Bayes Estimators & Ridge Regression

Readings Chapter 14 Christensen

STA721 Linear Models Duke University

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How Good are Estimators?

Quadratic loss for estimating $\boldsymbol{\beta}$ using estimator $\mathbf{a}$

$$L(\boldsymbol{\beta}, \mathbf{a}) = (\boldsymbol{\beta} - \mathbf{a})^T(\boldsymbol{\beta} - \mathbf{a})$$

- Consider our expected loss (before we see the data) of taking an action $\mathbf{a}$
- Under OLS or the Reference prior the Expected Mean Square Error

$$\begin{aligned} \mathsf{E}_{\mathbf{Y}}[(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) &= \sigma^2 \text{tr}[(\mathbf{X}^T\mathbf{X})^{-1}] \\ &= \sigma^2 \sum_{j=1}^{p} \lambda_j^{-1} \end{aligned}$$

- If smallest $\lambda_j \to 0$ then MSE $\to \infty$

Is g-prior any better?

Under the g-prior $\mathsf{E}_{\mathbf{Y}}[(\boldsymbol{\beta} - \frac{g}{1+g}\hat{\boldsymbol{\beta}})^T(\boldsymbol{\beta} - \frac{g}{1+g}\hat{\boldsymbol{\beta}})$

$$\begin{aligned} \mathsf{E}[L(\boldsymbol{\beta}, \frac{g}{1+g}\hat{\boldsymbol{\beta}})] &= \sigma^2 \left(\frac{g}{1+g}\right)^2 \operatorname{tr}[(\mathbf{X}^T\mathbf{X})^{-1}] + \frac{\boldsymbol{\beta}^T\boldsymbol{\beta}}{(1+g)^2} \\ &= \frac{1}{(1+g)^2}(\sigma^2 g^2 \sum \lambda_j^{-1} + \|\boldsymbol{\beta}\|^2) \end{aligned}$$

Aside: g prior is better than Reference Prior if

$$g > \frac{\|\boldsymbol{\beta}\|^2}{\sigma^2 \sum \lambda_j^{-1}} - 1$$

But still have risk going to infinity as $\lambda \to 0$

Assume that $\mathbf{X}$ has been centered and standardized so that $\mathbf{X}^T\mathbf{X} = \text{corr}(\mathbf{X})$ (use `scale` function in `R`)

- Write $\mathbf{X} = \mathbf{U}_p L \mathbf{V}^T$ Singular Value Decomposition where $\mathbf{U}_p^T \mathbf{U}_p = \mathbf{I}_p$ and $\mathbf{V}$ is $p \times p$ orthogonal matrix, L is diagonal

$$\mathbf{Y} = \mathbf{1}\alpha + \mathbf{U}_p L \mathbf{V}^T \boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- Let $\mathbf{U} = [\mathbf{1}\, \mathbf{U}_p\, \mathbf{U}_{n-p-1}]$ $n \times n$ orthogonal matrix
- Rotate by $\mathbf{U}^T$

$$\begin{aligned}
\mathbf{U}^T\mathbf{Y} &= \mathbf{U}^T\mathbf{1}\alpha + \mathbf{U}^T\mathbf{U}_p L \mathbf{V}^T\boldsymbol{\beta} + \mathbf{U}^T\boldsymbol{\epsilon} \\
\mathbf{Y}^* &= \begin{bmatrix} n & \mathbf{0}_p \\ 0 & L \\ \mathbf{0}_{n-p-1} & \mathbf{0}_{n-p-1 \times p} \end{bmatrix} \begin{pmatrix} \alpha \\ \gamma \end{pmatrix} + \boldsymbol{\epsilon}^*
\end{aligned}$$

Orthogonal Regression

$$
\begin{aligned}
\mathbf{U}^T\mathbf{Y} &= \mathbf{U}^T\mathbf{1}\alpha + \mathbf{U}^T\mathbf{U}_p L \mathbf{V}^T\boldsymbol{\beta} + \mathbf{U}^T\boldsymbol{\epsilon} \\
\mathbf{Y}^* &= \left[\begin{array}{cc} n & \mathbf{0}_p \\ 0 & L \\ \mathbf{0}_{n-p-1} & \mathbf{0}_{n-p-1\times p} \end{array}\right] \left(\begin{array}{c} \alpha \\ \gamma \end{array}\right) + \boldsymbol{\epsilon}^*
\end{aligned}
$$

- $\hat{\alpha} = \bar{y}$
- $\hat{\gamma} = (L^T L)^{-1} L^T \mathbf{U}_p^T \mathbf{Y}$ or $\hat{\gamma}_i = y_i^*/l_i$ for $i = 1, \ldots, p$
- $\text{Var}(\hat{\gamma}_i) = \sigma^2/l_i^2$

Directions in $\mathbf{X}$ space $\mathbf{U}_j$ with small eigenvectors l_i have the largest variances. Unstable directions.

