Statistics 452: Statistical Learning and Prediction

Chapter 6, Part 2: Shrinkage Methods

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Shrinkage Methods

- Fit a model that contains all p predictors using a method that shrinks the coefficient estimates towards zero.
- This biases the estimates, but reduces variance.
- We will discuss two shrinkage methods, ridge regression and the lasso.

Ridge Regression

- Penalize the criterion function, RSS, to favour smaller coefficient values.
- The ridge regression criterion function is

$$\text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2$$

  where $\lambda \geq 0$ is a tuning parameter.
- The ridge regression estimator $\hat{\beta}_\lambda^R$ is the minimizer of this criterion.
- The penalty term has two components, the tuning parameter and the sum of squared coefficients.

Tuning Parameter, λ

- We do **not** penalize the intercept.
- $\lambda = 0$ gives least squares
- $\lambda > 0$ will lead to estimates of $\beta_1, \ldots, \beta_p$ that are "shrunken" towards zero
- To be practical, we need a method for choosing the tuning parameter.

SS Coefficients, $\sum_{j=1}^{p} \beta_j^2$

- $\sum_{j=1}^{p} \beta_j^2$ is the square of the length of the vector $(\beta_1, \ldots, \beta_p)$ of non-intercept coefficients.
- The length is the Euclidean or ℓ_2 norm of the vector.
  - Sometimes ridge regression is called ℓ_2-penalized regression.

Scaling Predictors

- ▶ The least squares solution is said to be scale invariant.
  - ▶ If we multiply a predictor X_j by a constant c, the least squares solution $\hat{\beta}_j$ is multiplied by $1/c$ so that $X_j\hat{\beta}_j$ doesn't change.
- ▶ The same is not true for ridge regression.
  - ▶ $X_j\beta^R_{\lambda,j}$ depends on the scale of X_j; e.g., on the units X_j is measured in.
- ▶ We typically standardize each predictor by subtracting its mean and dividing by its sample SD.
  - ▶ Then the units of each X_j don't matter.
- ▶ Aside: If we also standardize the response, then it turns our the fitted intercept is zero.

Application to Credit Data

```
uu <- url("http://www-bcf.usc.edu/~gareth/ISL/Credit.csv")
Credit <- read.csv(uu,row.names=1)
head(Credit,n=3)
```

```
##     Income Limit Rating Cards Age Education Gender Student Married
## 1  14.891  3606    283     2  34        11   Male      No     Yes
## 2 106.025  6645    483     3  82        15 Female     Yes     Yes
## 3 104.593  7075    514     4  71        11   Male      No      No
##    Ethnicity Balance
## 1 Caucasian     333
## 2     Asian     903
## 3     Asian     580
```

Least Squares for Comparison

▶ Set up the design matrix and response ourselves and pass to the `lm.fit()` function, which does the fitting for `lm()`.

```
Xfull <- model.matrix(Balance ~ ., data=Credit)
head(Xfull,n=3)
```

```
##   (Intercept)  Income Limit Rating Cards Age Education GenderFemale
## 1           1  14.891  3606    283     2  34        11            0
## 2           1 106.025  6645    483     3  82        15            1
## 3           1 104.593  7075    514     4  71        11            0
##   StudentYes MarriedYes EthnicityAsian EthnicityCaucasian
## 1          0          1              0                  1
## 2          1          1              1                  0
## 3          0          0              1                  0
```

```
Y <- Credit$Balance
```

```r
# Standardize predictors
predInds <- 2:ncol(Xfull) # exclude intercept
Xfull[,predInds] <- scale(Xfull[,predInds])
Y <- Credit$Balance
lsfit <- lm.fit(Xfull,Y)
lsfit$coefficients
```

```
##       (Intercept)            Income             Limit
##        520.015000       -275.014651        440.650711
##            Rating             Cards               Age
##        175.848092         24.305139        -10.589809
##         Education        GenderFemale        StudentYes
##         -3.434150         -5.330027        127.884163
##        MarriedYes    EthnicityAsian EthnicityCaucasian
##         -4.162747          7.333463          5.059778
```

