# New Directions in Bayesian Shrinkage for Sparse and Structured Data 

Jyotishka Datta

September 14, 2021
Virginia Tech

## Outline of My Talk

## New Directions in Bayesian Shrinkage for Sparse and Structured Data

Part I: Global-Local Shrinkage: Overview

1. Sparse signal recovery
2. Horseshoe prior
3. Optimality properties
4. Global-local family

Part II: New Directions

1. Grouped sparsity/shrinkage
2. Precision matrix estimation
3. Future directions

## Global-Local Shrinkage: A Brief Overview

## Common Theme: High-dimensional Data

Sparsity: Needles in haystack!

## High-dimensional Inference

Normal Means: $\left(Y_{i} \mid \theta_{i}\right) \stackrel{\text { ind }}{\sim} \mathcal{N}\left(\theta_{i}, \sigma^{2}\right), i=1, \ldots, n$,
Regression: $\mathbf{Y}=\mathbf{X} \boldsymbol{\theta}+\boldsymbol{\epsilon}, p \gg n, \boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \sigma^{2} \mathbf{I}\right)$.
Sparsity: $\theta \in \ell_{0}\left[p_{n}\right] \equiv\left\{\theta: \#\left(\theta_{i} \neq 0\right) \leq p_{n}\right\}, p_{n} / n \rightarrow 0$


Theoretical Model
Fitted Model
$y=\beta_{0}+\beta_{1} X_{1}+\cdots \beta_{p} X_{p}+\epsilon$
$\hat{y}=\hat{\beta}_{0}+\hat{\beta}_{1} X_{1}+\cdots \hat{\beta}_{p} X_{p}$

## High-dimensional Inference

Normal Means: $\left(Y_{i} \mid \theta_{i}\right) \stackrel{\text { ind }}{\sim} \mathcal{N}\left(\theta_{i}, \sigma^{2}\right), i=1, \ldots, n$,
Regression: $\mathbf{Y}=\mathbf{X} \boldsymbol{\theta}+\boldsymbol{\epsilon}, p \gg n, \boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \sigma^{2} \mathbf{I}\right)$.
Sparsity: $\theta \in \ell_{0}\left[p_{n}\right] \equiv\left\{\theta: \#\left(\theta_{i} \neq 0\right) \leq p_{n}\right\}, p_{n} / n \rightarrow 0$


$$
\begin{array}{cc}
\text { Theoretical Model } & \text { Fitted Model } \\
y=\beta_{0}+\beta_{1} X_{1}+\cdots \beta_{p} X_{p}+\epsilon & \hat{y}=\hat{\beta}_{0}+\hat{\beta}_{1} X_{1}+\cdots \hat{\beta}_{p} X_{p}
\end{array}
$$

Grouped covariates: $\mathbf{y} \sim \mathcal{N}\left(\boldsymbol{C} \alpha+\sum_{g=1}^{G} \boldsymbol{X}_{g} \boldsymbol{\beta}_{g}, \sigma^{2} \boldsymbol{I}_{n}\right)$ where $g=1, \ldots, G$ indexes the groups.
Precision matrix: $\mathbf{X}^{(n)} \sim \mathcal{N}_{p}(\mathbf{0}, \boldsymbol{\Sigma})$, Estimate $\boldsymbol{\Omega}=\boldsymbol{\Sigma}^{-1}$.

## Goals:

1. Recovery: provide estimator $\hat{\boldsymbol{\theta}}$ or $\hat{\boldsymbol{\Omega}}$.
2. Multiple Testing: Test whether each $\theta_{i}\left(\right.$ or $\left.\omega_{i j}\right)$ is zero or non-zero.
3. Variable selection.
4. Prediction.

## The Two-groups Model i

- Natural hierarchical Bayesian solution: two-groups model.

1. Assume each $\theta_{i}$ is non-zero with a prior probability $\pi$, and the non-zero $\theta_{i}$ 's come from a common density $f_{A}(\cdot)$.
2. Use Bayes' rule to calculate posterior probabilities that each $\theta_{i} \sim f_{A}(\cdot)$.

- Automatically adjusts for multiplicity and sparsity without any regularization.
- Carry out tests using the posterior inclusion probabilities (PIP).

$$
\text { Posterior Inclusion Probability }=\omega_{i}=P\left(\theta_{i} \neq 0 \mid y_{i}\right)
$$

- Induce sparsity through a 'spike and slab' prior.


## The Two-groups Model ii

- Spike \& Slab

$$
\begin{aligned}
& Y_{i} \sim \mathcal{N}\left(\theta_{i}, \sigma^{2}\right), i=1, \ldots, n \\
& \theta_{i} \sim(1-p) \underbrace{\delta_{\{0\}}}_{\text {Spike }}+p \overbrace{\mathcal{N}\left(0, \psi^{2}\right)}^{\text {Slab }}
\end{aligned}
$$

Multiple testing:

$$
H_{0 i}: \theta_{i}=0 \text { vs. } H_{A i}: \theta_{i} \neq 0, i=1, \ldots, n .
$$

- Need (latent) indicators for MCMC:

$$
\gamma_{i}= \begin{cases}0 & \text { if } \theta_{i}=0 \\ 1 & \text { if } \theta_{i} \neq 0\end{cases}
$$

- $\gamma$ indexes $2^{\text {model dimension }}$ possible models: exploring the full posterior is computationally expensive.


