6.2 Shrinkage Methods

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Shrinkage Methods

- Subset selection methods use least squares to fit a linear model that contains a subset of the predictors.
- Instead, we can it a model using all p predictors, with some of the coefficients shrunken toward zero.
- It turns out that shrinking the coefficient estimates can significantly reduce their variance.

Least Squares

Recall: least squares regression estimates the coefficients by minimizing

$$\mathrm{RSS} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

Ridge Regression

In *ridge regression*, we instead minimize

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2=\mathrm{RSS}+\lambda\sum_{j=1}^{p}\beta_j^2$$

where $\lambda > 0$ is a *tuning parameter*

Ridge Regression

- Ridge regression still finds parameters which fit the data well by making RSS small.
- However, it now has to balance that with the *shrinkage penalty* $\lambda \sum_{j=1}^{p} \beta_j^2$
  - This term will be small when all the βs are close to 0.

Ridge Regression

- Balancing RSS with the penalty term shrinks the coefficients toward 0.
  - Less useful coefficients will have values closer to 0.
- The tuning parameter λ controls the relative impact of these two terms.
  - We use cross-validation to select select λ

Ridge Regression

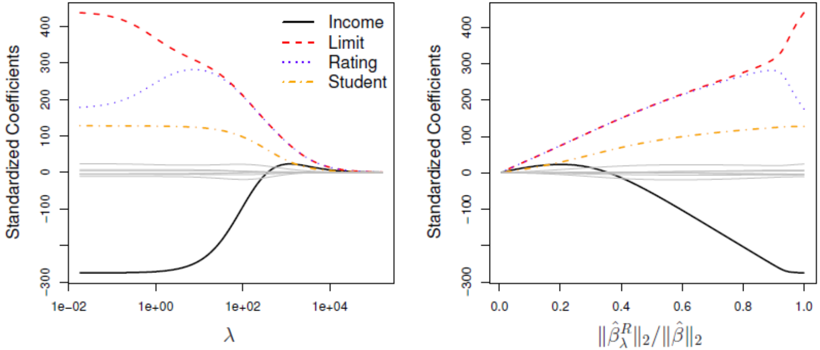


FIGURE 6.4. *The standardized ridge regression coefficients are displayed fo the* `Credit` *data set, as a function of λ and $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$.*

More on Previous Figure

- LHS shows ridge regression coefficient estimates plotted as a function of λ
- RHS shows coefficient estimates as a function of

$$||\hat{\beta}_\lambda^R||_2/||\hat{\beta}||_2$$

  - $\hat{\beta}$ is the least squares coefs; $\hat{\beta}_\lambda^R$ the ridge regression coefs
  - $||\beta||_2$ is the l_2 norm ("L-2") of a vector $||\beta||_2 = \sqrt{\sum_{j=1}^p \beta_j^2}$

Predictor Scaling

- Least squares estimates are *scale equivariant*
  - Multiplying X_j by a constant c scales the coef estimates by $1/c$ (and so $X_j\hat{\beta}_j$ will not change)
- Ridge regression coefficients are not
  - Coef estimates can change dramatically depending on variable scale.
  - To deal with this, we often standardize the predictors using

$$x_{ij}^* = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2}}$$

Example

```r
data("Credit")
x <- model.matrix(Balance ~ ., Credit)[, -1]
y <- Credit$Balance

library(glmnet)
grid <- 10^seq(10, -2, length = 100)
ridge.mod <- glmnet(x, y, alpha = 0, lambda = grid)
```

- `glmnet` will create a grid automatically, or we can create or own.
- For ridge regression, `glmnet` automatically scales the predictor variables.
- You will see more details in the lab.

Why Ridge Regression?

The bias variance tradeoff strikes again

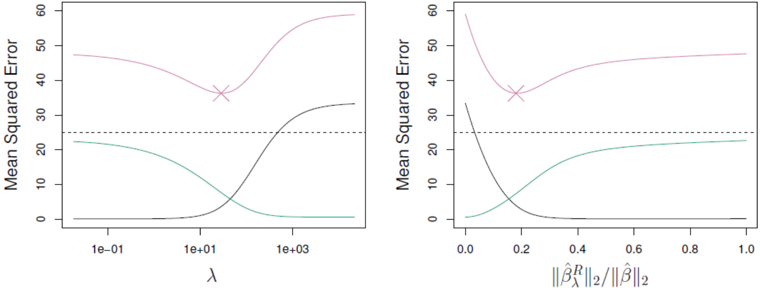


FIGURE 6.5. *Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of λ and $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.*

Ridge Regression

Disadvantage:

- Although it shrinks coefficients *toward* zero, it is unable to set coefficents equal to 0.
- So all p predictors will always be included in the model.

