Shrinkage Estimation & Ridge Regression

Readings Chapter 15 Christensen

STA721 Linear Models Duke University

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How Good are Bayes Estimators?

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

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

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where λ_j are eigenvalues of $\mathbf{X}^T\mathbf{X}$.

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  where λ_j are eigenvalues of $\mathbf{X}^T\mathbf{X}$.
- If smallest $\lambda_j \to 0$ then MSE $\to \infty$
- Note: estimate is unbiased!

Is the g-prior better?

-
- Explore Frequentist properties of using a Bayesian estimator

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- HW: show that there is a value of g prior such that the g-prior is always better than the Reference prior/OLS
- Potential problem: MSE also blows up if smallest eigenvalue goes to zero!

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  - other shrinkage estimators

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$$\mathbf{U} = [\mathbf{U}_0 \,|\, \mathbf{U}_p \,|\, \mathbf{U}_{n-p-1}]$$

where $\mathbf{U}_0 = \mathbf{1}/\sqrt{n}$

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  where $\mathbf{U}_0 = \mathbf{1}/\sqrt{n}$
- $\mathbf{U}_0^T\mathbf{U}_p = 0$, $\mathbf{U}_0^T\mathbf{U}_{n-p-1} = 0$ and $\mathbf{U}_p^T\mathbf{U}_{n-p-1} = 0$ (orthogonal columns)

Orthogonal Regression

Rotate by multiplyting by $\mathbf{U}^T$:

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

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$$
\begin{aligned}
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\mathbf{Y}^* &= \begin{bmatrix} \sqrt{n} & \mathbf{0}_p^T \\ \mathbf{0}_p & 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}
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- $\hat{\gamma} = (L^T L)^{-1} L^T \mathbf{U}_p^T \mathbf{Y}$ or $\hat{\gamma}_i = y_i^*/l_i$ for $i = 1, \ldots, p$

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

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 γ:

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Posterior mean

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

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

- 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.

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- Choice of k?

MSE

Can show that

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

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- $\mathrm{Var}(\tilde{\gamma}_i) = \sigma^2 l_i^2/(l_i^2 + k)^2$

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- Bias of $\tilde{\boldsymbol{\gamma}}$ is $-k\gamma_i/(l_i^2 + k)$

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- 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.

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

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

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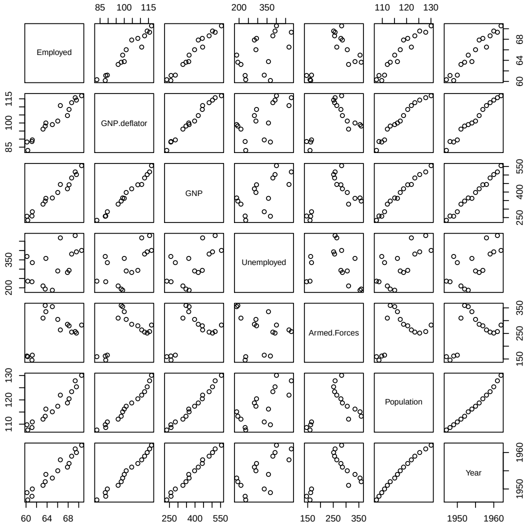
Picture

Longley Data



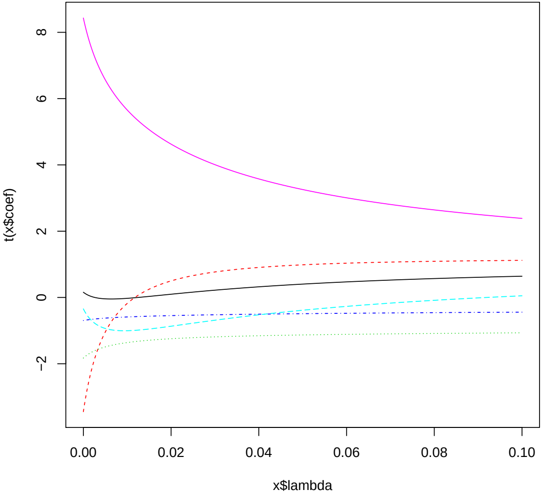
OLS

```
> 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,^^IAdjusted 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. $\frac{\gamma_i^2}{\mathrm{Var}(\hat{\gamma}_i)} < \frac{1+h_i}{1-h_i}$

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

Case: If $\gamma_j < \mathrm{Var}(\hat{\gamma}_i) = \sigma^2 / l_i^2$ 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 $\gamma_j \overset{\text{iid}}{\sim} \mathsf{N}(0, \sigma^2/k)$ take

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

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

Then Condition of Goldstein & Smith becomes

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

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

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- 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