

A Convex-Nonconvex Strategy for Grouped Variable Selection

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1 Convex-Nonconvex Penalization

- Motivation
- Generalized Minimax Concave (GMC) penalty

2 Group GMC for Grouped Variable Selection

- The group GMC estimator
- Algorithms for the group GMC model
- Error bound for the group GMC estimator
- Simulations and a real data application

3 Discussion

Recover a sparse representation:

$$\text{minimize } F(\boldsymbol{\beta}) = \frac{1}{2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda\psi(\boldsymbol{\beta}) \quad (1)$$

- Statistics – penalized linear regression
 - $\mathbf{y} \in \mathbb{R}^n$: response
 - $\mathbf{X} \in \mathbb{R}^{n \times p}$: design matrix
 - $\boldsymbol{\beta} \in \mathbb{R}^p$: vector of coefficients
- Signal processing – signal recovery/denoising
 - $\mathbf{y} \in \mathbb{R}^n$: vector of observations
 - $\mathbf{X} \in \mathbb{R}^{n \times p}$: linear operator
 - $\boldsymbol{\beta} \in \mathbb{R}^p$: signal vector
- $\psi : \mathbb{R}^p \mapsto \mathbb{R}$ – penalty function promoting sparsity in $\boldsymbol{\beta}$.

Convex penalization

Commonly used convex penalties:

- $\psi(\beta) = \|\beta\|_1$
 - Lasso (Tibshirani, 1996)
 - Basis Pursuit (Chen and Donoho, 1994)
- $\psi(\beta) = \alpha\|\beta\|_1 + (1 - \alpha)\|\beta\|_2^2$
 - Elastic Net (Zou and Hastie, 2005)

Characteristics of convex penalties:

- + no suboptimal local minimizers
- **underestimate** large magnitude components

Nonconvex penalization

Commonly used nonconvex penalties:

- the smoothly clipped absolute deviations (SCAD) penalty
 - (Fan and Li, 2001)
- the minimax concave penalty (MCP)
 - (Zhang et al., 2010)

Characteristics of nonconvex penalties:

- + more accurate estimation
- **existence** of suboptimal local minimizers

Introduction

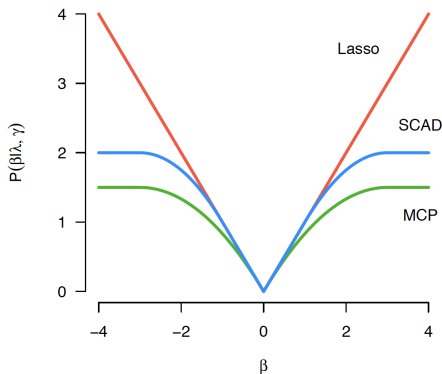


Figure: Visualization of Lasso, SCAD and MCP (Adopted from Patrick Breheny's lecture on BIOS 7240).

- non-differentiability at the origin \rightarrow sparsity

Introduction

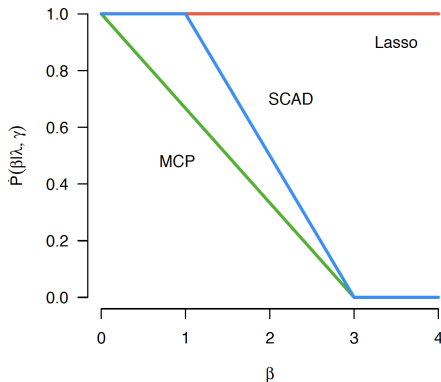


Figure: Visualization of derivatives of Lasso, SCAD and MCP (Adopted from Patrick Breheny's lecture on BIOS 7240)

- derivative \rightarrow penalization rate (estimation bias)

The GMC penalization

A convex-nonconvex strategy:

Design a nonconvex penalty but maintain the convexity of the problem.

