# Optimal Shrinkage/Selection and Oracle Properties

STA 721: Lecture 12

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# Outline

- Bounded Influence and Posterior Mean
- Shrinkage properties and nonconcave penalties
- conditions for optimal shrinkage and selection . . .
- Readings (see reading link)
  - Tibshirani (JRSS B 1996)
  - Carvalho, Polson & Scott (Biometrika 2010)
  - Armagan, Dunson & Lee (Statistica Sinica 2013)
  - Fan & Li (JASA 2001)

# Horseshoe Priors

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

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

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

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

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

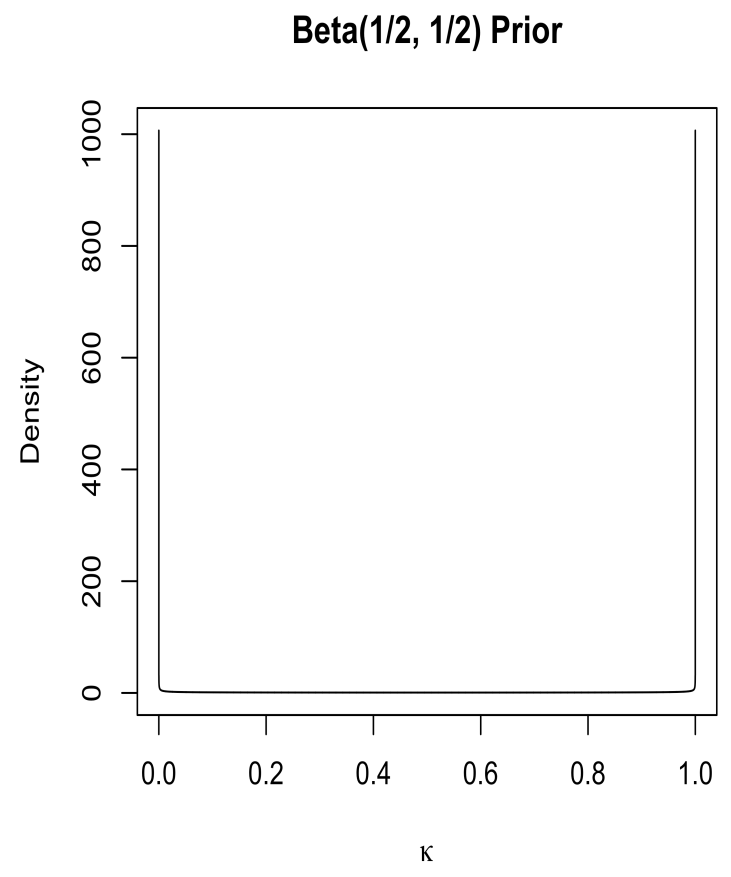
# Special Case: Orthonormal Regression

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)

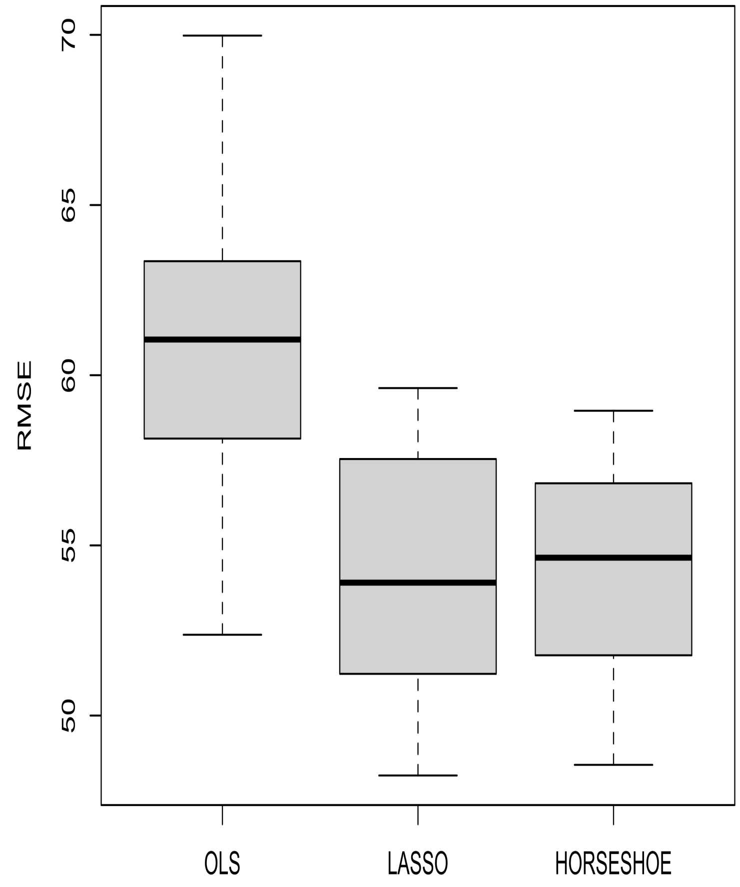
- Half-Cauchy prior induces a Beta(1/2, 1/2) distribution on $\kappa_i$ a priori (change of variables)
- marginal prior (after integrating out )



