Ch 6: Linear Model Selection and Regularization

This material is prepared by following the context of James et al. (2013) and slides at https://www.r-bloggers.com/in-depth-introduction-to-machine-learning-in-15-hours-of-expert-videos/

6.0 Introduction

- Recall the linear model

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon$$

- Despite its simplicity, the linear model has distinct advantages in terms of its interpretability and often shows good predictive performance.

- Hence we discuss some ways in which the simple linear model can be improved, by replacing ordinary least squares fitting with some alternative fitting procedures.

- Why consider alternatives to least squares ?

  - Prediction accuracy: especially when $p > n$, to control the variance.

  - Model interpretability: By removing irrelevant features – that is, by setting the corresponding coefficient estimates to zero – we can obtain a model that is more easily interpreted. We will present some approaches for automatically performing feature selection.

- Three classes of methods

  - Subset selection: We identify a subset of the p predictors that we believe to be related to the response. We then fit a model using least squares on the reduced set of variables.

  - Shrinkage: We fit a model involving all p predictors, but the estimated coefficients are shrunken towards zero relative to the least squares estimates. This shrinkage (also known as regularization) has the effect of reducing variance and can also perform variable selection.

- Dimension reduction: We project the p predictors into a M-dimensional subspace, where $M < p$. This is achieved by computing M different linear combinations, or projections, of the variables. Then these M projections are used as predictors to fit a linear regression model by least squares.

6.1 Subset Selection

6.1.1 Best Subset Selection

- To perform best subset selection, we fit a separate least squares regression best subset selection for each possible combination of the p predictors.

- The problem of selecting the best model from among the 2^p possibilities considered by best subset selection is not trivial.

- Best subset selection algorithm

  1. Let $\mathcal{M}_0$ denote the null model, which contains no predictors. This model simply predicts the sample mean for each observation.
  2. For $k = 1, 2, \ldots, p$:
     (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.
     (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Here best is defined as having the smallest RSS, or equivalently largest R^2.
  3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p, AIC, or BIC.

- Although we have presented best subset selection here for least squares regression, the same ideas apply to other types of models, such as logistic regression. The deviance–negative two times the maximized log-likelihood–plays the role of RSS for a broader class of models.

6.1.2 Stepwise Selection

- For computational reasons, best subset selection cannot be applied with very large p.

- Best subset selection may also suffer from statistical problems when p is large: larger the search space, the higher the chance of finding models that look good on the training data, even though they might not have any predictive power on future data.
- Thus, an enormous search space can lead to overfitting and high variance of the coefficient estimates.
- For both of these reasons, stepwise methods, which explore a far more restricted set of models, are attractive alternatives to best subset selection.

Forward Stepwise Selection

1. Let $\mathcal{M}_0$ denote the null model, which contains no predictors.
2. For $k = 0, 1, \ldots, p-1$:

   2.1 Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor.

   2.2 Choose the best among these $p-k$ models, and call it $\mathcal{M}_{k+1}$. Here best is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p, AIC, or BIC.