## Towards the one-group model $\mathbf{i}$

- The two-groups model leads to a shrinkage rule linear in $y_{i}$.
- If $\theta_{i} \sim(1-p) \delta_{\{0\}}+p \mathcal{N}\left(0, \psi^{2}\right)$, the posterior mean is:

$$
\begin{equation*}
\mathbb{E}\left(\theta_{i} \mid y_{i}\right)=\omega_{i} \frac{\psi^{2}}{1+\psi^{2}} y_{i}=\omega_{i}^{*} y_{i} \tag{1}
\end{equation*}
$$

where $\omega_{i}$ is the posterior inclusion probability $P\left(\theta_{i} \neq 0 \mid y_{i}\right)$.

- If $\psi^{2} \rightarrow \infty$ as the number of tests $n \rightarrow \infty$ :

$$
\left.E\left(\theta_{i} \mid y_{i}\right) \approx \omega_{i} y_{i} \text { (linear in } y_{i}\right)
$$

- The one-group model takes a different route:
- Directly models the posterior inclusion probability $\omega_{i}$


## The One-group model

Global-local shrinkage priors: Horseshoe [Carvalho et al., 2010]

$$
\begin{aligned}
& Y_{i} \mid \theta_{i} \sim \mathcal{N}\left(\theta_{i}, \sigma^{2}\right) ; \quad \theta_{i} \mid \lambda_{i} \sim \mathcal{N}\left(0, \lambda_{i}^{2} \tau^{2}\right) \\
& \underbrace{\lambda_{i}}_{\text {local }} \stackrel{\text { ind }}{\sim} \mathcal{C}^{+}(0,1), \underbrace{\tau}_{\text {global }} \sim \mathcal{C}^{+}(0, \sigma) \quad \text { (Heavy-tailed prior) }
\end{aligned}
$$

Posterior mean:
$\mathbb{E}\left(\theta_{i} \mid y_{i}\right)=\left\{1-\mathbb{E}\left(1 / 1+\lambda_{i}^{2} \tau^{2} \mid y_{i}\right)\right\} y_{i} \doteq\left(1-\mathbb{E}\left(\kappa_{i} \mid y_{i}\right)\right) y_{i}$.

## The One-group model

Global-local shrinkage priors: Horseshoe [Carvalho et al., 2010]

$$
\begin{aligned}
Y_{i} \mid \theta_{i} & \sim \mathcal{N}\left(\theta_{i}, \sigma^{2}\right) ; \quad \theta_{i} \mid \lambda_{i} \sim \mathcal{N}\left(0, \lambda_{i}^{2} \tau^{2}\right) \\
\underbrace{\lambda_{i}}_{\text {local }} & \stackrel{\text { ind }}{\sim} \mathcal{C}^{+}(0,1), \underbrace{\tau}_{\text {global }} \sim \mathcal{C}^{+}(0, \sigma) \text { (Heavy-tailed prior) }
\end{aligned}
$$

Posterior mean:
$\mathbb{E}\left(\theta_{i} \mid y_{i}\right)=\left\{1-\mathbb{E}\left(1 / 1+\lambda_{i}^{2} \tau^{2} \mid y_{i}\right)\right\} y_{i} \doteq\left(1-\mathbb{E}\left(\kappa_{i} \mid y_{i}\right)\right) y_{i}$.

| Two-groups Model | One-group Model |
| :---: | :---: |
| $\mathbb{E}\left(\theta_{i} \mid y_{i}\right) \approx \omega_{i} y_{i}, \omega_{i}=\mathrm{PIP}$ | $\mathbb{E}\left(\theta_{i} \mid Y_{i}\right)=\left\{1-\mathbb{E}\left(\kappa_{i} \mid y_{i}\right)\right\} y_{i}$ |

$1-\mathbb{E}\left(\kappa_{i} \mid y_{i}\right)$ mimics the posterior inclusion probability $\omega_{i}$.
$\mathbb{E}\left(\kappa_{i} \mid y_{i}\right) \approx 0$ for large $y_{i}($ signal $), \mathbb{E}\left(\kappa_{i} \mid y_{i}\right) \approx 1$ for small $y_{i}$ (noise)

## How to Build a Sparsity Prior

- $\mathbb{E}\left(\kappa_{i} \mid y_{i}\right) \approx 0$ for large $y_{i}, \mathbb{E}\left(\kappa_{i} \mid y_{i}\right) \approx 1$ for small $y_{i}$.

$$
\kappa \text {-scale: } \underbrace{p\left(\kappa_{i} \mid y_{i}\right)}_{\text {posterior }} \propto \underbrace{p\left(y_{i} \mid \kappa_{i}\right)}_{\text {likelihood }} \underbrace{p\left(\kappa_{i}\right)}_{\text {prior }} \propto \kappa_{i}^{\frac{1}{2}} \exp \left\{-\kappa_{i} \frac{y_{i}^{2}}{2}\right\} p\left(\kappa_{i}\right)
$$

- Likelihood doesn't concentrate near 1 for $y_{i} \approx 0$.
- Horseshoe: Push density towards $1 \rightarrow$ replace $\kappa_{i}^{\frac{1}{2}}$ with $\left(1-\kappa_{i}\right)^{-\frac{1}{2}}$.
- Achieved by 'horseshoe': $p\left(\kappa_{i}\right) \propto 1 / \sqrt{\kappa_{i}\left(1-\kappa_{i}\right)}$.


$$
\lambda_{i}^{2} \sim C^{+}(0,1) \equiv \kappa_{i} \sim \operatorname{Be}\left(\frac{1}{2}, \frac{1}{2}\right) \Rightarrow \text { "Horseshoe" }
$$

## Global-Local priors

Global-local scale mixtures[Polson and Scott, 2010b]:

$$
\begin{gathered}
(\mathbf{y} \mid \boldsymbol{\theta}) \sim \mathcal{N}\left(\mathbf{X} \boldsymbol{\theta}, \sigma^{2} \mathbf{I}\right) ; \theta_{i} \sim \mathcal{N}\left(0, \lambda_{i}^{2} \tau^{2}\right) \\
\lambda_{i}^{2} \sim \pi\left(\lambda_{i}^{2}\right) ;\left(\tau^{2}\right) \sim \pi\left(\tau^{2}\right), i=1, \ldots, n
\end{gathered}
$$