The **GMC penalty** (Selesnick, 2017):

$$\psi_{\mathbf{B}}(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_1 - \min_{\mathbf{v} \in \mathbb{R}^p} \left\{ \|\mathbf{v}\|_1 + \frac{1}{2} \|\mathbf{B}(\boldsymbol{\beta} - \mathbf{v})\|_2^2 \right\}, \quad (2)$$

where $\mathbf{B} \in \mathbb{R}^{n \times p}$ is a matrix parameter.

The GMC penalization

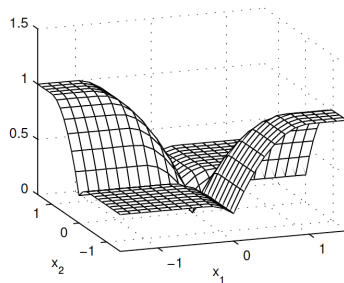
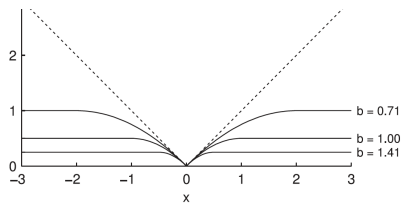


Figure: Visualization of the GMC penalty in the univariate case (left) and the multivariate case (right). Adopted from Selesnick (2017).

The GMC penalization

The optimization problem

$$\text{minimize } F(\boldsymbol{\beta}) = \frac{1}{2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \psi_{\mathbf{B}}(\boldsymbol{\beta}) \quad (3)$$

maintains convex if

$$\mathbf{X}^T \mathbf{X} \succeq \lambda \mathbf{B}^T \mathbf{B}. \quad (4)$$

- **Convexity-preserving condition** for the GMC model (3).

The GMC penalization

An open question for the GMC penalization:

how to set the matrix parameter \mathbf{B} ?

An approach in (Selesnick, 2017):

$$\mathbf{B} = \sqrt{\theta/\lambda} \mathbf{X}, \quad \text{with } \theta \in (0, 1),$$

then $\lambda \mathbf{B}^\top \mathbf{B} = \theta \mathbf{X}^\top \mathbf{X}$, which satisfies condition (4).

Grouped variable selection

The classical linear regression setting:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- $\mathbf{y} \in \mathbb{R}^n$: response vector
- $\mathbf{X} \in \mathbb{R}^{n \times p}$: design matrix whose columns are p covariate variables
with natural group structures
e.g. categorical data analysis
- $\boldsymbol{\epsilon} \in \mathbb{R}^n$: vector of noise variables with mean zero and variance σ^2

grouped variable selection and coefficient estimation

Grouped variable selection

- Convex penalization

Group Lasso (Yuan and Lin, 2006) and its variants

$$\hat{\beta}_{\text{grLasso}} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|\mathbf{y} - \sum_{j=1}^J \mathbf{X}_j \beta_j\|_2^2 + \lambda \sum_{j=1}^J K_j \|\beta_j\|_2 \quad (5)$$

- $\beta = (\beta_1^T, \dots, \beta_J^T)^T \in \mathbb{R}^p$ with $\beta_j \in \mathbb{R}^{p_j}$ and $\sum_{j=1}^J p_j = p$
- \mathbf{X}_j : submatrix of $\mathbf{X} \rightarrow$ variables in the j -th group
- K_j s: adjusting for the group sizes, e.g. $K_j = \sqrt{p_j}$

- Nonconvex penalization

Group SCAD (Wang et al., 2007), Group MCP (Huang et al., 2012)

The group GMC estimator

The **group GMC penalty** (Liu et al., 2021):

$$\phi_{\mathbf{B}}(\boldsymbol{\beta}) = \sum_{j=1}^J K_j \|\boldsymbol{\beta}_j\|_2 - \min_{\mathbf{v} \in \mathbb{R}^p} \left\{ \sum_{j=1}^J K_j \|\mathbf{v}_j\|_2 + \frac{1}{2n} \|\mathbf{B}(\boldsymbol{\beta} - \mathbf{v})\|_2^2 \right\} \quad (6)$$

