

Lecture 6 Model Selection II

STAT 441/505: Applied Statistical Methods in Data Mining

Linglong Kong

Department of Mathematical and Statistical Sciences
University of Alberta

Winter, 2016

Outline

Ridge Regression

The LASSO

Ridge regression and the LASSO

Summary and Remark

Ridge Regression

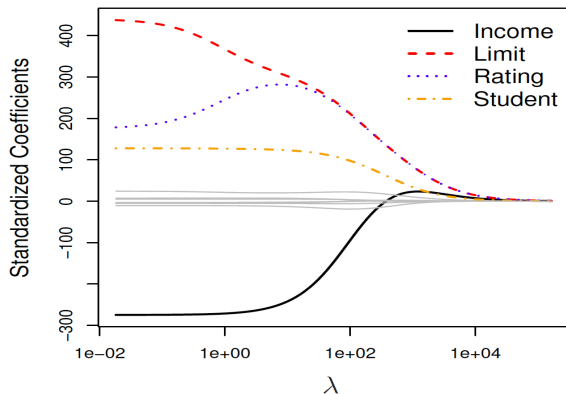
- ▶ The **ridge regression coefficient** estimates $\hat{\beta}^R$ are the values that minimize

$$\sum_i \left(y_i - \beta_0 - \sum_j \beta_j x_{ij} \right)^2 + \lambda \sum_j \beta_j^2,$$

where λ is a **tuning parameter**, to be determined separately.

- ▶ The second term $\lambda \sum_j \beta_j^2$ called a **shrinkage penalty**, is small when β_j , $j \geq 1$ are close to zero, and so it has the effect of shrinking the estimates of β_j towards zero.
- ▶ The tuning parameter λ serves to control the relative impact of these two terms on the regression coefficient estimates.
- ▶ Selecting a good value for λ is critical; **cross-validation** is used for this.

Credit data example



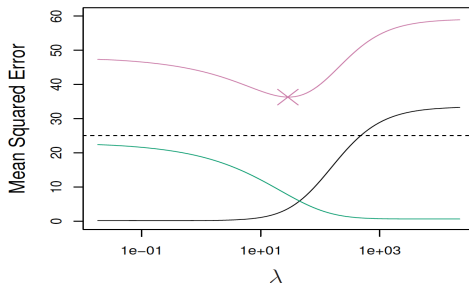
As λ increases, the coefficients are shrunk to zeros.

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 j -th 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 coefficient 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

$$\tilde{x}_{ij} = x_{ij} / \sqrt{\sum_i (x_{ij} - \bar{x}_j)^2 / n}.$$

Credit data example



Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficient. Squared bias (black), **variance (green)**, and **test mean squared error (purple)** for the ridge regression predictions on a simulated data set. The horizontal dashed lines indicate the minimum possible MSE. The **purple crosses** indicate the ridge regression models for which the MSE is smallest.

The LASSO

- ▶ Ridge regression, unlike subset selection, 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 coefficient $\hat{\beta}^L$ minimize the quantity

$$\sum_i \left(y_i - \beta_0 - \sum_j \beta_j x_{ij} \right)^2 + \lambda \sum_j |\beta_j|,$$

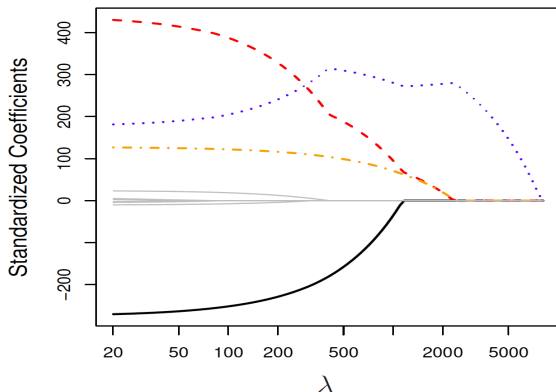
where λ is a **tuning parameter**.

- ▶ The LASSO uses l_1 penalty instead of l_2 (ridge regression).

