### **SLOPE**

### Malgorzata Bogdan<sup>1,2</sup>

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May, 2020

► Research with J.K.Ghosh - mBIC and asymptotic optimality of the Benjamini-Hochberg procedure

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- Screening Rules for SLOPE
- SLOPE for graphical models

# Modified version of BIC (1)

M. B, J.K. Ghosh, R.W. Doerge, Genetics (2004)





## Statistical problem

Selecting important genetic markers based on the multiple regression model:

 $X_{n \times p}$  - matrix of genotypes of genetic markers,

 $Y_{n\times 1}$  - vector of trait values.

Goal: Identify the best model of the form

$$Y = \beta_0 1 + X_I \beta_I + \varepsilon,$$

I - a subset of  $\{1,\ldots,p\}$ , k=|I|,  $\varepsilon \sim N(0,\sigma^2I)$ .

mBIC: Select the model minimizing

$$\log RSS + k \log(n) + 2k \log\left(\frac{p}{C}\right),\,$$

where RSS is the residual sum of squares,

C is the prior expected value of the number of genetic effects.

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mBIC results from supplementing BIC with the Binomial prior B(p, C/p) on the number of genetic effects.

 $2 \log p$  term plays a role of the Bonferroni for multiple testing (see e.g. Bogdan, Ghosh, Żak-Szatkowska, QREI, 2008).

M.B, J.K.G., S.T.Tokdar, *IMS Collections, 2008* M.B, J.K.G, A.Ochman, S.T.Tokdar, *QREI*, 2007





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 - independent,  $X_i \sim N(\mu_i, \sigma^2)$ 

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Benjamini-Hochberg procedure:

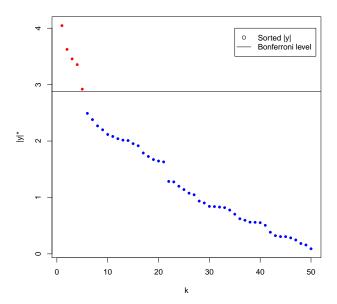
- (1)  $|X|_{(1)} \ge |X|_{(2)} \ge \ldots \ge |X|_{(p)}$
- (2) Find the largest index *i* such that

$$|X|_{(i)} \ge \sigma \Phi^{-1}(1 - \alpha_i), \quad \alpha_i = \alpha \frac{i}{2p}.$$
 (1)

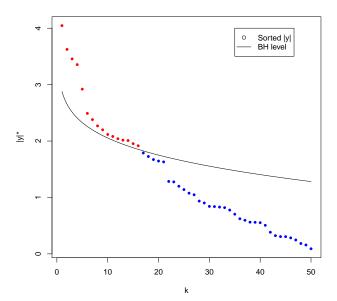
Call this index i<sub>SU</sub>.

(3) Reject all  $H_{(i)}$ 's for which  $i \leq i_{SU}$ .

### Bonferroni correction



## Benjamini and Hochberg correction



[B, Ghosh, Tokdar, *IMS Collections* 2008] and [B, Ghosh, Ochman, Tokdar *QREI*, 2007]: empirical comparison of BH with several Bayesian multiple testing procedures with respect to minimizing the Bayes classification risk.

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Bayes oracle  $\rightarrow$  Bayes classifier

M.B, A.Chakrabarti, F.Frommlet, JKG, Ann.Statist. 2011: The rule is Asymptotically Bayes Optimal under Sparsity (ABOS) if  $\lim \frac{R}{R_{opt}} \to 1$  (as  $p \to \infty$ )

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$$mBIC2 := \log RSS + k \log n + 2k \log(p/4) - 2 \log(k!)$$

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Problem - numerical complexity of identifying the model minimizing mBIC2.

Different search strategies implemented in the package *bigstep by P.Szulc.* 



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When  $\beta_i = 0$  then  $X_i'Y \sim N(0, \sigma^2)$  and the control of FWER is provided by the Bonferroni correction

$$\lambda = \sigma \Phi^{-1} \left( 1 - \frac{\alpha}{2p} \right) \approx \sqrt{2 \log p}$$

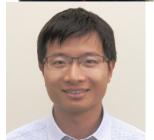
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### Sorted L-One Penalized Estimation

M.B., E.van den Berg, W.Su, E.J.Candès, arxiv 2013 M.B., E.van den Berg, C.Sabatti, W.Su, E.J.Candès, AOAS 2015









#### Sorted L-One Penalized Estimation

$$\hat{\beta} = \operatorname{argmin}_{b \in P} \|y - Xb\|_{\ell_2}^2 + \sum_{i=1}^p \lambda_i |b|_{(i)}.$$

where  $|b|_{(1)} \ge \ldots \ge |b|_{(p)}$  are ordered magnitudes of coefficients of b and  $\lambda_1 \ge \ldots \ge \lambda_p \ge 0$  is the sequence of tuning parameters.

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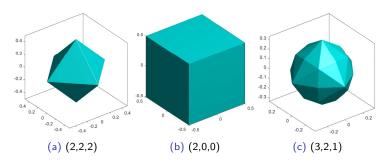
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Sorted L-One Norm: 
$$J_{\lambda}(b) = \sum_{i=1}^{p} \lambda_{i} |b|_{(i)}$$
 reduces to  $||b||_{1}$  if  $\lambda_{1} = \ldots = \lambda_{p}$  and to  $||b||_{\infty}$  if  $\lambda_{1} > \lambda_{2} = \ldots = \lambda_{p} = 0$ .

