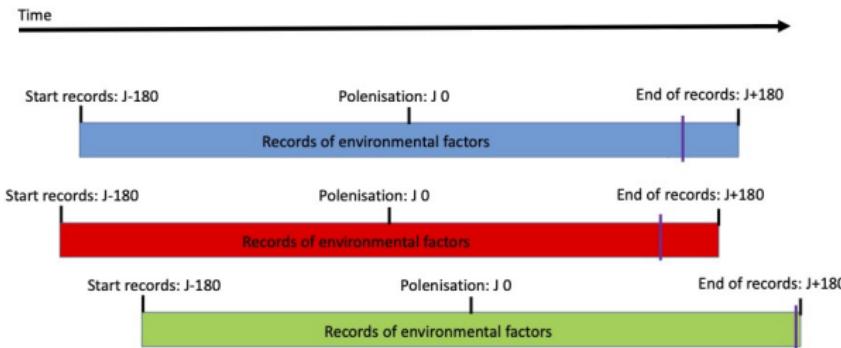
Biological motivation

Objective: to understand the impact of environmental variables on the process of fruit abscission in oil palm.

Dataset provided by "le Centre de Recherches Agricoles-Plantes Pérennes (CRA-PP)" ([Tisné et al., 2020](#))



Oil palm: fruit abscission process

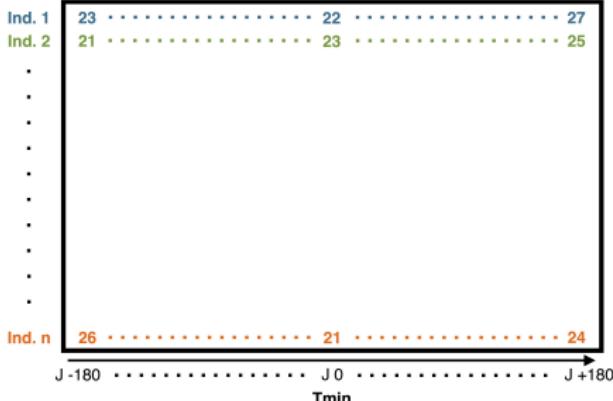


- **Climatic factors:**

Temperature, rainfall, ...

