Consistent high-dimensional Bayesian variable selection via penalized credible regions

Howard Bondell

bondell@stat.ncsu.edu

NC STATE UNIVERSITY

Joint work with Brian Reich

Outline

- High-Dimensional Variable Selection
- Bayesian Variable Selection
- Selection via Credible Sets
  - Joint / Marginal
- Asymptotic Properties
- Examples
- Conclusion

Variable Selection Setup

- Linear regression model $y_i = \mathbf{x}_i^T \boldsymbol{\beta} + \epsilon_i$
  - n observations and p predictor variables
  - y_i: response for observation i
  - $\mathbf{x}_i$: (column) vector of p predictors for observation i
  - $\boldsymbol{\beta}$: (column) vector of p regression parameters
  - ϵ_i iid errors - mean zero, constant variance
- Ultra-high dimensional data, $p \gg n$
- Only subset of predictors are relevant
- If $\beta_j = 0$ then variable j is effectively removed from the model

Variable Selection Methods

- All Subsets - 2^p !!!!
- Forward Selection
- Backward Elimination - Not possible for $p > n$
- Stepwise
- Penalization Methods
- Bayesian Methods

Penalization Methods

- Minimize:

$$\|\mathrm{y} - X\beta\|^2 + \lambda J(\beta)$$

- LASSO: $J(\beta) = \sum_{j=1}^{p} |\beta_j|$
- Elastic Net: $J(\beta) = (1-c)\sum_{j=1}^{p} \beta_j^2 + c\sum_{j=1}^{p} |\beta_j|$
- Adaptive LASSO, SCAD, MCP, OSCAR, ...
- λ and c chosen by AIC, BIC, Cross-Val, GCV
- Shrinkage creates bias
  - Reduces variance
  - Achieves selection by setting exact zeros

Ultra High-Dimensional Data

- When $p \gg n$, before performing penalization methods, common to screen down first
- Sure Independence Screening
  - Rank by marginal correlations
  - Reduce typically to $p < n$
- Perform forward selection sequence
  - Again reduce to $p < n$
- Then perform penalized regression

Bayesian Variable Selection

- Each candidate model indexed by $\boldsymbol{\delta} = (\delta_1, \cdots, \delta_p)^T$

$$\delta_j = \begin{cases} 1 & \text{if } \mathbf{x}_j \text{ is included in the model,} \\ 0 & \text{if } \mathbf{x}_j \text{ is excluded from the model.} \end{cases}$$

- $p(\boldsymbol{\delta})$ is prior over model space
- Most common $p(\boldsymbol{\delta}) \propto \pi^{p_\delta}(1-\pi)^{p-p_\delta}$
  - $p_{\boldsymbol{\delta}} = \sum_{j=1}^{p} \delta_j$ - number of predictors
  - π is prior inclusion probability for each
  - Uniform prior over model space $\Leftrightarrow \pi = 1/2$
  - π set to apriori guess of proportion of important predictors
  - Put prior on π - Beta (a, b)

Bayesian Variable Selection

- Given $\boldsymbol{\delta}$, we have $\Pi(\boldsymbol{\beta}|\boldsymbol{\delta}, \sigma^2, \tau)$
  - Typically, σ^2 gets diffuse prior (Inverse Gamma)
  - τ are other hyperparameters needed
- Most common $\Pi(\boldsymbol{\beta}|\boldsymbol{\delta}, \sigma^2, \tau) = N\left(0, \frac{\sigma^2}{\tau}V\right)$
  - $V = I_{p_{\boldsymbol{\delta}}}$ or $V = (X_{\boldsymbol{\delta}}^T X_{\boldsymbol{\delta}})^{-1}$
  - But $p_{\boldsymbol{\delta}} > n \Rightarrow X_{\boldsymbol{\delta}}^T X_{\boldsymbol{\delta}}$ not invertible
  - Focus on $V = I$
- τ either fixed, or given Gamma prior
- Equivalent to Spike-and-Slab, i.e. $\boldsymbol{\beta}$ is mixture of mass at zero and Normal