Ridge Regression

- Find the ridge regression solution for each λ on a grid.

```r
library(glmnet) # install.packages("glmnet"), if necessary
Xfull <- Xfull[,-1] # glmnet will add intercept and scale X's
lambdas <- 10^{seq(from=-2,to=5,length=100)}
rrfit <- glmnet(Xfull,Y,alpha=0,lambda=lambdas)
round(cbind(coef(rrfit,s=lambdas[1]),coef(rrfit,s=lambdas[50])),4)
```

```
## 12 x 2 sparse Matrix of class "dgCMatrix"
##                          1         1
## (Intercept)        520.0150  520.0150
## Income            -274.9070 -202.0820
## Limit              407.0633  276.0537
## Rating             209.3416  266.0201
## Cards               22.8687   21.2405
## Age                -10.6288  -15.4669
## Education           -3.2623   -1.7511
## GenderFemale        -5.3312   -3.0400
## StudentYes         127.6673  117.6251
## MarriedYes          -4.4077   -5.7662
## EthnicityAsian       7.4978    6.2090
## EthnicityCaucasian   5.0805    4.7190
```
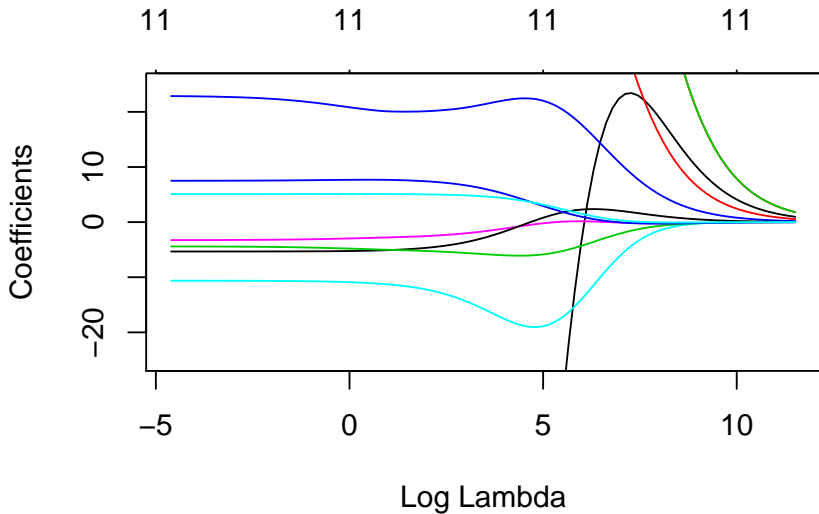
Plotting coefficient "paths"

- It is customary to plot the estimated coefficients for each λ as a function of λ or $\log \lambda$.

```
plot(rrfit,xvar="lambda")
```
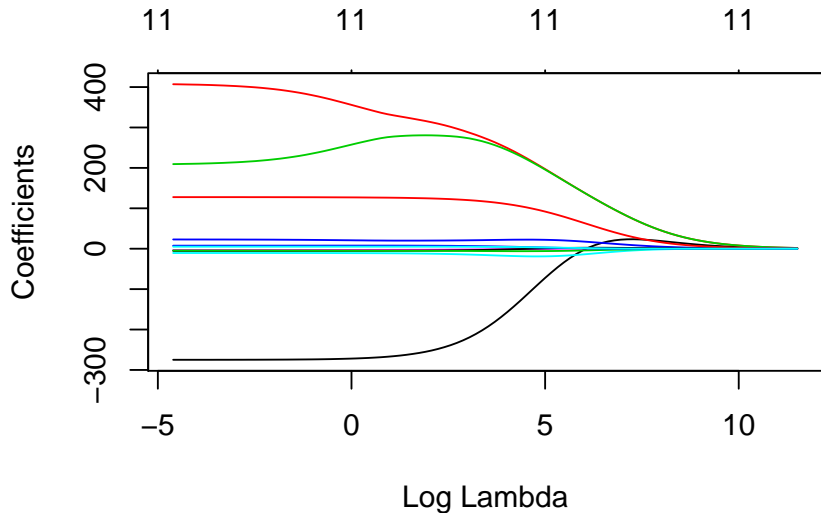
```
plot(rrfit,xvar="lambda",ylim=c(-25,25))
```