Ridge Regression & Independent Prior

(Another) Normal Conjugate Prior Distribution on $\boldsymbol{\gamma}$:

$$\boldsymbol{\gamma} \mid \phi \sim \mathsf{N}(\mathbf{0}_p, \frac{1}{\phi k}\mathbf{I}_p)$$

Posterior mean

$$\tilde{\gamma} = (L^T L + k\mathbf{I})^{-1} L^T \mathbf{U}_p^T \mathbf{Y} = (L^T L + k\mathbf{I})^{-1} L^T L \hat{\gamma}$$

$$\tilde{\gamma}_i = \frac{l_i^2}{l_i^2 + k}\hat{\gamma}_i = \frac{\lambda_i}{\lambda_i + k}\hat{\gamma}_i$$

- When $\lambda_i \to 0$ then $\tilde{\gamma}_i \to 0$
- When $k \to 0$ we get OLS back but if k gets too big posterior mean goes to zero.

Transform

- Transform back $\tilde{\boldsymbol{\beta}} = \mathbf{V}\tilde{\gamma}$

$$\tilde{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X} + k\mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}}$$

- importance of standardizing
- Is there a value of k for which ridge is better in terms of Expected MSE than OLS?
- Choice of k?

MSE

Can show that

$$\mathsf{E}[(\boldsymbol{\beta} - \tilde{\boldsymbol{\beta}})^T(\boldsymbol{\beta} - \tilde{\boldsymbol{\beta}})] = \mathsf{E}[(\boldsymbol{\gamma} - \tilde{\boldsymbol{\gamma}})^T(\boldsymbol{\gamma} - \tilde{\boldsymbol{\gamma}})]$$

- $\mathsf{Var}(\gamma_i - \tilde{\gamma}_i) = \sigma^2 l_i^2/(l_i^2 + k)^2$
- Bias of $\tilde{\gamma}$ is $-k/(l_i^2 + k)$
- MSE

$$\sigma^2 \sum_i \frac{l_i^2}{(l_i^2 + k)^2} + k^2 \sum_i \frac{\gamma_i^2}{(l_i^2 + k)^2}$$

The derivative with respect to k is negative at $k = 0$, hence the function is decreasing.

Since $k = 0$ is OLS, this means that is a value of k that will always be better than OLS

Alternative Motivation

- If $\hat{\beta}$ is unconstrained expect high variance with nearly singular $\mathbf{X}$
- Let $\mathbf{Y}^c = (\mathbf{I} - \mathrm{P}_1)\mathbf{Y}$ and $\mathbf{X}^c$ the centered and standardized $\mathbf{X}$ matrix
- Control how large coefficients may grow

$$\min_{\boldsymbol{\beta}} (\mathbf{Y}^c - \mathbf{X}^c \beta)^T (\mathbf{Y}^c - \mathbf{X}^c \beta)$$

  subject to

$$\sum \beta_j^2 \leq t$$

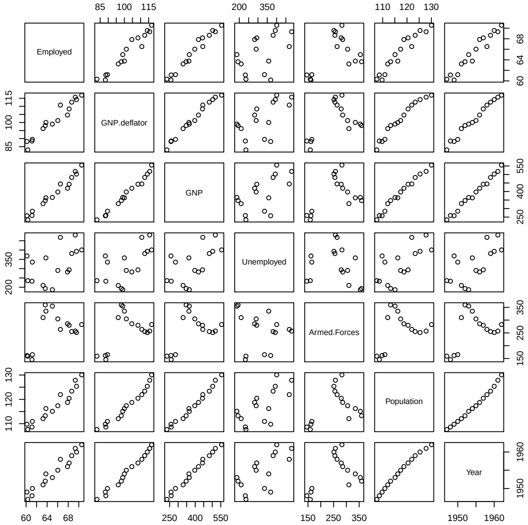
- Equivalent Quadratic Programming Problem

$$\min_{\boldsymbol{\beta}} \|\mathbf{Y}^c - \mathbf{X}^c \boldsymbol{\beta}\|^2 + k\|\boldsymbol{\beta}\|^2$$

