James-Stein Estimation and Shrinkage

STA 721: Lecture 10

Merlise Clyde (clyde@duke.edu)
Duke University

Outline

- Frequentist Risk in Orthogonal Regression
- James-Stein Estimation

Readings:

- Seber & Lee Chapter Chapter 12

Orthogonal Regression

- Consider the model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$ where $\mathbf{X}$ is $n \times p$ with $n > p$ and $\mathbf{X}^T\mathbf{X} = \mathbf{I}_p$.
- If $\mathbf{X}$ has orthogonal columns, then $\hat{\boldsymbol{\beta}} = \mathbf{X}^T\mathbf{Y}$ is the OLS estimator of $\boldsymbol{\beta}$.
- The OLS estimator is unbiased and has minimum variance among all
- The MSE for estimating $\boldsymbol{\beta}$ is $\mathsf{E}_{\mathbf{Y}}[(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})] = \sigma^2 \mathbf{tr}[(\mathbf{X}^T\mathbf{X})^{-1}] = p\sigma^2$
- Can always take a general regression problem and transform design so that the model matrix has orthogonal columns

  $$\mathbf{X}\boldsymbol{\beta} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^T\boldsymbol{\beta} = \mathbf{U}\boldsymbol{\alpha}$$

  where new parameters are $\boldsymbol{\alpha} = \boldsymbol{\Delta}\mathbf{V}^T\boldsymbol{\beta}$ and $\mathbf{U}^T\mathbf{U} = \mathbf{I}_p$.
- Orthogonal polynomials, Fourier bases and wavelet regression are other examples.
- $\hat{\boldsymbol{\alpha}} = \mathbf{U}^T\mathbf{Y}$ and MSE of $\hat{\boldsymbol{\alpha}}$ is $p\sigma^2$
- so WLOG we will assume that $\mathbf{X}$ has orthogonal columns

Shrinkage Estimators

- the g-prior and Ridge prior are equivalent in the orthogonal case

$$\boldsymbol{\beta} \sim \mathsf{N}(\mathbf{0}_p, \sigma^2 \mathbf{I}_p/\kappa)$$

  using the ridge parameterization of the prior $\kappa = 1/g$

- Bayes estimator in this case is

$$\hat{\boldsymbol{\beta}}_\kappa = \frac{1}{1+\kappa}\hat{\boldsymbol{\beta}}$$

- MSE of $\hat{\boldsymbol{\beta}}_\kappa$ is

$$\textsf{MSE}(\hat{\boldsymbol{\beta}}_\kappa) = \frac{1}{(1+\kappa)^2}\sigma^2 p + \frac{\kappa^2}{(1+\kappa)^2}\sum_{j=1}^{p}\beta_j^2$$

