Linear Model Selection and Regularization

ISLR 2nd Ed., Chapter 06

Outline

Subset Selection

- Best Subset Selection
- Stepwise Selection
- Choosing the Optimal Model

Shrinkage Methods

- Ridge Regression
- The Lasso

Improving on the Least Squares Regression Estimates?

We want to improve the Linear Regression model,

- by replacing the least square fitting with some alternative fitting procedure,
- i.e., the values that minimize the mean square error (MSE)

There are 2 reasons we might not prefer to just use

- the ordinary least squares (OLS) estimates

- Prediction Accuracy
- Model Interpretability

1. Prediction Accuracy

The least squares estimates have relatively low bias and low variability

- especially when the relationship between Y and X is linear
- and the number of observations n is way bigger
  - than the number of predictors p $(n >> p)$

But, when $n \approx p$**,**

- then the least squares fit can have high variance
- and may result in over fitting
- and poor estimates on unseen observations,

And, when $n < p$ **,**

- then the variability of the least squares fit increases dramatically,
- and the variance of these estimates in infinite

2. Model Interpretability

When we have a large number of variables X in the model

- there will generally be many that have little or no effect on Y

Leaving these variables in the model

- makes it harder to see the “big picture”,
- i.e., the effect of the “important variables”

The model would be easier to interpret

- by removing (i.e. setting the coefficients to zero)
- the unimportant variables

Solution

Subset Selection

- Identifying a subset of all p predictors X
  that we believe to be related to the response Y,
  and then fitting the model using this subset
- E.g. best subset selection and stepwise selection

Shrinkage

- Involves shrinking the estimates coefficients towards zero
  This shrinkage reduces the variance
- Some of the coefficients may shrink to exactly zero,
  and hence shrinkage methods can also perform variable selection
- E.g. Ridge regression and the Lasso

Dimension Reduction

- Involves projecting all p predictors into an M-dimensional space where M < p,
  and then fitting linear regression model
- E.g. Principle Components Regression

6.1 Subset selection

6.6.1 Best Subset Selection

In this approach, we run a linear regression

- for each possible combination of the X predictors

How do we judge which subset is the “best”?

One simple approach is to take the subset

- with the smallest RSS
- or the largest R^2

Unfortunately, one can show that the model that includes all the variables

- will always have the largest R^2
- (and smallest RSS)