- "penalized" likelihood

Picture

Longley Data



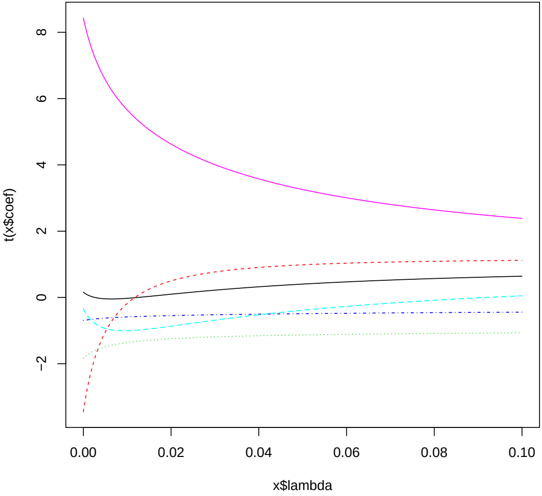
OLS

```
> longley.lm = lm(Employed ~ ., data=longley)
> summary(longley.lm)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  -3.482e+03  8.904e+02  -3.911 0.003560 **
GNP.deflator  1.506e-02  8.492e-02   0.177 0.863141
GNP          -3.582e-02  3.349e-02  -1.070 0.312681
Unemployed   -2.020e-02  4.884e-03  -4.136 0.002535 **
Armed.Forces -1.033e-02  2.143e-03  -4.822 0.000944 ***
Population   -5.110e-02  2.261e-01  -0.226 0.826212
Year          1.829e+00  4.555e-01   4.016 0.003037 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.3049 on 9 degrees of freedom
Multiple R-squared: 0.9955,Adjusted R-squared: 0.9925
F-statistic: 330.3 on 6 and 9 DF,  p-value: 4.984e-10
```

Ridge Trace



Generalized Cross-validation

```
> select(lm.ridge(Employed ~ ., data=longley,
         lambda=seq(0, 0.1, 0.0001)))

modified HKB estimator is 0.004275357
modified L-W estimator is 0.03229531
smallest value of GCV  at 0.0028

> longley.RReg = lm.ridge(Employed ~ ., data=longley,
                                 lambda=0.0028)
> coef(longley.RReg)
           GNP.deflator     GNP     Unemployed  Armed.Forces
-2.950e+03 -5.381e-04   -1.822e-02  -1.76e-02 -9.607e-03

 Population     Year
-1.185e-01  1.557e+00
```

Testimators

Goldstein & Smith (1974) have shown that if

1. $0 \leq h_i \leq 1$ and $\tilde{\gamma}_i = h_i \hat{\gamma}_i$
2. $\frac{\gamma_i^2}{\text{Var}(\hat{\gamma}_i)} < \frac{1+h_i}{1-h_i}$

then $\tilde{\gamma}_i$ has smaller MSE than $\hat{\gamma}_i$

Case: If $\gamma_j < \text{Var}(\hat{\gamma}_i) = \sigma^2 / l_i^2$ then $h_i = 0$ and $\tilde{\gamma}_i$ is better.

Apply: Estimate σ^2 with SSE/(n - p - 1) and γ_i with $\hat{\gamma}_i$. Set $h_i = 0$ if t-statistic is less than 1.

"testimator" - see also Sclove (JASA 1968) and Copas (JRSSB 1983)

Generalized Ridge

Instead of $\gamma_j \stackrel{\text{iid}}{\sim} \mathsf{N}(0, \sigma^2/k)$ take

$$\gamma_j \stackrel{\text{ind}}{\sim} \mathsf{N}(0, \sigma^2/k_i)$$

Then Condition of Goldstein & Smith becomes

$$\gamma_i^2 < \sigma^2 \left[\frac{2}{k_j} + \frac{1}{l_i^2} \right]$$

- If l_i is small almost any k_i will improve over OLS
- if l_i^2 is large then only very small values of k_i will give an improvement
- Prior on k_i?
- Induced prior on $\boldsymbol{\beta}$?

$$\gamma_j \stackrel{\text{ind}}{\sim} \mathsf{N}(0, \sigma^2/k_i) \Leftrightarrow \boldsymbol{\beta} \sim \mathsf{N}(\mathbf{0}, \sigma^2 \mathbf{V} K^{-1} \mathbf{V}^T)$$

which is not diagonal. Loss of invariance.

Summary

- OLS can clearly be dominated by other estimators
- Lead to Bayes like estimators
- choice of penalities or prior hyperparameters
- hierarchical model with prior on k_i