Fast and General Best Subset Selection using Data Depth and Resampling

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December 21, 2017

Summary

Consider the linear model:

$$Y = X\beta + \epsilon; \quad Y \in \mathbb{R}^n, X \in \mathbb{R}^{n \times p}, \beta \in \mathbb{R}^p \tag{1}$$

- Variable selection in (1) is a fundamental problem in statistics. There are two ways to do this- sparse penalized regression and best subset selection.
- Sparse methods have inferential and algorithmic issues. Best subset selection is computationally demanding.
- Best subset selection in other models with dependent or structured ϵ, e.g. mixed effect models is poorly explored.
- *Our method:* We propose a fast and general algorithm for best subset selection in a wide range of statistical models. Our method trains only a single model, and evaluates a model selection criterion at $p + 1$ models (p = no. of predictors) to come up with a selected set of variables.

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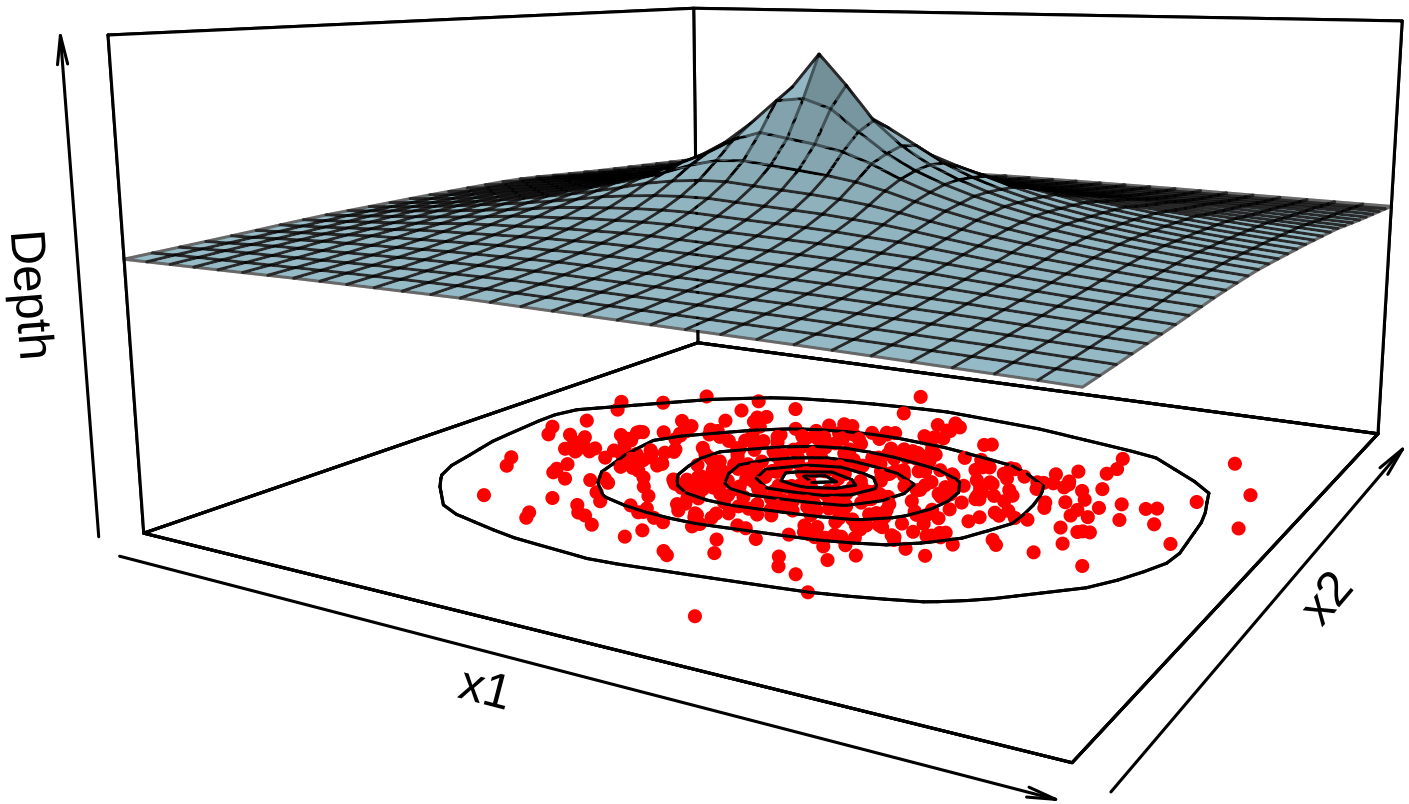
Outline

Data Depth

Example: 500 points from $\mathcal{N}_2((0,0)^T, \text{diag}(2,1))$.



Data depth is a **scalar measure of how much inside a point is with respect to a data cloud**. Denote it by $D(\mathbf{x}, F)$.

Our model selection criterion

- Parameters are estimated based on a finite random sample from sample space. So the estimates have their own probability distributions- these are called *sampling distributions*;
  e.g. in linear regression, $\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2(X^T X)^{-1}) \equiv [\hat{\beta}]$.