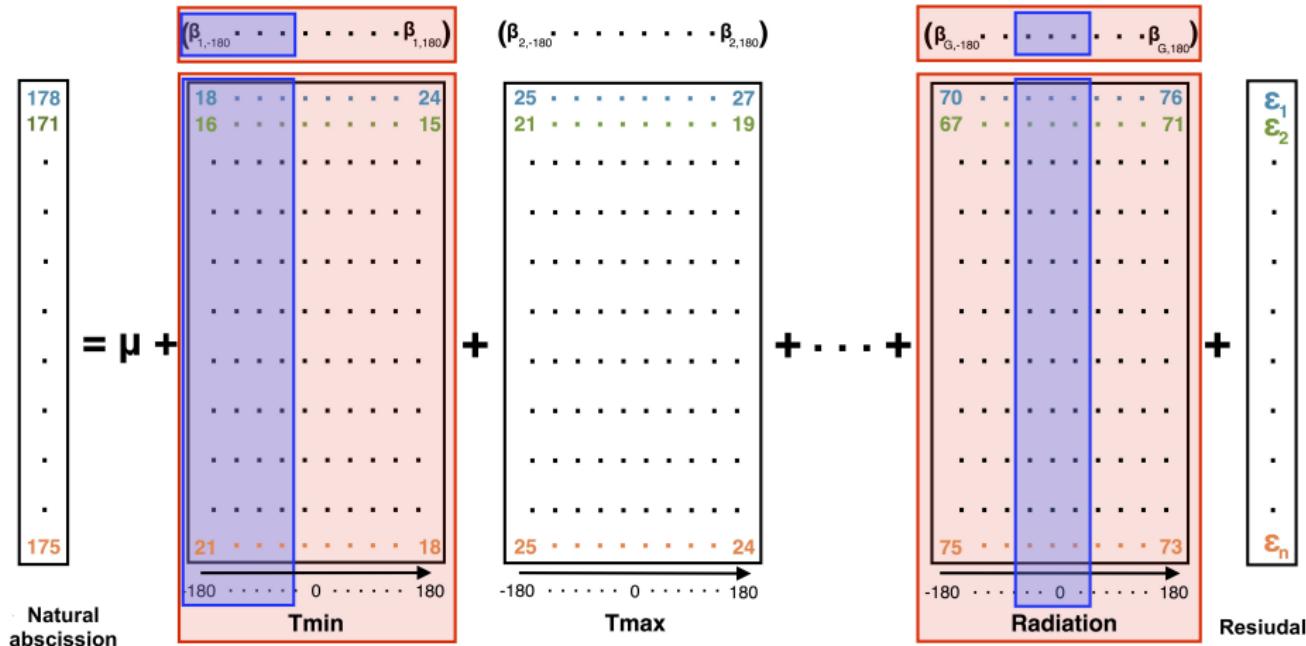
- **Ecophysiological factors:**

Evapotranspiration, photosynthesis, ...



Oil palm: fruit abscission process

To identify the **environmental variables** and the **time periods** affecting the oil palm fruit abscission process



Statistical questions

Linear model:

$$\mathbf{y} = \mu + \sum_{g=1}^G \mathbf{X}_g \boldsymbol{\beta}_g + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}_n(0, \sigma^2 I_n)$$

Selection:

- To identify **environmental variables** → Selection of grouped variables
↳ Selection of grouped parameters: $(\beta_{g,-180}, \dots, \beta_{g,180})' = (0, \dots, 0)'$?
- To identify **time periods** → Selection of variables
↳ Selection of parameters $\beta_{g,t} = 0$?

Double structure:

- Grouped variables
↳ Integration of group structure
- Repeated measures over time for each environmental variables
↳ High correlation between successive variables: to integrate natural order of variables on regression coefficients $\boldsymbol{\beta}_g = (\beta_{g,-180}, \dots, \beta_{g,180})'$

Group fused horseshoe prior

To combine the horseshoe and the fused (Tibshirani et al., 2005) priors.

$$\beta_g | \tau^2, \lambda_g^2, \omega_g^2, v_g^2, \sigma^2 \sim \mathcal{N}_T \left(0, \sigma^2 \left(\frac{\mathbf{D}'_g \Omega_g^{-1} \mathbf{D}_g}{\tau^2 \lambda_g^2} + \boldsymbol{\Upsilon}_g^{-1} \right)^{-1} \right)$$

$$\tau, \lambda_g, \omega_{g,t}, v_{g,t} \sim \mathcal{C}^+(0, 1)$$

1st matrix: to penalize differences while allowing abrupt changes

- τ^2 : global hyperparameter
- λ_g^2 : local hyperparameters specific to each group (environmental variables)
- $\omega_{g,t}^2$: local hyperparameter specific to difference $\beta_{g,t+1} - \beta_{g,t}$

2nd matrix: to add an additional level of penalization to shrink towards zero small effects

- $v_{g,t}^2$ local hyperparameter specific to the effect $\beta_{g,t}$

→ Extension of priors: *sparse group horseshoe* (Xu et al., 2016), *fusion horseshoe* (Faulkner and Minin, 2018), *fused Laplace* (Kyung et al., 2010)

Inference: Gibbs algorithm (Markov chain Monte Carlo method). R code available at: <https://github.com/Heuclin/GroupFusedHorseshoe>

Simulation study

- Different profiles over time:
smooth or with abrupt changes
- Comparisons with usual
approaches:
- Sparse PLS, Elastic-net, Penalized
regression with composite MCP
penalty, Penalized regression with
composite MCP + ridge

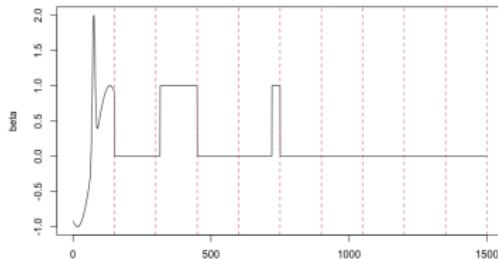


Figure 6: Simulated profiles for $G=10$ groups over $T=150$ time points

Results

- Group fused horseshoe outperforms other approaches in terms of selection, estimation, and prediction
- Robust: no sensitive to the ratio sample size / number of variables
- Stable: low variability between repetitions