$\lambda_{i}$ : local shrinkage - tags signal, $\tau$ : global shrinkage - adjusts to sparsity.

| Global-local shrinkage priors | Authors |
| :---: | :---: |
| Normal Exponential Gamma | Griffin and Brown [2010] |
| Horseshoe | Carvalho et al. [2010, 2009] |
| Hypergeometric Inverted Beta | Polson and Scott [2010a] |
| Generalized Double Pareto | Armagan et al. [2011] |
| Generalized Beta | Armagan et al. [2013] |
| Dirichlet-Laplace | Bhattacharya et al. [2015] |
| Horseshoe+ | Bhadra et al. [2017b] |
| Horseshoe-like | Bhadra et al. [2017a] |
| Spike-and-Slab Lasso | Ročková and George [2016] |
| R2-D2 | Zhang et al. [2016] |
| Inverse-Gamma-Gamma | Bai and Ghosh [2017] |
| Heavy-tailed Horseshoe | Womack and Yang [2019] |
| Log-adjusted prior | Hamura et al. [2020] |
| Gauss-Hypergeometric | Datta and Dunson [2016] |
| Extremely heavy-tailed (EH) prior | Hamura et al. [2019] |

## Shape of G-L priors



## Horseshoe > Bayesian Lasso


(a) Shrinkage profile for Horseshoe, Horseshoe+, and Laplace prior.

(b) Shrinkage Profiles

Lasso overshrinks, Horseshoe doesn't
Castillo et al. [2015]: the full Lasso posterior distribution does not contract at the same speed as the posterior mode $\Rightarrow$ Poor uncertainty quantification.

## Theory for general G-L prior

$$
\theta_{i} \sim \mathcal{N}\left(0, \lambda_{i}^{2} \tau^{2}\right), \lambda_{i}^{2} \stackrel{\text { ind }}{\sim} \pi_{1}\left(\lambda_{i}^{2}\right) ;\left(\tau^{2}\right) \sim \pi_{2}\left(\tau^{2}\right), i=1, \ldots, n .
$$

- Ghosh et al. [2016]: Bayes oracle for G-L priors.
- Ghosh and Chakrabarti [2017]: Asymptotic Minimaxity for G-L priors.
- Key idea: local shrinkage priors should have regularly varying tails.
- Up to $O(1)$ can be relaxed: G-L priors can be exactly minimax and ABOS [Ghosh et al., 2016, Bai and Ghosh, 2017].

Grouped shrinkage

## Exposure Correlation Structure (NHANES 2003-2004)



Source: National Health and Nutrition Examination Survey (NHANES).

## Simple multipollutant model

- Consider a Bayesian sparse linear regression model

$$
\begin{equation*}
\left[\boldsymbol{y} \mid \boldsymbol{\alpha}, \boldsymbol{\beta}, \sigma^{2}\right] \sim N\left(\boldsymbol{C} \alpha+\sum_{g=1}^{G} \boldsymbol{X}_{g} \boldsymbol{\beta}_{g}, \sigma^{2} \boldsymbol{I}_{n}\right), \quad \pi(\boldsymbol{\alpha}) \propto 1, \quad \boldsymbol{\beta} \sim \pi(\boldsymbol{\beta}) \tag{2}
\end{equation*}
$$

where $g=1, \ldots, G$ indexes the groups, $\boldsymbol{y}$ is an $n \times 1$ vector of centered continuous responses, $\boldsymbol{C}$ is a matrix of adjustment covariates,

- and $\ldots \boldsymbol{X}_{g}$ is an $n \times p_{g}$ matrix of standardized covariates in the $g$-th group, $\beta_{g}=\left(\beta_{g 1}, \ldots, \beta_{g p_{g}}\right)^{\top}$ is a $p_{g} \times 1$ vector of regression coefficients corresponding to the $g$-th group,
- and $\ldots \boldsymbol{\beta}=\left(\boldsymbol{\beta}_{1}^{\top}, \ldots, \boldsymbol{\beta}_{G}^{\top}\right)^{\top}$ is a $p \times 1$ vector of regression coefficients to employ shrinkage on.


## Group Inverse-Gamma Gamma (GIGG) Shrinkage

Global-Group-Local Shrinkage Priors [ Xu et al., 2016]

$$
\left[y_{g j} \mid \beta_{g j}, \sigma^{2}\right] \sim N\left(\beta_{g j}, \sigma^{2}\right), \quad\left[\beta_{g j} \mid \tau^{2}, \gamma_{g}^{2}, \lambda_{g j}^{2}\right] \sim N\left(0, \tau^{2} \gamma_{g}^{2} \lambda_{g j}^{2}\right),
$$

where $g j$ indexes the $j$-th mean in the $g$-th group, $\lambda_{g}^{2}=\left(\lambda_{g 1}^{2}, \ldots, \lambda_{g p_{g}}^{2}\right)$, and $p_{g}$ denotes the number of observations in the $g$-th group.