- $\boldsymbol{\beta} = (\boldsymbol{\beta}_1^T, \dots, \boldsymbol{\beta}_J^T)^T \in \mathbb{R}^p$
- $\mathbf{v} = (\mathbf{v}_1^T, \dots, \mathbf{v}_J^T)^T \in \mathbb{R}^p$
- For each j , $\boldsymbol{\beta}_j, \mathbf{v}_j \in \mathbb{R}^{p_j}$ with $\sum_{j=1}^J p_j = p$

The group GMC estimator

The group GMC model:

$$\arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \phi_{\mathbf{B}}(\beta), \quad (7)$$

- $\lambda \geq 0$: tuning parameter representing the degree of penalization
- \mathbf{B} : matrix parameter controlling the concavity of the penalty

The group GMC estimator

The group GMC problem (7) is convex if

$$\mathbf{X}^T \mathbf{X} \succeq \lambda \mathbf{B}^T \mathbf{B} \quad (8)$$

- **convexity-preserving condition** for group GMC

The group GMC estimator

Set matrix \mathbf{B} for group GMC:

$$\lambda \mathbf{B}^T \mathbf{B} = \theta \mathbf{X}^T \mathbf{X}, \quad \theta \in [0, 1]. \quad (9)$$

- θ : the **convexity-preserving parameter** of the group GMC model
 - $\theta = 0$: group GMC \rightarrow group Lasso
 - $\theta = 1$: a maximally nonconvex penalty

The group GMC estimator

Relation between group GMC and group MCP (Huang et al., 2012):

Remark

The group GMC method is equivalent to the group MCP method when $\mathbf{B}^T \mathbf{B}$ is diagonal and the diagonal elements are suitably designed. This equivalence also holds for the GMC and MCP.

The group GMC estimator

Properties of the solution path:

Theorem

Suppose $\mathbf{X}^\top \mathbf{X} \succ \lambda \mathbf{B}^\top \mathbf{B}$, then the solution path $\beta^(\lambda)$ to the group GMC problem (7) exists, is unique, and is continuous in λ .*

- Problem (7) is well-posed
- Warm start when solving a sequence of problems over a grid of λ values

The group GMC estimator

Properties of the solution path:

Theorem

The group GMC problem (7) has a unique solution $\beta^(\lambda) = \mathbf{0}$ for all λ greater than $\lambda_0 = \max_j \left\{ \frac{\|\mathbf{x}_j^T \mathbf{y}\|_2}{nK_j} \right\}$, where \mathbf{x}_j and K_j are as defined in (5) for $j = 1, \dots, J$.*

- A precise range of λ , $[0, \lambda_0]$, to sample the full dynamic range of the coefficient estimation

Algorithms for the group GMC model

Recast problem (7) as a saddle-point problem

$$\min_{\beta \in \mathbb{R}^p} \max_{\mathbf{v} \in \mathbb{R}^p} f(\beta) + \beta^\top \mathbf{Z} \mathbf{v} - g(\mathbf{v}), \quad (10)$$

where

$$f(\beta) = \frac{1}{2n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \sum_{j=1}^J K_j \|\beta_j\|_2 - \frac{\lambda}{2n} \|\mathbf{B}\beta\|_2^2,$$

$$g(\mathbf{v}) = \frac{\lambda}{2n} \|\mathbf{B}\mathbf{v}\|_2^2 + \lambda \sum_{j=1}^J K_j \|\mathbf{v}_j\|_2,$$

$$\mathbf{Z} = \frac{\lambda}{n} \mathbf{B}^\top \mathbf{B}.$$

- Primal-Dual Hybrid Gradient (PDHG) method (Goldstein et al., 2013, 2015a)

Algorithm 1 Basic PDHG steps for problem (10)