Bayesian Variable Selection

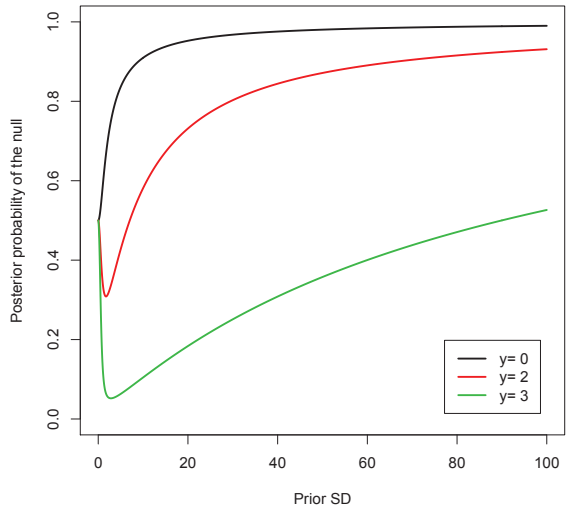
- Crank out Bayes' rule and get posterior probability for each configuration of δ
- Instead, use stochastic search (SSVS) to visit models with MCMC chain
  - Estimate posterior probabilities by proportion of times visited
- Search for highest posterior model
- Alternative: Use marginal posterior for each variable
  - Include variable in final model if $P(\delta_j = 1|X, y) > t$ for some threshold
    - Median probability model (Barbieri and Berger, 2004) use $t = 1/2$
    - Optimal predictive model under certain conditions

Drawbacks

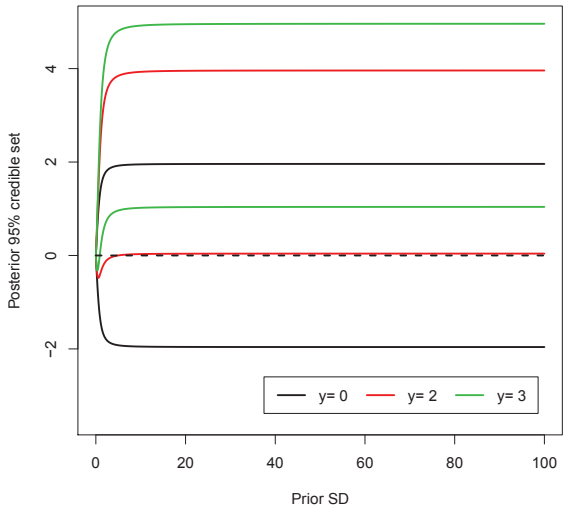
- Typical SSVS approach requires:
  - Proper prior distribution
  - Choice of prior on model space
  - Posterior threshold choice
  - MCMC chains to estimate posterior probabilities (often need very long runs)
- Results can be sensitive to each choice
- Marginal inclusion probabilities may be poor under high correlation
  - Highly correlated predictors may each show up equally often
  - But each only a small number of times

Further Drawback: Lindley's Paradox

- Problem with using posterior probabilities
- Diffuse prior typical in practice
- Simple case
  - Sample of size 1, from $N(\mu, 1)$
  - $\mu = 0$ vs. $\mu \neq 0$ - More diffuse prior $\Rightarrow$ Prob of $H_0 \rightarrow 1$



(a) Posterior Probability in favor of Null for various prior standard deviations.



(b) 95% Posterior Credible Set for various prior standard deviations.

Joint Credible Regions

- Specify prior only on parameters in full model

$$\Pi(\boldsymbol{\beta}|\sigma^2, \tau) = N\left(0, \frac{\sigma^2}{\tau} I\right)$$

$$p(\sigma^2) = IG(0.01, 0.01)$$

- $\mathcal{C}_\alpha$ is $(1-\alpha) \times 100\%$ credible region
- For fixed hyperparameter, τ, get elliptical regions