Key Idea: Need $\pi\left(\gamma_{g}^{2}, \lambda_{g}^{2}\right)$ such that

$$
\gamma_{g}^{2} \lambda_{g j}^{2} \sim \beta^{\prime}\left(a_{g}, b_{g}\right), \quad \forall j \in\left\{1, \ldots, p_{g}\right\} .
$$

## Group Inverse-Gamma Gamma (GIGG) Shrinkage

Global-Group-Local Shrinkage Priors [ Xu et al., 2016]

$$
\left[y_{g j} \mid \beta_{g j}, \sigma^{2}\right] \sim N\left(\beta_{g j}, \sigma^{2}\right), \quad\left[\beta_{g j} \mid \tau^{2}, \gamma_{g}^{2}, \lambda_{g j}^{2}\right] \sim N\left(0, \tau^{2} \gamma_{g}^{2} \lambda_{g j}^{2}\right),
$$

where $g j$ indexes the $j$-th mean in the $g$-th group, $\lambda_{g}^{2}=\left(\lambda_{g 1}^{2}, \ldots, \lambda_{g p_{g}}^{2}\right)$, and $p_{g}$ denotes the number of observations in the $g$-th group.

Key Idea: Need $\pi\left(\gamma_{g}^{2}, \lambda_{g}^{2}\right)$ such that

$$
\gamma_{g}^{2} \lambda_{g j}^{2} \sim \beta^{\prime}\left(a_{g}, b_{g}\right), \quad \forall j \in\left\{1, \ldots, p_{g}\right\} .
$$

Proposition: If $U \sim G(a, \eta)$ and $V \sim I G(b, \eta)$ are independent, then

$$
U V \sim \beta^{\prime}(a, b) .
$$

## Group Inverse-Gamma Gamma (GIGG) Prior [Boss, Datta, Wang, Park, Kang, and Mukherjee, 2021]

## Formulation

$$
\left[\beta_{g j} \mid \tau^{2}, \gamma_{g}^{2}, \lambda_{g j}^{2}\right] \sim N\left(0, \tau^{2} \gamma_{g}^{2} \lambda_{g j}^{2}\right), \quad \gamma_{g}^{2} \sim G\left(a_{g}, 1\right), \quad \lambda_{g j}^{2} \sim I G\left(b_{g}, 1\right)
$$

Here, the index $g j$ refers to the $j$-th mean in the $g$-th group.
Posterior Distribution of Shrinkage Factors

$$
\begin{gathered}
\pi\left(\kappa_{g 1}, \ldots, \kappa_{g p_{g}} \mid y_{g 1}, \ldots, y_{g p_{g}}, \tau^{2}, \sigma^{2}, a_{g}, b_{g}\right) \propto \\
\left(1+\frac{\tau^{2}}{\sigma^{2}} \sum_{j=1}^{p_{g}} \frac{\kappa_{g j}}{1-\kappa_{g j}}\right)^{-\left(a_{g}+p_{g} b_{g}\right)}\left(\prod_{j=1}^{p_{g}} \kappa_{g j}^{b_{g}-1 / 2}\left(1-\kappa_{g j}\right)^{-\left(b_{g}+1\right)} e^{-\frac{y_{g j}^{2}}{2 \sigma^{2}} \kappa_{g j}}\right),
\end{gathered}
$$

where $0<\kappa_{g j}<1$ for all $1 \leq j \leq p_{g}$ ( $p_{g}$ is the size of the $g$-th group).
Reduces to usual horseshoe prior for $p_{g}=1$ (groups of size 1 ).

## Posterior Mean (GIGG Prior)

Illustrative Model: $\left[y_{g 1} \mid \beta_{g 1}\right] \sim N\left(\beta_{g 1}, 1\right), \quad\left[y_{g 2} \mid \beta_{g 2}\right] \sim N\left(\beta_{g 2}, 1\right)$


Here $a_{g}$ effectively controls the overall strength of the shrinkage, whereas $b_{g}$ generally controls the dependence of the within-group shrinkage.

## Theoretical Results

## Posterior Concentration (Sparse Normal Means)

- $\left|y_{g j}\right| \rightarrow \infty \Longrightarrow$ posterior distribution of $\kappa_{g j}$ concentrates near 0 .
- $\tau \rightarrow 0 \Longrightarrow$ posterior distribution of $\kappa_{g j}$ concentrates near 1 .

Posterior Concentration (Linear Regression with $p<n$ )

- $\tau \rightarrow 0 \Longrightarrow$ posterior distribution of $\left\|\hat{\boldsymbol{\beta}}^{O L S}-E[\boldsymbol{\beta} \mid \cdot]\right\|_{2}$ concentrates near $\left\|\hat{\boldsymbol{\beta}}^{O L S}\right\|_{2}(E[\boldsymbol{\beta} \mid \cdot]$ is the full conditional mean).
- For block diagonal correlation structure, $b_{g} \rightarrow \infty$ and $\tau^{2} / \sigma^{2}$ small $\Longrightarrow$ shrinkage of $g$-th group close to zero.


## Posterior Consistency (Linear Regression)

- Assumes that $p=o(n)$ and fixed values of $a_{g}$ and $b_{g}$.


## Simulations ( $n=500, p=50$ )

## Simulation Settings


(a) Concentrated Signal

(b) Distributed Signal

In the diagram, the $g j$-th box is the $j$-th exposure in the $g$-th group. The boxes corresponding to non-null regression coefficients are filled in.

## Exposure Correlation Structure

- Correlations within exposure class are $\rho=0.8$.
- Correlations between exposure classes are 0.2.