- 1: Set $\beta_0 \in \mathbb{R}^p$, $\mathbf{v}_0 \in \mathbb{R}^p$, $\sigma_k > 0$, $\tau_k > 0$
 - 2: **for** $k = 1$ to K **do**
 - 3: $\hat{\beta}_{k+1} = \beta_k - \tau_k \mathbf{Z}^T \mathbf{v}_k$
 - 4: $\beta_{k+1} = \arg \min_{\beta \in \mathbb{R}^p} f(\beta) + \frac{1}{2\tau_k} \|\beta - \hat{\beta}_{k+1}\|_2^2$
 - 5: $\hat{\mathbf{v}}_{k+1} = \mathbf{v}_k + \sigma_k \mathbf{Z}(2\beta_{k+1} - \beta_k)$
 - 6: $\mathbf{v}_{k+1} = \arg \min_{\mathbf{v} \in \mathbb{R}^p} g(\mathbf{v}) + \frac{1}{2\sigma_k} \|\mathbf{v} - \hat{\mathbf{v}}_{k+1}\|_2^2$
 - 7: **end for**
-

Algorithms for the group GMC model

Updating β_{k+1} and \mathbf{v}_{k+1} :

$$\beta_{k+1} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{2n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 - \frac{\lambda}{2n} \|\mathbf{B}\beta\|_2^2 + \frac{1}{2\tau_k} \|\beta - \hat{\beta}_{k+1}\|_2^2 \right\} \\ + \lambda \sum_{j=1}^J K_j \|\beta_j\|_2$$

$$\mathbf{v}_{k+1} = \operatorname{argmin}_{\mathbf{v} \in \mathbb{R}^p} \left\{ \frac{\lambda}{2n} \|\mathbf{B}\mathbf{v}\|_2^2 + \frac{1}{2\sigma_k} \|\mathbf{v} - \hat{\mathbf{v}}_{k+1}\|_2^2 \right\} + \lambda \sum_{j=1}^J K_j \|\mathbf{v}_j\|_2$$

- group Lasso penalized problems
- Fast Adaptive Shrinkage/Thresholding Algorithm (FASTA) (Goldstein et al., 2014, 2015b)

Error bound for the group GMC estimator

Some definitions:

- $\mathbf{v}^* = \operatorname{argmin}_{\mathbf{v} \in \mathbb{R}^p} \left\{ \sum_{j=1}^J K_j \|\mathbf{v}_j\|_2 + \frac{1}{2n} \|\mathbf{B}(\boldsymbol{\beta}^* - \mathbf{v})\|_2^2 \right\}$
- $\mathcal{S} := \{j : \|\boldsymbol{\beta}_j^*\|_2 \neq 0, j \in [J]\}$ and $\mathcal{S}^c := [J] \setminus \mathcal{S}$
- $$\nu_j = \begin{cases} K_j + n^{-1} \|[\mathbf{B}^\top \mathbf{B}]_{j,\cdot}(\boldsymbol{\beta}^* - \mathbf{v}^*)\|_2, & j \in \mathcal{S} \\ K_j - n^{-1} \|[\mathbf{B}^\top \mathbf{B}]_{j,\cdot}(\boldsymbol{\beta}^* - \mathbf{v}^*)\|_2, & j \in \mathcal{S}^c \end{cases}$$
- $\bar{\nu} := \max_{j \in \mathcal{S}} \nu_j$ and $\underline{\nu} := \min_{k \in \mathcal{S}^c} \nu_k$

Error bound for the group GMC estimator

Conditions and assumptions:

- \mathbf{X} satisfies a “block-normalization” condition:

$$\|\mathbf{X}_{\cdot,j}\| \leq \sqrt{n}, \quad j \in [J]$$

- **A1.** (Subgaussian errors). The data are generated from (12) where $\epsilon \in \mathbb{R}^n$ has independent entries which are σ -subgaussian random variables for $0 < \sigma < \infty$. That is, $\mathbb{E}(\epsilon_i) = 0$ and for all $t \in \mathbb{R}$, $\mathbb{E}\{\exp(t\epsilon_i)\} \leq \exp(t^2\sigma^2/2)$ for each $i \in [n]$.
- **A2.** (Convexity) The matrix \mathbf{B} is chosen so that $\mathbf{X}^\top \mathbf{X} \succeq \lambda \mathbf{B}^\top \mathbf{B}$.
- **A3.** (Sample size) The sample size n is sufficiently large so that $\nu_k > 0$ for all $k \in \mathcal{S}^c$.