The Lasso

- More recent alternative to ridge regression that is able to shrink coefficients *to* 0.
- Now we minimize

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \mathrm{RSS} + \lambda\sum_{j=1}^{p}|\beta_j|$$

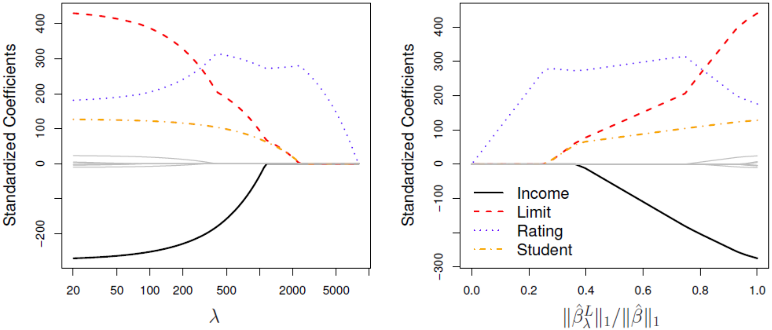
- This uses an l_1 ("L-1") penalty instead of an l_2 penalty:

$$||\beta||_1 = \sum_{j=1}^{p}|\beta_j|$$

The Lasso

- The l_1 penalty forces some coefficient estimates to exactly 0 when λ is sufficiently large.
- So the Lasso is a variable selection method.
- We say the Lasso yields *sparse* models since they involve only a subset of the variables.
- We again use cross-validation to select good values for λ.

Example: Credit Dataset



Variable Selection and Lasso

Why does the l_1 penalty force coefficients to 0 (and the l_2 penalty does not)?

Ridge regression minimizes

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2$$

with the constraint that

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

Variable Selection and Lasso

Lasso minimizes

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

with the constraint that

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

Variable Selection and Lasso

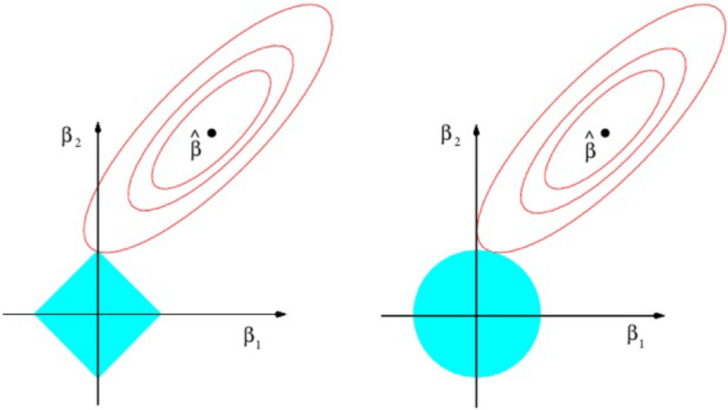


FIGURE 6.7. *Contours of the error and constraint functions for the lasso* (left) *and ridge regression* (right). *The solid blue areas are the constraint regions,* $|\beta_1| + |\beta_2| \le s$ *and* $\beta_1^2 + \beta_2^2 \le s$, *while the red ellipses are the contours of the RSS.*

Variable Selection and Lasso

- Each ellipses represents a contour on which all points have the same RSS value.
- The blue areas are the constraint regions.
- The ridge/lasso estimates are where the ellipses meets the constraint region.
  - With ridge, this generally does not occur on an axis.
  - With lasso, this is likely to occur at an axis, and so at least one of the coefficient estimates will be zero.

Example

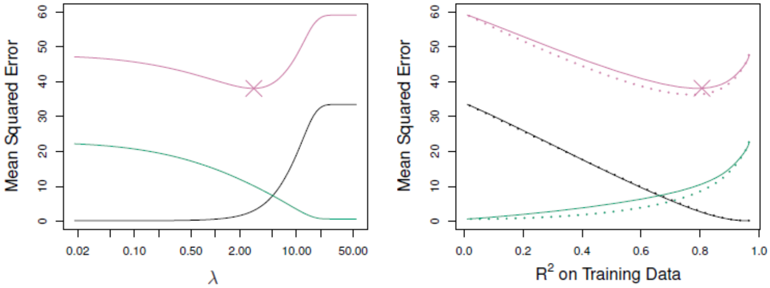
```
lasso.mod <- glmnet(x, y, alpha = 1, lambda = grid)
```

- The only difference from ridge regression is that, to get `glmnet` to do a ridge regression, we set `alpha=1`.

Ridge or Lasso?