- squared bias term grows with κ and variance term decreases with κ

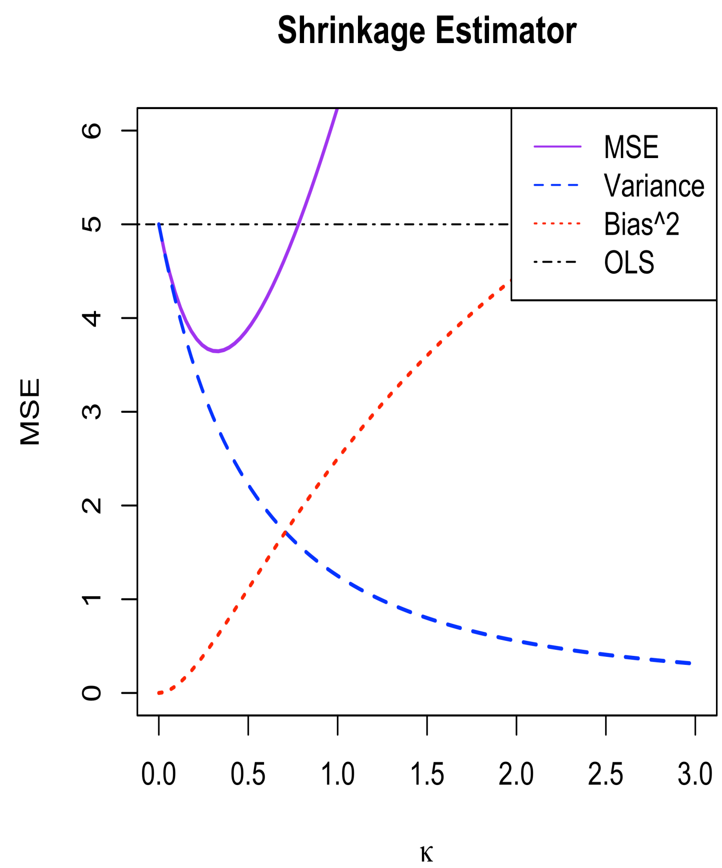
Shrinkage

- in principle, with the right choice of κ we can get a better estimator and reduce the MSE
- while not unbiased, what we pay for bias we can make up for with a reduction in variance
- the variance-bias decomposition of MSE based on the plot suggests there is an optimal value of κ the improves over OLS in terms of MSE
- "optimal" κ

$$\kappa = \frac{p\sigma^2}{\|\boldsymbol{\beta}^*\|^2}$$

where $\boldsymbol{\beta}^*$ is the true value of $\boldsymbol{\beta}$

- but never know that in practice!



Estimating κ

James-Stein Estimators

in James and Stein (1961) proposed a shrinkage estimator that dominated the MLE for the mean of a multivariate normal distribution

$$\tilde{\boldsymbol{\beta}}_{JS} = \left(1 - \frac{(p-2)\sigma^2}{\|\hat{\boldsymbol{\beta}}\|^2}\right)\hat{\boldsymbol{\beta}}$$

(equivalent to our orthogonal regression case; just multiply everything by $\mathbf{X}^T$ to show)

- they showed that this is the best (in terms of smallest MSE) of all estimators of the form $\left(1 - \frac{b}{\|\hat{\boldsymbol{\beta}}\|^2}\right)\hat{\boldsymbol{\beta}}$
- it is possible to show that the MSE of the James-Stein estimator is

$$\textsf{MSE}(\tilde{\boldsymbol{\beta}}_{JS}) = 2\sigma^2$$

which is less than the MSE of the OLS estimator if $p > 2$! (more on this in STA732)

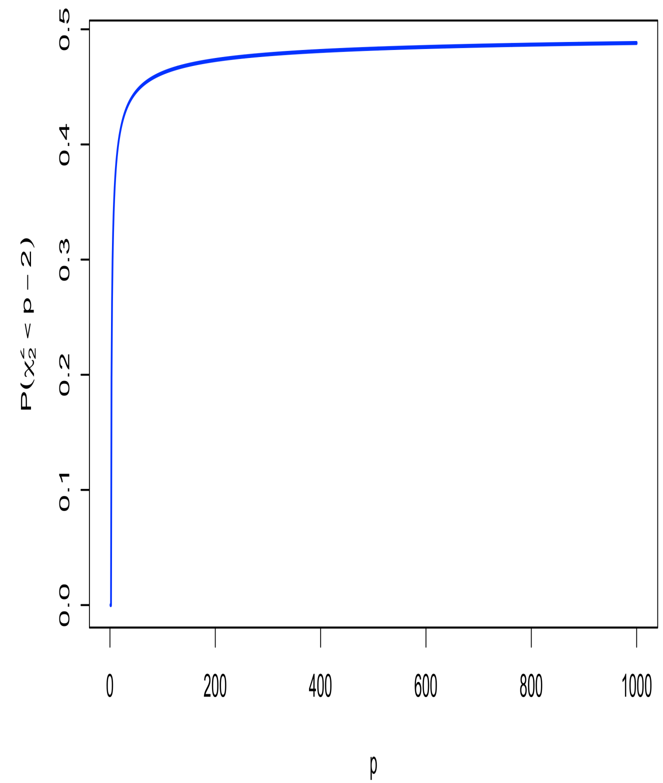
Negative Shrinkage?