#### Unit balls for different SLOPE sequences by D.Brzyski



Clustering in the context of portfolio optimization - P. Kremmer, S. Lee, MB and S. Paterlini "Journal of Banking and Finance", 2019

The class of models attainable by SLOPE - U.Schneider and P.Tardivel, arxiv 2020

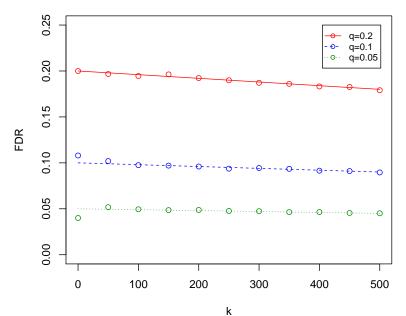
#### FDR control with SLOPE

Theorem (B,van den Berg, Su and Candès (2013)) When  $X^TX = I$  SLOPE with

$$\lambda_i := \sigma \Phi^{-1} \Big( 1 - i \cdot \frac{q}{2p} \Big)$$

controls FDR at the level  $q \frac{p_0}{p}$ .

# Orthogonal design, n = p = 5000



Let  $k = ||\beta||_0$  and consider the setup where  $k/p \to 0$  and  $\frac{k \log p}{n} \to 0$ . X is standardized so that each column has a unit  $L_2$  norm.

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SLOPE with the BH related sequence of tuning parameters attains minimax rate for the estimation error  $||\hat{\beta} - \beta||^2$ .

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SLOPE rate of the estimation error -  $k \log(p/k)$ 

LASSO rate of the estimation error -  $k \log p$ 

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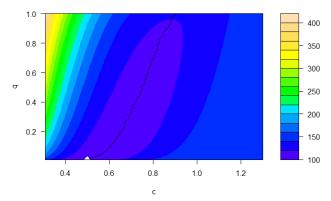
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Extension to logistic regression by Abramovich and Grinshtein (2018, IEEE Trans. Inf. Theory)

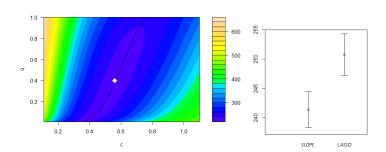
# Predictive properties of SLOPE, Independent predictors

Heat map of 
$$MSE(X\hat{\beta})$$
  $\lambda_i = c\Phi\left(1-\frac{iq}{2p}\right), \quad n=p=1000, k=20$  for  $i\in S, \quad \beta_i = \sqrt{2\log\frac{p}{k}}$ 



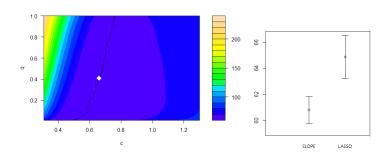
# Independent predictors

$$n = p = 1000, k = 100$$



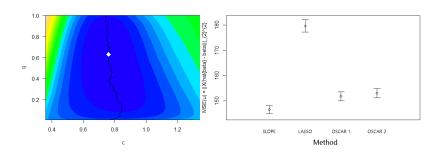
# Correlated predictors

$$n = p = 1000, k = 20, \rho(X_i, X_j) = 0.5$$
 for  $i \neq j$ 



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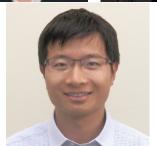


Group SLOPE, (D.Brzyski, A.Gossmann, W.Su and MB,

JASA, 2019)







Identification of groups of predictors:

$$[[\beta]]_{I} := \left( \|X_{I_{1}}\beta_{I_{1}}\|_{2}, \ldots, \|X_{I_{m}}\beta_{I_{m}}\|_{2} \right)^{\mathsf{T}} \ .$$

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$$\beta^{gS} := \operatorname{argmin}_{b} \left\{ \frac{1}{2} \left\| y - Xb \right\|_{2}^{2} + \sigma J_{\lambda} \left( W[[b]]_{I} \right) \right\},$$

where W is a diagonal matrix with  $W_{i,i} := w_i$ , for i = 1, ..., m.

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Selection of

$$\lambda_i^{\max} := \max_{j=1,\dots,m} \left\{ \frac{1}{w_j} F_{\chi_{l_j}}^{-1} \left( 1 - \frac{q \cdot i}{m} \right) \right\}$$

allows to control group FDR and obtain a minimax rate of estimation of  $[[\beta]]_I$  if variables in different groups are orthogonal to each other.

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Heuristic adjustment for the situation when variables in different groups are independent.

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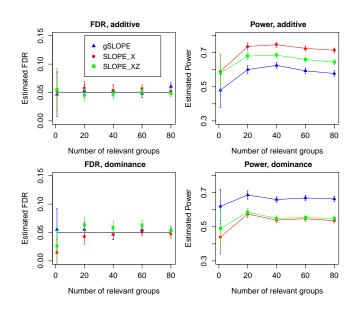
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Scenario 2: modeling dominance

$$Z_{ij} = \begin{cases} -1 & \text{for } aa, AA \\ 1 & \text{for } aA \end{cases},$$

$$y = [X, Z][\beta'_X, \beta'_Z]' + \epsilon .$$
(3)

#### Simulation results



# Robust regression with SLOPE

A. Virouleau, A. Guilloux, S. Gaiffas, MB (arxiv, 2017)







Candes and Randall (2006), Gannaz (2006) and McCann and Welsch (CSDA, 2007) ,

$$y = X\beta + I\mu + \varepsilon \tag{4}$$

 $\mu \in R^n$  is the sparse vector of outliers' effects and  $\varepsilon \sim N(0, \sigma^2 I)$ 