The LASSO

- ▶ As with ridge regression, the lasso shrinks the coefficient estimates towards zero as λ increases.
- ▶ 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. Thus **performs variable selection**.
- ▶ We say that the lasso yields **sparse models** — that is, models that involve only a subset of the variables.
- ▶ Selecting a good value for λ is critical; **cross-validation** is again used for this.

Credit data example



As λ increases, the coefficients are shrunk to exact zeros.

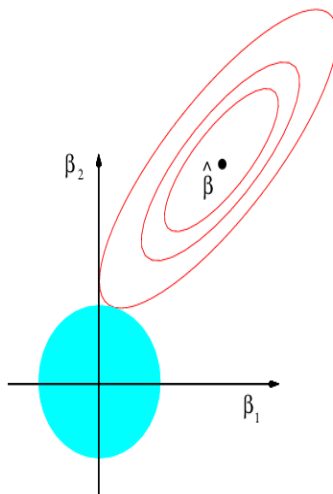
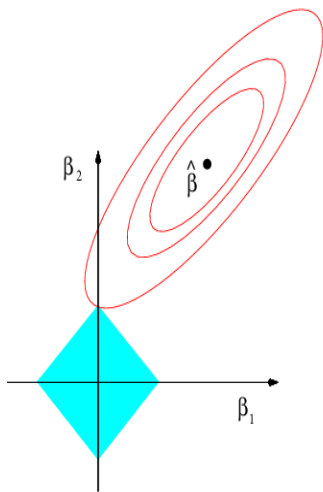
Ridge regression and the LASSO

- ▶ Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?
- ▶ One can show that the lasso and ridge regression coefficient estimates solve the problems

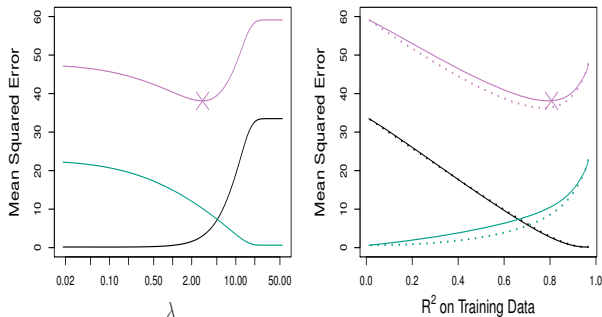
$$\min_{\beta} \sum_i \left(y_i - \beta_0 - \sum_j \beta_j x_{ij} \right)^2, \text{ subject to } \sum_j |\beta_j| \leq c;$$

$$\min_{\beta} \sum_i \left(y_i - \beta_0 - \sum_j \beta_j x_{ij} \right)^2, \text{ subject to } \sum_j \beta_j^2 \leq c;$$

Ridge regression and the LASSO

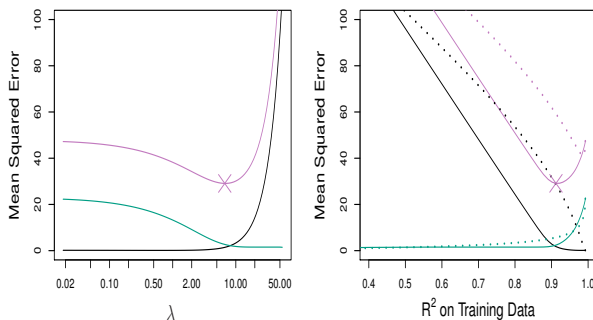


Credit data example



Left: Plots of squared bias (black), **variance (green)**, and **test mean squared error (purple)** for the LASSO on a simulated data set. **Right:** Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed). The **purple crosses** indicate the LASSO models for which the MSE is smallest.

Credit data example



Left: Plots of squared bias (black), **variance** (green), and **test mean squared error** (purple) for the LASSO on another simulated data set. **Right:** Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed). The **purple crosses** indicate the LASSO models for which the MSE is smallest.

Conclusions

- ▶ 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.

Summary and Remark

- ▶ Ridge Regression
- ▶ The LASSO
- ▶ Ridge Regression and the LASSO
- ▶ Read textbook Chapter 3
- ▶ Do R lab