  $\mathcal{C}_\alpha = \{\boldsymbol{\beta} : (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T \Sigma^{-1} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \leq C_\alpha\}$, for some C_α
- $\hat{\boldsymbol{\beta}}$, Σ - posterior mean, variance
  - Closed form if τ fixed —- $\hat{\boldsymbol{\beta}} = \left(X^T X + \tau I\right)^{-1} X^T y$
  - Otherwise, simple short MCMC run used
- Prior on $\tau \Rightarrow$ elliptical contours still valid credible sets

Joint Credible Regions

- All points within region may be feasible parameter values
- Among these, we seek a sparse solution
- Search within the region for the ‘sparsest’ point

$$\tilde{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} ||\boldsymbol{\beta}||_0$$
$$\text{subject to}$$
$$\boldsymbol{\beta} \in \mathcal{C}_\alpha$$

- Chosen model for given α defined by set of indices, $\mathcal{A}_n^\alpha = \{j \ : \ \tilde{\beta}_j \neq 0\}$.

Joint Credible Regions

- Problems with searching for sparsest solution
  - High dimensional region - combinatorial search
  - Also Non-unique
- Replace L_0 by smooth bridge between L_0 and L_1 (Lv and Fan, 2009)

$$\sum_{j=1}^{p} \rho_a(|\beta_j|),$$

$$\rho_a(t) = \frac{(a+1)t}{a+t} = \left(\frac{t}{a+t}\right) I(t \neq 0) + \left(\frac{a}{a+t}\right) t, \qquad t \in [0, \infty),$$

$$\rho_0(t) = lim_{a \to 0^+} \rho_a(t) = I(t \neq 0)$$

$$\rho_\infty(t) = lim_{a \to \infty} \rho_a(t) = t$$

- Interest on $\rho_a(t)$ for $a \approx 0$.

Computation

- Non-convex penalty function
- Local linear approximation to penalty

$$\rho_a(|\beta_j|) \approx \rho_a(|\hat{\beta}_j|) + \rho'_a(|\hat{\beta}_j|)\left(|\beta_j| - |\hat{\beta}_j|\right),$$

$$\text{with } \rho'_a(|\hat{\beta}_j|) = \frac{a(a+1)}{\left(a+|\hat{\beta}_j|\right)^2}$$

- $\hat{\boldsymbol{\beta}}$ is posterior mean
- Using Lagrangian gives

$$\tilde{\boldsymbol{\beta}} = \arg\min\left\{(\boldsymbol{\beta}-\hat{\boldsymbol{\beta}})^T\Sigma^{-1}(\boldsymbol{\beta}-\hat{\boldsymbol{\beta}}) + \lambda_\alpha \sum_{j=1}^{p} \frac{|\beta_j|}{\left(a+|\hat{\beta}_j|\right)^2}\right\}$$

- Constant absorbed into λ_α
- One-to-one correspondence between λ_α and α

Computation

- Optimization becomes

$$\tilde{\boldsymbol{\beta}} = \arg\min \left\{ (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T \Sigma^{-1} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) + \lambda_\alpha \sum_{j=1}^{p} \frac{|\beta_j|}{\left(a + |\hat{\beta}_j|\right)^2} \right\}$$

- For $a \to 0$,

$$\tilde{\boldsymbol{\beta}} \approx \arg\min \left\{ (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T \Sigma^{-1} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) + \lambda_\alpha \sum_{j=1}^{p} \frac{|\beta_j|}{|\hat{\beta}_j|^2} \right\}$$

- Adaptive Lasso form
  - LARS algorithm gives full path as vary α

Selection Consistency

- Sequence of credible sets $(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T \Sigma^{-1} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \leq C_n$
- Sequence of models $\mathcal{A}_n^{\alpha_n}$
- One-to-one correspondence between α_n and C_n
- True model $\mathcal{A}$

THEOREM 1. *Under general conditions, if* $C_n \to \infty$ *and* $n^{-1} C_n \to 0$, *then the credible set method is consistent in variable selection, i.e.* $P(\mathcal{A}_n^{\alpha_n} = \mathcal{A}) \to 1$