Backward Stepwise Selection

1. Let $\mathcal{M}_0$ denote the full model, which contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:

   2.1 Consider all k models that contain all but one of the predictors in M_k, for a total of $k-1$ predictors.

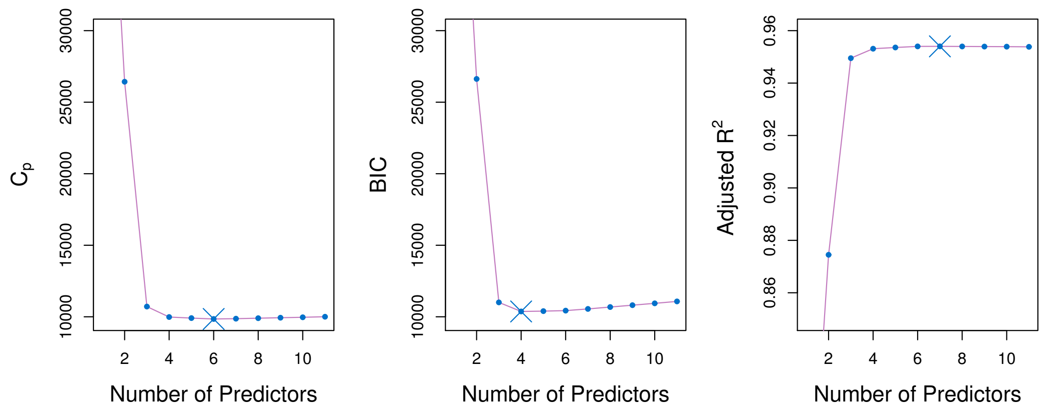
   2.2 Choose the best among these k models, and call it $\mathcal{M}_{k-1}$. Here best is defined as having smallest RSS or highest R^2.

3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p, AIC, or BIC.

Note that backward selection requires that the number of samples n is larger than the number of variables p (so that the full model can be fit). In contrast, forward stepwise can be used even when $n < p$, and so is the only viable subset method when p is very large.

6.1.3 Choosing the Optimal Model

- The model containing all of the predictors will always have the smallest RSS and the largest R^2, since these quantities are related to the training error.
- We wish to choose a model with low test error, not a model with low training error. Recall that training error is usually a poor estimate of test error.
- Therefore, RSS and R^2 are not suitable for selecting the best model among a collection of models with different numbers of predictors.
- Estimating test error: two approaches
  - We can indirectly estimate test error by making an adjustment to the training error to account for the bias due to overfitting.
  - We can directly estimate the test error, using either a validation set approach or a cross-validation approach, as discussed in previous lectures.
- C_p, AIC, BIC, and Adjusted R^2
  - These techniques adjust the training error for the model size, and can be used to select among a set of models with different numbers of variables.
  - Mallow's C_p:
$$C_p = \frac{1}{n}(RSS + 2d\hat{\sigma}^2)$$
    where d is the total # of parameters used and $\hat{\sigma}^2$ is an estimate of the variance of the error associated with each response measurement.



- The AIC criterion is defined for a large class of models fit by maximum likelihood:

$$\text{AIC} = -2 \log L + 2d$$

  where L is the maximized value of the likelihood function for the estimated model.

- In the case of the linear model with Gaussian errors, maximum likelihood and least squares are the same thing, and C_p and AIC are equivalent.

- BIC=$\frac{1}{n}(RSS + \log(n)d\hat{\sigma}^2)$

  * Like C_p, the BIC will tend to take on a small value for a model with a low test error, and so generally we select the model that has the lowest BIC value.

  * Notice that BIC replaces the $2d\hat{\sigma}^2$ used by C_p with a $\log(n)d\hat{\sigma}^2$ term, where n is the number of observations.

  * Since $\log n > 2$ for any $n > 7$, the BIC statistic generally places a heavier penalty on models with many variables, and hence results in the selection of smaller models than C_p.

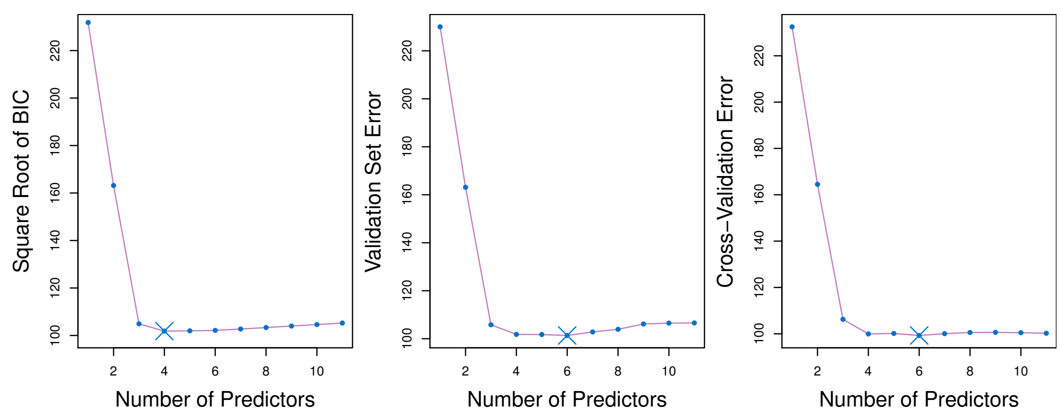
- Adjusted $R^2 = 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)}$ with total sum of squares

