Ridge Regression

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Ridge regression: Definition

- As mentioned in the previous lecture, ridge regression penalizes the size of the regression coefficients
- Specifically, the ridge regression estimate $\widehat{\boldsymbol{\beta}}$ is defined as the value of $\boldsymbol{\beta}$ that minimizes

$$\sum_i (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

Ridge regression: Solution

Theorem: The solution to the ridge regression problem is given by

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Note the similarity to the ordinary least squares solution, but with the addition of a "ridge" down the diagonal

Corollary: As $\lambda \to 0$, $\widehat{\boldsymbol{\beta}}^{\text{ridge}} \to \widehat{\boldsymbol{\beta}}^{\text{OLS}}$

Corollary: As $\lambda \to \infty$, $\widehat{\boldsymbol{\beta}}^{\text{ridge}} \to \mathbf{0}$

Ridge regression: Solution (Cont'd)

Corollary: In the special case of an orthonormal design matrix,

$$\hat{\beta}_J^{\text{ridge}} = \frac{\hat{\beta}_J^{\text{OLS}}}{1+\lambda}$$

- This illustrates the essential feature of ridge regression: *shrinkage*
- Applying the ridge regression penalty has the effect of shrinking the estimates toward zero – introducing bias but reducing the variance of the estimate

Ridge vs. OLS in the presence of collinearity

The benefits of ridge regression are most striking in the presence of multicollinearity, as illustrated in the following example:

```
> x1 <- rnorm(20)
> x2 <- rnorm(20,mean=x1,sd=.01)
> y <- rnorm(20,mean=3+x1+x2)
> lm(y~x1+x2)$coef
(Intercept)          x1          x2
   2.582064   39.971344  -38.040040
> lm.ridge(y~x1+x2,lambda=1)
                 x1        x2
2.6214998 0.9906773 0.8973912
```

Invertibility

- Recall from BST 760 that the ordinary least squares estimates do not always exist; if $\mathbf{X}$ is not full rank, $\mathbf{X}^T\mathbf{X}$ is not invertible and there is no unique solution for $\widehat{\boldsymbol{\beta}}^{\text{OLS}}$
- This problem does not occur with ridge regression, however
- **Theorem:** For any design matrix $\mathbf{X}$, the quantity $\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}$ is always invertible; thus, there is always a unique solution $\widehat{\boldsymbol{\beta}}^{\text{ridge}}$

Bias and variance

- **Theorem:** The variance of the ridge regression estimate is

$$\mathrm{Var}(\widehat{\boldsymbol{\beta}}) = \sigma^2 \mathbf{W}\mathbf{X}^T\mathbf{X}\mathbf{W},$$

  where $\mathbf{W} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}$

- **Theorem:** The bias of the ridge regression estimate is

$$\mathrm{Bias}(\widehat{\boldsymbol{\beta}}) = -\lambda\mathbf{W}\boldsymbol{\beta}$$

- It can be shown that the total variance ($\sum_j \mathrm{Var}(\hat{\beta}_j)$) is a monotone decreasing sequence with respect to λ, while the total squared bias ($\sum_j \mathrm{Bias}^2(\hat{\beta}_j)$) is a monotone increasing sequence with respect to λ

Existence theorem

Existence Theorem: There always exists a λ such that the MSE of $\widehat{\boldsymbol{\beta}}_\lambda^{\text{ridge}}$ is less than the MSE of $\widehat{\boldsymbol{\beta}}^{\text{OLS}}$

This is a rather surprising result with somewhat radical implications: even if the model we fit is exactly correct and follows the exact distribution we specify, we can *always* obtain a better estimator by shrinking towards zero

Bayesian interpretation

As mentioned in the previous lecture, penalized regression can be interpreted in a Bayesian context:

Theorem: Suppose $\boldsymbol{\beta} \sim N(\mathbf{0}, \tau^2\mathbf{I})$. Then the posterior mean of $\boldsymbol{\beta}$ given the data is

$$\left(\mathbf{X}^T\mathbf{X} + \frac{\sigma^2}{\tau^2}\mathbf{I}\right)^{-1}\mathbf{X}^T\mathbf{y}.$$

