Day 6: Model Selection II

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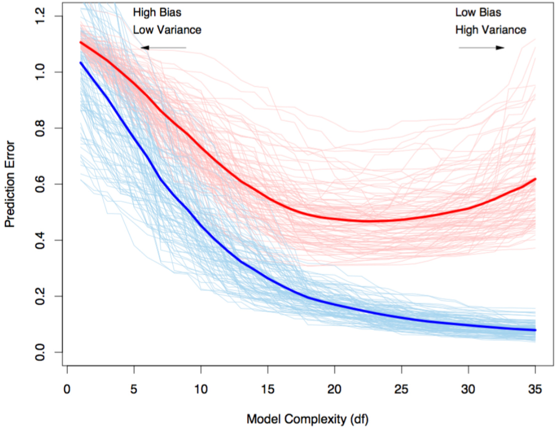
Essex Summer School

Introduction to Statistical Learning

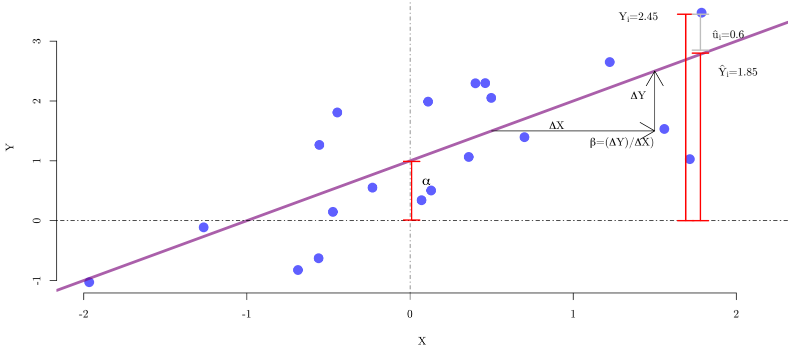
Repetition: Fundamental Problem



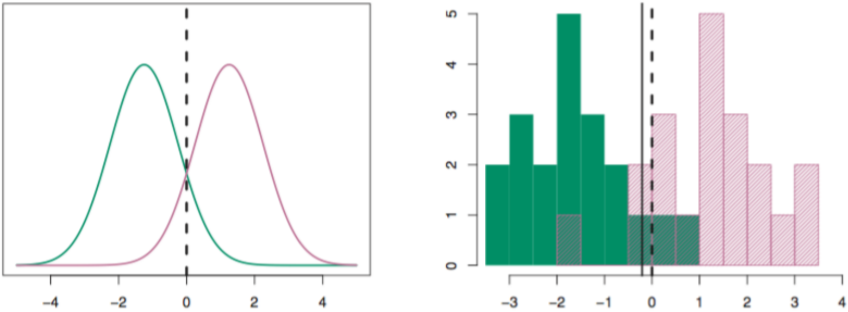
Red: Test error.
Blue: Training error.

(Hastie et al, 2008: 220)

Tuesday: Linear Models

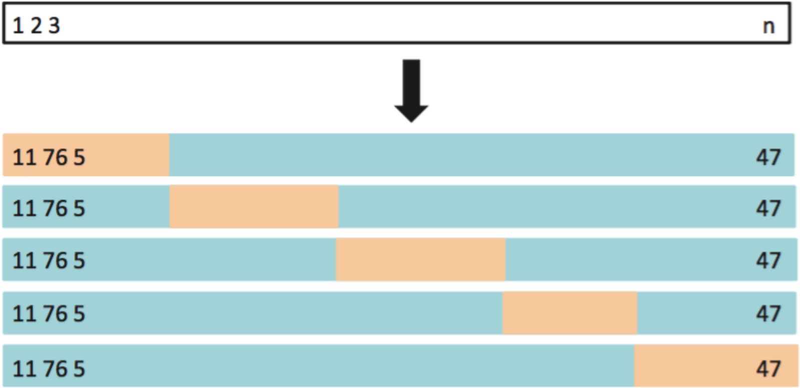


Wednesday: Classification



(James et al, 2013: 140)