- one potential problem with the James-Stein estimator

$$\tilde{\boldsymbol{\beta}}_{JS} = \left(1 - \frac{(p-2)\sigma^2}{\|\hat{\boldsymbol{\beta}}\|^2}\right)\hat{\boldsymbol{\beta}}$$

  is that the term in the parentheses can be negative if $\|\hat{\boldsymbol{\beta}}\|^2 < (p-2)\sigma^2$

- How likely is this to happen?
- Suppose that each of the parameters β_j are actually zero, then $\hat{\boldsymbol{\beta}} \sim \mathsf{N}(\mathbf{0}_p, \sigma^2 \mathbf{I}_p)$ then $\|\hat{\boldsymbol{\beta}}\|^2/\sigma^2 \sim \chi^2_p$
- compute the probability that $\chi^2_p < (p-2)$
- so if the model is full of small effects, the James-Stein can lead to negative shrinkage!



Positive Part James-Stein Estimator

Bayes and Admissibilty

- Bayes rules based on proper priors are generally always admissible (see Christian Robert (2007) The Bayesian Choice for more details)
- unique Bayes rules are admissible
- Generalized Bayes rules based on improper priors may not be inadmissible, but this will depend on the loss function and the prior
- under regularity conditions, limits of Bayes rules will be admissible
- the Positive-Part James-Stein estimator fails to be admissible under squared error loss as Bayes risk is not continuous

Positive Part James-Stein Estimator and Testimators

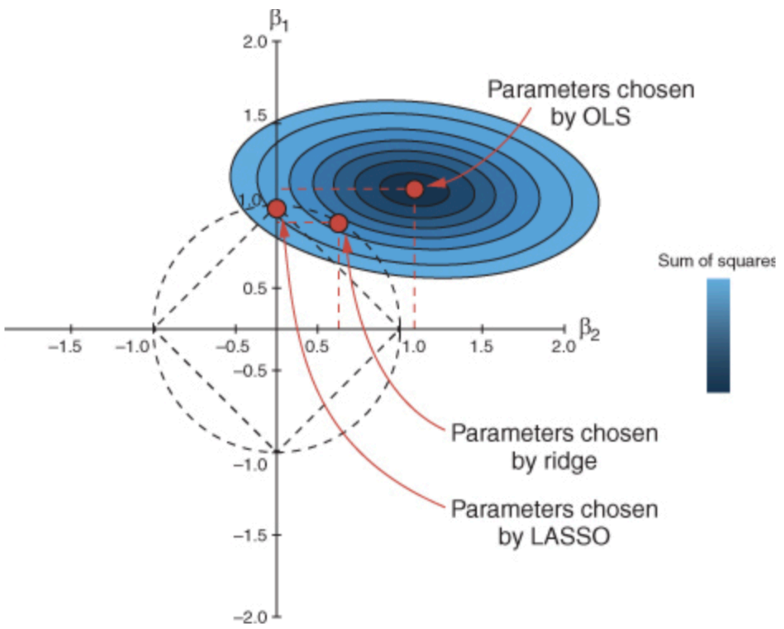
- the positive part James-Stein estimator can be shown to be related to **testimators** where if we fail to reject the hypothesis that all the β_j are zero at some level, we set all coefficients to zero, and otherwise we shrink the coefficients by an amount that depends on how large the test statistic ($\|\hat{\boldsymbol{\beta}}\|^2$) is.
- note this can shrink all the coefficients to zero if the majority are small so increased bias for large coefficients that are not zero!
- this is a form of **model selection** where we are selecting the model that has all the coefficients zero!

LASSO Estimator

- an alternative estimator that allows for shrinkage and selection is the LASSO (Least Absolute Shrinkage and Selection Operator).
- the LASSO replaces the penalty term in the ridge regression with an L_1 penalty term

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

- the LASSO can also be shown to be the posterior mode of a Bayesian model with independent Laplace or double exponential prior distributions on the coefficients.
- as the double exponential prior is a "scale" mixture of normals, this provides a generalization of the ridge regression.



from Machine Learning with R