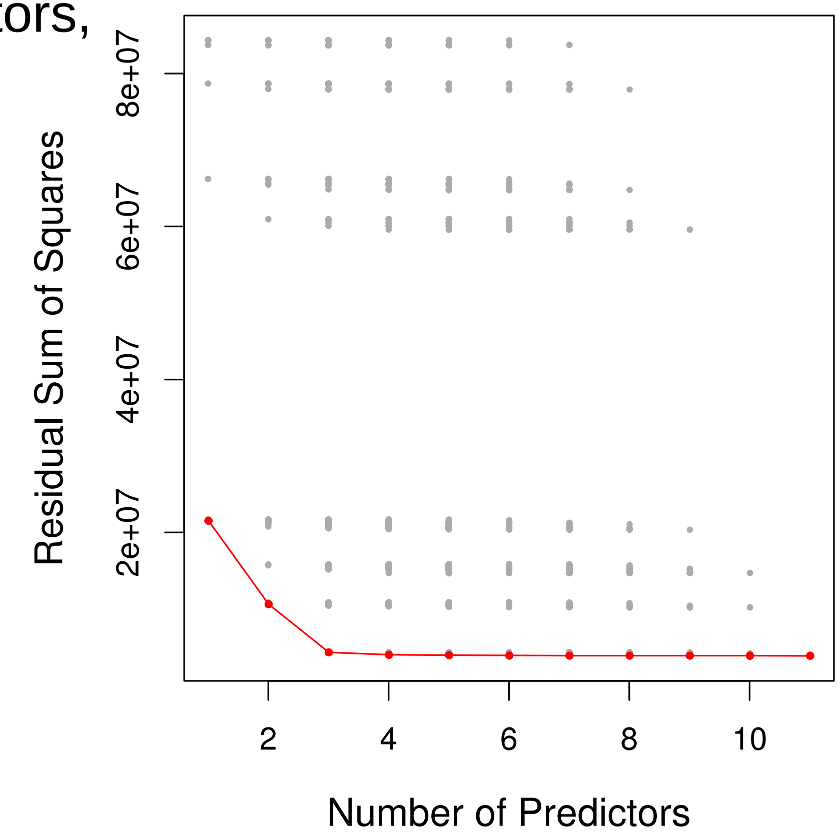
Credit Data: R^2 vs. Subset Size

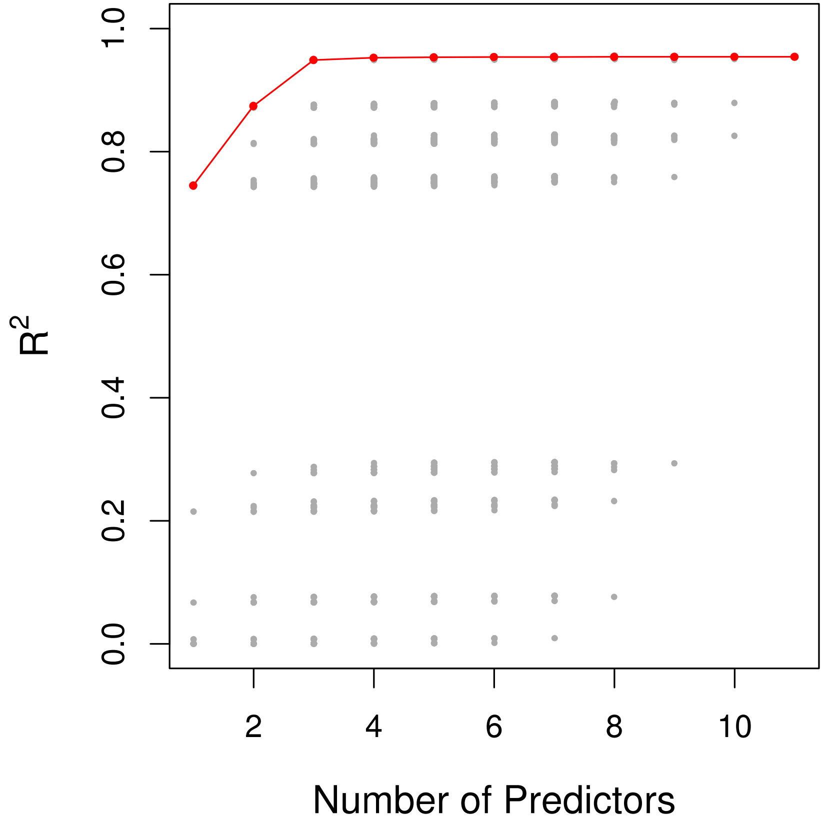
The RSS/R^2 will always decline/increase

- as the number of variables increase
- so they are not very useful

The red line tracks the best model

- for a given number of predictors,
- according to RSS and R^2





Other Measures of Comparison

To compare different models, we can use other approaches:

- Adjusted R^2
- AIC (Akaike information criterion)
- BIC (Bayesian information criterion)
- C_p (equivalent to AIC for linear regression)