- We compare sampling distributions of parameter estimates in a candidate model with that of a baseline model using a generic quantity called the ***e*-value**.

- Given some depth function $D(.,.)$ we define the e-value as

$$e(\mathcal{M}) = \mathbb{E}D(\hat{\beta}_{\mathcal{M}}, [\hat{\beta}])$$

  i.e. the expected depth of the model estimates with respect to the sampling distribution of $\hat{\beta}$.

The fast variable selection 'algorithm'

1. Obtain e-value for the full model:

$$e(\mathcal{M}_{full}) = \mathbb{E}D(\hat{\beta}, [\hat{\beta}])$$

2. Set $\mathcal{S}_{select} = \phi$.

3. For $j = 1, 2, \ldots, p$
   Replace j^{th} index of $\hat{\beta}$ by 0, name it $\hat{\beta}_{-j}$.
   Obtain $e(\mathcal{M}_{-j}) = \mathbb{E}D(\hat{\beta}_{-j}, [\hat{\beta}])$.
   If $e(\mathcal{M}_{-j}) < e(\mathcal{M}_{full})$
      Set $\mathcal{S}_{select} \leftarrow \{\mathcal{S}_{select}, j\}$.

For large enough n, $\mathcal{S}_{select}$ is the set of non-zero indices in the true parameter vector.

	DroppedVar	Cn
1	**- x2**	**0.2356008**
2	**- x3**	**0.2428004**
3	**- x4**	**0.2448785**
4	**- x1**	**0.2473548**
5	**- x5**	**0.2486610**
6	**- x20**	**0.2503475**
7	<none>	0.2505000
8	- x9	0.2522873
9	- x21	0.2538186
10	- x22	0.2547132
11	- x14	0.2548410
12	- x17	0.2554293
13	- x13	0.2559990
14	- x10	0.2564211
15	- x24	0.2566334
16	- x19	0.2568725
17	- x25	0.2573902
18	- x8	0.2578656
19	- x16	0.2588032
20	- x12	0.2590218
21	- x6	0.2595048
22	- x23	0.2598039
23	- x15	0.2605307
24	- x11	0.2606763
25	- x18	0.2610460
26	- x7	0.2613168

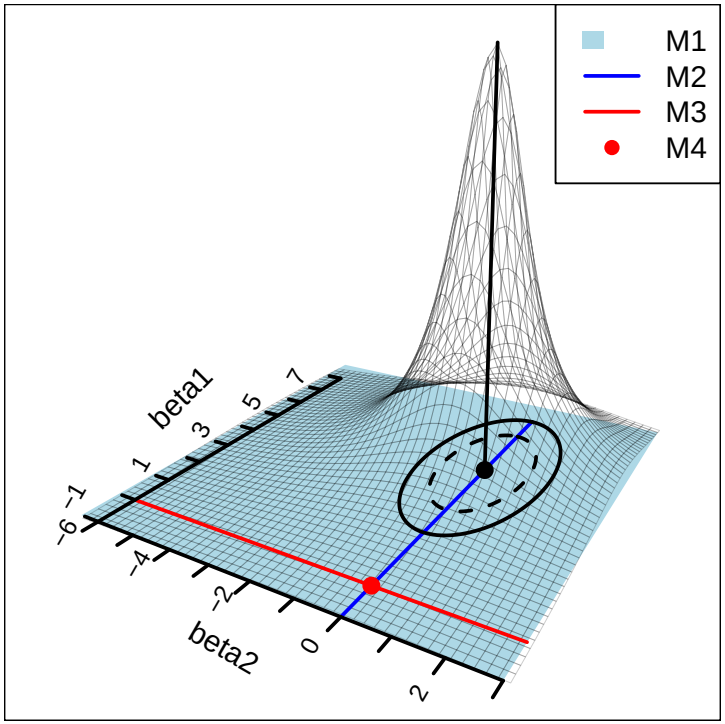
The idea- an example

Consider a linear model with $p = 2$, and true coefficient vector $\beta_0 = (5, 0)^T$. Here we have the following choice of models:

$$\begin{aligned}
\mathcal{M}_1 : &\quad Y = X_1\beta_1 + X_2\beta_2 + \epsilon; &\quad \Theta_1 &= \mathbb{R}^2 \\
\mathcal{M}_2 : &\quad Y = X_1\beta_1 + \epsilon; &\quad \Theta_2 &= \mathbb{R} \times \{0\} \\
\mathcal{M}_3 : &\quad Y = X_2\beta_2 + \epsilon; &\quad \Theta_3 &= \{0\} \times \mathbb{R} \\
\mathcal{M}_4 : &\quad Y = \epsilon; &\quad \Theta_4 &= (0, 0)^T
\end{aligned}$$

Some are good models, some are bad models.

The idea- an example



As n grows, the full model sampling distribution concentrates around β_0, so mean depths at $\mathcal{M}_3$ and $\mathcal{M}_4$ vanish.
However, both depth and density contours scale down by the same multiple as n goes down, so that mean depths at $\mathcal{M}_1$ and $\mathcal{M}_2$ remain constant.