# Bounded Influence $(\mathbf{X}^T\mathbf{X} = \mathbf{I})$

# 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
- both Lasso and Horseshoe much better than OLS



# Duality for Modal Estimators

# Properties for Modal Estimates

Fan & Li (JASA 2001) discuss variable selection via nonconcave penalties and oracle properties in the context of penalized likelihoods in this setting

- with duality of the negative log prior as their penalty we can extend to Bayesian modal estimates where the prior is a function of $|\beta_j|$

$$\frac{1}{2}\sum(\beta_i - y_i^*)^2 + \frac{1}{2}\sum_j(\beta_j - \hat{\beta}_j)^2 + \sum_j \textsf{pen}_\lambda(|\beta_j|)$$

- Requirements on penality
  - Unbiasedness: The resulting estimator is nearly unbiased when the true unknown parameter is large (avoid unnecessary modeling bias).
  - Sparsity: thresholding rule sets small coefficients to 0 (avoid model complexity)
  - Continuity: continuous in the data $\hat{\beta}_j = y_i^*$ (avoid instability in model prediction)

# Conditions for Unbiasedness

To find the optimal estimator take derivative of $\frac{1}{2}\sum_j(\beta_j - \hat{\beta}_j)^2 + \sum_j \textsf{pen}_\lambda(|\beta_j|)$ componentwise and set to zero

- Derivative is

$$\frac{d}{d\,\beta_j}\left\{\frac{1}{2}(\beta_j - \hat{\beta}_j)^2 + \textsf{pen}_\lambda(|\beta_j|)\right\} = (\beta_j - \hat{\beta}_j) + \mathrm{sgn}(\beta_j)\textsf{pen}'_\lambda(|\beta_j|)$$
$$= \mathrm{sgn}(\beta_j)\left\{|\beta_j| + \textsf{pen}'_\lambda(|\beta_j|)\right\} - \hat{\beta}_j$$

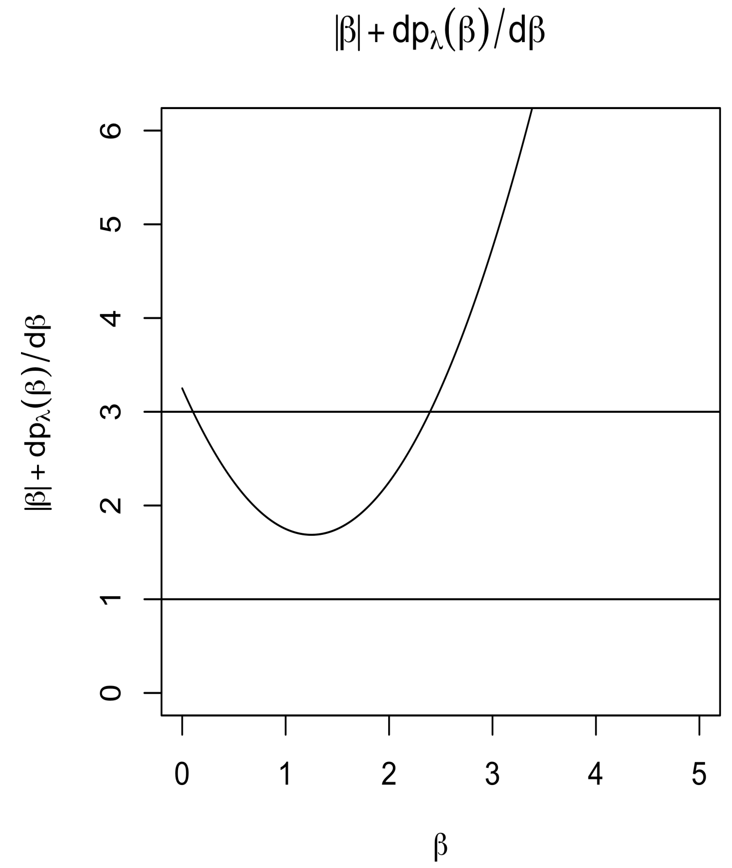
- setting derivative to zero gives $\hat{\beta}_j = \mathrm{sgn}(\beta_j)\left\{|\beta_j| + \textsf{pen}'_\lambda(|\beta_j|)\right\}$
- if $\lim_{|\beta_j|\to\infty} p'_\lambda(|\beta|) = 0$ then $\hat{\beta}_j = \mathrm{sgn}(\beta_j)|\beta_j| = \beta_j$
- for large $|\beta_j|$, $|\hat{\beta}_j|$ is large with high probability
- as MLE is unbiased, the optimal estimator is approximately unbiased for large $|\beta_j|$