These methods add penalty to RSS

- for the number of variables (i.e. complexity) in the model

None are perfect

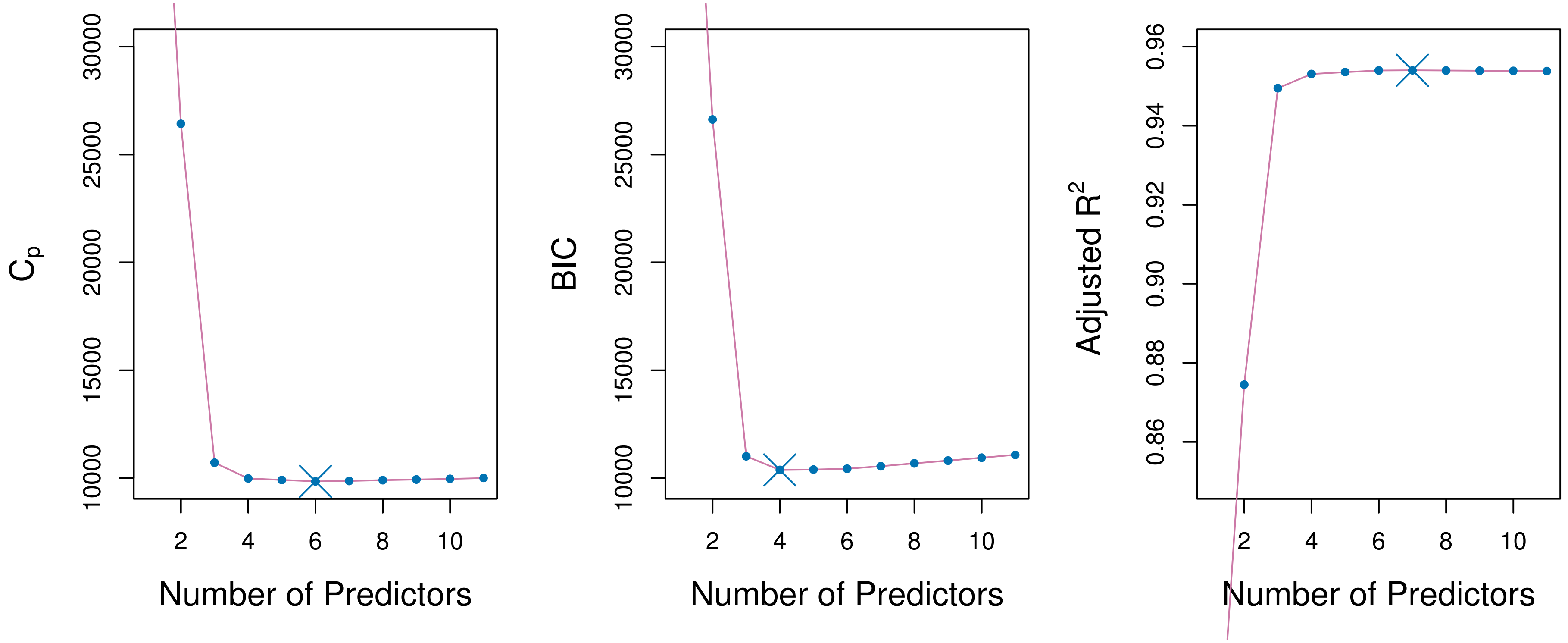
Credit Data: Cp, BIC, and Adjusted R2

A small value of C_p and BIC

- indicates a low error,
- and thus a better model

A large value for the Adjusted R^2

- indicates a better model



6.1.2 Stepwise Selection

Best Subset Selection is computationally intensive

- especially when we have a large number of predictors (large p)

More attractive methods:

- Forward Stepwise Selection:
  Begins with the model containing no predictor,
  and then adds one predictor at a time that improves the model the most
  until no further improvement is possible
- Backward Stepwise Selection:
  Begins with the model containing all predictors,
  and then deleting one predictor at a time that improves the model the most
  until no further improvement is possible

6.2 Shrinkage Methods

6.2.1 Ridge Regression

Ordinary Least Squares (OLS) estimates $\beta's$ 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 uses a slightly different equation

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

Ridge Regression Adds a Penalty on $\beta's$!