Application on oil palm

Data

- 1,173 bunches (statistical unit)
- Outcome (y): number of days from pollination to fruit drop
- 5 climatic variables: Tmax, Tmin, Relative air humidity (RH), Rainfall (R), Solar radiation (SR)
- 5 ecophysiological variables: Maximum daily vapor pressure deficit (VPD), Fraction of transpirable soil water (FTSW), Supply-demand ratio (SD), Daily reproductive demand (DRD)
- 121 time points for each environmental variables: $p = 1,210$ predictors greater than $n = 1,173$ observations

Application on oil palm

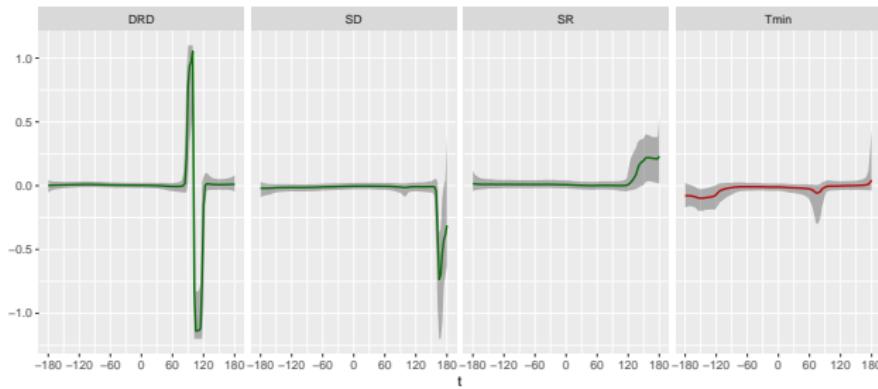


Figure 7: Estimated coefficient profiles for DRD, SD, SR, Tmin. Gray shadows represent the 95% credible interval.

- Identification of 4 environmental variables: DRD, SD, SR, Tmin
- Identification of relevant time periods
 - Tmin: smooth effect during the inflorescence development
 - DRD and SD: punctual effects at the end of the fruit bunch development
 - SR: smooth effect at the end of the fruit bunch development

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Motivations

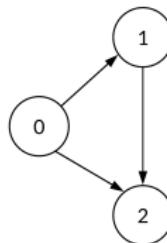
Most of the dependence structures between variables may be encoded by an undirected graph

Undirected graph

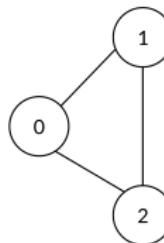
A **graph** is a pair $\mathcal{G} = (V, E)$ where $V = \{1, \dots, p\}$ is a finite set of vertices (nodes), and the set of edges E is a subset of the set $V \times V$. Two types of commonly used graphs:

- **directed graph** where edges are denoted by ordered pairs $(i, j) \in E$
- **undirected graph** where edges are denoted by unordered pairs $(i, j) \in E \iff (j, i) \in E$.

Directed Graph



Undirected Graph

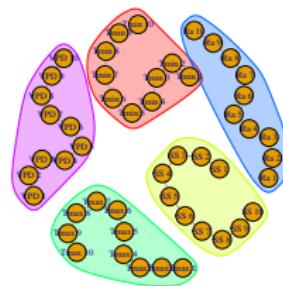


Motivations

Most of the dependence structures between variables may be encoded by an undirected graph

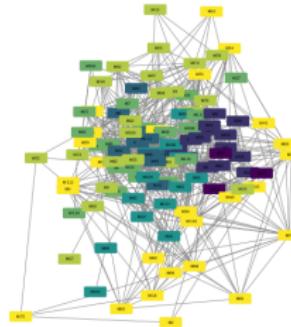
Fruit abscission process

- nodes = climatic variables
- edges = linked when temporally dependent



Gene network

- nodes = genes
- edges = linked when co-expressed



Proposed model

We propose to extend the approach proposed by [Faulkner and Minin \(2018\); Faulkner \(2019\)](#) to the more general context of graph-structured variables by combining:

- ➊ The **efficiency and flexibility** of the horseshoe (HS) prior in terms of selection and estimation:
- ➋ With a Gaussian Markov random field (GMRF) for its **appealing connection** with undirected graphs ([Rue and Held, 2005](#)):
 - allows to impose the dependence structure between the parameters via the precision matrix of a conditionally Gaussian prior thus leading to sparse matrices and to smooth coefficients over the graph with possible abrupt changes

Focus on the appealing connection of GMRF with undirected graphs

In a Gaussian assumption, conditional independence is implied by the form of the precision matrix:

Fruit abscission process

- nodes = climatic variables
- edges = linked when temporally structured

For each environmental variable the structure of the precision matrix is given by:

$$\mathbf{B} = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & \dots & 1 & 1 \end{pmatrix}$$

The global structure of the precision matrix is a block diagonal matrix given by :

$$\begin{pmatrix} \mathbf{B} & & & & 0 \\ \vdots & \mathbf{B} & & & \vdots \\ & & \mathbf{B} & & \\ & & & \mathbf{B} & \\ 0 & & \dots & & \mathbf{B} \end{pmatrix}$$

Bayesian hierarchical model

We assume that $\mathcal{G} = \bigcup_{i=1}^I \mathcal{G}_i = \bigcup_{i=1}^I (V_i, E_i)$ a disjoint union of I subgraphs and \mathcal{S} the set of indices associated to one representative of each of the I subgraphs.

HS-GMRF model

$$\mathbf{y} | \boldsymbol{\beta}, \sigma^2 \sim \mathcal{N}_n(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n)$$

$$\beta_j - s_{jj'}\beta_{j'}|\tau_{jj'}^2, \lambda^2 \sim \mathcal{N}(0, \lambda^2 \tau_{jj'}^2) \text{ for } (j, j') \in \bigcup_{i=1}^I E_i$$

$$\beta_j |\tau_j^2, \lambda^2 \sim \mathcal{N}(0, \lambda^2 \tau_j^2) \text{ for } j \in \mathcal{S}$$

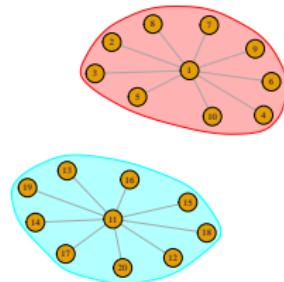
$$\tau_{jj'} \sim \mathcal{C}^+(0, 1) \text{ for } (j, j') \in \bigcup_{i=1}^I E_i; \tau_j \sim \mathcal{C}^+(0, 1) \text{ for } j \in \mathcal{S}$$

$$\lambda | \sigma \sim \mathcal{C}^+(0, \sigma); \sigma^2 \sim \text{IG}(a_0, b_0)$$

with $s_{jj'} = \text{sign}\{\text{cor}(X_j, X_{j'})\}$ to encourage regression coefficients of negatively correlated variables to take opposite signs.

Simulation study

- Different graphs: highly or moderately connected
- Comparisons with HS and spike-and-slab with Ising prior (structure information at the variable indicator level) and when the sample correlation sign is considered or not



Results

HS-GMRF-based approaches lead to the best results in terms of selection, estimation, and prediction:

- HS-GMRF outperforms HS-GMRF-nosign especially when $\rho = 0.9$
- Performances for non-connected predictors are similar for HS and HS-GMRF-based approaches
- For connected variables the integration of the dependence structure helps to select variables with small effects