Bias-Variance Tradeoff

- Recall that the MSE is the variance plus bias squared
- The least squares estimate of the regression coefficients is unbiased and therefore so are the predictions $X\hat{\beta}$.
- Penalizing introduces bias into the predictions, but reduces variance.
- Illustrated in the text for a "simulated dataset".
    - My guess is that they are evaluating variance and bias by simulating from a model.
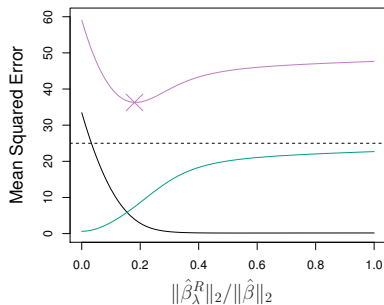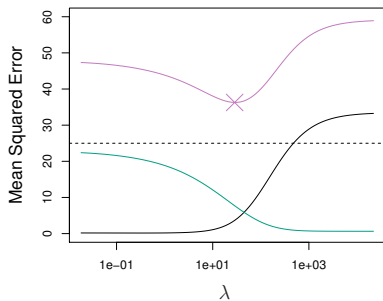
- ▶ Figure 6.5 of the text. The MSE is in purple, variance in green and squared bias in black.
 - ▶ Minimum MSE is at λ of about 30.

The Lasso

- ▶ A drawback of ridge regression is that it does not *select* a subset of predictors.
  - ▶ The final model includes all p coefficients, shrunken toward zero.
  - ▶ Not good for interpretation.
- ▶ An alternative called the lasso does model selection and shrinkage.
- ▶ The lasso replaces the ℓ_2 penalty of ridge regression with an ℓ_1 penalty; i.e., the lasso estimator $\hat{\beta}^L$ minimizes the criterion

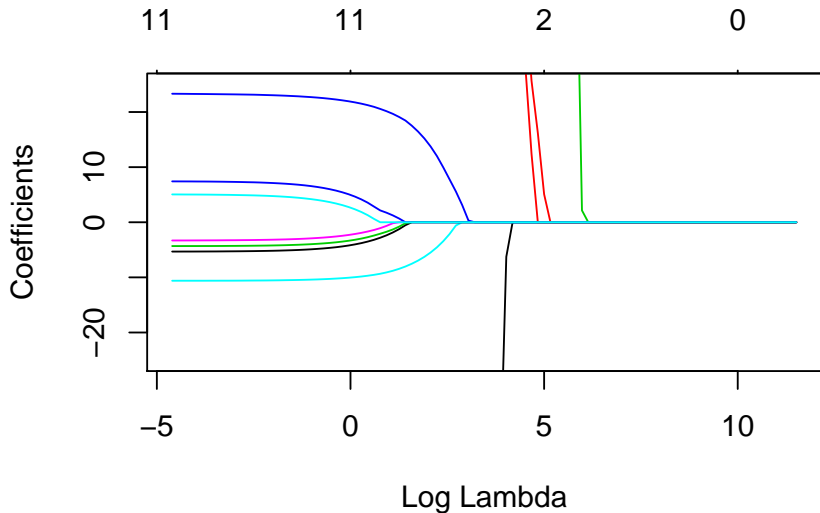$$\mathrm{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|$$

- ▶ It turns out that the lasso can shrink estimates to zero, and hence de-select predictors.
  - ▶ Variable-selected models are said to be sparse.