Degrees of freedom

- Information criteria are a common way of choosing among models while balancing the competing goals of fit and parsimony
- In order to apply AIC or BIC to the problem of choosing λ, we will need an estimate of the degrees of freedom
- Recall that in linear regression:
  - $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$, where $\mathbf{H}$ was the projection ("hat") matrix
  - $\text{tr}(\mathbf{H}) = p$, the degrees of freedom

Degrees of freedom (cont'd)

- Ridge regression is also a linear estimator ($\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$), with

$$\mathbf{H}_{\text{ridge}} = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T$$

- Analogously, one may define its degrees of freedom to be $\text{tr}(\mathbf{H}_{\text{ridge}})$
- Furthermore, one can show that

$$df_{\text{ridge}} = \sum \frac{\lambda_i}{\lambda_i + \lambda}$$

where $\{\lambda_i\}$ are the eigenvalues of $\mathbf{X}^T\mathbf{X}$

If you don't know what eigenvalues are, don't worry about it. The main point is to note that df is a decreasing function of λ with $df = p$ at $\lambda = 0$ and $df = 0$ at $\lambda = \infty$.

AIC and BIC

Now that we have a way to quantify the degrees of freedom in a ridge regression model, we can calculate AIC or BIC and use them to guide the choice of λ:

$$\begin{aligned} \mathrm{AIC} &= n \log(\mathrm{RSS}) + 2df \\ \mathrm{BIC} &= n \log(\mathrm{RSS}) + df \log(n) \end{aligned}$$

Introduction

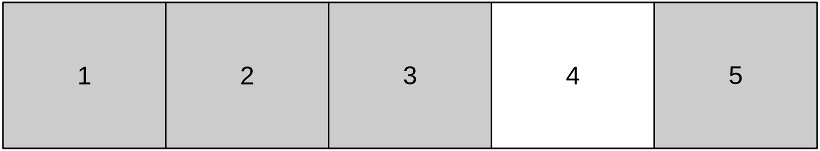
- An alternative way of choosing λ is to see how well predictions based on $\widehat{\beta}_\lambda$ do at predicting actual instances of Y
- Now, it would not be fair to use the data twice twice – once to fit the model and then again to estimate the prediction accuracy – as this would reward overfitting
- Ideally, we would have an external data set for validation, but obviously data is expensive to come by and this is rarely practical

Cross-validation

- One idea is to split the data set into two fractions, then use one portion to fit $\widehat{\boldsymbol{\beta}}$ and the other to evaluate how well $\mathbf{X}\widehat{\boldsymbol{\beta}}$ predicted the observations in the second portion
- The problem with this solution is that we rarely have so much data that we can freely part with half of it solely for the purpose of choosing λ
- To finesse this problem, *cross-validation* splits the data into K folds, fits the data on $K-1$ of the folds, and evaluates risk on the fold that was left out

Cross-validation figure

This process is repeated for each of the folds, and the risk averaged across all of these results:



Common choices for K are 5, 10, and n (also known as *leave-one-out* cross-validation)

Generalized cross-validation

- You may recall from BST 760 that we do not actually have to refit the model to obtain the leave-one-out ("deleted") residuals:

$$y_i - \hat{y}_{i(-i)} = \frac{r_i}{1 - H_{ii}}$$

- Actually calculating $\mathbf{H}$ turns out to be computationally inefficient for a number of reasons, so the following simplification (called *generalized cross validation*) is often used instead:

$$GCV = \frac{1}{n} \sum_i \left(\frac{y_i - \hat{y}_i}{1 - \mathrm{tr}(\mathbf{H})/n} \right)^2$$

Prostate cancer study

- An an example, consider the data from a 1989 study examining the relationship prostate-specific antigen (PSA) and a number of clinical measures in a sample of 97 men who were about to receive a radical prostatectomy
- PSA is typically elevated in patients with prostate cancer, and serves a biomarker for the early detection of the cancer
- The explanatory variables:
  - `lcavol`: Log cancer volume
  - `lweight`: Log prostate weight
  - age
  - `lbph`: Log benign prostatic hyperplasia
  - `svi`: Seminal vesicle invasion
  - `lcp`: Log capsular penetration
  - `gleason`: Gleason score
  - `pgg45`: % Gleason score 4 or 5

