Ridge, Bayesian Ridge and Shrinkage

Readings Chapter 15 Christensen

STA721 Linear Models Duke University

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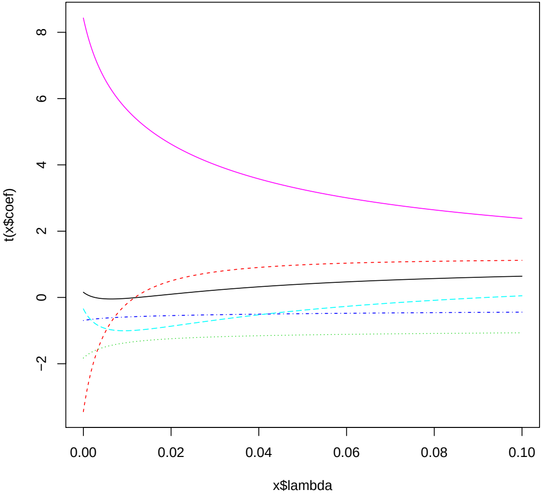
Ridge Trace



Generalized Cross-validation

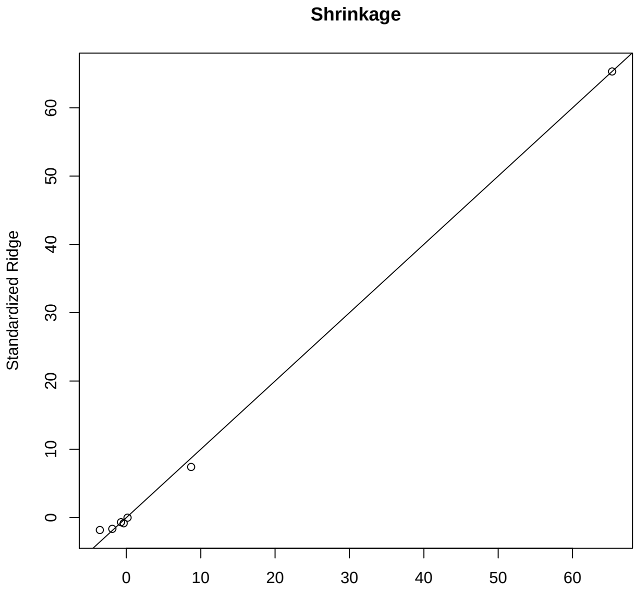
```
> select(lm.ridge(Employed ~ ., data=longley,
         lambda=seq(0, 0.1, 0.0001)))

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
```

Shrinkage


Shrinkage
Standardized Ridge
0
10
20
30
40
50
60
0
10
20
30
40
50
60

Bayesian Ridge: Prior on k

Reparameterization:

$$\begin{aligned}
\mathbf{Y} &= \mathbf{1}\alpha + (\mathbf{I} - \mathbf{P_1})\mathbf{X}S^{-1/2}S^{1/2}\boldsymbol{\beta} + \boldsymbol{\epsilon} \\
&= \mathbf{1}\alpha + \mathbf{X}^s\boldsymbol{\beta}^s + \boldsymbol{\epsilon} \\
\mathbf{Y}^c &= \mathbf{X}^s\boldsymbol{\beta}^s + \boldsymbol{\epsilon}^s \qquad \boldsymbol{\epsilon}^s \sim \mathrm{N}(\mathbf{0}, (\mathbf{I} - \mathbf{P}_1)/\phi) \\
\bar{\mathbf{Y}} \mid \alpha, \phi &\sim N(\alpha, 1/(n\phi)) \\
\mathbf{U}_p\mathbf{Y} &= L\boldsymbol{\gamma} + \boldsymbol{\epsilon}_p \qquad \boldsymbol{\epsilon}_p \sim \mathrm{N}(\mathbf{0}, \mathbf{I}_p/\phi) \\
\mathrm{SSE} \equiv \mathbf{Y}^T\mathbf{U}_{n-p-1}\mathbf{U}_{n-p-1}^T\mathbf{Y} &\sim \mathbf{G}((n-p-1)/2, \phi/2)
\end{aligned}$$

Hierarchical prior

- $p(\alpha \mid \phi, \boldsymbol{\gamma}, \kappa) \propto 1$
- $\boldsymbol{\gamma} \mid \phi, \kappa \sim \mathrm{N}(\mathbf{0}, \mathbf{I}(\phi\kappa)^{-1})$
- $p(\phi \mid \kappa) \propto 1/\phi$
- prior on κ? Take $\kappa \mid \phi \sim \mathbf{G}(1/2, 1/2)$