Thursday: Resampling



(James et al, 2013: 181)

Friday: Model Selection I

Subset Selection:

1. Generate an empty model and call it $\mathcal{M}_0$
2. For $k = 1....p$:
   i) Generate all $\binom{p}{k}$ possible models with k explanatory variables
   ii) determine the model with the best criteria value (e.g. R^2) and call it $\mathcal{M}_k$
3. Determine best model within the set of these models: $\mathcal{M}_0$, ..., $\mathcal{M}_p$
   - rely on a criteria like AIC, BIC, R^2, C_p or use CV and estimate test error

Regularization Approaches

Shrinkage Methods

Ridge regression and Lasso

- The subset selection methods use least squares to fit a linear model that contains a subset of the predictors.
- As an alternative, we can fit a model containing all p predictors using a technique that constrains or regularizes the coefficient estimates, or equivalently, that shrinks the coefficient estimates towards zero.
- It may not be immediately obvious why such a constraint should improve the fit, but it turns out that shrinking the coefficient estimates can significantly reduce their variance.

Regularization

- Recall that the least squares fitting procedure estimates $\beta_0, \beta_1, \ldots, \beta_p$ using the values that minimize

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

- In contrast, the regularization approach minimizes:

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

where $\lambda \geq 0$ is a tuning parameter, to be determined separately.

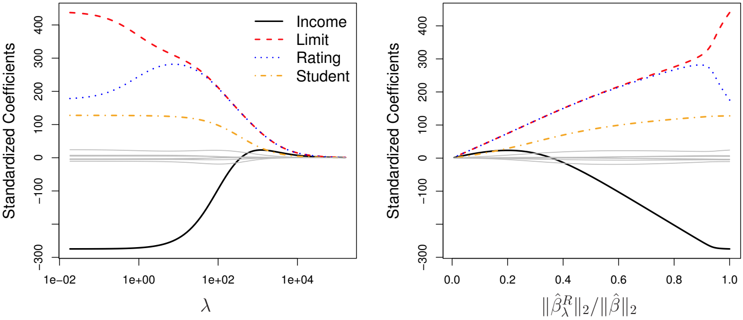
Ridge Regression

- Ridge Regression minimizes this expression:

$$\underbrace{\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{J}\beta_j x_{ij}\right)^2}_{standard\ \ OLS\ \ estimate} + \underbrace{\lambda \sum_{j=1}^{J}\beta_j^2}_{penalty}$$

- λ is a tuning parameter, i.e. different values of λ lead to different models and predictions.
    - When λ is very big the estimates get pushed to 0.
    - When λ is 0 the ridge regression and OLS are identical.
- We can find an optimal value for λ by relying on cross-validation.

Example: Credit data



$||\hat{\beta}||_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$

(James et al, 2013: 216)

Ridge Regression: Details

- Shrinkage is not applied to the model constant β_0, model estimate for conditional mean should be *un-shrunk*.
- Ridge regression is an example of ℓ_2 regularization:
  - $\ell_1 : f(\beta_j) = \sum_{j=1}^{J} |\beta_j|$
  - $\ell_2 : f(\beta_j) = \sum_{j=1}^{J} \beta_j^2$

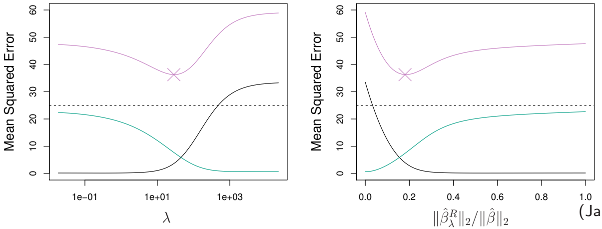
$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2}}$$

Ridge regression: scaling of predictors

- The standard least squares coefficient estimates are scale equivariant: multiplying X_j by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how the jth predictor is scaled, $X_j\hat{\beta}_j$ will remain the same.
- In contrast, the ridge regression coefficient estimates can change substantially when multiplying a given predictor by a constant, due to the sum of squared coefficients term in the penalty part of the ridge regression objective function.
- Therefore, it is best to apply ridge regression after standardizing the predictors, using the formula

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

Why Does Ridge Regression Improve Over Least Squares?



