Shrinkage Estimators and Hierarchical Bayes

STA 721: Lecture 11

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Outline

- Lasso
- Bayesian Lasso

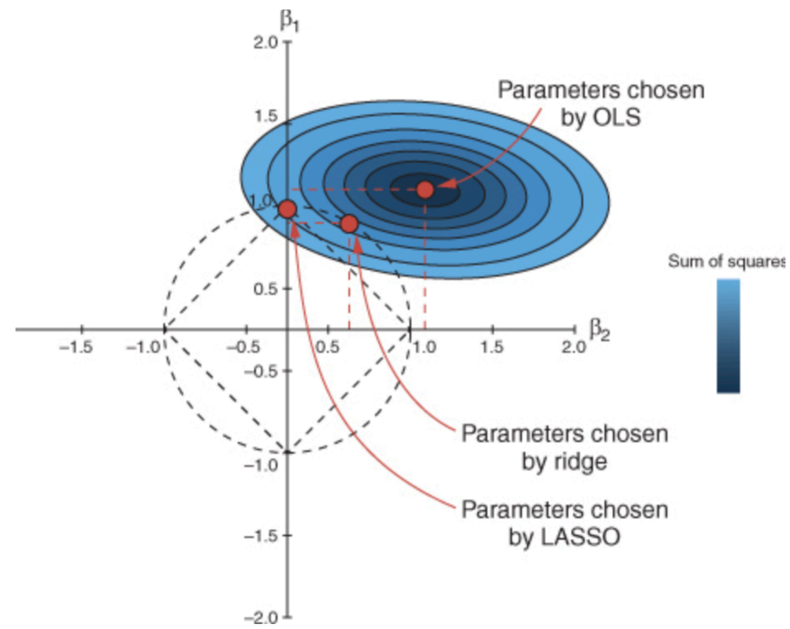
- Readings (see reading link)
  - Seber & Lee Chapter Chapter 12
  - Tibshirani (JRSS B 1996)
  - Park & Casella (JASA 2008)
  - Hans (Biometrika 2010)
  - Carvalho, Polson & Scott (Biometrika 2010)

LASSO Estimator

Tibshirani (JRSS B 1996) proposed estimating coefficients through L_1 constrained least squares via the **L**east **A**bsolute **S**hrinkage and **S**election **O**perator or *lasso*

$$\hat{\boldsymbol{\beta}}_L = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \left\{ \|\mathbf{Y}_c - \mathbf{X}_s \boldsymbol{\beta}\|^2 + \lambda \|\boldsymbol{\beta}\|_1 \right\}$$

- $\mathbf{Y}_c$ is the centered $\mathbf{Y}$, $\mathbf{Y}_c = \mathbf{Y} - \bar{\mathbf{Y}}\mathbf{1}$
- $\mathbf{X}_s$ is the centered and standardized $\mathbf{X}$ matrix so that the diagonal elements of $\mathbf{X}_s^T \mathbf{X}_s = c$.
- use the `scale` function but standardization usually handled within packages