Error bound for the group GMC estimator

Conditions and assumptions:

- **A4.** (Restricted eigenvalue condition) For a fixed $c > 1$, define

$$\mathbb{C}_n(\mathcal{S}, \nu, c) = \left\{ \boldsymbol{\Delta} \in \mathbb{R}^p : \boldsymbol{\Delta} \neq \mathbf{0}, \sum_{k \in \mathcal{S}^c} \left(\nu_k - \frac{\nu}{c} \right) \|\boldsymbol{\Delta}_k\|_2 \leq \sum_{j \in \mathcal{S}} \left(\nu_j + \frac{\nu}{c} \right) \|\boldsymbol{\Delta}_j\|_2 \right\}.$$

We assume there exists a constant $k > 0$ such that for all n and p ,

$$0 < k \leq \kappa_{\mathbf{B}}(\mathcal{S}, c) = \inf_{\boldsymbol{\Delta} \in \mathbb{C}_n(\mathcal{S}, \nu, c)} \frac{\boldsymbol{\Delta}^T (\mathbf{X}^T \mathbf{X} - \lambda \mathbf{B}^T \mathbf{B}) \boldsymbol{\Delta}}{2n \|\boldsymbol{\Delta}\|_2^2}.$$

Error bound for the group GMC estimator

Theorem

(Error bound for group GMC) Let $c > 1$ and $k_1 > 0$ be fixed constants. If assumptions **A1–A4** hold and

$$\lambda = \frac{2c\sigma}{\underline{\nu}} \left(\max_{j \in [J]} \sqrt{\frac{p_j}{n}} + \sqrt{\frac{k_1 \log(J)}{n}} \right),$$

then with probability at least $1 - 2 \exp(-2k_1 \log(J))$,

$$\|\hat{\beta}(\lambda) - \beta^*\|_2 \leq \frac{2c\sigma}{\kappa_{\mathbf{B}}(\mathcal{S}, c)} \left(\frac{\bar{\nu}}{\underline{\nu}} + \frac{1}{c} \right) \left\{ \left(\max_{j \in [J]} \sqrt{\frac{|\mathcal{S}| p_j}{n}} \right) + \sqrt{\frac{|\mathcal{S}| k_1 \log(J)}{n}} \right\},$$

where $\hat{\beta}(\lambda)$ is the group GMC estimator obtained from (7).

Error bound for the group GMC estimator

- Same asymptotic error rate as the group Lasso estimator
- Choose \mathbf{B} such that $\kappa_{\mathbf{B}}(\mathcal{S}, c)$ is large and $\bar{\nu}/\underline{\nu}$ is small

Error bound for the group GMC estimator

Theorem

(Error bound for GMC) Let $c > 1$ and $k_2 \in (0, 1/2)$ be fixed constants. Let $p_j = 1$ for $j \in [p]$ so that $\mathcal{S} = \{j : \beta_j^* \neq 0, j \in [p]\}$. If assumptions **A1–A4** hold and $\lambda = (c\sigma/\underline{\nu})\sqrt{2\log(p/k_2)/n}$, then with probability at least $1 - 2k_2$,

$$\|\hat{\beta}(\lambda) - \beta^*\|_2 \leq \frac{c\sigma}{\kappa_{\mathbf{B}}(\mathcal{S}, c)} \left(\frac{\bar{\nu}}{\underline{\nu}} + \frac{1}{c} \right) \sqrt{\frac{2|\mathcal{S}| \log(p/k_2)}{n}},$$

where $\hat{\beta}(\lambda)$ is the corresponding GMC estimator.