(James et al, 2013: 218)

- Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients.
- Squared bias (black), variance (green), and test mean squared error (purple).
- The purple crosses indicate the ridge regression models for which the MSE is smallest.
- OLS with p variables is low bias but high variance - shrinkage lowers variance at the price of bias.

The Lasso

- Ridge regression does have one obvious disadvantage: unlike subset selection, which will generally select models that involve just a subset of the variables, ridge regression will include all p predictors in the final model.
- The Lasso is a relatively recent alternative to ridge regression that overcomes this disadvantage. The lasso coefficients, $\hat{\beta}_\lambda^L$, minimize this quantity

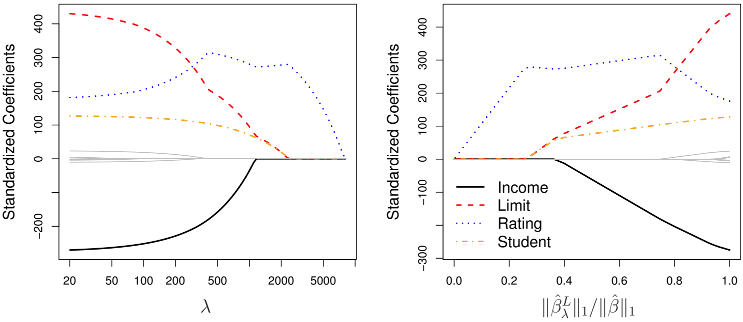
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = RSS + \lambda\sum_{j=1}^{p}|\beta_j|$$

- In statistical parlance, the lasso uses an ℓ_1 (pronounced “ell 1”) penalty instead of an ℓ_2 penalty. The ℓ_1 norm of a coefficient vector β is given by $\|\beta\|_1 = \sum|\beta_j|$.

The Lasso: continued

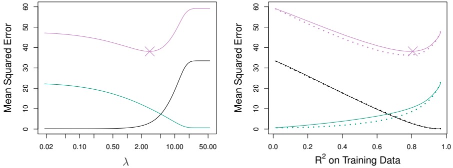
- As with ridge regression, the lasso shrinks the coefficient estimates towards zero.
- However, in the case of the lasso, the ℓ_1 penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter λ is sufficiently large.
- Hence, much like best subset selection, the lasso performs variable selection.
- We say that the lasso yields sparse models – that is, models that involve only a subset of the variables.
- As in ridge regression, selecting a good value of λ for the lasso is critical; cross-validation is again the method of choice.

Example: Credit data



(James et al, 2013: 220)

Comparing the Lasso and Ridge Regression



- Left: Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data set.
- Right: Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed).
- Both are plotted against their R^2 on the training data, as a common form of indexing.
- The crosses in both plots indicate the lasso model for which the MSE is smallest.

Comparing the Lasso and Ridge Regression: continued

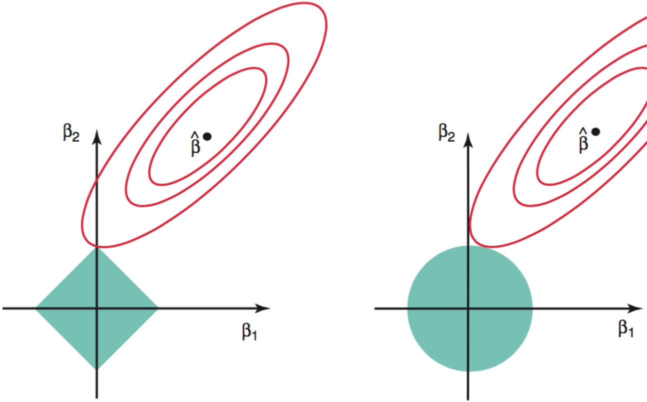


FIGURE 6.7. *Contours of the error and constraint functions for the lasso* (left) *and ridge regression* (right). *The solid blue areas are the constraint regions,* $|\beta_1| + |\beta_2| \leq s$ *and* $\beta_1^2 + \beta_2^2 \leq s$, *while the red ellipses are the contours of the RSS.*