The effect of this equation is to add a penalty of the form

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

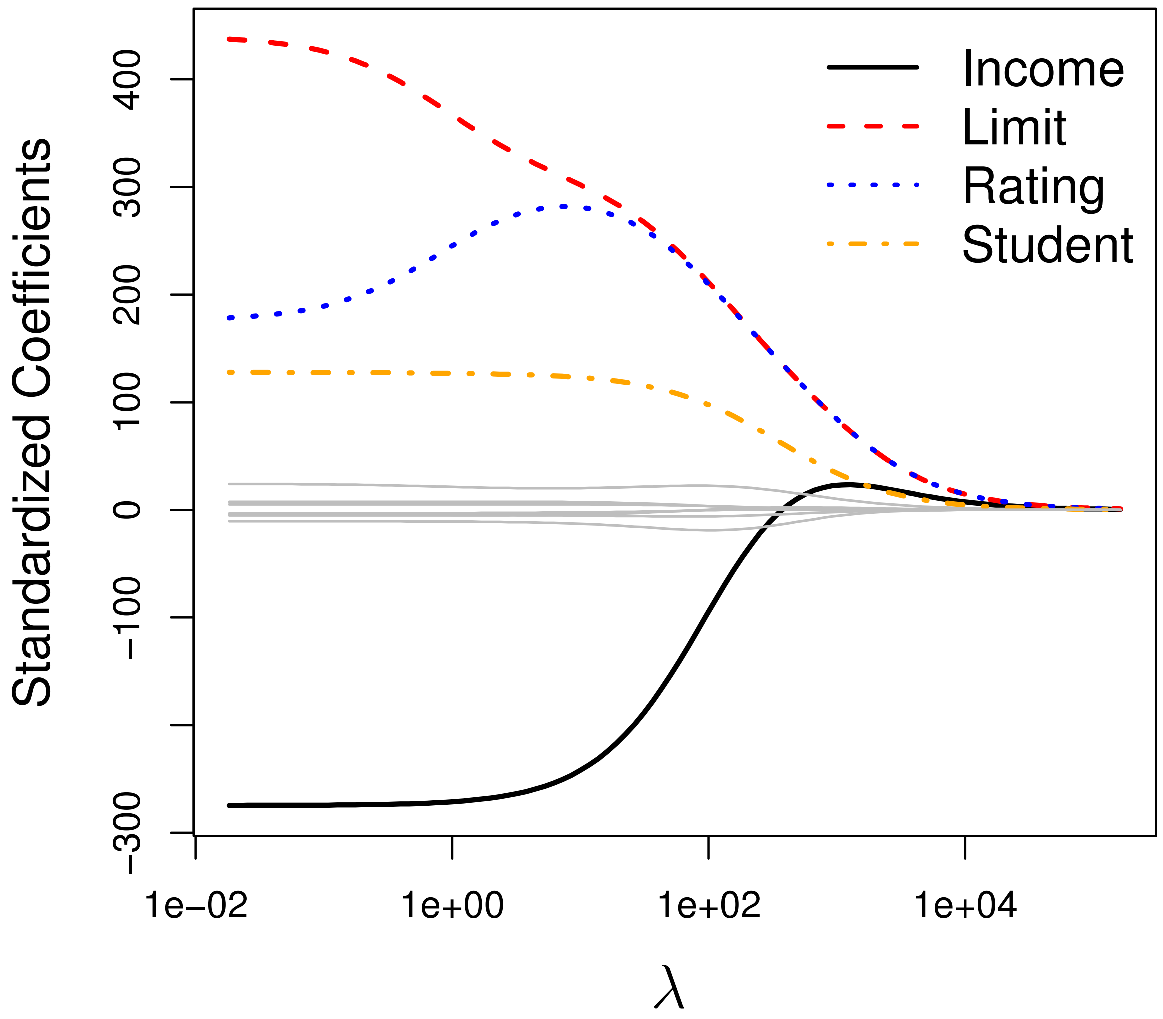
Where the tuning parameter λ is a positive value.

- This has the effect of “shrinking” large values of $\beta's$ towards zero.
- It turns out that such a constraint should improve the fit, because shrinking the coefficients can significantly reduce their variance
- Notice that when λ = 0, we get the OLS!

Credit Data: Ridge Regression

As λ increases,

- the standardized coefficients
- shrinks towards zero.



Why can shrinking towards zero be a good thing to do?

It turns out that the OLS estimates

- generally have low bias
- but can be highly variable.