The Lasso on the Credit Data

```r
lafit <- glmnet(Xfull,Y,alpha=1,lambda=lambdas) # notice alpha=1
plot(lafit,xvar="lambda")
```
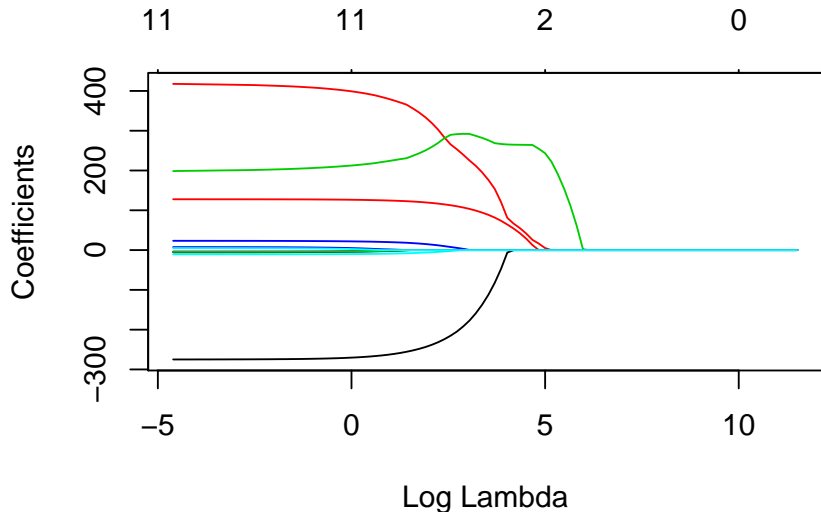
```
plot(lafit,xvar="lambda",ylim=c(-25,25))
```


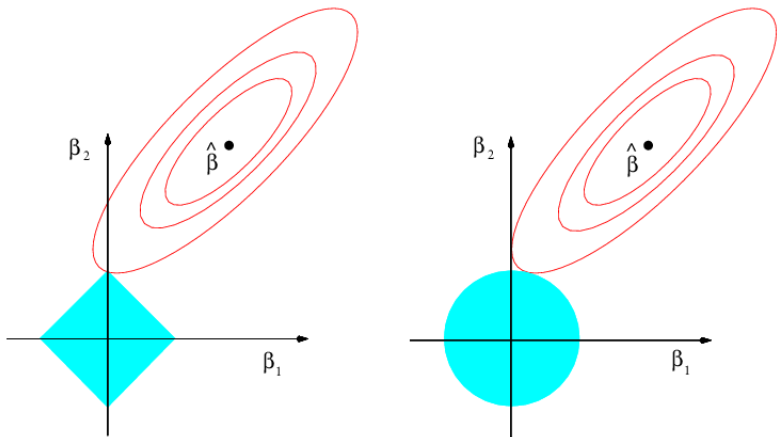- After $\log \lambda > 6$ or so all coefficients have been set to zero.

Equivalent Representation of Ridge and Lasso

- One can show that for a given λ there is an s such that the lasso solution $\hat{\beta}_\lambda^L$ is the solution to the constrained minimization of RSS subject to

$$\sum_{j=1}^{p} |\beta_j| \leq s$$

- Similarly, the ridge regression solution $\hat{\beta}_\lambda^R$ is the solution to the constrained minimization of RSS subject to

$$\sum_{j=1}^{p} \beta_j^2 \leq s$$

- Figure 6.7 of the text. The shaded regions are where the constraints are satisfied for the lasso (left) and ridge regression (right). The contours are of the RSS. The lasso solution zeroes out the β_1 coefficient.

Selecting the Tuning Parameter

- We can select the λ that minimizes estimated test set error over a grid of λ values.
    - Estimate test set error by cross-validation.
- Then fit the model with this best λ.
- Convenience function `cv.glmnet()` will do most of the work for us.