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Virouleau, Guilloux, Gaiffas, B (2017) use SLOPE penalties:

$$\min_{\beta \in {}^p,\mu \in {}^n} \left\{ \|y - X\beta - \mu\|_2^2 + 2\rho_1 J_{\tilde{\lambda}}(\beta) + 2\rho_2 J_{\lambda}(\mu) \right\}$$

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$$\lambda_i(\beta) = \sigma \sqrt{\log\left(\frac{2p}{i}\right)}, \ \ \lambda_i(\mu) = \sigma \sqrt{\log\left(\frac{2n}{i}\right)}$$

#### Estimation properties

Assumptions - restricted eigenvalue condition on X Satisfied with large probability e.g. if the rows of X are iid gaussian with a positive definite covariance matrix and the numbers of nonzero elements in  $\beta$  and  $\mu$  are sufficiently small

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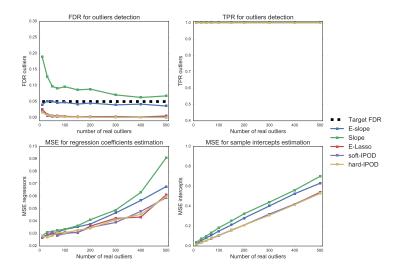
Rates of convergence for

$$\|\hat{\beta} - \beta\|_2^2 + \|\hat{\mu} - \mu\|_2^2$$

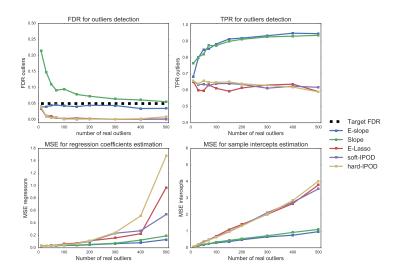
$$s=\#\{i:\mu_i\neq 0\}$$
 - number of outliers,

NO/SL1	$(p \lor s \log(n/s))/n$
L1/L1	$(k \log p \vee s \log n)/n$
L1/SL1	$(k \log p \vee s \log(n/s))/n$
SL1/SL1	$(k \log (p/k) \vee s \log (n/s))/n$

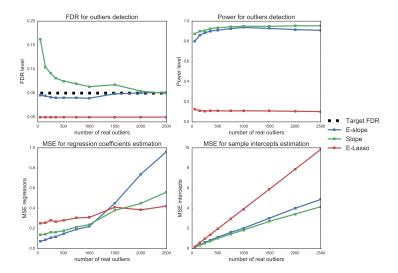
# Low dimensional set-up; large outliers



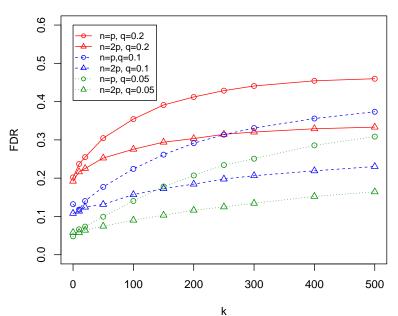
#### Low dimensional set-up; small outliers



#### High dimensional set-up; small outliers



# Gaussian design (1), n = p = 5000



#### Problems with FDR control

Similar problems occur for LASSO.

Intuitive explanation:

$$\hat{eta}_i = \eta_\lambda (eta_i + X_i'z + v_i)$$
  $v_i = X_i, \sum_{j 
eq i} X_j (eta_j - \hat{eta}_j)$   $\eta_\lambda(t) = sign(t)(|t| - \lambda)_+, \quad \text{applied componentwise}$ 

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LASSO can identify the true model only if a very stringent *irrepresentability* condition is satisfied.

Precise FDR-Power Tradeoff under asymptotic assumptions of AMP theory is provided in (Su, B, Candès, AOS 2017).

### Identifiability condition

### Definition (Identifiability)

Let X be a  $n \times p$  matrix. The vector  $\beta \in R^p$  is said to be identifiable with respect to the  $l^1$  norm if the following implication holds

$$X\gamma = X\beta \text{ and } \gamma \neq \beta \Rightarrow ||\gamma||_1 > ||\beta||_1.$$
 (5)

### Theorem (Tardivel, Bogdan, 2019)

For any  $\lambda > 0$  LASSO can separate well the causal and null features if and only if vector  $\beta$  is identifiable with respect to  $l_1$  norm and  $\min_{i \in I} |\beta_i|$  is sufficiently large.

#### Solutions:

- threshold LASSO estimates (see e.g. LCD knockoffs)
- use adaptive LASSO

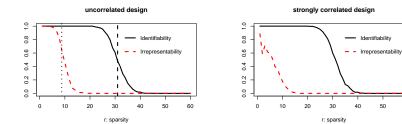


Figure: n = 100, p = 300, in the right panel  $\rho(X_i, X_j) = 0.9$ , vertical lines correspond to  $n/(2 \log p)$  and the transition curve of Donoho and Tanner (2009).

#### **Curves setting 2, positive components**

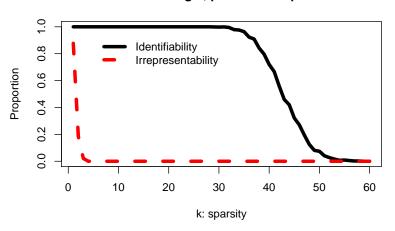


Figure: n = 100, p = 300, in the right panel  $\rho(X_i, X_j) = 0.9$  and all signs of nonzero elements of  $\beta$  are the same.