In particular when n and p are of similar size

- or when $n < p$,
- then the OLS estimates will be extremely variable

The penalty term makes the ridge regression estimates biased

- but can also substantially reduce variance

Thus, there is a bias / variance trade-off

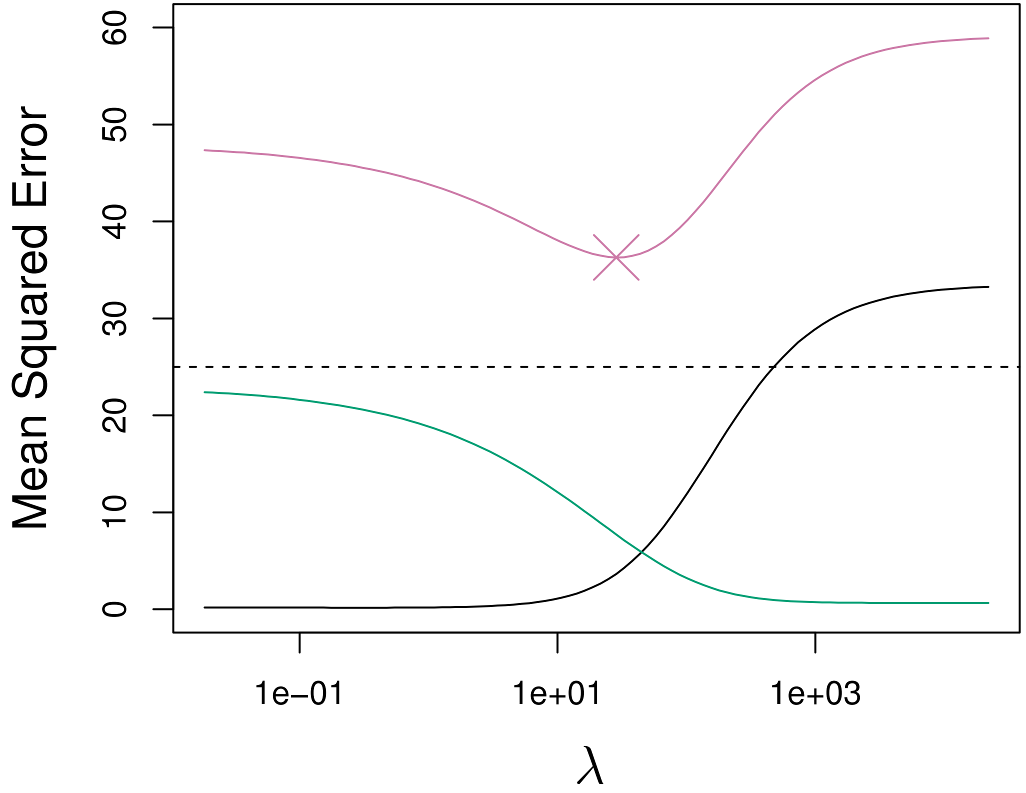
Ridge Regression Bias/ Variance

Black: Bias

Green: Variance

Purple: MSE

Increase λ increases bias but decreases variance



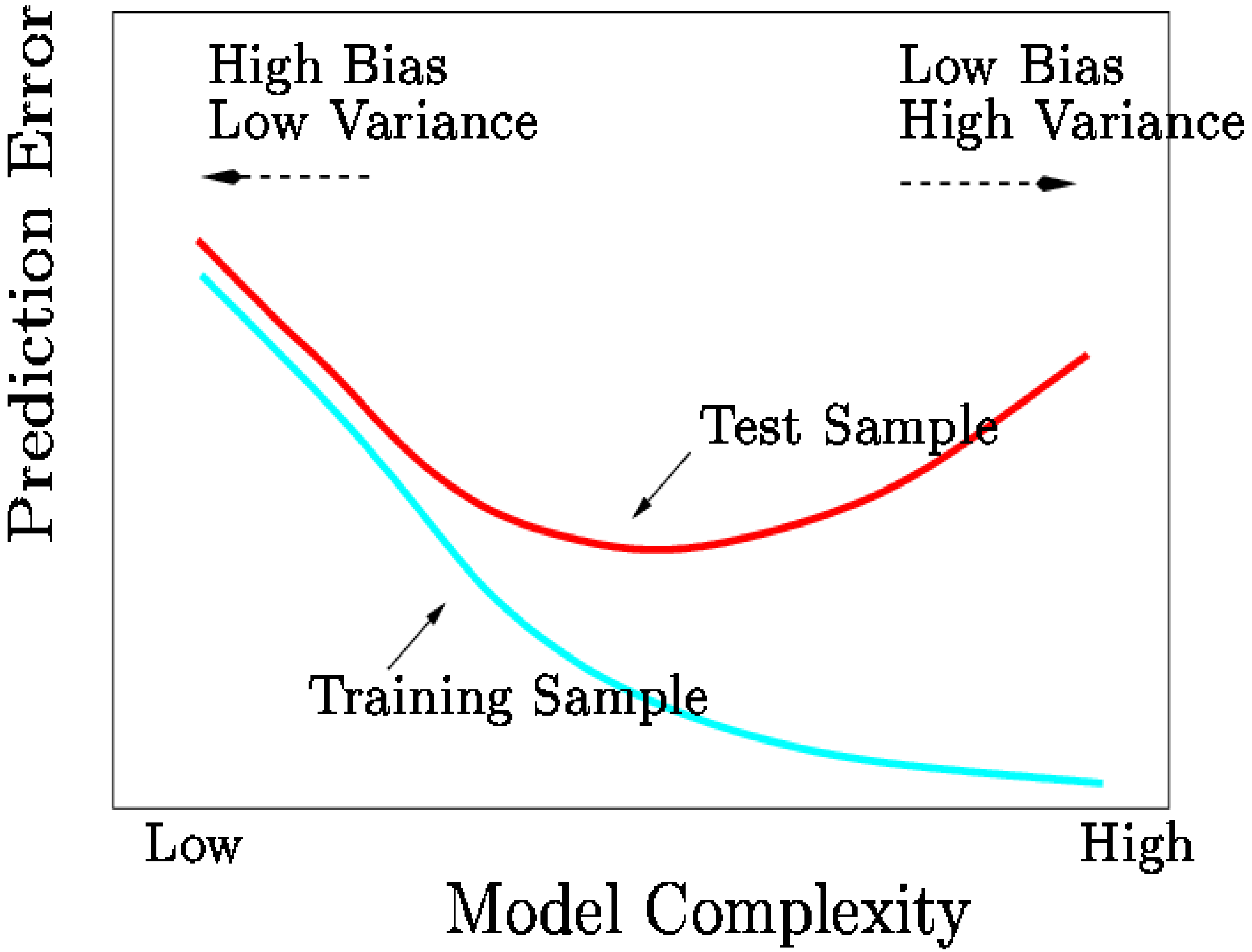
Bias/ Variance Trade-off

In general, the ridge regression estimates

- will be more biased than the OLS ones
- but have lower variance

Ridge regression will work best in situations

- where the OLS estimates
- have high variance



Computational Advantages of Ridge Regression

If p is large, then using the best subset selection approach

- requires searching through enormous numbers of possible models

With Ridge Regression, for any given λ,

- we only need to fit one model
- and the computations turn out to be very simple

Ridge Regression can even be used

- when p > n,
- a situation where OLS fails completely!

6.2.2. The LASSO

Ridge Regression isn't perfect

One significant problem is that the penalty term

- will never force any of the coefficients to be exactly zero.

Thus, the final model will include all variables,

- which makes it harder to interpret

A more modern alternative is the LASSO

The LASSO works

- in a similar way to Ridge Regression,
- except it uses a different penalty term

LASSO's Penalty Term

Ridge Regression minimizes

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

The LASSO estimates the β's by minimizing the

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

What's the Big Deal?

