Global-local shrinkage prior for variable selection in graph-structured models.

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Context

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

- Disease mapping: structure in space and time for variables measured over time at adjacent locations,
- Genomic studies: dependence structure between genes obtained from biological pathways or inferred computationally (e.g., based on co-expression),

$\hookrightarrow$ Most of the dependence structures between variables may be encoded by an undirected graph $\mathcal{G}$.

Objective:

To develop a unified Bayesian variable selection for graph-structured variables providing flexibility in the amount of shrinkage and smoothness over the graph.

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From a statistical point of view

Why incorporate the dependence structure into statistical models?

- helps the model building process,
- increases power to detect associations,
- improves the predictive power.

Why incorporate the dependence structure into variable selection methods?

- It encourages the identification of groups of dependent variables acting jointly on the response, especially those with subtle individual effects.

How to incorporate the dependence structure into variable selection methods?

- Penalized likelihood approaches
- Bayesian regularization via the specification of shrinkage priors.

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The proposed approach

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

1. The **efficiency and flexibility** of the Horseshoe (HS) (Carvalho et al., 2010) prior (global-local shrinkage prior) in terms of selection and estimation,
2. The **appealing connection** between Gaussian Markov random field (GMRF) and undirected graphs (nonzero elements in the precision matrix correspond to edges in the graph) (Rue and Held, 2005).

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Bayesian hierarchical models

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

$$
\begin{aligned}
y|\beta, \sigma^2 &\sim \mathcal{N}_n(X\beta, \sigma^2 I_n) \\
\beta_j - \beta_{j'}|\tau_{jj'}^2, \lambda^2 &\sim \mathcal{N}(0, \lambda^2\tau_{jj'}^2) \text{ for } (j, j') \in \bigcup_{i=1}^{I} E_i \\
\beta_j|\tau_j^2, \lambda^2 &\sim \mathcal{N}(0, \lambda^2\tau_j^2) \text{ for } j \in \mathcal{S} \\
\tau_{jj'} &\sim \mathcal{C}^+(0, 1) \text{ for } (j, j') \in \bigcup_{i=1}^{I} E_i \\
\tau_j &\sim \mathcal{C}^+(0, 1) \text{ for } j \in \mathcal{S} \\
\lambda|\sigma &\sim \mathcal{C}^+(0, \sigma), \ \sigma^2 \sim \mathcal{IG}(s, r)
\end{aligned}
$$

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Bayesian hierarchical models

To encourage the regression coefficients estimates to have opposite signs for situations where connected covariates have negative correlation

$\Rightarrow$ We propose to incorporate the sign of the sample correlation such that:

HS-GMRF-sign model

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

with $\eta_{jj'}$ the sign of the correlation between covariates j and j'

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MCMC implementation

MCMC implementation

A Gibbs sampling algorithm is straightforward used to fit the hierarchical models:

- by using the parametrization of a half-Cauchy as a mixture of inverse-gamma distributions, (Makalic and Schmidt, 2016),
- by introducing a q-dimensional vector $\phi = (\phi_1, \ldots, \phi_q)' = C\beta$ where $q = |E| + |\mathcal{S}|$ and C is a contrast matrix such that:

$$\phi \sim \mathcal{N}_q(0, \Sigma_\phi),$$

with $\Sigma_\phi = \text{diag}(\lambda^2 \boldsymbol{\tau}^2)$.

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Simulation studies

Objectives

- To evaluate the performances of the proposed approaches,
- To compare the results with two other approaches: the HS and the spike-and-slab with Ising prior (SS-Ising) (Smith and Fahrmeir, 2007; Li and Zhang, 2010).

$$Y = \sum_{g=1}^{G} \mathbf{X_g} \beta_g + \varepsilon \text{ with } X_{i,g} = (X_{i;g1}, \dots, X_{i;gk})' \sim \mathcal{N}_k(0, \Sigma_g) \text{ and } \varepsilon \sim \mathcal{N}_n(0, \sigma^2 I_n)$$

12 simulated scenarios

- Two covariance structures
- Two levels of correlation ($\rho = 0.5, 0.9$)
- Three regression coefficients

↬ Focus on the scenario where the half of groups with Σ_g and the rest independent, and with

$$\beta_g = (5, -\tfrac{5}{\sqrt{10}}, -\tfrac{5}{\sqrt{10}}, \underbrace{\frac{5}{\sqrt{10}}, \dots, \frac{5}{\sqrt{10}}}_{k-3})$$

Simulations:

- $n = 100$, $p = 140$
- $G = 14$ groups of $k = 10$ predictors,
- only the groups $g = 1, 3, 5, 8, 10$ have non-zero effects,
- $\sigma^2 = \sum_{g=1}^{G} \beta_g^2 / 5$
- repetitions: 50

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Simulation results

Performance criteria

- Variable selection criteria:
  - For HS-based: variable selected if 95% HPD interval does not contain 0,
  - For SS-Ising: variable selected if marginal inclusion posterior probabilitie greater than 0.5.
- Matthews correlation coefficient (MCC),
- Mean squared error (MSE) of the regression coefficients,
- Mean squared prediction error (MSPE).