Posterior Distributions

Joint Distribution

- $\alpha, \boldsymbol{\gamma}, \phi \mid \kappa, \mathbf{Y}$ Normal-Gamma family given $\mathbf{Y}$ and κ
- $\kappa \mid \mathbf{Y}$ not tractable

Obtain marginal for γ via

- Numerical integration
- MCMC: Full conditionals
  Pick initial values $\alpha^{(0)}, \boldsymbol{\beta}^{(0)}, \phi^{(0)}$,
  Set $t = 1$
  1. Sample $\kappa^{(t)} \sim p(\kappa \mid \alpha^{(t-1)}, \boldsymbol{\gamma}^{(t-1)}, \phi^{(t-1)}, \mathbf{Y})$
  2. Sample $\alpha^{(t)}, \boldsymbol{\gamma}^{(t)}, \phi^{(t)} \mid \kappa(t), \mathbf{Y}$
  3. Set $t = t + 1$ and repeat until $t > T$

  Use Samples $\alpha^{(t)}, \boldsymbol{\gamma}^{(t)}, \phi^{(t)}, \kappa^{(t)}$ for $t = B, \ldots, T$ for inference
  Change of variables to get back to $\boldsymbol{\beta}$

Rao-Blackwellization Model

What is "best" estimate of $\boldsymbol{\beta}$ from Bayesian perspective?

- Loss $(\boldsymbol{\beta} - \mathbf{a})^T(\boldsymbol{\beta} - \mathbf{a})$ under action $\mathbf{a}$
- Decision Theory: Take action $\mathbf{a}$ that minimizes posterior expected loss which is posterior mean of $\boldsymbol{\beta}$.
- Estimate of posterior mean is Ergodic average of MCMC: $\sum_i \boldsymbol{\beta}^{s(t)}/T \to$
- Posterior mean given κ

$$\tilde{\boldsymbol{\beta}}^s(\kappa) = (\mathbf{X}^{sT}\mathbf{X}^s + \kappa\mathbf{I})^{-1}\mathbf{X}^{sT}\mathbf{X}^s\hat{\boldsymbol{\beta}}^s$$

- Rao-Blackwell Estimate

$$\frac{1}{T}\sum_t (\mathbf{X}^{sT}\mathbf{X}^s + \kappa^{(t)}\mathbf{I})^{-1}\mathbf{X}^{sT}\mathbf{X}^s\hat{\boldsymbol{\beta}}^s$$

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

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

Then Condition of Goldstein & Smith becomes

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

- If l_i is small almost any κ_i will improve over OLS
- if l_i^2 is large then only very small values of κ_i will give an improvement
- Prior on κ_i?
- Prior that can capture the feature above?

- Induced prior on $\boldsymbol{\beta}$?

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

  which is not diagonal.
- Or start with

$$\boldsymbol{\beta} \mid \sigma^2, \mathbf{K} \sim \mathsf{N}(0, \sigma^2 K)$$

- loss of invarince with linear transformations of $\mathbf{X}^s$
- $\mathbf{X}^s \mathbf{A}\mathbf{A}^{-1} \beta = \mathbf{Z}\boldsymbol{\alpha}$ where $\mathbf{A}^{-1}\beta = \boldsymbol{\alpha}$

Related Regression on PCA

- Principal Components of $\mathbf{X}$ may be obtained via the Singular Value Decomposition:

$$\mathbf{X} = \mathbf{U}_p \mathbf{L} \mathbf{V}^T$$

- the l_i are the eigenvalues of $\mathbf{X}^T\mathbf{X}$

$$\begin{aligned} \mathbf{Y} &= \mathbf{1}\alpha + \mathbf{U}\mathbf{L}\mathbf{V}^T\boldsymbol{\beta} + \boldsymbol{\epsilon} \\ &= \mathbf{1}\alpha + \mathbf{F}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \end{aligned}$$

- Columns $\mathbf{F}_i \propto \mathbf{U}_i$ are the principal components of the data multivariate data $\mathbf{X}_1, \ldots, \mathbf{X}_p$
- If the direction $\mathbf{F}_i$ is ill-defined ($l_i = 0$ or $\lambda_i < \boldsymbol{\epsilon}$ then we may decide to not use $\mathbf{F}_i$ in the model.
- equivalent to setting
  - $\tilde{\gamma}_i = \hat{\gamma}_i$ if $l_i \geq \boldsymbol{\epsilon}$
  - $\tilde{\gamma}_i = 0$ if $l_i < \boldsymbol{\epsilon}$

Summary

- OLS can clearly be dominated by other estimators for extimating $\boldsymbol{\beta}$
- Lead to Bayes like estimators
- choice of penalties or prior hyper-parameters
- hierarchical model with prior on κ_i
- Shrinkage, dimension reduction & variable selection ?
- what loss function? Estimation versus prediction? Copas 1983