- Control how large coefficients may grow

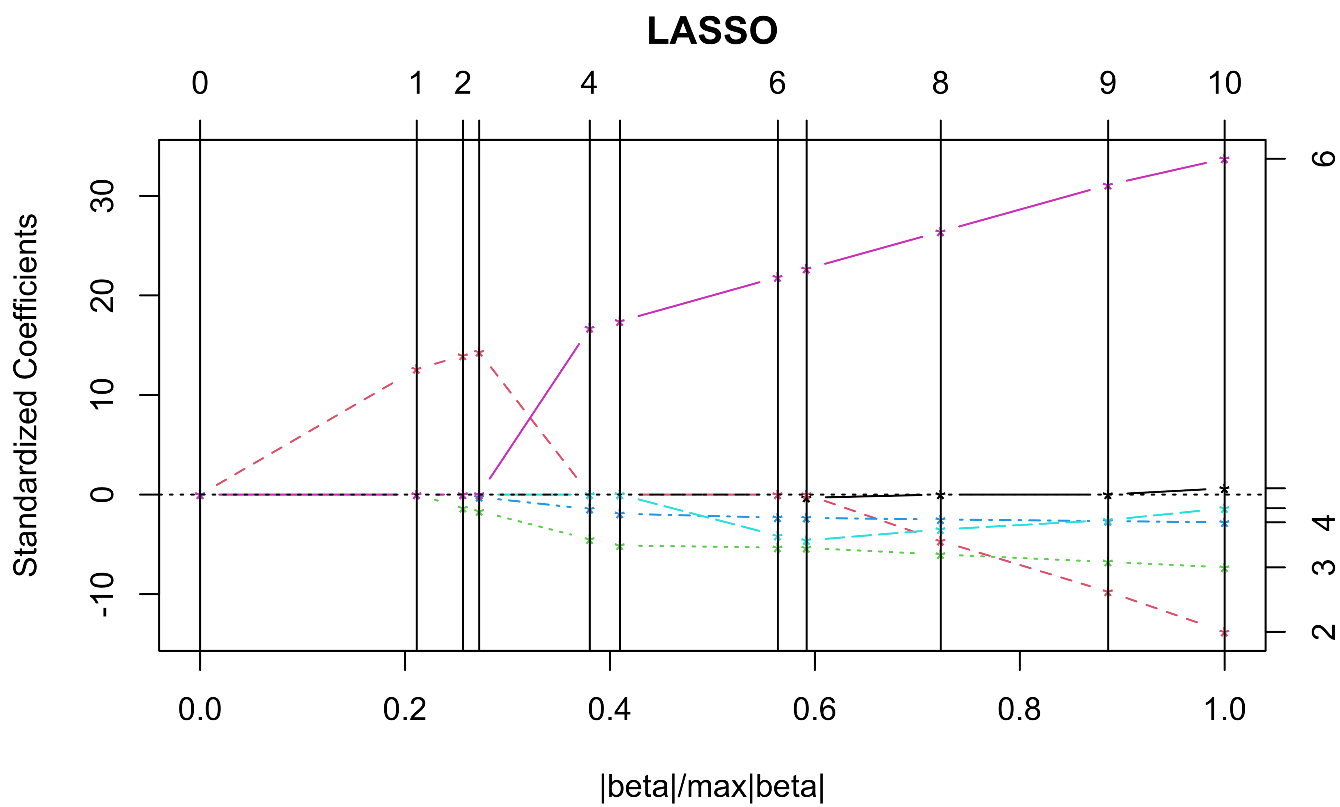
$$\underset{\boldsymbol{\beta}}{\arg\min} (\mathbf{Y}_c - \mathbf{X}_s \boldsymbol{\beta})^T (\mathbf{Y}_c - \mathbf{X}_s \boldsymbol{\beta}$$

$$\text{subject to } \sum |\beta_j| \le t$$

Lasso Solutions

The entire path of solutions can be easily found using the ``Least Angle Regression'' Algorithm of Efron et al (Annals of Statistics 2004)

```r
library(lars); datasets::longley
longley.lars = lars(as.matrix(longley[,-7]), longley[,7], type="l
```



Coefficients

```
1 round(coef(longley.lars),4)
```

```
      GNP.deflator     GNP Unemployed Armed.Forces Population   Year
 [1,]       0.0000  0.0000     0.0000       0.0000     0.0000 0.0000
 [2,]       0.0000  0.0327     0.0000       0.0000     0.0000 0.0000
 [3,]       0.0000  0.0362    -0.0037       0.0000     0.0000 0.0000
 [4,]       0.0000  0.0372    -0.0046      -0.0010     0.0000 0.0000
 [5,]       0.0000  0.0000    -0.0124      -0.0054     0.0000 0.9068
 [6,]       0.0000  0.0000    -0.0141      -0.0071     0.0000 0.9438
 [7,]       0.0000  0.0000    -0.0147      -0.0086    -0.1534 1.1843
 [8,]      -0.0077  0.0000    -0.0148      -0.0087    -0.1708 1.2289
 [9,]       0.0000 -0.0121    -0.0166      -0.0093    -0.1303 1.4319
[10,]       0.0000 -0.0253    -0.0187      -0.0099    -0.0951 1.6865
[11,]       0.0151 -0.0358    -0.0202      -0.0103    -0.0511 1.8292
```

Selecting a Solution from the Path

```r
summary(longley.lars)
```

```
LARS/LASSO
Call: lars(x =
as.matrix(longley[, -7]), y =
longley[, 7], type = "lasso")
   Df     Rss        Cp
0   1 185.009 1976.7120
1   2   6.642   59.4712
2   3   3.883   31.7832
3   4   3.468   29.3165
4   5   1.563   10.8183
5   4   1.339    6.4068
6   5   1.024    5.0186
7   6   0.998    6.7388
```

- For p predictors,

$$C_p = \frac{\text{SSE}_p}{s^2} - n + 2p$$

- s^2 is the residual variance from the full model
- SSE_p is the sum of squared errors for the model with p predictors (RSS)
- if the model includes all the predictors with non-zero coefficients, then $C_p \approx p$
- choose minimum $C_p \approx p$
- in practice use Cross-validation or Generalized Cross Validation (GCV) to choose λ