Outline

Definition of a model

At stage n there is a triangular array of functions

$$\{\Psi_{ni}(\theta_n, Z_{ni}) : 1 \leq i \leq k_n, n \geq 1\}$$

where $\mathcal{Z}_n = \{Z_{n1}, \ldots, Z_{nk_n}\}$ is an observable array of random variables, and $\theta_n \in \Theta_n \subseteq \mathbb{R}^p$.
The true unknown vector of parameters θ_{0n} is the unique minimizer of

$$\Psi_n(\theta_n) = \mathbb{E} \sum_{i=1}^{k_n} \Psi_{ni}(\theta_n, Z_{ni})$$

The common non-zero support of all estimable parameters is $\mathcal{S}_{*n} = \cup_{\theta_n \in \Theta_n} \text{support}(\theta_n)$.

In this general setup, we associate a candidate model $\mathcal{M}_n$ with two quantities:

(a) The set of indices $\mathcal{S}_n \subseteq \mathcal{S}_{*n}$ where the parameter values are unknown and **estimated from the data**, and

(b) an ordered vector of **known constants** $C_n = (C_{nj} : j \notin \mathcal{S}_n)$ for parameters not indexed by $\mathcal{S}_n$.

The generic parameter vector corresponding to this model, denoted by $\theta_{mn} \in \Theta_{mn} \subseteq \Theta_n := \prod_j \Theta_{nj}$, will thus have the structure

$$\theta_{mnj} = \begin{cases} \text{unknown } \theta_{mnj} \in \Theta_{nj} & \text{for } j \in \mathcal{S}_n, \\ \text{known } C_{nj} \in \Theta_{nj} & \text{for } j \notin \mathcal{S}_n. \end{cases}$$

The estimator $\hat{\theta}_{*n}$ of θ_{0n} is obtained as

$$\hat{\theta}_{*n} = \underset{\theta_n}{\operatorname{argmin}}\, \hat{\Psi}_n(\theta_n) = \underset{\theta_n}{\operatorname{argmin}} \sum_{i=1}^{k_n} \Psi_{ni}\left(\theta_n, Y_{ni}\right)$$

We assume an elliptical asymptotic distribution for $\hat{\theta}_{*n}$ with the conditions-

(A1) There exists a sequence of positive reals $a_n \uparrow \infty$ such that $a_n(\hat{\theta}_{*n} - \theta_{0n}) \rightsquigarrow \mathcal{E}(0_p, V, g)$, for some p.d. matrix $V \in \mathbb{R}^{p\times p}$ and density generator function g;

(A2) For almost every data sequence $\mathcal{Z}_n$, There exists a sequence of positive definite matrices $V_n \in \mathbb{R}^{p\times p}$ such that $\text{plim}_{n\to\infty} V_n = V$.

For any other model $\mathcal{M}_n$, we use the plugin estimate:

$$\hat{\theta}_{mnj} = \begin{cases} \hat{\theta}_{*nj} & \text{for } j \in \mathcal{S}_n, \\ C_{nj} & \text{for } j \notin \mathcal{S}_n. \end{cases}$$

‘Good’ and ‘bad’ models

- A model $\mathcal{M}_n$ is called *adequate* if

$$\lim_{n\to\infty} \sum_{j\notin \mathcal{S}_n} |C_{nj} - \theta_{0nj}| = 0$$

  A model that is not adequate, will be called an *inadequate* model.
- The model $\mathcal{M}_n$ is called *strictly adequate* if, for all n and $j \notin \mathcal{S}_n$, $C_{nj} = \theta_{0nj}$.

Covers obvious cases:

$$
\begin{aligned}
(1, 2, 3, 0, -1) &\quad - \quad \text{preferred parameter vector} \\
(*, 0, *, *, *) &\quad - \quad \text{inadequate model} \\
(*, *, *, *, *) &\quad - \quad \text{full model} \\
(*, *, *, 0, *) &\quad - \quad \text{strictly adequate model}
\end{aligned}
$$

Covers limiting cases:, e.g. $(*, *, *, \delta_n), \delta_n = o(1)$ will be an adequate model in our framework.

Such data generating models, e.g.

$$Y_{ni} = X_{1i}\beta_{01} + X_{2i}\delta_n + \epsilon; \quad \beta_{01} \in \mathbb{R}, \delta_n = o(1)$$

for linear regression, frequently arise from prior choices in bayesian variable selection techniques.

We now use a *data depth function*:

$$D : \mathbb{R}^p \times \tilde{\mathbb{R}}^p \mapsto [0, \infty)$$

to quantify the relative position of θ_{mn} with respect to the preferred model estimate distribution. Denote this by

$$D(\hat{\theta}_{mn}, [\hat{\theta}_{*n}])$$

***e*-value** is simply a functional of the distribution of this random evaluation function. Denote this by $e_n(\mathcal{M}_n)$.