- Models:
 - an ANOVA model with all two-way interactions
 - an additive model including both categorical and continuous variables
- Factors of interest:
 - signal-to-noise ratio (SNR) of the model
 - correlation among groups
 - problem dimension
 - convexity-preserving parameter (for the group GMC)

Data generation of the ANOVA model:

- Z_1, Z_2, Z_3 and Z_4 from a centered multivariate normal distribution
 - $\text{Cov}(Z_i, Z_j) = \rho^{|i-j|}$
- Z_1, \dots, Z_4 are trichotomized to 0, 1 or 2
 - 0 if smaller than $\Phi^{-1}(\frac{1}{3})$
 - 1 if larger than $\Phi^{-1}(\frac{1}{3})$
 - 2 if in between

Data generation of the ANOVA model:

$$y = 3\mathbb{1}(Z_1 = 1) + 2\mathbb{1}(Z_1 = 0) + 3\mathbb{1}(Z_2 = 1) + 2\mathbb{1}(Z_2 = 0) + \\ \mathbb{1}(Z_1 = 1, Z_2 = 1) + \mathbb{1}(Z_1 = 1, Z_2 = 0) + \\ 2\mathbb{1}(Z_1 = 0, Z_2 = 1) + 2.5\mathbb{1}(Z_1 = 0, Z_2 = 0) + \epsilon,$$

- $\mathbb{1}(\cdot)$ is the indicator function
- $\epsilon \sim N(0, \sigma^2)$
- 32 covariate variables from 10 groups

Simulation experiments

Performance in three aspects:

- Coefficient estimation

- $SE = \|\hat{\beta} - \beta\|_2^2$

- Prediction performance

- prediction error = $\frac{1}{n} \|\mathbf{X}\hat{\beta} - \mathbf{X}\beta\|_2^2$

- Support recovery

- $F1 \text{ score} = \frac{2TP}{2TP + FP + FN}$

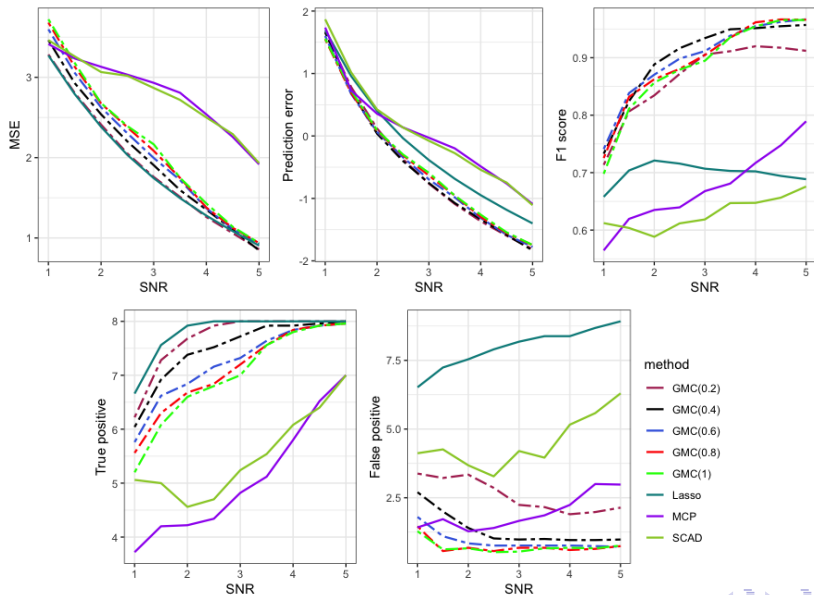
- true positive (TP) and false positive (FP)

| | | Estimation | |
|-------|------------------|------------------------|---------------------|
| | | $\hat{\beta}_j \neq 0$ | $\hat{\beta}_j = 0$ |
| Truth | $\beta_j \neq 0$ | TP | FN |
| | $\beta_j = 0$ | FP | TN |