Features and Issues

- Combines shrinkage (like Ridge Regression) with Variable Selection to deal with collinearity
- Can be used for prediction or variable selection
- not invariant under linear transformations of the predictors
- typically no uncertainty estimates for the coefficients or predictions
- ignores uncertainty in the choice of λ
- may overshrink large coefficients

Bayesian LASSO

- Equivalent to finding posterior mode with a Double Laplace Prior

$$\underset{\boldsymbol{\beta}}{\text{argmax}} - \frac{\phi}{2}\{\|\mathbf{Y}_c - \mathbf{X}_s\boldsymbol{\beta}\|^2 + \lambda^*\|\boldsymbol{\beta}\|_1\}$$

- Park & Casella (JASA 2008) and Hans (Biometrika 2010) propose Bayesian versions of the Lasso

$$\begin{aligned}
\mathbf{Y} \mid \alpha, \boldsymbol{\beta}, \phi &\sim \textsf{N}(\mathbf{1}_n\alpha + \mathbf{X}^s\boldsymbol{\beta}^s, \mathbf{I}_n/\phi) \\
\boldsymbol{\beta} \mid \alpha, \phi, \boldsymbol{\tau} &\sim \textsf{N}(\mathbf{0}, \textsf{diag}(\boldsymbol{\tau}^2)/\phi) \\
\tau_1^2 \ldots, \tau_p^2 \mid \alpha, \phi &\overset{\text{iid}}{\sim} \textsf{Exp}(\lambda^2/2) \\
p(\alpha, \phi) &\propto 1/\phi
\end{aligned}$$

- Generalizes Ridge Priors to allow different prior variances for each coefficient

Double Exponential or Double Laplace Prior

- Marginal distribution of β_j

$$
\begin{aligned}
\boldsymbol{\beta} \mid \alpha, \phi, \boldsymbol{\tau} &\sim \mathsf{N}(\mathbf{0}, \mathsf{diag}(\boldsymbol{\tau}^2)/\phi) \\
\tau_1^2 \ldots, \tau_p^2 \mid \alpha, \phi &\overset{\text{iid}}{\sim} \mathsf{Exp}(\lambda^2/2) \\
p(\beta_j \mid \phi, \lambda) &= \int_0^\infty p(\beta_i \mid \phi, \tau_j^2) p(\tau_j^2 \mid \phi, \lambda)\, d\tau^2
\end{aligned}
$$

- Can show that $\beta_j \mid \phi, \lambda \overset{\text{iid}}{\sim} DE(\lambda\sqrt{\phi})$

$$
\int_0^\infty \frac{1}{\sqrt{2\pi t}} e^{-\frac{1}{2}\phi\frac{\beta^2}{t}} \, \frac{\lambda^2}{2} e^{-\frac{\lambda^2 t}{2}}\, dt = \frac{\lambda \phi^{1/2}}{2} e^{-\lambda \phi^{1/2}|\beta|}
$$

- Scale Mixture of Normals (Andrews and Mallows 1974)

Gibbs Sampler

- Integrate out α: $\alpha \mid \mathbf{Y}, \phi \sim \mathsf{N}(\bar{y}, 1/(n\phi))$
- $\boldsymbol{\beta} \mid \boldsymbol{\tau}, \phi, \lambda, \mathbf{Y}_c \sim \mathsf{N}(,)$
- $\phi \mid \boldsymbol{\tau}, \boldsymbol{\beta}, \lambda, \mathbf{Y}_c \sim \mathbf{G}(,)$
- $1/\tau_j^2 \mid \boldsymbol{\beta}, \phi, \lambda, \mathbf{Y} \sim \textsf{InvGaussian}(,)$
- $X \sim \textsf{InvGaussian}(\mu, \lambda)$ has density

$$f(x) = \sqrt{\frac{\lambda^2}{2\pi}} x^{-3/2} e^{-\frac{1}{2}\frac{\lambda^2(x-\mu)^2}{\mu^2 x}} \qquad x > 0$$

- Homework: Derive the full conditionals for $\boldsymbol{\beta}^s, \phi, 1/\tau^2$
- see Casella & Park

Horseshoe Priors

Carvalho, Polson & Scott (2010) propose an alternative shrinkage prior

$$
\begin{aligned}
\boldsymbol{\beta} \mid \phi &\sim \mathsf{N}(\mathbf{0}_p, \frac{\mathsf{diag}(\tau^2)}{\phi}) \\
\tau_j^2 \mid \lambda &\overset{\text{iid}}{\sim} C^+(0, \lambda) \\
\lambda &\sim \mathsf{C}^+(0, 1/\phi) \\
p(\alpha, \phi) &\propto 1/\phi
\end{aligned}
$$