## Mean-Squared Error

| $\rho=\mathbf{0 . 8}$ | Concentrated |  | Distributed |  |
| :--- | :---: | :---: | :---: | :---: |
| Method | Null | Non-Null | Null | Non-Null |
| Ordinary Least Squares | 3.74 | 0.41 | 8.09 | 2.03 |
| Horseshoe | 0.51 | 0.41 | 0.85 | 2.14 |
| GIGG $\left(a_{g}=1 / n, b_{g}=1 / n\right)$ | $\mathbf{0 . 1 1}$ | $\mathbf{0 . 3 0}$ | 0.03 | 3.59 |
| GIGG $\left(a_{g}=1 / 2, b_{g}=1 / n\right)$ | $\mathbf{0 . 1 1}$ | $\mathbf{0 . 3 0}$ | 0.04 | 3.56 |
| GIGG $\left(a_{g}=1 / n, b_{g}=1 / 2\right)$ | 0.29 | 0.39 | $\mathbf{0 . 0 3}$ | $\mathbf{1 . 5 7}$ |
| *GIGG $\left(a_{g}=1 / 2, b_{g}=1 / 2\right)$ | 0.33 | 0.40 | 0.24 | 1.70 |
| GIGG $\left(a_{g}=1 / n, b_{g}=1\right)$ | 0.53 | 0.49 | $\mathbf{0 . 0 3}$ | $\mathbf{1 . 4 3}$ |
| GIGG $\left(a_{g}=1 / 2, b_{g}=1\right)$ | 0.58 | 0.49 | 0.26 | 1.43 |
| GIGG (MMLE) | $\mathbf{0 . 2 0}$ | $\mathbf{0 . 3 4}$ | $\mathbf{0 . 0 4}$ | $\mathbf{1 . 4 2}$ |
| Group Half Cauchy | 0.30 | 0.39 | 0.08 | 1.64 |
| Spike-and-Slab Lasso | $\mathbf{0 . 1 5}$ | $\mathbf{0 . 3 3}$ | 0.21 | 4.27 |
| BGL-SS | 2.01 | 0.80 | $\mathbf{0 . 0 4}$ | $\mathbf{1 . 3 1}$ |
| BSGS-SS | 0.23 | 0.42 | 0.04 | 1.84 |

*GIGG $\left(a_{g}=1 / 2, b_{g}=1 / 2\right)$ is equivalent to group horseshoe.
**Bolded entries indicate the top four performers.

## Illustrative Example from NHANES 2003-2004

## Study Details

- 990 adults with 35 measured environmental contaminants.
- Outcome of interest is Gamma-Glutamyl Transferase (GGT).


## Exposure Classes

- 3 Metals (cadmium, lead, and mercury)
- 7 Phthalates
- 8 Organochlorine Pesticides
- 7 Polybrominated Diphenyl Ethers (PBDEs)
- 10 Polycyclic Aromatic Hydrocarbons (PAHs)


## Illustrative Example from NHANES 2003-2004



## Precision matrix estimation

## Gaussian Graphical Model i

- Gaussian graphical model (GGM) remains popular as a fundamental building block for network estimation because of the ease of interpretation of the resulting precision matrix estimate:
- An inferred off-diagonal zero corresponds to conditional independence of the two corresponding nodes given the rest [see, e.g., Lauritzen, 1996].
- There are both Bayesian and frequentist approaches to this, it is difficult to obtain good Bayesian and frequentist properties under the same prior-penalty dual, complicating justification.
- Our contribution is a novel prior-penalty dual that closely approximates the popular graphical horseshoe prior and penalty, and performs well in both Bayesian and frequentist senses.


## Gaussian Graphical Model ii

- $\mathbf{X}^{(n)}=\left(\mathbf{X}_{1}, \ldots, \mathbf{X}_{n}\right)^{T} \sim \mathcal{N}_{p}(\mathbf{0}, \boldsymbol{\Sigma})$.
- The corresponding precision matrix: $\boldsymbol{\Omega}=\left(\left(\omega_{i j}\right)\right)$ is defined as $\Omega=\boldsymbol{\Sigma}^{-1}$.
- Assume that $\boldsymbol{\Omega}$ is sparse, in the sense that the number of non-zero off-diagonal elements is small.
- Goal: fully Bayesian inference on $\boldsymbol{\Omega}$, we need a suitable sparsity-favoring prior that also results in a penalty function with good frequentist properties.


## Horseshoe Regularization ${ }^{1}$

- Horseshoe prior: $p(\omega)$ not analytically tractable !

$$
\frac{1}{\tau(2 \pi)^{3 / 2}} \log \left(1+\frac{4 \tau^{2}}{\omega^{2}}\right)<p_{H S}(\omega \mid \tau)<\frac{2}{\tau(2 \pi)^{3 / 2}} \log \left(1+\frac{2 \tau^{2}}{\omega^{2}}\right)
$$

- Hindrance in learning via EM-type algorithms.


## Horseshoe Regularization ${ }^{1}$

- Horseshoe prior: $p(\omega)$ not analytically tractable !

$$
\frac{1}{\tau(2 \pi)^{3 / 2}} \log \left(1+\frac{4 \tau^{2}}{\omega^{2}}\right)<p_{H S}(\omega \mid \tau)<\frac{2}{\tau(2 \pi)^{3 / 2}} \log \left(1+\frac{2 \tau^{2}}{\omega^{2}}\right)
$$

- Hindrance in learning via EM-type algorithms.
- Solution: normalize the tight bounds: 'horseshoe-like' [Bhadra et al., 2017a].

$$
p_{\widetilde{H S}}(\omega \mid a)=\frac{1}{2 \pi a^{1 / 2}} \log \left(1+\frac{a}{\omega^{2}}\right) .
$$

- Extend this for precision matrix estimation (Sagar, Banerjee, D., \& Bhadra, 2021).