• Case I: effect of the SNR

- uncorrelated groups ($\rho = 0$)
- problem dimension $p = 32$
- sample size $n = 100$
- $\text{SNR} \in \{1, 2, \dots, 5\}$
- $\theta \in \{0.2, 0.4, 0.6, 0.8, 1\}$

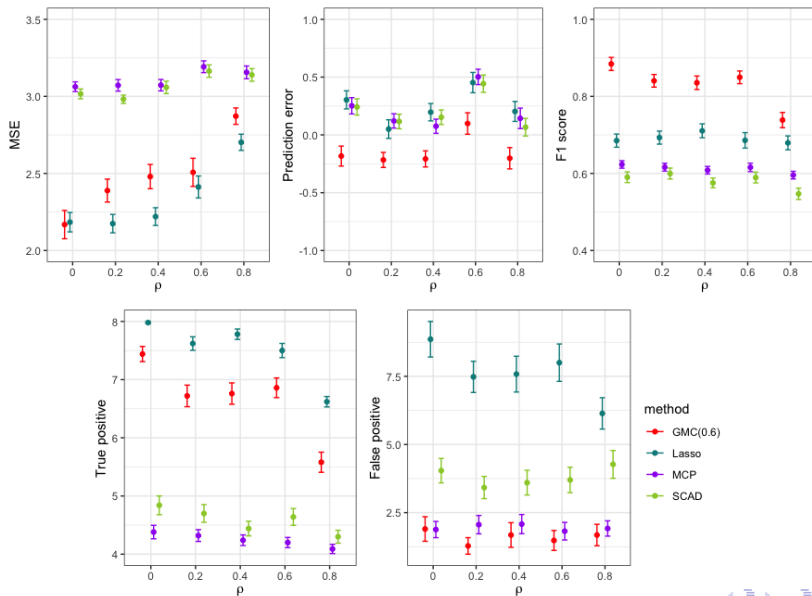
Simulation experiments



- **Case II: effect of the correlation among groups**

- $\text{SNR} = 2$
- problem dimension $p = 32$
- sample size $n = 100$
- $\theta = 0.6$
- correlation $\rho \in \{0, 0.2, 0.4, 0.6, 0.8\}$

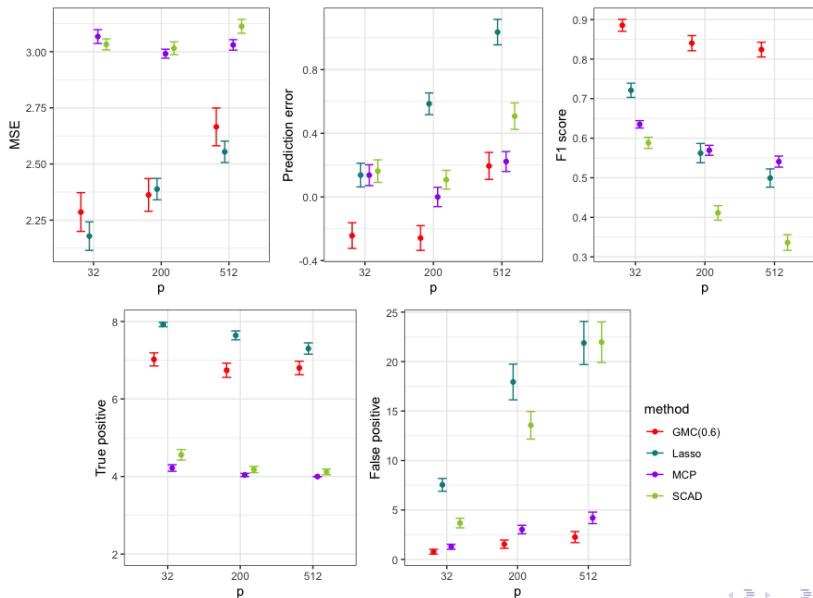
Simulation experiments



• Case III: effect of the problem dimension

- uncorrelated groups ($\rho = 0$)
- $\text{SNR} = 2$
- sample size $n = 100$
- $\theta = 0.6$
- $p \in \{32, 200, 512\}$