SAS/R syntax

To fit a ridge regression model in SAS, we can use `PROC REG`:

```
PROC REG DATA=prostate ridge=0 to 50 by 0.1 OUTEST=fit;
  MODEL lpsa = pgg45 gleason lcp svi lbph age lweight lcavol;
RUN;
```

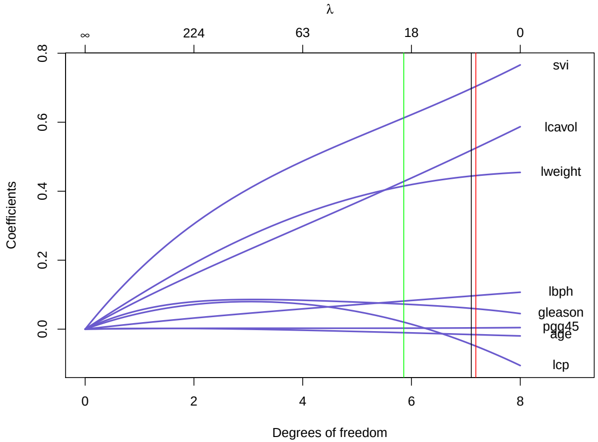
In R, we can use `lm.ridge` in the `MASS` package:

```
fit <- lm.ridge(lpsa~.,prostate,lambda=seq(0,50,by=0.1))
```

R (unlike SAS, unfortunately) also provides the GCV criterion for each λ:

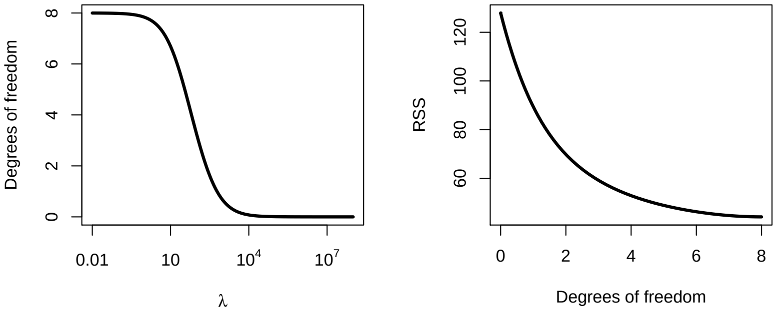
```
fit$GCV
```

Results



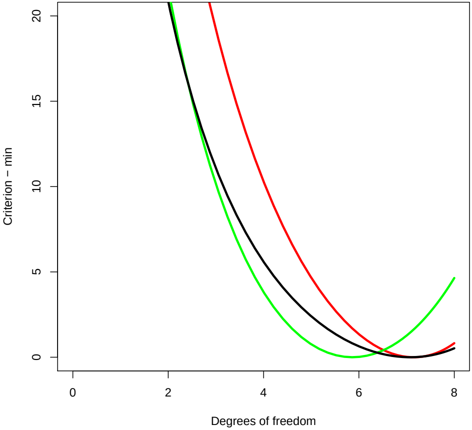
Red=AIC, black=GCV, green=BIC

Additional plots



Model selection criteria

Red=AIC, black=GCV, green=BIC:



Ridge vs. OLS

	Estimate		Std. Error		z-score	
	OLS	Ridge	OLS	Ridge	OLS	Ridge
lcavol	0.587	0.519	0.088	0.075	6.68	6.96
lweight	0.454	0.444	0.170	0.153	2.67	2.89
age	-0.020	-0.016	0.011	0.010	-1.76	-1.54
lbph	0.107	0.096	0.058	0.053	1.83	1.83
svi	0.766	0.698	0.244	0.209	3.14	3.33
lcp	-0.105	-0.044	0.091	0.072	-1.16	-0.61
gleason	0.045	0.060	0.157	0.128	0.29	0.47
pgg45	0.005	0.004	0.004	0.003	1.02	1.02