### Adaptive LASSO

Adaptive LASSO [Zou, *JASA* 2006], [Candès, Wakin and Boyd, *J. Fourier Anal. Appl.* 2008]

$$\beta_{aL} = \operatorname{argmin}_{b} \left\{ \frac{1}{2} \left\| y - Xb \right\|_{2}^{2} + \lambda \sum_{i=1}^{p} w_{i} |b|_{i} \right\}, \tag{6}$$

where  $w_i = \frac{1}{f(|\hat{\beta}_i|)}$ ,  $\hat{\beta}_i$  is some consistent estimator of  $\beta_i$  and f is an increasing function.

## Spike and Slab LASSO

V.Rockova, E. George, JASA 2018

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Spike and Slab LASSO uses a spike and slab Laplace prior:

$$\gamma = (\gamma_1, \ldots, \gamma_p)$$

 $\gamma_i = 1$  if  $\beta_i$  is "large" and  $\gamma_i = 0$  if  $\beta_i$  is "small"

$$\pi(eta|\lambda,\gamma) \propto c^{\sum_{i=1}^{
ho} 1(\gamma_i=1)} \prod_{i=1}^{
ho} e^{-w_i|eta_i|\lambda_0},$$

where  $w_i = 1$  if  $\gamma_i = 0$  and  $w_i = c \in (0,1)$  if  $\gamma_i = 1$ .

# Spike and Slab LASSO (2)

The maximum aposteriori rule is given by reweighted LASSO

$$\hat{\beta}(\gamma) = \operatorname{argmin}_{b \in R^p} \frac{1}{2} ||y - Xb||_2^2 + \lambda_0 \sum_{i=1}^p w_i |b_i|$$

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In consecutive iterations  $\gamma_i$  is replaced with

$$\pi_i^t = P(\gamma_i = 1 | \beta^t, c) = \frac{c\theta e^{-c|\beta_i^t|\lambda_0}}{c\theta e^{-c|\beta_i^t|\lambda_0} + (1-\theta)e^{-|\beta_i^t|\lambda_0}}$$

and then a new estimate  $\hat{\beta}^{t+1}$  is calculated by solving reweighted LASSO with the vector  $\gamma$  replaced with the vector  $\pi^t$ .



## Borrowing information

When updating  $i^{th}$  variable  $\theta$  is replaced by  $E(\theta|\beta_{-i})$ 

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SSL package creates the path of SSL solutions for the sequence of  $100\ \lambda_0$  values

# Adaptive SLOPE with missing values (1)

W. Jiang, MB, J.Josse, B.Miasojedow, V.Rockova, TraumaBase Group,

arxiv 2019











## Motivation: Paris Hospital

► Traumabase<sup>®</sup> data: 20000 major trauma patients × 250 measurements...

Accident type	Age	Sex	Blood pressure	Lactate	Temperature	Platelet (G/L)
Falling	50	М	140		35.6	150
Fire	28	F		4.8	36.7	250
Knife	30	M	120	1.2		270
Traffic accident	23	M	110	3.6	35.8	170
Knife	33	M	106		36.3	230
Traffic accident	58	F	150		38.2	400

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#### ► Challenge :

How to select relevant measurements with missing values?

### Adaptive Bayesian SLOPE

We propose an adaptive version of Bayesian SLOPE (ABSLOPE). After standardizing X so each column has a unit  $L_2$  norm, the prior for  $\beta$  is

$$p(\beta \mid \gamma, c, \sigma^2; \lambda) \propto c^{\sum_{j=1}^{p} \mathbb{I}(\gamma_j = 1)} \prod_{j} \exp \left\{ -w_j |\beta_j| \frac{1}{\sigma} \lambda_{r(W\beta, j)} \right\},$$

#### Interpretation of the model:

- ▶  $\beta_i$  is large enough  $\Rightarrow$  **true signal**;  $0 \Rightarrow$  noise.
- ▶  $\gamma_j \in \{0,1\}$  signal indicator.  $\gamma_j | \theta \sim Bernoulli(\theta)$  and  $\theta$  the **sparsity**.
- ▶  $1/c \in [1, \infty)$ : proportional to the average signal magnitude.
- $W = \text{diag}(w_1, w_2, \dots, w_p)$  and its diagonal element:

$$w_j = c\gamma_j + (1-\gamma_j) = egin{cases} c, & \gamma_j = 1 \ 1, & \gamma_j = 0 \end{cases}.$$

### Adaptive Bayesian SLOPE

#### Advantage of introducing W:

- when  $\gamma_j = 0$ ,  $w_j = 1$ , i.e., the null variables are treated with the regular SLOPE penalty
- when  $\gamma_j=1$ ,  $w_j=c<1$ , i.e, **smaller penalty**  $\lambda_{r(W\beta,j)}$  for true predictors than the regular SLOPE one

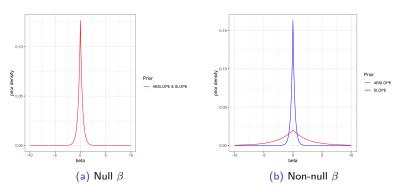


Figure: comparison of SLOPE prior and ABSLOPE prior

## Major difference between SSL and ABSLOPE

ABSLOPE spike prior is "fixed" and frequentist motivated, with the aim of FDR control

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ABSLOPE spike prior is "fixed" and frequentist motivated, with the aim of FDR control

Slab component is "estimated" via the estimation of the average signal magnitude

# Model selection with missing values

**Decomposition:**  $X = (X_{obs}, X_{mis})$ 

Pattern: matrix M with  $M_{ij} = \begin{cases} 1, & \text{if } X_{ij} \text{ is observed} \\ 0, & \text{otherwise} \end{cases}$ 

Assumption 1: Missing at random (MAR)