We shall now elaborate on the following choice of the *e*-value:

$$e_n(\mathcal{M}_n) = \mathbb{E} D(\hat{\theta}_{mn}, [\hat{\theta}_{*n}])$$

Resampling approximation of *e*-values

- We use resampling to approximate the distributions of the random quantities $\hat{\theta}_{mn}$ and $\hat{\theta}_{*n}$. The resampling estimate of a model *e*-value is defined using two bootstrap samples:

$$e_{rn}(\mathcal{M}_n) = \mathbb{E}_{r_1} D\big(\hat{\theta}_{r_1 mn}, [\hat{\theta}_{r*n}]\big)$$

- For $\hat{\theta}_{*n}$, we use *Generalized bootstrap* (Chatterjee and Bose, 2005) that is based on the following approximation:

$$\hat{\theta}_{r*n} = \hat{\boldsymbol{\theta}}_{*n} - \frac{\tau_n}{a_n}\left[\sum_{i=1}^{n} W_i \Psi''_{ni}(\hat{\boldsymbol{\theta}}_{*n}, Z_{ni})\right]^{-1} \sum_{i=1}^{n} W_i \Psi'_{ni}(\hat{\boldsymbol{\theta}}_{*n}, Z_{ni}) + R_{rn};$$

$$\mathbb{E}_r \|R_{rn}\|^2 = o_P(1), \tau_n \to \infty, \tau_n = o(a_n)$$

- For $\hat{\theta}_{mn}$ we use the plugin estimate

$$\hat{\theta}_{r_1 mnj} = \begin{cases} \hat{\theta}_{r_1 * nj} & \text{for } j \in \mathcal{S}_n; \\ C_{nj} & \text{for } j \notin \mathcal{S}_n \end{cases}$$

Fast algorithm for variable selection

1. (Dropping n in all subscripts except e) Fix resampling standard deviation τ.
2. Obtain bootstrap samples: $\mathcal{T} = \{\hat{\theta}_{1*}, ..., \hat{\theta}_{R*}\}$, and $\mathcal{T}_1 = \{\hat{\theta}_{1*}, ..., \hat{\theta}_{R_1*}\}$.
3. Calculate $\hat{e}_{rn}(\mathcal{M}_*) = \frac{1}{R_1} \sum_{r_1=1}^{R_1} D(\hat{\theta}_{r_1*}, [\mathcal{T}_1])$.
4. Set $\hat{\mathcal{S}}_0 = \phi$.
5. For j in $1 : p$
   For r_1 in $1 : R_1$
      Replace j^{th} index of $\hat{\theta}_{*r_1}$ by 0 to get $\hat{\theta}_{r_1,-j}$.
   Calculate $\hat{e}_{rn}(\mathcal{M}_{-j}) = \frac{1}{R_1} \sum_{r_1=1}^{R_1} D(\hat{\theta}_{r_1,-j}, [\mathcal{T}_1])$.
   If $\hat{e}_{rn}(\mathcal{M}_{-j}) < \hat{e}_{rn}(\mathcal{M}_*)$
      Set $\hat{\mathcal{S}}_0 \leftarrow \{\hat{\mathcal{S}}_0, j\}$.

Corollary

Consider two sets of bootstrap estimates of $\hat{\theta}_*$*:* $\mathcal{T} = \{\hat{\theta}_{r*} : r = 1, \ldots, R\}$ *and* $\mathcal{T}_1 = \{\hat{\theta}_{r_1*} : r_1 = 1, \ldots, R_1\}$*. Obtain sample e-value estimates as*

$$\hat{e}_{rn}(\mathcal{M}) = \frac{1}{R_1} \sum_{r_1=1}^{R_1} D(\hat{\theta}_{r_1 m}, [\mathcal{T}])$$

where $[\mathcal{T}]$ *is the empirical distribution of the corresponding bootstrap samples. Consider the set of predictors* $\hat{\mathcal{S}}_0 = \{\hat{e}_{rn}(\mathcal{M}_{-j}) < \hat{e}_{rn}(\mathcal{M}_*)\}$*. Then as* $n, R, R_1 \to \infty$*,*

$$P_2(\hat{\mathcal{S}}_0 = \mathcal{S}_0) \to 1$$

where P_2 *is the probability conditional on the data and bootstrap samples, and* $\mathcal{S}_0$ *is the true index set of non-zero predictors.*

Outline

Simulation: linear models

Methods compared:

(a) Mixed Integer Optimization (MIO) (Bertsimas et al., 2016)
(b) Lasso penalized regression
(c) SCAD penalized regression
(d) BIC forward selection

Comparison metrics:

$$\text{Sparsity}(\hat{\beta}) = \|\hat{\beta}\|_0; \quad \text{PE}(\hat{\beta}) = \frac{\|X_{\text{test}}\hat{\beta} - X_{\text{test}}\beta_0\|}{\|X_{\text{test}}\beta_0\|}$$