Simulation experiments



The birth weight data set investigated in Yuan and Lin (2006):

- risk factors associated with low rank infant birth weight
- 189 observations of a response variable (infant birth weight)
- 8 explanatory variables (continuous and categorical)

Table 1. *Description of the birth weight data set*

| Name | Type | Variable description |
|----------------------|-------------|--|
| Birth weight | Continuous | Infant birth weight in kilograms |
| Mother's age | Continuous | Mother's age in years |
| Mother's weight | Continuous | Mother's weight in pounds at last menstrual period |
| Race | Categorical | Mother's race (white, black or other) |
| Smoking | Categorical | Smoking status during pregnancy (yes or no) |
| # Premature | Categorical | Previous premature labors (0, 1, or more) |
| Hypertension | Categorical | History of hypertension (yes or no) |
| Uterine irritability | Categorical | Presence of uterine irritability (yes or no) |
| # Phys. visits | Categorical | Number of physician visits during the first trimester (0, 1, 2, or more) |

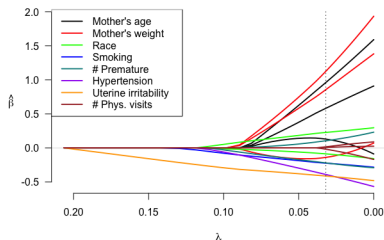
- 16 covariate variables from 8 groups

Table 2. *Summarized results for the birth weight data*

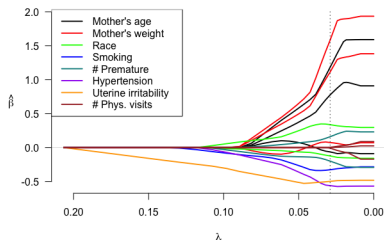
| | Prediction error | # nonzero groups | Excluded groups |
|-------------|------------------|------------------|-----------------|
| Group Lasso | 0.36 | 8 | none |
| Group SCAD | 0.35 | 8 | none |
| Group MCP | 0.35 | 7 | # Phys. visits |
| Group GMC | 0.35 | 7 | # Phys. visits |

Real data application

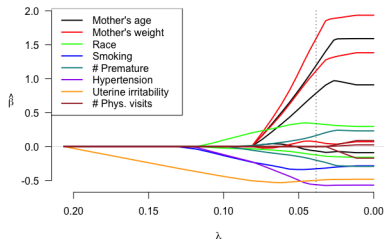
Group Lasso



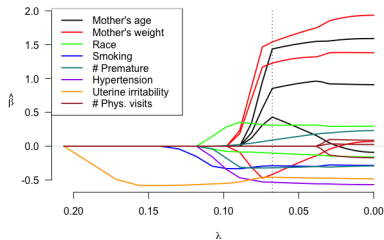
Group SCAD



Group MCP



Group GMC



Summary:

- A group GMC method for grouped variable selection and coefficient estimation in linear regression
- Convexity preserving condition, relation to existing methods, and properties of solution path
- Algorithms for computing the solution path
- Error bounds of the (group) GMC estimator
- Simulations and a real data application

Future directions:

- Guidance on setting the matrix parameter \mathbf{B}
- Extension to generalized linear models
- Computation of the (group) GMC problem

Please reach out if you have any questions:

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Useful links:

- The original GMC paper:
<https://ieeexplore.ieee.org/document/7938377>
- Matlab code for GMC:
<https://codeocean.com/capsule/2729219/tree/v1>
- Our group GMC paper:
<https://arxiv.org/abs/2111.15075>
- An R package for group GMC will be available on CRAN soon

Thank You!

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