Application

Objective

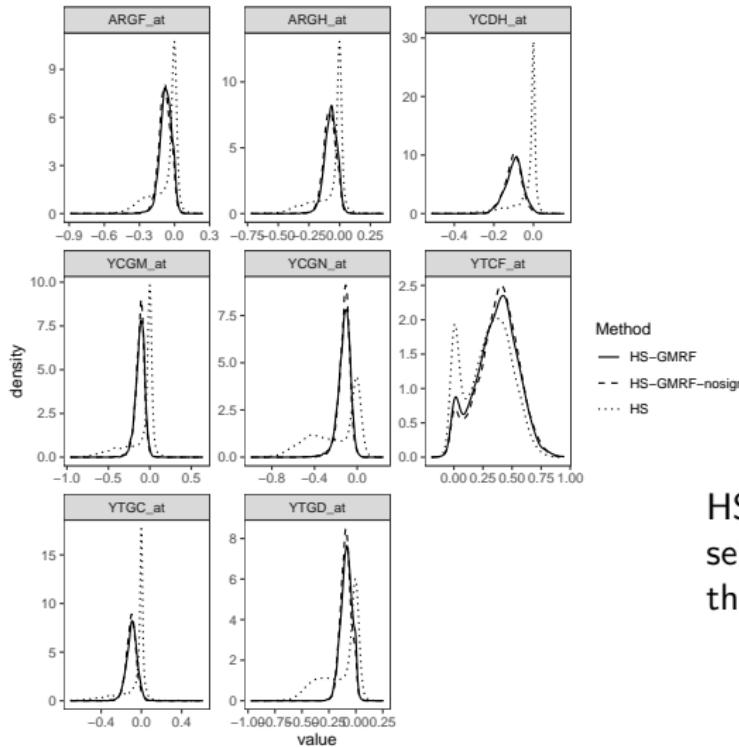
To identify gene expressions involved in the variability of riboflavin production using data on 71 samples

- A total of 142 gene expressions considered
- Estimation of an undirected graph with 157 edges
- 5-fold cross-validation procedure

| Methods | CV-MSPE | Selected genes |
|----------------|-------------|--|
| HS-GMRF | 0.29 | 4 (90% HPD) 8 (80% HPD) |
| HS-GMRF-nosign | 0.31 | 4(90% HPD) 6 (80% HPD) |
| HS | 0.33 | 0(90% HPD) 0 (80% HPD) |
| SS-Ising | 0.37 | 21 ($PPI > 0.5$) 16 ($PPI > 0.8$) |
| Lasso | 0.41 | 16 |

→ HS-GMRF yields the smallest CV-MSPE

Application



For moderate non-zero effects:

- HS estimates densities concentrated around 0 with long tails or bimodal densities with one of the modes around 0,
- HS-GMRF-based methods estimate unimodal densities or bimodal densities with the mode around 0 less than with HS.

HS-GMRF-based approaches select groups of genes involved in the same biological pathway.

Application

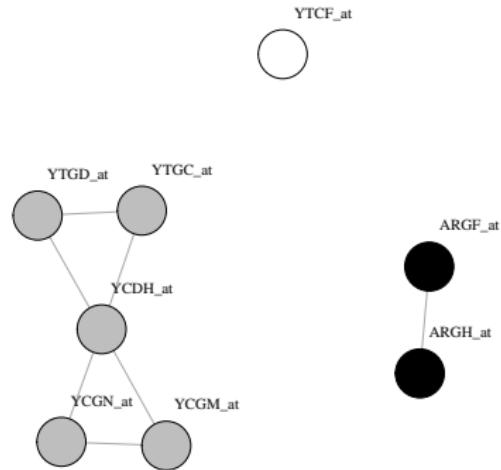


Figure 8: The estimated network

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Conclusion

Two priors proposed to select structured variables:

- Efficient combination and extension of existing approaches to deal with high-dimensional structured predictors,
- Flexibility and efficiency of horseshoe prior, via the local and global shrinkage hyperparameters, to handle different structures and to select relevant variables and/or groups of variables,
- Encompass a broad type of dependence structures : applicable in various applications (varying coefficient models, near infrared spectroscopy context (NIRS), QTL mapping, ...)

Perspectives

- To integrate prior knowledge on strengths of connections,
- To integrate dependence structures between observations,
- To extend to multivariate case (Y multivariate),
- To consider a multi-dimensional indexation.

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