## Normal Scale Mixture Representation!

- Frullani's identity [Jeffreys and Swirles, 1972, pp. 406-407]:

$$
\int_{0}^{\infty} \frac{f(a x)-f(b x)}{x} d x=\{f(0)-f(\infty)\} \log (b / a)
$$

- $f(x)=\exp (-x)$ yields a latent variable representation:

$$
\frac{1}{2 \pi a^{1 / 2}} \log \left(1+\frac{a}{\omega^{2}}\right)=\int_{0}^{\infty} \exp \left(-\frac{u \omega^{2}}{a}\right) \frac{\left(1-e^{-u}\right)}{2 \pi a^{1 / 2} u} d u
$$

- Normal scale mixture:

$$
(\omega \mid u, a) \stackrel{i n d}{\sim} \mathcal{N}\left(0, \frac{a}{2 u}\right), p(u)=\frac{1-e^{-u}}{2 \pi^{1 / 2} u^{3 / 2}}
$$

- Reparametrize $\left(t^{2}=2 u\right.$ and $\left.\tau^{2}=a\right)$ :

$$
(\omega \mid i, \tau) \sim \mathcal{N}\left(0, \frac{\tau^{2}}{t^{2}}\right), p(t)=\frac{\left(1-e^{-\frac{1}{2} t^{2}}\right)}{\sqrt{2 \pi} t^{2}}
$$

- This $p(t)$ is the standard Slash-Normal density that can be written as a Normal variance mixture with a $\operatorname{Pareto}\left(\frac{1}{2}\right)$ mixing density.


## Details

- For the fully Bayesian model, the element-wise prior specification induced by the horseshoe-like prior is,

$$
\omega_{i j} \mid a \sim \pi\left(\omega_{i j} \mid a\right), 1 \leq i<j \leq p ; \quad \omega_{i i} \propto 1,1 \leq i \leq p
$$

where $\pi\left(\omega_{i j} \mid a\right)$ is the density of the horseshoe-like prior.

- The horseshoe-like prior above can be expressed as a Gaussian scale-mixture [Bhadra et al., 2017a], thus giving us a global-local shrinkage prior:

$$
\begin{equation*}
\omega_{i j} \mid v_{i j}, a \sim \mathcal{N}\left(0, \frac{a}{2 v_{i j}}\right), \pi\left(v_{i j}\right) \sim \frac{1-\exp \left(-v_{i j}\right)}{2 \pi^{1 / 2} v_{i j}^{3 / 2}} \tag{3}
\end{equation*}
$$

- Only $v_{i j}$ is considered to be latent and the global scale parameter a is considered to be fixed.
- Can estimate $a$ by the effective model size approach of Piironen et al. [2017] to avoid it collapsing to zero.


## Details

- We restrict the prior on a subspace of symmetric positive definite matrices, $\mathcal{M}_{p}^{+}(L)$, where

$$
\begin{equation*}
\mathcal{M}_{p}^{+}(L)=\left\{\boldsymbol{\Omega} \in \mathcal{M}_{p}^{+}: 0<L^{-1} \leq \operatorname{eig}_{1}(\boldsymbol{\Omega}) \leq \cdots \leq \operatorname{eig}_{p}(\boldsymbol{\Omega}) \leq L<\infty\right\} \tag{4}
\end{equation*}
$$

- Only necessary for arriving at the theoretical results involving the posterior convergence rate of $\Omega$. We assume that $L$ is a fixed constant, which can be large.
- However, this condition does not affect the practical implementation of our proposed method, and is used purely as a technical requirement.
- Beyond this, no structural assumption (e.g., decomposability) is placed on either $\boldsymbol{\Omega}$ or $\boldsymbol{\Sigma}$.


## Joint prior

- Combining the unrestricted prior as in (3) and (3), along with the prior space restriction as in (4), the joint prior distribution on $\boldsymbol{\Omega}$ is given by,

$$
\pi(\boldsymbol{\Omega} \mid v, a) \pi(v) \propto \prod_{i, j: i<j}\left(1-\exp \left(-v_{i j}\right)\right) v_{i j}^{-1} \exp \left(\frac{-v_{i j} \omega_{i j}^{2}}{a}\right) \mathbb{1}_{\mathcal{M}_{p}^{+}(L)}(
$$

- With the prior specification as in (5), the log-posterior $\mathcal{L}$ thus becomes,
$\mathcal{L} \propto \frac{n}{2} \log |\boldsymbol{\Omega}|-\frac{n}{2} \operatorname{tr}(\mathbf{S} \boldsymbol{\Omega})+\sum_{i, j: i<j}\left\{\log \left(1-\exp \left(-v_{i j}\right)\right)-\log v_{i j}-\frac{v_{i j} \omega_{i j}^{2}}{a}\right\}$


## Estimation

- Utilize the Gaussian mixture representation to devise an Expectation Conditional Maximization (ECM) [Meng and Rubin, 1993] approach to MAP estimation.
- For updating the elements of the precision matrix, we use the coordinate descent technique proposed by Wang [2014].
- E Step: Following Bhadra et al. [2017a], we calculate the conditional expectation of the latent variable $v_{i j}, 1 \leq i<j \leq p$, at current iteration $(t)$ as follows:

$$
\begin{equation*}
\mathbb{E}\left(v_{i j} \mid \omega_{i j}^{(t)}, a\right)=\left\{\log \left(1+\frac{a}{\left(\omega_{i j}^{(t)}\right)^{2}}\right)\right\}^{-1} \frac{a^{2}}{\left(\left(\omega_{i j}^{(t)}\right)^{2}+a\right)\left(\left(\omega_{i j}^{(t)}\right)^{2}\right)} \tag{7}
\end{equation*}
$$

- CM Steps: Having updated the latent parameters in the E-Step, the coordinate descent approach of Wang [2014] is used to update one column of the precision matrix at a time.