MCMC settings:

- iterations : 6000,
- burn-in: 1000.

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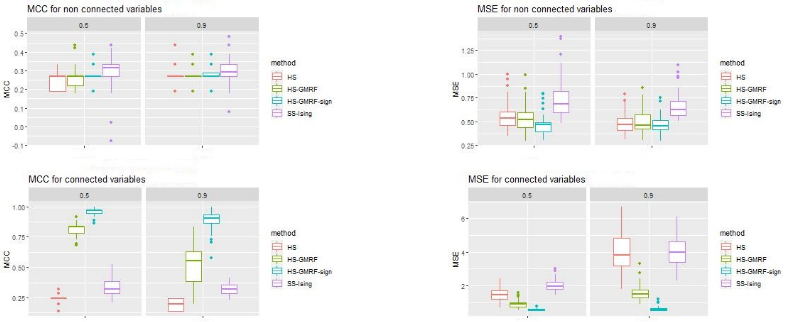
Results



- HS-GMRF-based approaches lead to the best results in terms of MCCs and MSEs with HS-GMRF-sign outperforming the other methods,
- Performances for non-connected predictors are similar for HS and HS-GMRF-based approaches.

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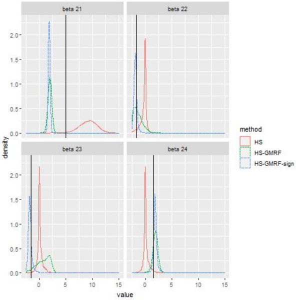
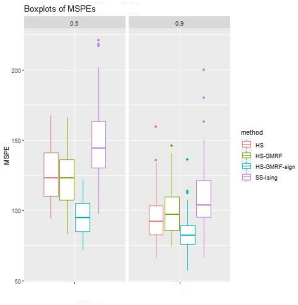
Results





- Posterior densities of β:
  - HS tends to select one representative of a group of correlated variables,
  - HS-GRMF-based approaches encourage similar values for connected variables,
- For predictive performance when correlated variables of effects of different signs: HS-GMRF-sign gives better results.

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Results with estimated graphs

In situations where the true graph structure is not known.

- For a moderate level of correlation: graph is underestimated $\Rightarrow$ slightly poorer selection and estimation,
- For a high level of correlation: graph is overestimated $\Rightarrow$ improved selection and estimation.

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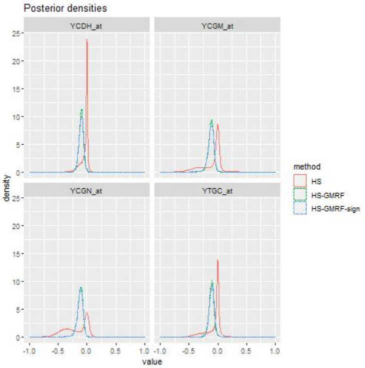
Application

Objective: To identify genes involved in the variability of riboflavin production

Data/Settings

- 71 samples, 142 gene expression
- Undirected graph with 157 edges,
- 5-fold cross-validation procedure.

Methods	MSPEs
HS	0.33
HS-GMRF	0.31
HS-GMRF-sign	0.29
SS-Ising	0.37



↬ selection of groups of correlated variables

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Conclusion/Perspective

The proposed approaches allow to:

- consider a broad type of dependence structures,
- achieve flexibility in the estimation and the selection due to the local and global shrinkage hyperparameters,
- need to consider the sign of the sample correlation,
- give better predictive performances notably by selecting groups of connected variables,
- give good results even when true graph is unknown and needs to be estimated.

Limitation:

- tend to encourage similar values fo connected variables, especially for highly correlated variables or overestimated graphs.

For future research:

- Extension to non-Gaussian distributions,
- Integration of prior knowledge on strengths of connections between variables.

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Outline

1. Bibliography

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