 $\begin{array}{ll} p(\textit{M} \mid \textit{X}_{\rm obs}, \textit{X}_{\rm mis}) = p(\textit{M} \mid \textit{X}_{\rm obs}) & \Rightarrow & \text{ignorable missing patterns} \\ \text{e.g. People at older age didn't tell his income at larger probability.} \end{array}$ 

**Assumption 2:** Distribution of covariates

 $\label{eq:continuity} X_i \!\sim_{\mathrm{i.i.d.}} \! \mathcal{N}_p(\mu, \Sigma), \quad i = 1, \cdots, n.$ 

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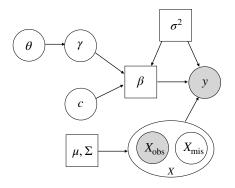
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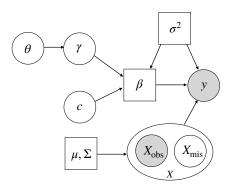
**Problem:** With NA, only a few methods are available to select a model, and their performances are limited. For example,

- Claeskens and Consentino, 2008) adapts AIC to missing values ⇒ Impossible to deal with high dimensional analysis.
- ► (Loh and Wainwright, 2012) LASSO with NA
  - $\Rightarrow$  Non-convex optimization; requires to know bound of  $\|\beta\|_1$
  - ⇒ difficult in practice

# ABSLOPE with missingness: Summary



### ABSLOPE with missingness: Summary



$$\begin{split} \ell_{\text{comp}} &= \log \mathtt{p}(y, X, \gamma, c; \ \beta, \theta, \sigma^2) \\ &= \log \left\{ \mathtt{p}(X; \ \mu, \Sigma) \, \mathtt{p}(y \mid X; \ \beta, \sigma^2) \, \mathtt{p}(\beta; \ \gamma, c) \, \mathtt{p}(\gamma; \ \theta) \, \mathtt{p}(c) \right\} \end{split}$$

**Objective:** Maximize  $\ell_{\rm obs} = \iiint \ell_{\rm comp} \, dX_{\rm mis} \, dc \, d\theta \, d\gamma$ .

# EM algorithm

E step: evaluate

$$Q^t = \mathbb{E}(\ell_{\text{comp}}) \quad \text{wrt} \quad p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^t, \sigma^t, \mu^t, \Sigma^t).$$

► *M step:* update

$$\beta^t, \sigma^t, \mu^t, \Sigma^t = \arg\max Q^t$$

**Problem:** The function Q is not tractable.  $\Rightarrow$ 

1. Monte Carlo EM ? (Wei and Tanner 1990)



## EM algorithm

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**Problem:** The function Q is not tractable.  $\Rightarrow$ 

- Monte Carlo EM ?
   Expensive to generate a large number of samples.
- 2. Stochastic Approximation EM (book, Lavielle 2014)
  - One sample in each iteration;

### Adapted SAEM algorithm

E step:

$$Q^t = \mathbb{E}(\ell_{\text{comp}})$$
 wrt  $p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^t, \sigma^t, \mu^t, \Sigma^t)$ .

• Simulation: draw one sample  $(X_{\min}^t, \gamma^t, c^t, \theta^t)$  from

$$p(X_{\text{mis}}, \gamma, c, \theta \mid y, X_{\text{obs}}, \beta^{t-1}, \sigma^{t-1}, \mu^{t-1}, \Sigma^{t-1});$$
 [Gibbs sampling]

Stochastic approximation: update function Q with

$$Q^t = Q^{t-1} + \eta_t \left( \ell_{\text{comp}}(X_{\text{mis}}^t, \gamma^t, c^t, \theta^t) - Q^{t-1} \right).$$

 $\begin{array}{l} \blacktriangleright \; \textit{M step:} \; \beta^{t+1}, \sigma^{t+1}, \mu^{t+1}, \Sigma^{t+1} = \arg\max Q^{t+1}. \\ [\text{When } \eta_t = 1 \text{: Reweighted SLOPE, Shrinkage of covariance}] \end{array}$ 

Details of initialization, generating samples and optimization are in the draft (arXiv:1909.06631)

### **SLOBE**

Instead of using Gibbs sampling  $\gamma$  and c are replaced with the approximation to their conditional expectations given data,  $\beta$  and  $\sigma$ 

### R package: ABSLOPE

### Install package:

```
library(devtools)
install_github("wjiang94/ABSLOPE")
```

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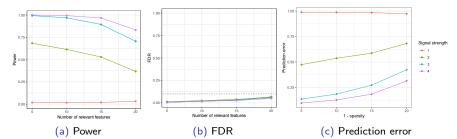
```
library(devtools)
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```

### Main algorithm:

```
lambda = create_lambda_bhq(ncol(X),fdr=0.10)
list.res = ABSLOPE(X, y, lambda)
```

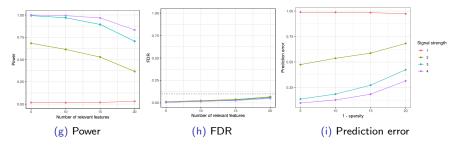
## Simulation study (200 rep. $\Rightarrow$ average)

n=p=100, no correlation and 10% missingness

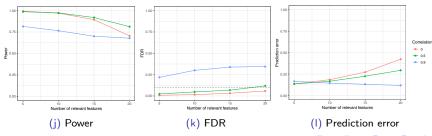


# Simulation study (200 rep. $\Rightarrow$ average)

n=p=100, no correlation and 10% missingness



n=p=100, with 10% missingness and strong signal

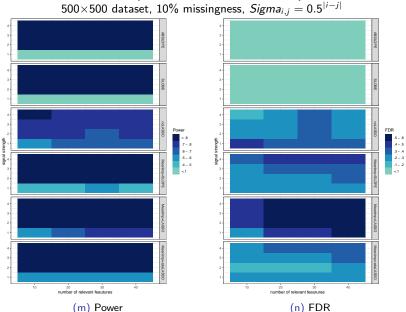


### Method comparison

- ABSLOPE and SLOBE
- ▶ ncLASSO: non convex LASSO (Loh and Wainwright, 2012)
- **MeanImp** + **SLOPE**: Mean imputation followed by SLOPE with known  $\sigma$
- ▶ MeanImp + LASSO: Mean imputation followed by LASSO, with  $\lambda$  tuned by cross validation
- ► MeanImp + adaLASSO: Mean imputation followed by adaptive LASSO (Zou, 2006)

In the SLOPE type methods,  $\lambda={\sf BH}$  sequence which controls the FDR at level  ${\bf 0.1}$ 

# Method comparison (200 rep. $\Rightarrow$ average)



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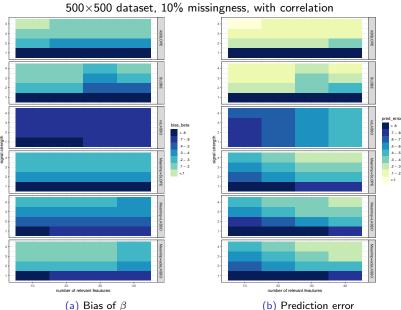
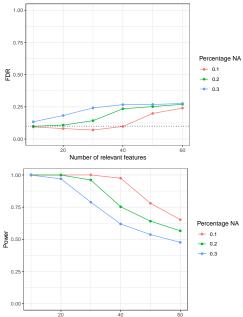


Figure: Comparison of power (a) FDR (b) bias of  $\beta$  (c) and prediction error

# n = p = 500, $\Sigma_{ij} = 0.5^{|i-j|}$ , FDR and Power



Number of relevant features

## Variables in the TraumaBase data set (APHP)

#### Goal - quick prediction of the level of platelets

- ► Age: Age
- SI: Shock index indicates level of occult shock based on heart rate (FC) and systolic blood pressure (PAS).  $SI = \frac{FC}{PAS}$ . Evaluated on arrival of hospital.
- ▶ *PAM:* Mean arterial pressure is an average blood pressure in an individual during a single cardiac cycle, based on systolic blood pressure (PAS) and diastolic blood pressure (PAD).  $PAM = \frac{2PAD + PAS}{3}$ . Evaluated on arrival of hospital.
- delta\_Hemocue: The difference between the hemoglobin on arrival at hospital and that in the ambulance.
- Temps.lieux.hop: Time spent in hospital i.e., medicalization time, in minutes.
- Lactates: The conjugate base of lactic acid.
- ▶ Temperature: Patient's body temperature.

#### **Variables**

- FC: heart rate measured on arrival of hospital.
- Remplissage: A volume expander is a type of intravenous therapy that has the function of providing volume for the circulatory system.
- CGR.dechoc: A binary index which indicates whether the transfusion of Red Blood Cells Concentrates is performed.
- SI.SMUR: Shock index measured on ambulance.
- ► PAM.SMUR: Mean arterial pressure measured in the ambulance.
- FC.max: Maximum value of measured heart rate in the ambulance.
- PAS.min: Minimum value of measured systolic blood pressure in the ambulance.
- PAD.min: Minimum value of measured diastolic blood pressure in the ambulance.

### Percentage of missing values

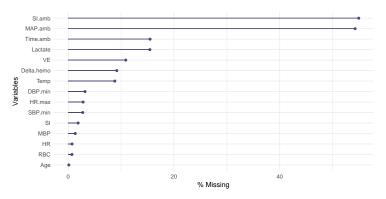
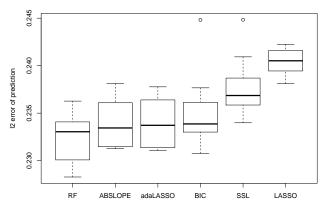


Figure: Percentage of missing values in each pre-selected variable from TraumaBase.

#### Results

 $\label{eq:problem} TraumaBase: \ Measurements \stackrel{Predict}{\longrightarrow} Platelet \\ Cross-validation: \ random \ splits \ to \ training \ and \ test \ sets \ \times \ 10$ 



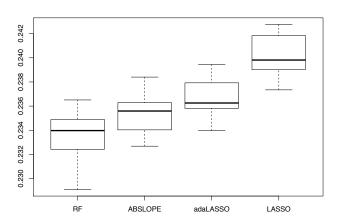
- Comparable to random forest
- ▶ Interpretable model selection and estimation results

#### Selected variables

Figure: Number of times that each variable is selected over 10 replications. Bold numbers indicate which variables are included in the model selected by ABSLOPE.

Variable	ABSLOPE	SLOPE	LASSO	adaLASSO	BIC
Age	10	10	4	10	10
SI	10	2	0	0	9
MBP	1	10	1	10	1
Delta.hemo	10	10	8	10	10
Time.amb	2	6	0	4	0
Lactate	10	10	10	10	10
Temp	2	10	0	0	0
HR	10	10	1	10	10
VE	10	10	2	10	10
RBC	10	10	10	10	10
SI.amb	0	0	0	0	0
MBP.amb	0	0	0	0	0
HR.max	3	9	0 .	A + 4 1 + 4 =	. 0∍
CDD :		10	10		

### With interactions



### Selected variables

Method	Variables selected			
ABSLOPE	Age * MBP.amb, Delta.hemo * Lactate			
	Lactate * RBC, HR * SBP.min			
	RBC, SBP.min			
	Age * Lactate, Age * VE			
LASSO	Delta.hemo * Lactate, Delta.hemo * VE			
	Lactate * VE, Lactate * RBC			
	Age * Time.amb, Age * HR			
	Age * MBP.amb, Age * SBP.min			
adaLASSO	MBP * HR, Delta.hemo * VE			
	Lactate * VE,HR * HR.max			