  * Unlike C_p, AIC, and BIC, for which a small value indicates a model with a low test error, a large value of adjusted R^2 indicates a model with a small test error.

  * Maximizing the adjusted R^2 is equivalent to minimizing RSS$/(n-d-1)$. While RSS always decreases as the number of variables in the model increases, RSS$/(n-d-1)$ may increase or decrease, due to the presence of d in the denominator.

* Unlike the R^2 statistic, the adjusted R^2 statistic pays a price for the inclusion of unnecessary variables in the model.

- Validation and Cross-Validation
  - Each of the procedures returns a sequence of models $\mathcal{M}_k$ indexed by model size $k = 0, 1, 2, \ldots$. Our job here is to select $\hat{k}$. Once selected, we will return model $\mathcal{M}_{\hat{k}}$.
  - We compute the validation set error or the cross-validation error for each model $\mathcal{M}_k$ under consideration, and then select the k for which the resulting estimated test error is smallest.
  - This procedure has an advantage relative to AIC, BIC, C_p, and adjusted R^2, in that it provides a direct estimate of the test error, and doesn't require an estimate of the error variance $\hat{\sigma}^2$.
  - It can also be used in a wider range of model selection tasks, even in cases where it is hard to pinpoint the model degrees of freedom (e.g. the number of predictors in the model) or hard to estimate the error variance σ^2.



6.2 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.

6.2.1 Ridge regression

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

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

- In contrast, the ridge regression coefficient estimates $\hat{\beta}^R$ are the values that minimize

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

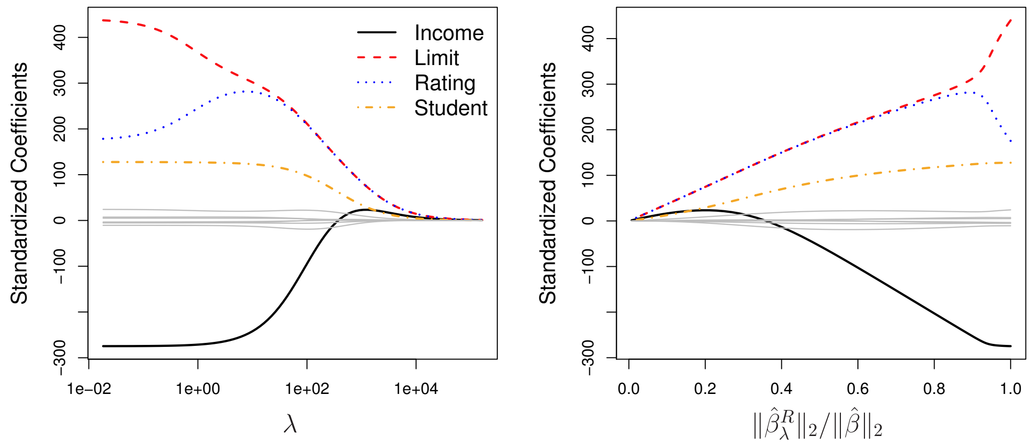
  where $\lambda \geq 0$ is a tuning parameter, to be determined separately.

- As with least squares, ridge regression seeks coefficient estimates that fit the data well, by making the RSS small.

