Ridge Regression Readings Chapter 15 Christensen

STA721 Linear Models Duke University

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October 17, 2017

Quadratic loss for estimating β using estimator **a**

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

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- If smallest $\lambda_j \rightarrow 0$ then MSE $\rightarrow \infty$
- Similar problem with g prior or mixtures of g-priors

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

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• Let $\mathbf{U} = [\mathbf{1}/\sqrt{n} \mathbf{U}_p \mathbf{U}_{n-p-1}] n \times n$ orthogonal matrix

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$$\mathbf{Y}^{*} = \begin{bmatrix} \sqrt{n} & \mathbf{0}_{p} \\ 0 & L \\ \mathbf{0}_{n-p-1} & \mathbf{0}_{n-p-1\times p} \end{bmatrix} \begin{pmatrix} \alpha \\ \gamma \end{pmatrix} + \epsilon^{*}$$

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

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$$\hat{\alpha} = \bar{y}$$

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

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

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(Another) Normal Conjugate Prior Distribution on γ :

$$\gamma \mid \phi \sim \mathsf{N}(\mathbf{0}_{p}, rac{1}{\phi k} \mathbf{I}_{p})$$

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Posterior mean

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

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

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

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

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

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- Choice of k?

Can show that

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

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► 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.

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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

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Alternative Motivation

 \blacktriangleright If $\hat{\beta}$ is unconstrained expect high variance with nearly singular ${\bf X}$

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- Let Y^c = (I − P₁)Y and X^c the centered and standardized X matrix

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Control how large coefficients may grow

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- Let Y^c = (I − P₁)Y and X^c the centered and standardized X matrix
- Control how large coefficients may grow

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

subject to

$$\sum eta_j^2 \leq t$$

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subject to

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Equivalent Quadratic Programming Problem

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

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- If $\hat{\beta}$ is unconstrained expect high variance with nearly singular
 X
- Let Y^c = (I − P₁)Y and X^c the centered and standardized X matrix
- Control how large coefficients may grow

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

subject to

$$\sum eta_j^2 \leq t$$

Equivalent Quadratic Programming Problem

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

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"penalized" likelihood

- If $\hat{\beta}$ is unconstrained expect high variance with nearly singular
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$$\min_{\beta} (\mathbf{Y}^{c} - \mathbf{X}^{c}\beta)^{T} (\mathbf{Y}^{c} - \mathbf{X}^{c}\beta)$$

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Equivalent Quadratic Programming Problem

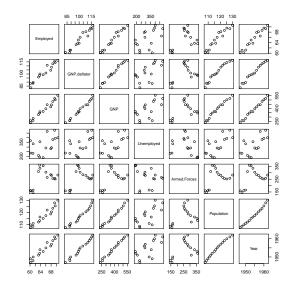
$$\min_{\boldsymbol{\beta}} \|\mathbf{Y}^{c} - \mathbf{X}^{c}\boldsymbol{\beta}\|^{2} + k\|\boldsymbol{\beta}\|^{2}$$

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"penalized" likelihood

Picture

Longley Data



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OLS

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

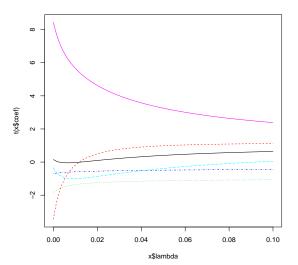
> summary(longley.lm)

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	s: 0 '***'	0.001 '**'	0.01 '*	' 0.05 '.'	0.1 ''

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

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

Population Year -1.185e-01 1.557e+00

Testimators

Goldstein & Smith (1974) have shown that if

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

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

Case: If $\gamma_j < Var(\hat{\gamma}_i) = \sigma^2/l_i^2$ 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)

$\begin{array}{l} \mbox{Generalized Ridge} \\ \mbox{Instead of } \gamma_j \overset{\rm iid}{\sim} {\sf N}(0,\sigma^2/k) \mbox{ take} \end{array}$

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

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

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

Then Condition of Goldstein & Smith becomes

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

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• If I_i is small almost any k_i will improve over OLS

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

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- If I_i is small almost any k_i will improve over OLS
- if l_i² is large then only very small values of k_i will give an improvement

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

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

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_i² is large then only very small values of k_i will give an improvement

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▶ Prior on k_i?

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

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

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_i² is large then only very small values of k_i will give an improvement
- Prior on k_i?
- ▶ Induced prior on *β*?

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

which is not diagonal. Loss of invariance. $\Box_{D} : (\overline{D}) : (\overline{D$

Summary

OLS can clearly be dominated by other estimators

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- Lead to Bayes like estimators
- choice of penalities or prior hyperparameters
- hierarchical model with prior on k_i