	HR * SBP.min, $VE * RBC$			

#### Conclusion & Future research

#### Conclusion:

- ► ABSLOPE reduces the estimation bias of large regression coefficients.
- This allows for
  - 1. Improved estimation and prediction properties
  - FDR control under much wider range of scenarios than for regular SLOPE
- Modeling in a Bayesian framework allows for the estimation of the structure of predictors such as the signal sparsity and the signal strength;

#### Future research:

- Deal with other missing mechanisms
- Application for other statistical models (e.g. GLM or Gaussian Graphical Models)
- Theoretical analysis of statistical properties (asymptotic FDR control, minimaxity)
- Speeding the SLOPE algorithm

# Strong screening rule for SLOPE

J. Larsson, MB, J. Wallin (2020)





### Predictor screening rules

#### Goal

Constructing the SLOPE solution path corresponding to the sequence  $\lambda^j$ ,  $j \in \{1, \dots, m\}$  such that for all  $i \in \{1, \dots, p\}$ ,  $\lambda^j_i > \lambda^{j+1}_i$ 

### Predictor screening rules

#### Goal

Constructing the SLOPE solution path corresponding to the sequence  $\lambda^j$ ,  $j \in \{1,\ldots,m\}$  such that for all  $i \in \{1,\ldots,p\}$ ,  $\lambda^j_i > \lambda^{j+1}_i$ 

#### Basic idea

Use the solution at the step j to construct a relatively cheap test to determine which predictors will be inactive before fitting the model for the step j+1.

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#### Safe and Heuristic Rules

safe rules certifies that discarded predictors are not in model heuristic rules may incorrectly discard some predictors, which means problem must sometimes be solved several times (in practice never more than twice)

## Motivation for lasso strong rule

Assume we are solving the lasso, i.e. minimizing

$$g(\beta) + h(\beta), \qquad h(\beta) := \lambda \sum_{i=1}^{p} |\beta_i|.$$

KKT stationarity condition is

$$\mathbf{0} \in \nabla g(\hat{\beta}) + \partial h(\hat{\beta}),$$

where  $\partial h(\hat{\beta})$  is the subdifferential for the  $\ell_1$  norm with elements given by

$$\partial h(\hat{\beta})_i = \begin{cases} \operatorname{sign}(\hat{\beta}_i)\lambda & \hat{\beta}_i \neq 0 \\ [-\lambda, \lambda] & \hat{\beta}_i = 0, \end{cases}$$

which means that  $|\nabla g(\hat{\beta})_i| < \lambda \implies \hat{\beta}_i = 0.$ 

#### Gradient estimate

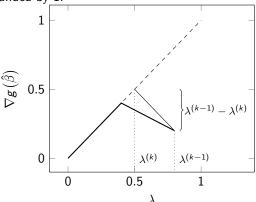
Assume that we are fitting a regularization path and have  $\hat{\beta}(\lambda^{(k-1)})$ —the solution for  $\lambda^{(k-1)}$ —and want to discard predictors corresponding to the problem for  $\lambda^{(k)}$ .

Basic idea: replace  $\nabla g(\hat{\beta})$  with an estimate and apply the KKT stationarity criterion, discarding predictors that are estimated to be zero.

What estimate should we use?

### The unit slope bound

A simple (and usually conservative) estimate turns out to be  $\lambda^{(k-1)} - \lambda^{(k)}$ , i.e. assume that the gradient is piece-wise linear function with slope bounded by 1.

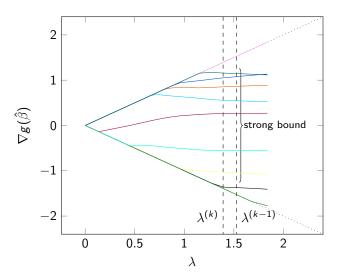


### The strong rule for the lasso

Discard the jth predictor if

Empirical results show that the strong rule leads to remarkable performance improvements in  $p \gg n$  regime (and no penalty otherwise) (tibshirani2012).

### Strong rule for lasso in action



### Strong rule for SLOPE

Exactly the same idea as for lasso strong rule.

The subdifferential for SLOPE is is the set of all  $g \in \mathbb{R}^p$  such that

$$g_{\mathcal{A}_i} = \left\{ s \in \mathbb{R}^{\operatorname{card} \mathcal{A}_i} \mid egin{aligned} \operatorname{cumsum}(|s|_{\downarrow} - \lambda_{R(s)_{\mathcal{A}_i}}) \preceq \mathbf{0} & ext{if } eta_{\mathcal{A}_i} = \mathbf{0}, \\ \operatorname{cumsum}(|s|_{\downarrow} - \lambda_{R(s)_{\mathcal{A}_i}}) \preceq \mathbf{0} & \\ \wedge \sum_{j \in \mathcal{A}_i} \left(|s_j| - \lambda_{R(s)_j} \right) = 0 & ext{otherwise}. \end{aligned} 
ight\}$$

 $A_i$  defines a cluster containing indices of coefficients equal in absolute value.

R(x) is an operator that returns the ranks of elements in |x|.

 $|x|_{\downarrow}$  returns the absolute values of x sorted in non-increasing order.

## Strong rule algorithm for SLOPE