## Posterior sampling

- Posterior sampling strategy combines ideas from [Bhadra et al., 2017a] and [Li et al., 2017].
- With substitutions $2 v_{i j} \mapsto t_{i j}^{2}$ and $a \mapsto \tau^{2}$, the prior can be written as:
$\omega_{i j} \mid v_{i j}, \tau \sim \mathcal{N}\left(0, \tau^{2} / t_{i j}^{2}\right), \pi\left(t_{i j}\right)=\frac{1-\exp \left(-t_{i j}^{2} / 2\right)}{(2 \pi)^{1 / 2} t_{i j}^{2}}, t_{i j} \in \mathbb{R}, \tau^{2}>0$,
where $\pi\left(t_{i j}\right)$ above is known as the the slash normal density, expressed as $\left(\phi(0)-\phi\left(t_{i j}\right)\right) / t_{i j}^{2}$ [Bhadra et al., 2017a].
- Introducing a further local latent variable $r_{i j}$, the density for $t_{i j}$ can also be written as a normal scale mixture, where the scale follows a Pareto distribution, that is,

$$
t_{i j} \mid r_{i j} \sim \mathcal{N}\left(0, r_{i j}\right), r_{i j} \sim \text { Pareto }(1 / 2) .
$$

- Remaining steps are similar to the graphical horseshoe sampler of Li et al. [2017].


## Posterior consistency

- Posterior contraction rate of the precision matrix $\boldsymbol{\Omega}$ around the true precision matrix $\Omega_{0}$ with respect to the Frobenius norm under the graphical horseshoe-like prior.
- We make certain assumptions on the true precision matrix, the dimension and sparsity, and the prior space.
- Assumptions: True underlying graph is sparse, effective dimension of the parameter $\Omega_{0}, p+s$ satisfies $(p+s) \log p / n=o(1)$, the prior space contains the true precision matrix, and the prior puts sufficient mass around the true zero elements in the precision matrix.


## Theorem

The posterior distribution of $\Omega$ satisfies

$$
\mathbb{E}_{0}\left[P\left\{\left\|\boldsymbol{\Omega}-\mathbf{\Omega}_{0}\right\|_{2}>M \epsilon_{n} \mid \mathbf{X}^{(n)}\right\}\right] \rightarrow 0
$$

for $\epsilon_{n}=n^{-1 / 2}(p+s)^{1 / 2}(\log p)^{1 / 2}$ and a sufficiently large constant $M>0$.

## MAP estimator

- We can prove that the extended real-valued penalty function $\operatorname{pen}_{a}(x)=-\log \log \left(1+a / x^{2}\right), a>0$, is strongly concave, and hence strictly concave, for all $x \in \operatorname{dom}\left(\right.$ pen $\left._{a}\right)$, separately for $x>0$ and $x<0$.
- Strict concavity of penalty function guarantees that the LLA algorithm will satisfy an ascent property, that is, $Q\left(\boldsymbol{\Omega}^{(t+1)}\right)>Q\left(\boldsymbol{\Omega}^{(t)}\right)$.


## Theorem

Under the conditions of Theorem 1, the MAP estimator of $\boldsymbol{\Omega}$, given by $\hat{\mathbf{\Omega}}^{\mathrm{MAP}}$ is consistent, in the sense that

$$
\left\|\hat{\mathbf{\Omega}}^{\mathrm{MAP}}-\mathbf{\Omega}_{0}\right\|_{2}=O_{P}\left(\epsilon_{n}\right)
$$

where $\epsilon_{n}$ is the posterior convergence rate as defined in Theorem 1.

- Converges to the true precision matrix $\boldsymbol{\Omega}_{0}$ at the same rate as the posterior convergence rate in the Frobenius norm.


## Simulation: selected

Hubs. The rows/columns are partitioned into $K$ disjoint groups $G_{1}, \ldots, G_{K}$. The off-diagonal entries $\omega_{i j}^{0}$ are set to 0.25 if $i \neq j$ and $i, j \in G_{k}$ for $k=1, \ldots, K$. In our simulations we consider $p / 10$ groups with equal number of elements in each group.

Table 1: 50 data sets generated with precision matrix $\Omega_{0}$, where $n=120$ and $p=100$. Candidates: frequentist graphical lasso with penalized diagonal elements (GL1) and with unpenalized diagonal elements (GL2), graphical SCAD (GSCAD), Bayesian graphical lasso (BGL), the graphical horseshoe (GHS), graphical horseshoe-like ECM (ECM) and graphical horseshoe-like MCMC (MCMC).

|  | Hubs90 nonzero pairs out of 4950 nonzero elements $=0.25$ |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | GL1 | GL2 | GSCAD | BGL | GHS | ECM | MCMC |
| Stein's loss | 5.255 | 6.328 | 5.213 | 43.042 | 5.101 | 4.22 | 5.310 |
|  | (0.263) | (0.414) | (0.261) | (0.802) | (0.455) | (0.369) | (0.485) |
| F norm | 3.018 | 3.432 | 3.003 | 4.295 | 2.544 | 2.415 | 2.687 |
|  | (0.091) | (0.112) | (0.093) | (0.156) | (0.126) | (0.103) | (0.141) |
| TPR | . 995 | . 986 | . 998 | . 995 | . 872 | 0.985 | 0.754 |
|  | (.007) | (.017) | (.002) | (.008) | (.04) | (.014) | (0.004) |
| FPR | . 101 | . 045 | . 983 | . 186 | . 003 | . 062 | 0.003 |
|  | (.016) | (.008) | (.012) | (.007) | (.001) | (0.005) | (0.001) |
| MCC | 0.373 | 0.523 | 0.016 | 0.27 | 0.85 | 0.458 | 0.775 |
|  | (.027) | (.039) | (.006) | (.006) | (.027) | (.015) | (.033) |
| Avg CPU time | 1.739 | 1.76 | 48.54 | 549.196 | 252.94 | 5.811 | 537.604 |