# Conditions for Thresholding & Continuity

As sufficient condition for a thresholding rule $\hat{\beta}_\lambda = 0$ is if

$$0 < \min\left\{|\beta_j| + p'_\lambda(|\beta_j|)\right\}$$

- if $|\hat{\beta}_j| < \min\left\{|\beta_j| + p'_\lambda(|\beta_j|)\right\}$ then the derivative is positive for all positive $\beta_j$ and negative for all negative $\beta_j$ so $\hat{\beta}_j^\lambda = 0$ is a local minimum
- if $|\hat{\beta}_j| > \min\left\{|\beta_j| + p'_\lambda(|\beta_j|)\right\}$ multiple crossings (local roots)
- a sufficient and necessary condition for continuity is that the minimum of $|\beta_j| + p'_\lambda(|\beta_j|)$ is obtained at zero

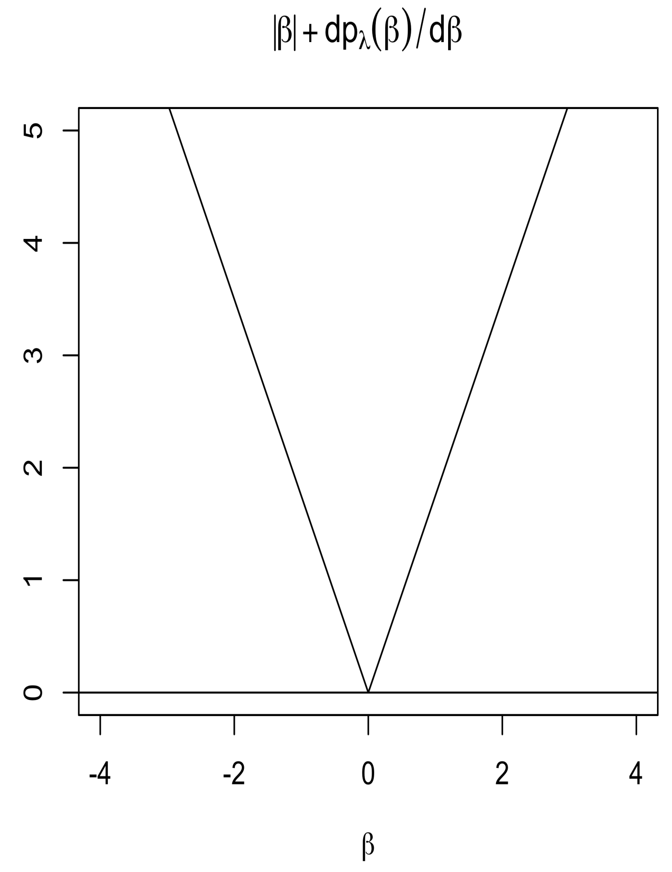


# Example: Gaussian Prior

- Prior N$(0, 1/\lambda^2)$
- Penalty: **pen**$_\lambda(|\beta_j|) = \frac{1}{2}\lambda|\beta_j|^2$
- Unbiasedness: for large $|\beta_j|$?
  - Derivative of **pen**$_\lambda(|\beta_j|) = \lambda\beta_j = \text{sgn}(\beta_j)\lambda|\beta_j|$
  - does not go to zero as $|\beta_j| \to \infty$
  - No! (bias towards zero)
- not a thresholding rule as