- $C^+(0, \lambda)$ is the half-Cauchy distribution with scale λ

$$
p(\tau_j^2 \mid \lambda) = \frac{2}{\pi} \frac{\lambda}{\lambda^2 + \tau_j^2}
$$

- $\mathsf{C}^+(0, 1/\phi)$ is the half-Cauchy distribution with scale $1/\phi$

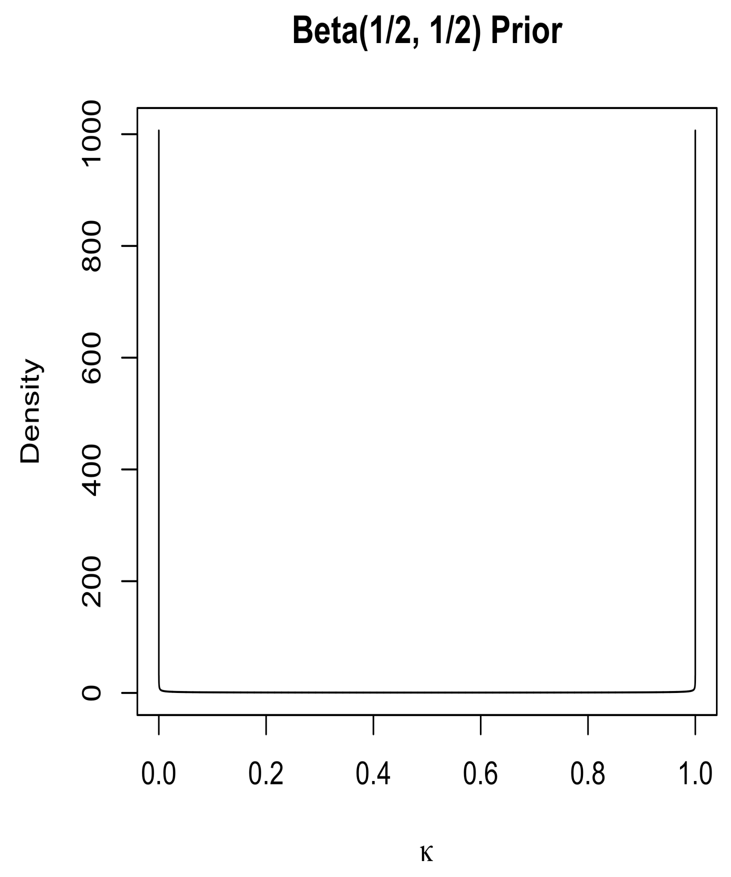
Special Case

In the case $\lambda = \phi = 1$ and with $\mathbf{X}^t\mathbf{X} = \mathbf{I}$, $\mathbf{Y}^* = \mathbf{X}^T\mathbf{Y}$

$$\begin{aligned} E[\beta_i \mid \mathbf{Y}] &= \mathsf{E}_{\kappa_i \mid \mathbf{Y}}[\mathsf{E}_{\beta_i \mid \kappa_i, \mathbf{Y}}[\beta_i \mid \mathbf{Y}] \\ &= \int_0^1 (1 - \kappa_i) y_i^* p(\kappa_i \mid \mathbf{Y}) \, d\kappa_i \\ &= (1 - \mathsf{E}[\kappa \mid y_i^*]) y_i^* \end{aligned}$$

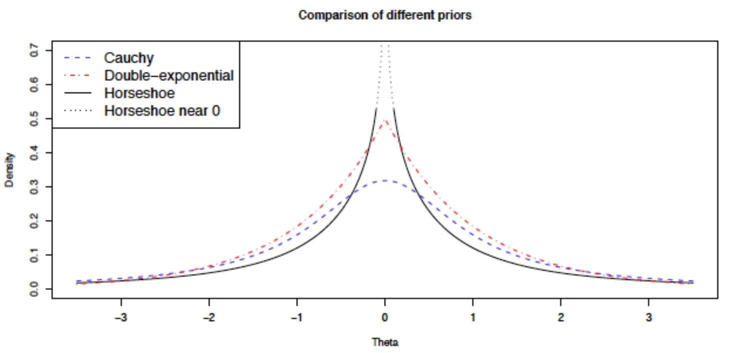
where $\kappa_i = 1/(1 + \tau_i^2)$ is the shrinkage factor (like in James-Stein)