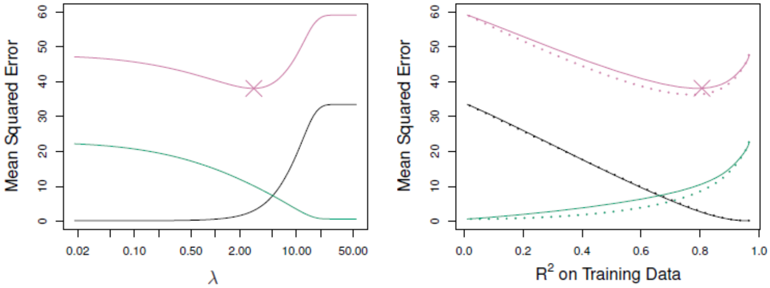
- Lasso has at least one clear advantage over ridge regression: variable selection.
- Is Lasso always better? We consider variance, squared bias, and MSE of both methods.

Ridge or Lasso?



- Simulation setting: all 45 predictors are related to the response.
- LHS: squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data
- RHS: comparison between lasso (solid) and ridge (dotted)

Ridge or Lasso?



- Simulation setting: only 2 of the 45 predictors are related to the response.
- LHS: squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data
- RHS: comparison between lasso (solid) and ridge (dotted)

Ridge or Lasso?

So which is better? It depends.

- In general, ridge regression will perform better if all coefficients are related to the response
- . . . and lasso will perform better if relatively few are related to the response.

but in practice we don't know this.

- We can use cross-validation to determine which approach to use for a particular dataset.

A Simple Special Case

We build intuition by considering the following:

- Let $n = p$ and X be the identity matrix I_n.
- We will build our model without an intercept.
- Then the least squares problem minimizes

$$\sum_{j=1}^{p}(y_j - \beta_j)^2$$

- The least squares solution is given by

$$\hat{\beta}_j = y_j$$

A Simple Special Case

Ridge regression amounts to minimizing

$$\sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

and lasso to minimizing

$$\sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

A Simple Special Case

Here, the ridge estimates take the form

$$\hat{\beta}_j^R = y_j/(1+\lambda)$$

and the lasso estimates take the form

$$\hat{\beta}_j^R = \begin{cases} y_j - \lambda/2 & \text{if} \quad y_j > \lambda/2 \\ y_j + \lambda/2 & \text{if} \quad y_j < -\lambda/2 \\ 0 & \text{if} \quad |y_j| \leq \lambda/2 \end{cases}$$

A Simple Special Case

- Notice that ridge shrinks all coefficients by the same proportion.
- but lasso shrinks each by a constant amount *or* sets the coefficient to 0.
- A more realistic X matrix results in a more complex setup, but the ideas are *basically* the same.

Selecting the Tuning Parameter

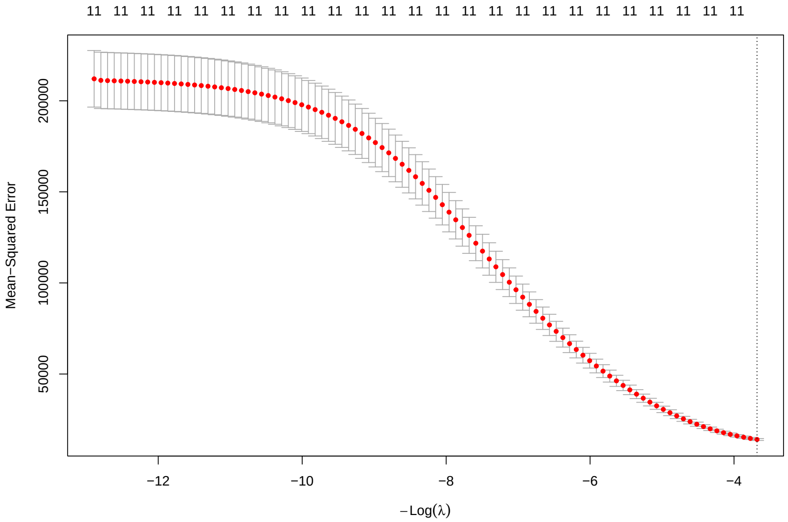
- One challenge of ridge regression and lasso is that λ is user-defined.
- Cross-validation provides a straightforward way to tackle this problem.
  - Choose a grid of λ values and compute the CV error rate at each.
  - Select the tuning parameter for which the cross-validation error is smallest.
  - Fit the model using all available observations using the selected tuning parameter.

Example

```
set.seed(1)
cv.out <- cv.glmnet(x, y, alpha = 0)
plot(cv.out)
bestlam <- cv.out$lambda.min
bestlam
log(bestlam)
```

- Here, we run a ridge regression, using cross-validation to select λ.
- This can be done fairly simply in R!
- Again, you will spend some time with this in the Ch 6 lab.

Example



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Mean−Squared Error
50000
100000
150000
200000
−12
−10
−8
−6
−4
−Log(λ)