Results: $n = 1000, p = 60$

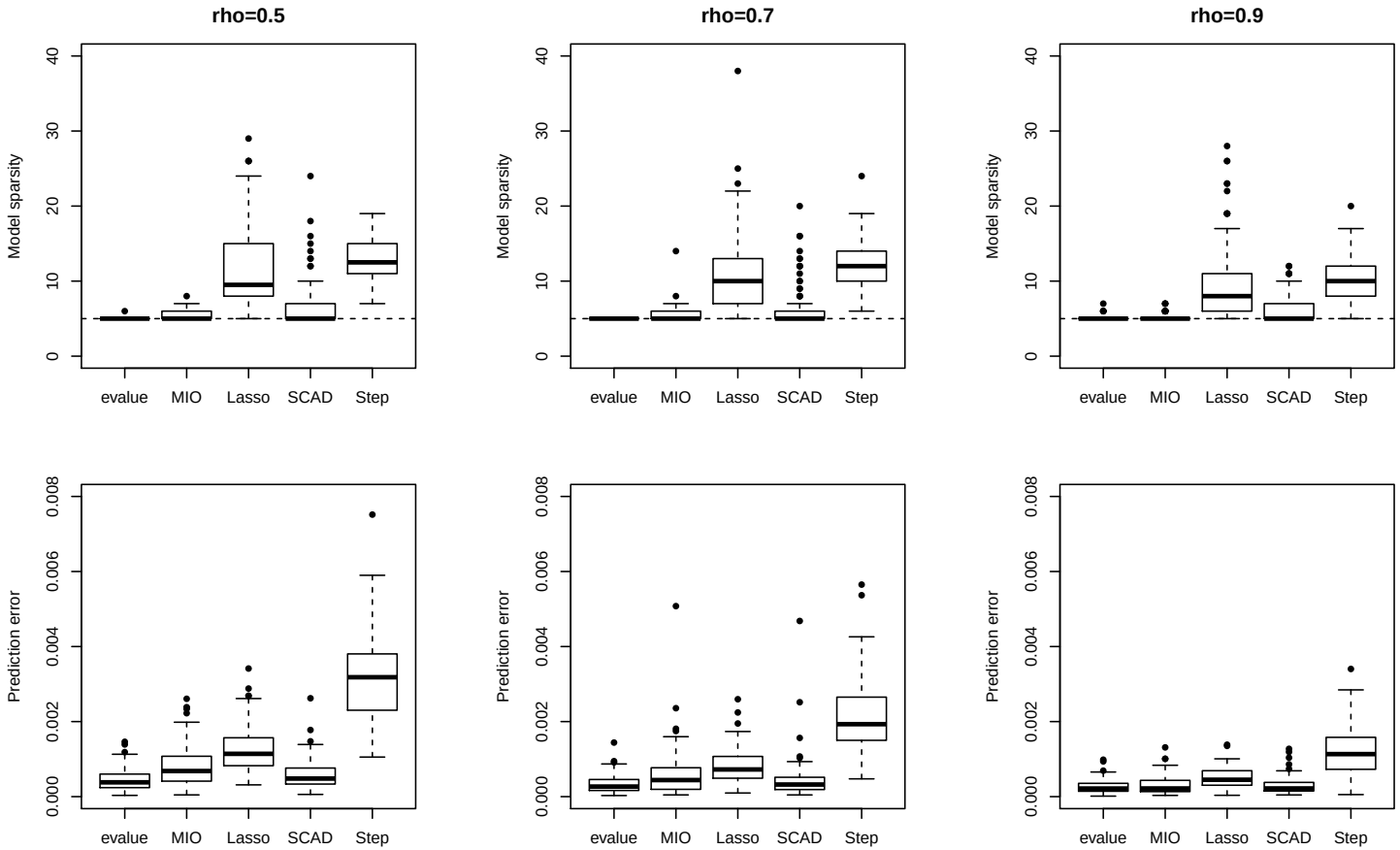


Figure: Model sparsity (top row) and prediction performance (bottom row) for all methods in $n = 60, p = 1000$ setup.