Credit Data Example, Ridge Regression
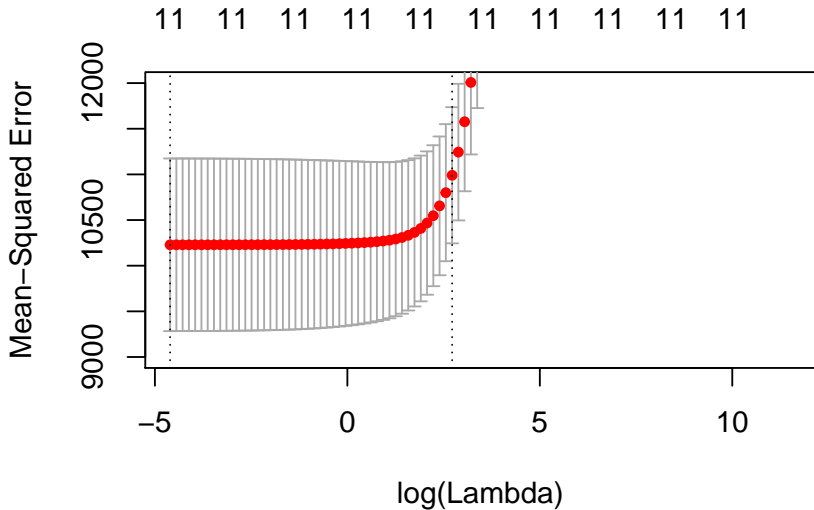
```
# Ridge regression
cv.rrfit <- cv.glmnet(Xfull,Y,alpha=0,lambda=lambdas)
plot(cv.rrfit)
```
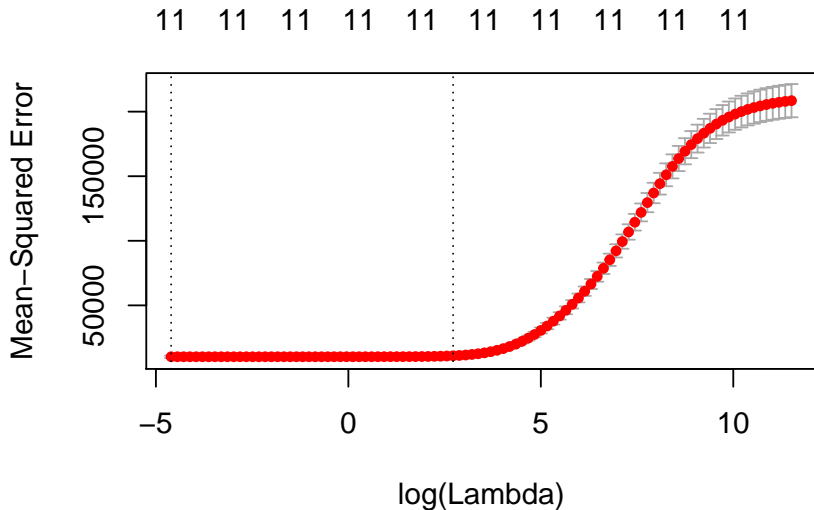
```
plot(cv.rrfit,ylim=c(9000,12000))
```

Error Bars

- The error bars are $\pm$ one SD of the MSE estimates across the ten folds.
- Hastie & co. (ESL, page 216) advocate the "one-standard-error" rule: Use the most parsimonious model (largest λ) whose error is no more than one SD above the error of the best model.
- Acknowledges that the MSEs are only estimates.
    - Rather *ad hoc* rule though.

```
cv.rrfit$lambda.min; cv.rrfit$lambda.1se
```

```
## [1] 0.01
```

```
## [1] 15.19911
```