This seems like a very similar idea but there is a big difference

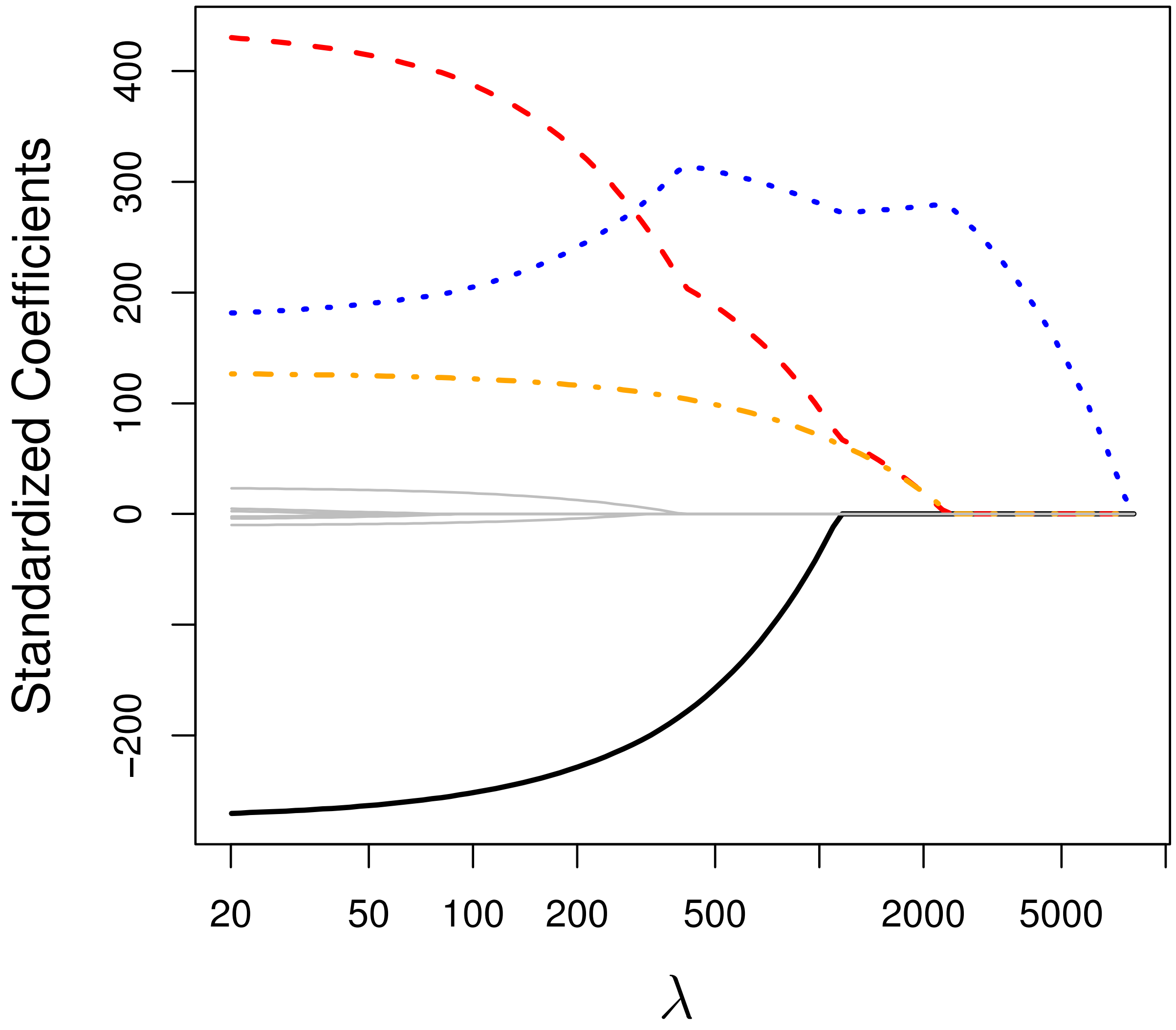
Using this penalty, it could be proven mathematically

- that some coefficients end up being set to exactly zero

With LASSO,

- we can produce a model that has high predictive power
- and it is simple to interpret

Credit Data: LASSO



6.2.3 Selecting the Tuning Parameter λ

We need to decide on a value for λ

Select a grid of potential values,

- **use cross validation to estimate the error rate on test data**
  - (for each value of λ)
- **and select the value that gives the least error rate**