Results: $n = 60, p = 1000$

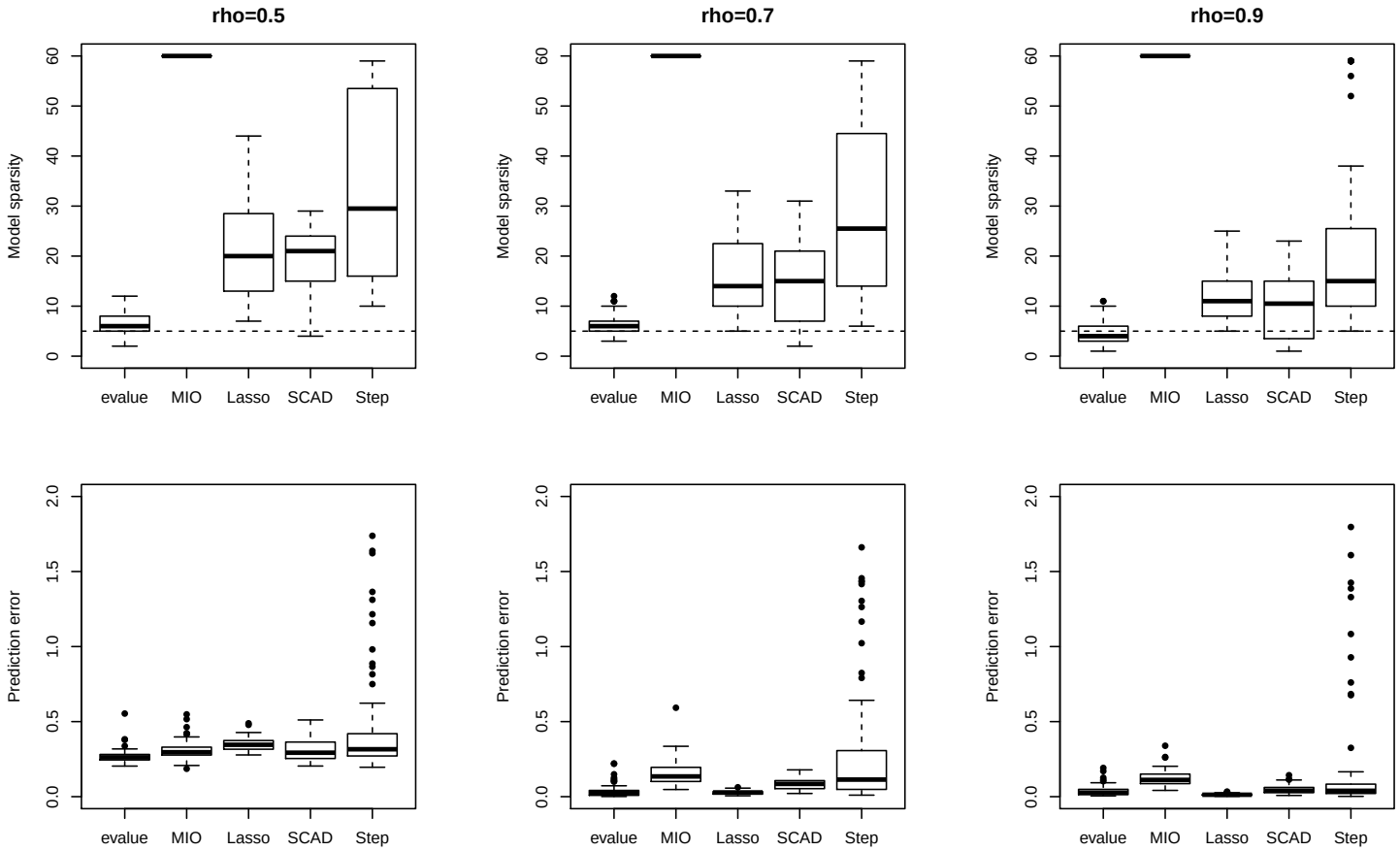


Figure: Model sparsity (top row) and prediction performance (bottom row) for all methods in $n = 60, p = 1000$ setup.

Results: effect of tuning parameter

Setting 1: $n = 1000, p = 60$						
Choice of τ_n	$\rho = 0.5$		$\rho = 0.7$		$\rho = 0.9$	
	Sparsity	PE ($\times 10^{-4}$)	Sparsity	PE ($\times 10^{-4}$)	Sparsity	PE ($\times 10^{-4}$)
$\tau_n = \log n$	5.01	4.5	5.00	3.3	5.06	2.6
$\tau_n = n^{0.1}$	16.16	33.6	16.85	23.3	17.89	16.3
$\tau_n = n^{0.2}$	5.74	8.1	6.03	5.7	6.75	4.8
$\tau_n = n^{0.3}$	5.01	4.5	5.01	3.3	4.96	5.0
$\tau_n = n^{0.4}$	5.00	4.4	5.00	3.3	3.14	633.6
Setting 2: $n = 60, p = 1000$						
Choice of τ_n	$\rho = 0.5$		$\rho = 0.7$		$\rho = 0.9$	
	Sparsity	PE ($\times 10^{-2}$)	Sparsity	PE ($\times 10^{-2}$)	Sparsity	PE ($\times 10^{-2}$)
$\tau_n = \log n$	6.63	4.5	6.34	3.4	4.79	3.7
$\tau_n = n^{0.1}$	7.57	4.6	7.24	3.0	7.16	2.1
$\tau_n = n^{0.2}$	7.38	4.6	7.23	3.0	6.61	2.3
$\tau_n = n^{0.3}$	6.94	4.6	6.58	3.0	5.44	3.0
$\tau_n = n^{0.4}$	6.08	4.1	5.66	3.9	3.90	6.0

Table: Model sparsity and prediction errors for different choices of τ

Simulation: linear mixed models

$$Y_i = X_i\beta + \epsilon \in \mathbb{R}^{n_i}$$
$$epsilon \sim N(0, V_i); \quad V_i = \sigma^2 I_{n_i} + Z_i \Delta Z_i^T$$

- m subjects, n_i observations per subject, $n = m \times n_i$ total observations;
- $p = 9, \beta = (1, 1, 0, 0, 0, 0, 0, 0, 0)^T$;
- Elements of $X_1, \ldots, X_m$ chosen from Unif$(-2, 2)$, random effect design matrix Z_i is first 4 columns of X_i;
- $$\Delta = \begin{pmatrix} 9 & & & \\ 4.8 & 4 & & \\ 0.6 & 1 & 1 & \\ 0 & 0 & 0 & 0 \end{pmatrix}$$
- Two settings: (i) $m = 30, n_i = 5$, (ii) $m = 60, n_i = 10$;
- We use i.i.d. draws of Gamma(1,1) as bootstrap weights $W_i + 1$.