```
 \begin{array}{llll} \textbf{Input:} & c \in \mathbb{R}^p, \ \lambda \in \mathbb{R}^p, \ \text{where} \ \lambda_1 \geq \cdots \geq \lambda_p \geq 0. \\ 0: & \mathcal{S}, \mathcal{B} \leftarrow \varnothing \\ 0: & \textbf{for} \ i \leftarrow 1, \ldots, p \ \textbf{do} \\ 0: & \mathcal{B} \leftarrow \mathcal{B} \cup \{i\} \\ 0: & \textbf{if} \ \sum_{j \in \mathcal{B}} \left( c_j - \lambda_j \right) \geq 0 \ \textbf{then} \\ 0: & \mathcal{S} \leftarrow \mathcal{S} \cup \mathcal{B} \\ 0: & \mathcal{B} \leftarrow \varnothing \\ 0: & \textbf{end if} \\ 0: & \textbf{Return} \ \mathcal{S} = 0 \\ \end{array}
```

Set

$$c := |\nabla g(\hat{\beta}) + \lambda^{(k-1)} - \lambda^{(k)}|_{\downarrow} \qquad \lambda := \lambda^{(k)},$$

and run the algorithm above; the result is the predicted support for  $\hat{\beta}(\lambda^{(k)})$  (subject to a permutation).

### Efficiency for simulated data

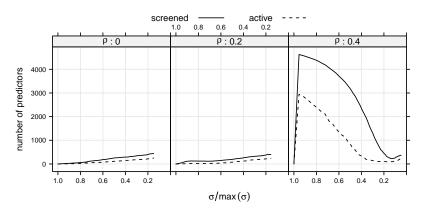


Figure: Gaussian design,  $X \in \mathbb{R}^{200 \times 5000}$ , predictors pairwise correlated with correlation  $\rho$ . There were no violations of the strong rule here.

### Efficiency for real data

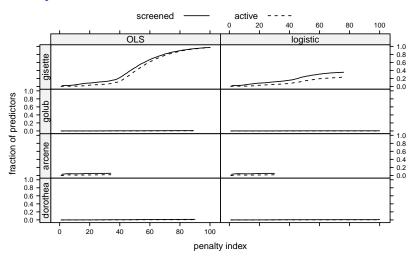


Figure: Efficiency for real data sets. The dimensions of the predictor matrices are  $100 \times 9920$  (arcene),  $800 \times 88119$  (dorothea),  $6000 \times 4955$  (gisette), and  $38 \times 7129$  (golub).

#### **Violations**

Violations may occur if the unit slope bound fails, which can occur if ordering permutation of absolute gradient changes, or any predictor becomes active between  $\lambda^{(k-1)}$  and  $\lambda^{(k)}$ .

Thankfully, such violations turn out to be rare.

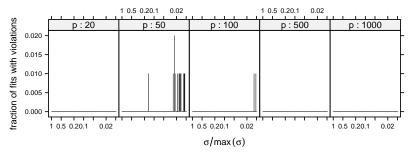


Figure: Violations for sorted  $\ell_1$  regularized least squares regression with predictors pairwise correlated with  $\rho=0.5.~X\in\mathbb{R}^{100\times p}$ .

#### Performance

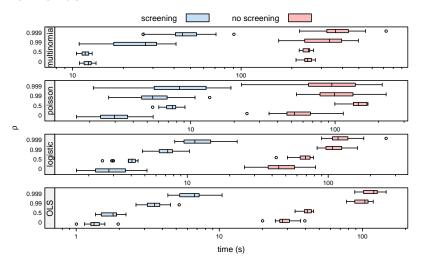


Figure: Performance benchmarks for various generalized linear models with  $X \in \mathbb{R}^{200 \times 20000}$ . Predictors are autocorrelated through an AR(1) process with correlation  $\rho$ .

### Algorithms

The original strong rule paper (tibshirani2012) presents two strategies for using the screening rule. For SLOPE, we have two slightly modified versions of these algorithms

### strong set algorithm

initialize  ${\mathcal E}$  with strong rule set

- 1. fit SLOPE to predictors in  ${\mathcal E}$
- 2. check KKT criteria against  $\mathcal{E}^{\mathcal{C}}$ ; if there are any failures, add predictors that fail the check to  $\mathcal{E}$  and go back to 1

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#### previous set algorithm

initialize  ${\mathcal E}$  with ever-active predictors

- 1. fit SLOPE to predictors in  $\mathcal{E}$
- 2. check KKT criteria against predictors in strong set
  - $\blacktriangleright$  if there are any failures, include these predictors in  ${\mathcal E}$  and go back to 1
  - if there are no failures, check KKT criteria against remaining predictors; if there are any failures, add these to ε and go back to 1



### Comparing algorithms

Strong set strategy marginally better for low–medium correlation

Previous set strategy starts to become useful for high correlation

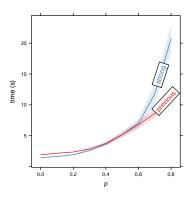


Figure: Performance of strong and previous set strategies for OLS problems with varying correlation between predictors.

#### Limitations

- ▶ the unit slope bound is generally very conservative
- does not use second-order structure in any way
- current methods for solving SLOPE (FISTA, ADMM) do not make as good use of screening rules as coordinate descent does (for the lasso)

### The SLOPE package for R

Strong screening rule for SLOPE has been implemented in the R package SLOPE (https://CRAN.R-project.org/package=SLOPE).

#### Features include

- ▶ OLS, logistic, Poisson, and multinomial models
- support for sparse and dense predictors
- cross-validation
- efficient codebase in C++

Proximal Newton solver for SLOPE will be implemented this summer with the Google Summer of Code program.