$$\min\left\{|\beta_j| + p'_\lambda(|\beta_j|)\right\} = (1+\lambda)|\beta_j|$$

  is zero
- is continuous as minimum is at zero

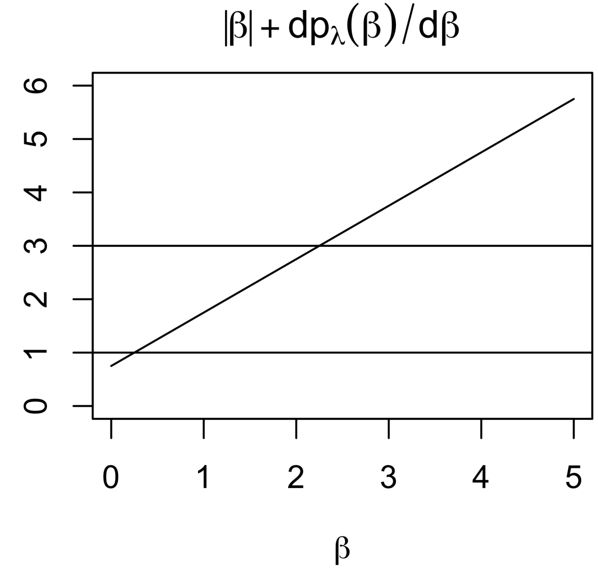


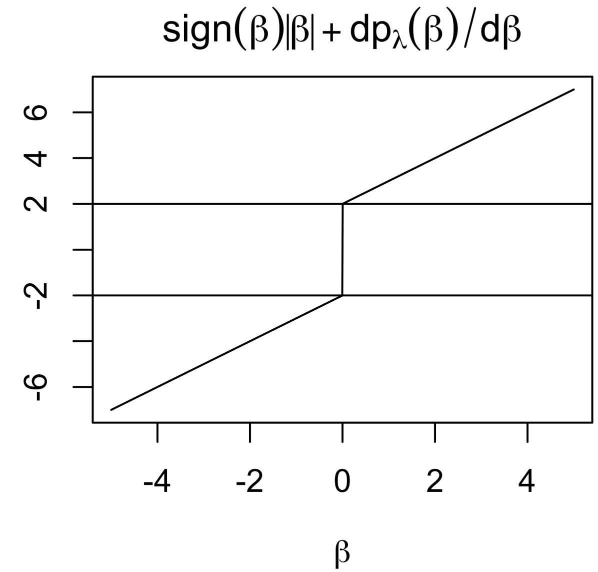
# Example: Lasso Prior

- Penalty: **pen**$_\lambda(|\beta_j|) = \lambda|\beta_j|$
- Unbiasedness: for large $|\beta_j|$?
  - Derivative of **pen**$_\lambda(|\beta_j|) = \lambda\,\mathrm{sgn}(\beta_j)$
  - does not go to zero as $|\beta_j| \to \infty$
  - No! (bias towards zero)
- Is a thresholding rule as

$$\min\left\{|\beta_j| + p'_\lambda(|\beta_j|)\right\} = (|\beta_j| + \lambda) > 0$$

- is continuous as minimum is at $\beta_j = 0$



# Generalized Double Pareto Prior

The Generalized Double Pareto of Armagan, Dunson & Lee (2013) has a prior density for $\beta_j$ of the form

$$p(\beta_j \mid \xi, \alpha) = \frac{1}{2\xi}\left(1 + \frac{\beta_j}{\alpha\xi}\right)^{-(1+\alpha)}$$

# Choice of Penalty/Prior and Conditions

- Ridge: none
- Lasso: does not satisfy conditions for unbiasedness
- GDP: Can show that Generalized Double Pareto does for some choices of hyperparameters
- Horseshoe: need marginal distribution of $\beta_j$ for penalty
  - marginal generally not available in closed form
  - can show for a special case where there is an analytic expression for the marginal density ($\lambda = \phi = 1$)

$$p(\beta) = k \exp(\beta^2/2) E_1(\beta^2/2)$$

- where $E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt$ for $n = 1, 2, \ldots$
- $E_n'(x) = -E_{n-1}(x)$ for $n = 1, 2, \ldots$

# Shrinkage Estimators

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

- Ridge
- Lasso
- 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)

# Selection and Uncertainty

- Prior/Posterior do not put any probability on the event $\beta_j = 0$
- Uncertainty that the coefficient is zero?
- Selection solved as a post-analysis decision problem
- Selection part of model uncertainty
  - add prior probability that $\beta_j = 0$
  - combine with decision problem