Simulation results

Method	Tuning	FPR%	FNR%	Model size	FPR%	FNR%	Model size
		$n_i = 5, m = 30$			$n_i = 10, m = 60$		
e-value based	$\tau_n/\sqrt{n} = 1$	57.4	0.0	5.24	43.8	0.0	4.03
	2	30.4	0.0	3.32	12.3	0.0	2.42
	3	15.6	0.0	2.54	3.2	0.0	2.10
	4	7.3	0.0	2.24	1.0	0.0	2.03
	5	3.0	0.0	2.09	0.7	0.0	2.02
	6	1.7	0.0	2.05	0.3	0.0	2.01
	7	1.0	0.0	2.03	0.0	0.0	2.00
	8	0.7	0.0	2.02	0.0	0.0	2.00
	9	0.0	0.0	2.00	0.0	0.0	2.00
	10	0.0	0.0	2.00	0.0	0.0	2.00
Peng and Lu (2012)	BIC	21.5	9.9	2.26	1.5	1.9	2.10
	AIC	17	11.0	2.43	1.5	3.3	2.20
	GCV	20.5	6	2.30	1.5	3	2.18
	$\sqrt{\log n/n}$	21	15.6	2.67	1.5	4.1	2.26

Comparison between our method and that proposed by Peng and Lu (2012) through average false positive percentage, false negative percentage and model size

Simulation results

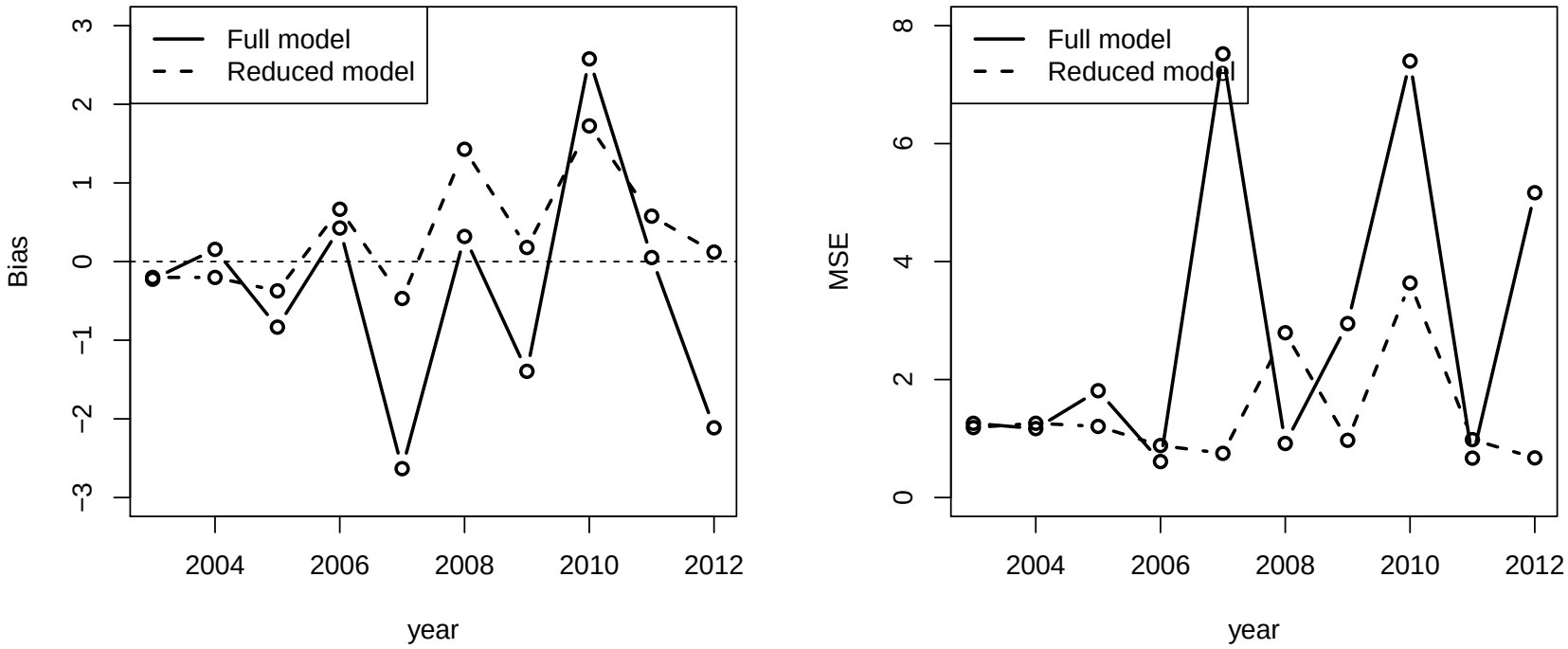
Method	$\tau_n/\sqrt{n}$	Setting 1	Setting 2
e-value based	1	2	16
	2	36	67
	3	60	91
	4	80	97
	5	91	98
	6	95	99
	7	97	100
	7	98	100
	8	100	100
	10	100	100
Bondell et al. (2010)		73	83
Peng and Lu (2012)		49	86
Fan and Li (2012)		90	100