- Also holds for $p \to \infty$, but $p/n \to 0$

Selection Consistency

- What about $p \gg n$?
- Asymptotics with $p/n \to 0$ not entirely relevant
- Posterior mean - Ridge Regression form
- $\hat{\boldsymbol{\beta}} = \left(X^T X + \tau I\right)^{-1} X^T y$
- If $\lim_{n,p\to\infty} \; p/n > 0$, can show that $\hat{\boldsymbol{\beta}}$ not mean square consistent

$$\lim_{n,p\to\infty} \; E\left\{\left(\hat{\beta} - \beta^0\right)^T \left(\hat{\beta} - \beta^0\right)\right\} > 0$$

Selection Consistency

- Consider rectangular credible regions - not elliptical
- Just use diagonal elements of Σ ignoring covariances
- Construct credible sets separately for each parameter
- Simple componentwise thresholding on posterior mean (t-statistics)

THEOREM 2. *Let* $\tau \to \infty$ *and* $\tau = O\left(\left(n^2 \log p\right)^{1/3}\right)$ *then the posterior thresholding approach is consistent in selection when the dimension* p *satisfies* $\log p = O\left(n^c\right)$ *for some* $0 \leq c < 1$.

- Selection consistency for exponential growing dimension, $\log p = o(n)$
- Also applies to ridge regression with ridge parameter τ

Simulation Study

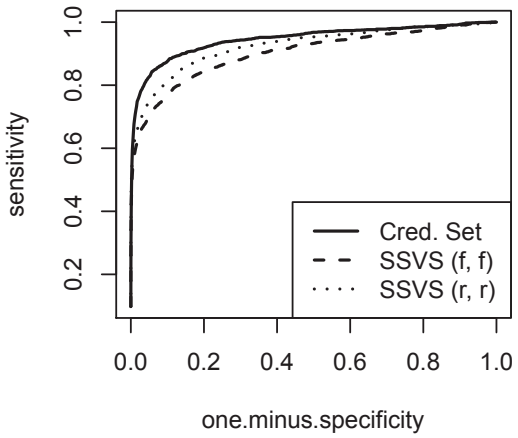
- Linear Regression Model with $N(0,1)$ errors
- $n = 60$ observations (same as real data example)
- $p \in \{500, 2000\}$ also $N(0,1)$ with $AR(1), \rho \in \{0.5, 0.9\}$
- Results based on 200 datasets for each of the 4 setups

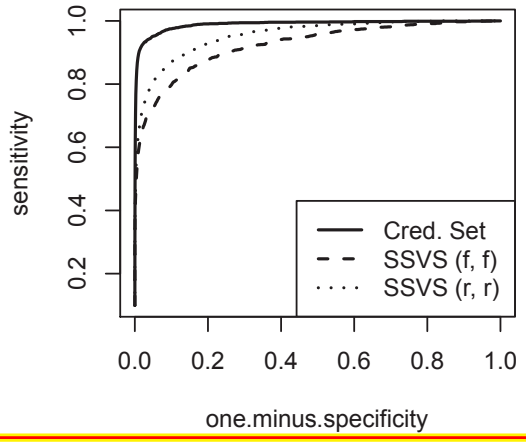
Simulation Study

- Consider ordering of predictors induced by:
  - Joint credible regions
  - Marginal posterior thresholding
  - Stochastic Search (with various choices of prior)
  - LASSO (L_1 penalization)
- To measure reliability of ordering:
  - ROC curve - measures sensitivity vs. specificity

Simulation Study

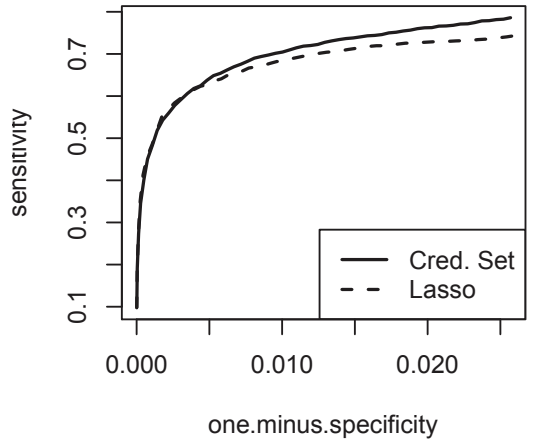
- $p = 500$, $n = 60$ $\rho = 0.5$ (Top) and $\rho = 0.9$ (Bottom)