## Summary and Scopes (Part I)

- Global-local priors: state-of-the-art Bayesian tool for sparse signal recovery.
- Can be extended to sparse + structured covariates: GIGG and graphical-horseshoe.
- Scale mixture: allows for MCMC + EM and LLA algorithms.
- Can be interpreted as non-convex penalty (horseshoe-like)
- Scopes:

1. Selection for bi-level sparsity (still Oracle?)
2. Multiple graphical models.
3. Extend beyond Gaussian set-up (e.g. [Datta and Dunson, 2016]).
4. An appealing new direction is Bayesian neural net, e.g. [Ghosh and Doshi-Velez, 2017] ['Model selection in Bayesian neural networks via horseshoe priors']

## References

## References (for this talk)

- Graphical horseshoe-like prior: Sagar, Ksheera, Banerjee, S., Datta, J., and Bhadra, A.. "Precision Matrix Estimation under the Horseshoe-like Prior-Penalty Dual." arXiv preprint arXiv:2104.10750 (2021).
- GIGG shrinkage: Boss, J., Datta, J., Wang, X., Park, S. K., Kang, J., \& Mukherjee, B. (2021). Group Inverse-Gamma Gamma Shrinkage for Sparse Regression with Block-Correlated Predictors. arXiv preprint arXiv:2102.10670.
- Horseshoe-like prior: Bhadra, A., Datta, J., Polson, N. G., \& Willard, B. (2019). Horseshoe regularization for feature subset selection. Sankhya B. [preprint]
- Graphical horseshoe: Li, Y., Craig, B. A., \& Bhadra, A. (2019). The graphical horseshoe estimator for inverse covariance matrices. Journal of Computational and Graphical Statistics, 28(3), 747-757.


## References (General global-Local)

- Bhadra, A., Datta, J., Li, Y., Polson, N. G., \& Willard, B. (2019). Prediction risk for global-local shrinkage regression. 20 (78), 1-39, Journal of Machine Learning Research. arXiv:1605.04796.
- Bhadra, A., Datta, J., Polson, N. G., \& Willard, B. T. (2019). Lasso Meets Horseshoe: A Survey. 34(3), 405-427. Statistical Science.
- Bhadra, Datta, Li and Polson (2019). "Horseshoe Regularization for Machine Learning in Complex and Deep Models". Published, International Statistical Review. Discussed paper [preprint].
- Bhadra, Datta, Polson, and Willard (2019), (*alphabetical), "Global-local mixtures - A Unifying Framework". Accepted, Sankhya A.
- Bhadra, A., Datta, J., Polson, N. G., \& Willard, B. (2017). The horseshoe+ estimator of ultra-sparse signals. Bayesian Analysis, 12(4), 1105-1131.
- Datta, J., \& Dunson, D. B. (2016). Bayesian inference on quasi-sparse count data. Biometrika, 103(4), 971-983.
- Bhadra, A., Datta, J., Polson, N. G., \& Willard, B. (2016). Default Bayesian analysis with global-local shrinkage priors. Biometrika, 103(4), 955-969.
- Datta, J., \& Ghosh, J. K. (2013). Asymptotic properties of Bayes risk for the horseshoe prior. Bayesian Analysis, 8(1), 111-132.
- Li, Datta, Craig, and Bhadra, (2020+). "Joint Mean-Covariance Estimation via the Horseshoe with an Application in Genomic Data Analysis". submitted. [preprint].


## Thank you!



Resources for Horseshoe Prior

## Learning $\tau$

1. Maximum marginal likelihood estimator (MMLE)
2. Full Bayes estimator: half-Cauchy prior truncated to the interval $[1 / n, 1]$.
3. Cross-validation.
4. By studying the prior for $m_{\text {eff }}=\sum_{i=1}^{n}\left(1-\kappa_{i}\right)$ [Piironen and Vehtari, 2016]

- MMLE beats simple thresholding:

$$
\hat{\tau}_{s}\left(c_{1}, c_{2}\right)=\max \left\{\frac{\sum_{i=1}^{n} \mathbf{1}\left\{\left|y_{i}\right| \geq \sqrt{\left.c_{1} \log (n)\right\}}\right.}{c_{2} n}, \frac{1}{n}\right\} .
$$

- Empirical Bayes estimate of $\tau$ can replace a full Bayes estimate of $\tau$.
- Caution to prevent the estimator from getting too close to zero.


## Computation for Horseshoe

1. MCMC : block-updating $\boldsymbol{\theta}, \boldsymbol{\lambda}$ and $\tau$ using either a Gibbs or parameter expansion or slice sampling strategy.
2. Makalic and Schmidt [2016]: Inverse-gamma scale mixture for Gibbs sampling scheme for horseshoe and horseshoe+ prior for linear regression and logistic and negative binomial regression.
3. Hahn et al. [2016]: Elliptical slice sampler - wins over Gibbs strategies!
4. Bhattacharya et al. [2016]: Gaussian sampling alternative to the naïve Cholesky decomposition to reduce the computational burden from $O\left(p^{3}\right)$ to $O\left(n^{2} p\right)$.

## Implementation

Table 2: Implementations of Horseshoe and Other Shrinkage Priors

| Implementation (Package/URL) | Authors |
| :---: | :---: |
| R package: monomvn | Gramacy and Pantaleo [2010] |
| R code in paper | Scott [2010] |
| R package: horseshoe | van der Pas et al. [2016] |
| R package: fastHorseshoe | Hahn et al. [2016] |
| MATLAB code | Bhattacharya et al. [2016] |
| GPU accelerated Gibbs sampling | Terenin et al. [2016] |
| bayesreg + MATLAB code in paper | Makalic and Schmidt [2016] |
| MATLAB code | Johndrow and Orenstein [2017] |