Comparison of our method and three sparsity-based methods of mixed effect model selection through accuracy of selecting correct fixed effects

Application: selection of important predictors in Indian monsoon

- Annual median observations for 1978-2012;
- Local measurements across 36 weather stations (e.g. elevation, latitude, longitude), as well as global variables (e.g. El-Nino, tropospheric temperature variations) : total 35 predictors;
- Aim is two-fold: (i) Selecting important predictors, (ii) providing good predictions using the reduced model.

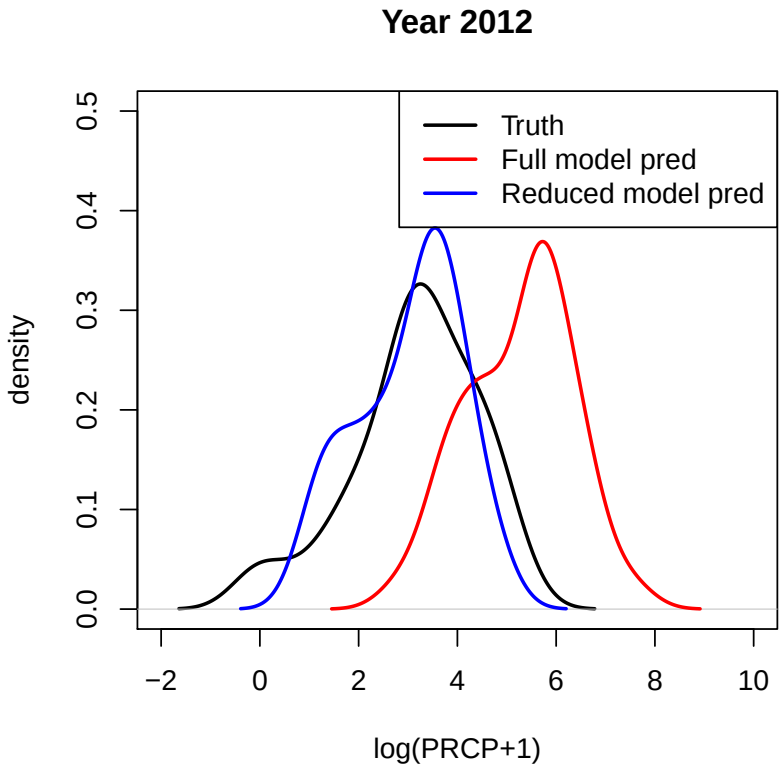
Application: results



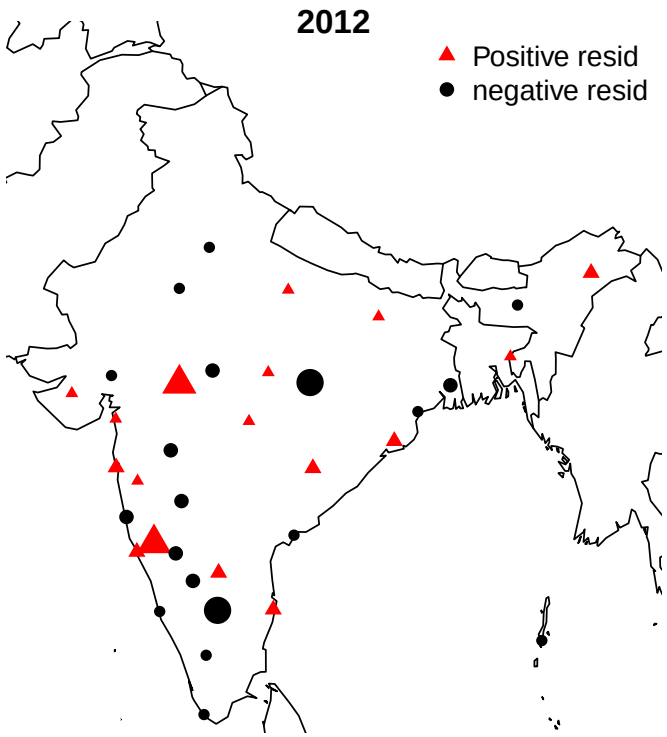
(a) (b)

Figure: Comparing full model rolling predictions with reduced models: (a) Bias across years, (b) MSE across years

Application: results



(a)



(b)

Figure: Comparing full model rolling predictions with reduced models: (a) density plots for 2012, (b) stationwise residuals for 2012

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THANK YOU!

https://arxiv.org/abs/1706.02429

Questions?