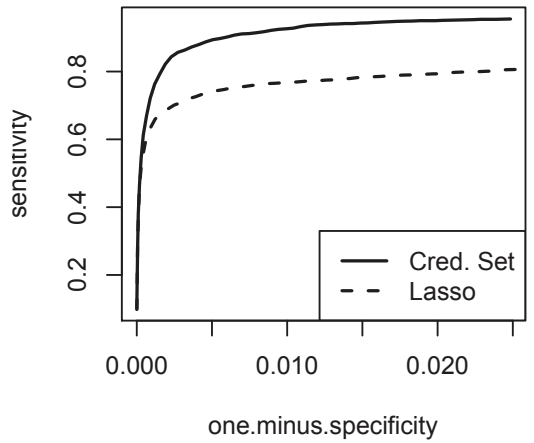




Simulation Study

- $p = 2000$, $n = 60$ $\rho = 0.5$ (Top) and $\rho = 0.9$ (Bottom)





Ultra High-Dimension

Table 1: Selection performance for $p = 10,000$ with 3 important predictors for various choices of n based on 100 datasets. The entries in the table denote Correct Selection Proportion (CS), Coverage Proportion (COV), Average Model Size (MS), and Average Number of Important Predictors out of the 3 Included (IP).

	$n = 100$				$n = 200$				$n = 500$			
	CS	COV	MS	IP	CS	COV	MS	IP	CS	COV	MS	IP
Marginal Sets	9.0	31.0	3.22	2.06	24.0	47.0	3.37	2.38	39.0	54.0	3.01	2.49
SIS + SCAD	1.0	15.0	4.08	1.82	5.0	35.0	6.06	2.28	6.0	59.0	11.62	2.56
	$n = 1000$				$n = 2000$							
	CS	COV	MS	IP	CS	COV	MS	IP				
Marginal Sets	45.0	61.0	2.98	2.58	62.0	74.0	2.89	2.71				
SIS + SCAD	12.0	64.0	14.62	2.62	23.0	79.0	17.96	2.78				

Real Data Analysis

- Mouse Gene Expression (Lan et al., 2006)
- 60 arrays (31 female, 29 male mice)
- 22,575 genes + gender $(p = 22,576)$
- Fit with $n = 55$, leave out 5 for testing

Table 1: Mean squared prediction error and model size based on 100 random splits of the real data, with standard errors in parenthesis. The 3 response variables are PEPCK, GPAT, and SCD1.

	PEPCK		GPAT		SCD1	
	MSPE	Model Size	MSPE	Model Size	MSPE	Model Size
Marginal Sets $(p = 22,576)$	2.14 (0.15)	7.1 (0.41)	4.70 (0.45)	9.3 (0.59)	3.54 (0.26)	7.6 (0.54)
SIS + SCAD $(p = 22,576)$	2.82 (0.18)	2.3 (0.09)	5.88 (0.44)	2.6 (0.10)	3.44 (0.22)	3.2 (0.14)
Joint Sets $(p = 2,000)$	2.03 (0.14)	9.6 (0.46)	3.83 (0.34)	4.2 (0.43)	3.04 (0.22)	22.0 (0.56)
Marginal Sets $(p = 2,000)$	1.84 (0.14)	23.3 (0.67)	5.33 (0.41)	21.8 (0.72)	3.27 (0.21)	19.1 (0.71)
LASSO $(p = 2,000)$	3.03 (0.19)	7.7 (0.96)	5.03 (0.42)	3.3 (0.79)	3.25 (0.31)	19.7 (0.77)

Conclusion

- Variable selection via Bayesian Credible sets
  - Sparse solution within set
  - Elliptical regions consistent if $p/n \to 0$
  - Rectangular regions consistent if $\log p = o(n)$
- Computationally feasible even in high dimensions
- Excellent finite sample performance
- Extensions to other models