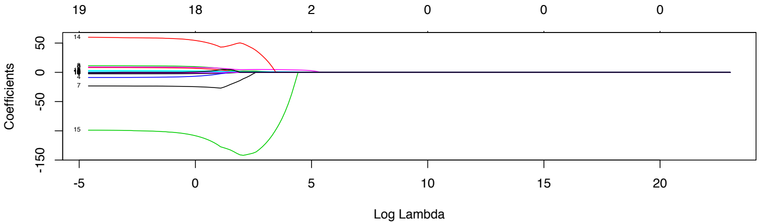
Take away message

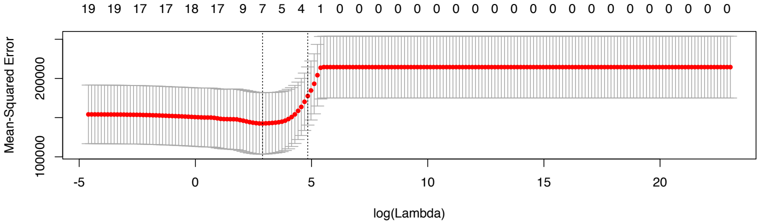
- These two examples illustrate that neither ridge regression nor the lasso will universally dominate the other.
- In general, one might expect the lasso to perform better when the response is a function of only a relatively small number of predictors.
- However, the number of predictors that is related to the response is never known *a priori* for real data sets.
- A technique such as cross-validation can be used in order to determine which approach is better on a particular data set.

Selecting the Tuning Parameter for Ridge Regression and Lasso

- As for subset selection, for ridge regression and lasso we require a method to determine which of the models under consideration is best.
- That is, we require a method selecting a value for the tuning parameter λ or equivalently, the value of the constraint s.
- Cross-validation provides a simple way to tackle this problem. We choose a grid of λ values, and compute the cross-validation error rate for each value of λ.
- We then select the tuning parameter value for which the cross-validation error is smallest.
- Finally, the model is re-fit using all of the available observations and the selected value of the tuning parameter.

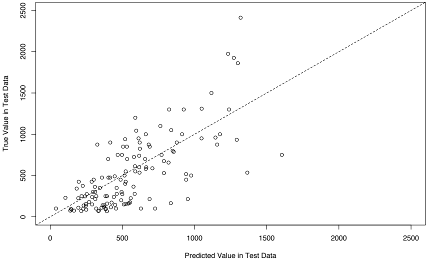
Example: Baseball Data





Lasso Example 4

```
> lasso.pred <- predict(lasso.mod, s = log(cv.out$lambda.1se), newx = x[test, ])
> plot(lasso.pred, y[test], ylim=c(0,2500), xlim=c(0,2500), ylab="True Value in Test Data", xlab="Predicted Va
> abline(coef = c(0,1),lty=2)
```



Ridge vs Lasso

- Ridge is preferred when some features are (strongly) correlated – Lasso tends to only pick one.
- As mentioned: CV to pick one of the two approaches.
- Elastic net: Combining Lasso and Ridge:

$$\tilde{\beta} \;=\; \text{argmin}\Big(RSS - \lambda \sum_{j=1}^{J} (\alpha\beta_j^2 + (1-\alpha)|\beta_j|\Big)$$

  we now have two tuning parameters: α and λ
- Details: Hastie et al. 2008. *The Elements of Statistical Learning*. Springer.