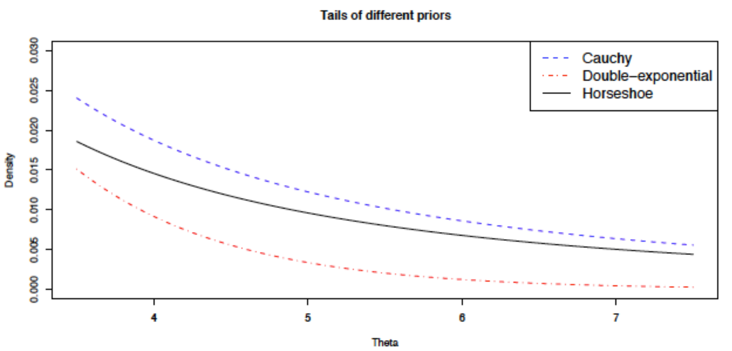
- Half-Cauchy prior induces a Beta(1/2, 1/2) distribution on κ_i a priori (change of variables)



Features and Issues

- the posterior mode also induces shrinkage and variable selection if the mode is at zero
- the posterior mean is a shrinkage estimator (no selection)
- the tails of the distribution are heavier than the Laplace prior (like a Cauchy distribution) so that there is less shrinkage of large $|\hat{\beta}|$.
- Desirable in the orthogonal case, where lasso is more like ridge regression (related to bounded influence)
- MCMC is slow to mix using programs like `stan` but specialized `R` packages like `horseshoe` and `monomvm::bhs`are available

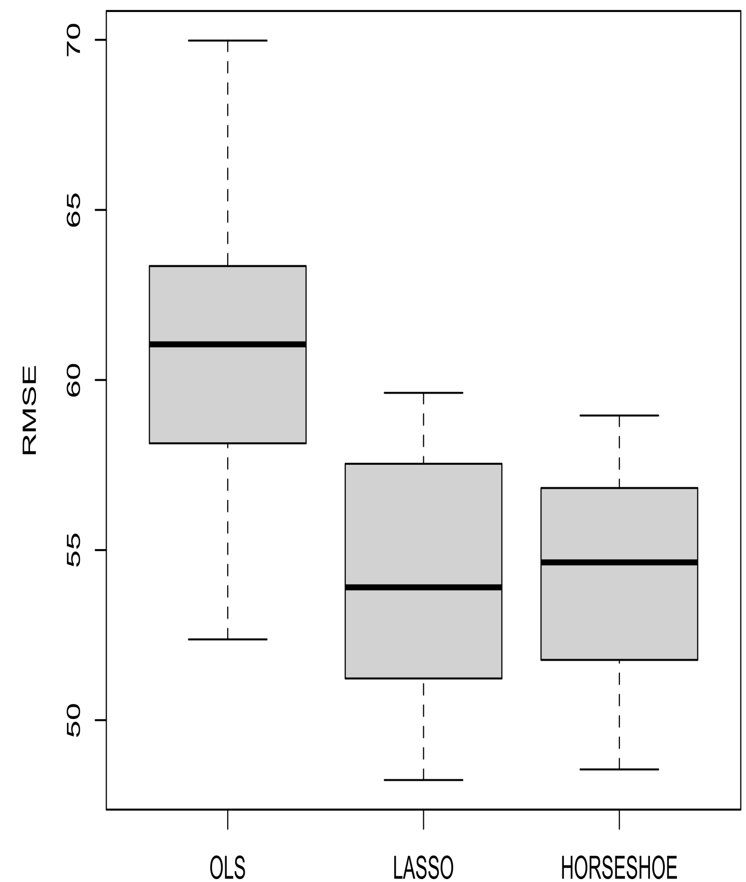




Bounded Influence and Posterior Mean

Comparison

- Diabetes data (from the `lars` package)
- 64 predictors: 10 main effects, 2-way interactions and quadratic terms
- sample size of 442
- split into training and test sets
- compare MSE for out-of-sample prediction using OLS, lasso and horseshoe priors
- Root MSE for prediction for left out data based on 25 different random splits with 100 test cases



Summary

The literature on shrinkage estimators (with or without selection) is vast

- Elastic Net (Zou & Hastie 2005)
- SCAD (Fan & Li 2001)
- Generalized Double Pareto Prior (Armagan, Dunson & Lee 2013)
- Spike-and-Slab Lasso (Rockova & George 2018)

For Bayes, choice of estimator

- posterior mean (easy via MCMC)
- posterior mode (optimization)
- posterior median (via MCMC)

Properties?

- Fan & Li (JASA 2001) discuss variable selection via non-concave penalties and oracle properties (next time …)