Fitted Model with Best λ

```r
rr.best.lam <- cv.rrfit$lambda.1se
rr.best.lam
```

```
## [1] 15.19911
```
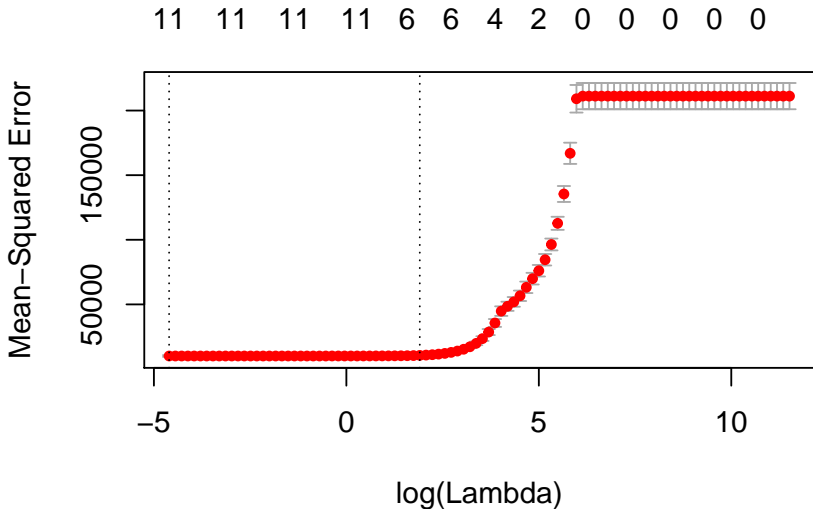
```r
rr.best <- glmnet(Xfull,Y,alpha=0,lambda=rr.best.lam)
coef(rr.best)
```

```
## 12 x 1 sparse Matrix of class "dgCMatrix"
##                             s0
## (Intercept)         520.015000
## Income             -233.139235
## Limit               296.872561
## Rating              277.415633
## Cards                20.509865
## Age                 -13.599096
## Education            -2.202829
## GenderFemale         -4.013911
## StudentYes          121.929679
## MarriedYes           -5.483194
## EthnicityAsian        6.943371
## EthnicityCaucasian    4.923224
```
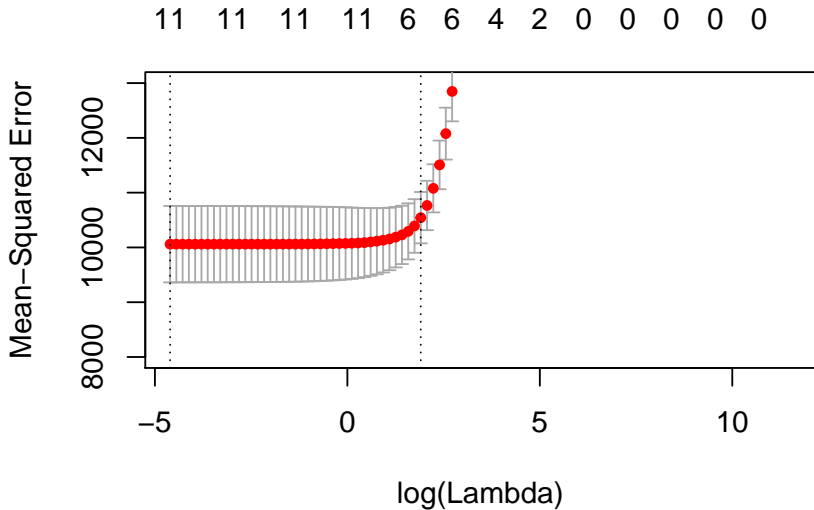
- Now lasso

```
cv.lafit <- cv.glmnet(Xfull,Y,alpha=1,lambda=lambdas)
plot(cv.lafit)
```

```r
plot(cv.lafit,ylim=c(8000,13000))
```

```r
la.best.lam <- cv.lafit$lambda.1se
la.best.lam
```

```
## [1] 6.734151
```

```r
la.best <- glmnet(Xfull,Y,alpha=1,lambda=la.best.lam)
coef(la.best)
```

```
## 12 x 1 sparse Matrix of class "dgCMatrix"
##                            s0
## (Intercept)        520.015000
## Income            -243.832313
## Limit              399.897411
## Rating             184.556182
## Cards               18.046488
## Age                 -6.232961
## Education             .
## GenderFemale         .
## StudentYes         120.195769
## MarriedYes           .
## EthnicityAsian       .
## EthnicityCaucasian   .
```

Summary of Credit Data

- Ridge regression shrinks, but is not very interpretable.
- Lasso shrinks and selects variables.
  - The lasso solution is similar to the best model found by model selection methods (see week 6 exercises).