- However, the second term, $\lambda \sum_j \beta_j^2$, called a shrinkage penalty, is small when $\beta_1, \ldots, \beta_p$ 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.

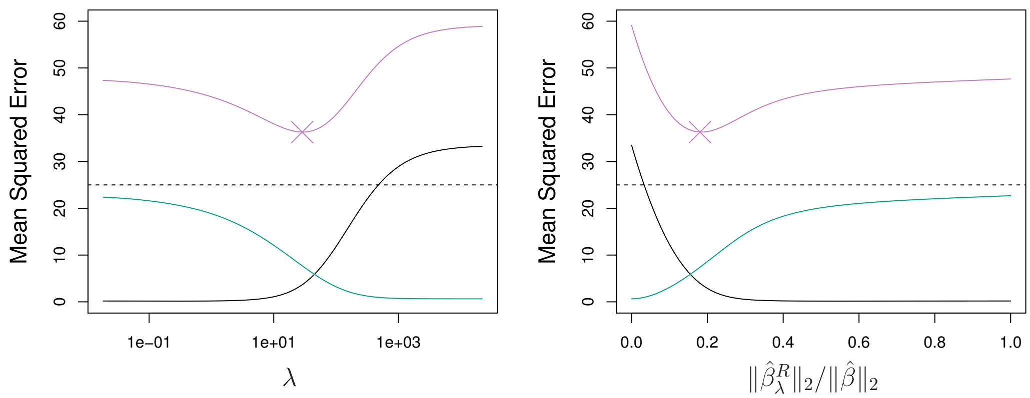
- Selecting a good value for λ is critical; cross-validation is used for this.



- Credit data example
  - In the left-hand panel, each curve corresponds to the ridge regression coefficient estimate for one of the ten variables, plotted as a function of λ.
  - The right-hand panel displays the same ridge coefficient estimates as the left-hand panel, but instead of displaying λ on the x-axis, we now display $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$ where $\hat{\beta}$ denotes the vector of least squares coefficient estimates. The notation $\|\beta\|$ denotes the ℓ_2 norm of a vector, and is defined as $\|\beta\|_2 = \sqrt{\sum_{j=1}^p \beta_j^2}$.
- 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 ?



Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients. 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 $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.

6.2.2 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, $\hat{\beta}^L_\lambda$, minimize the quantity

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

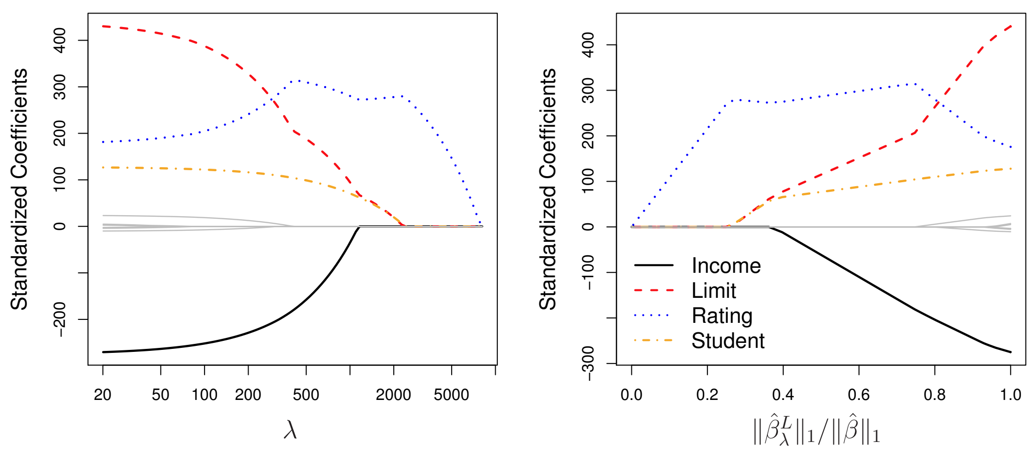
- As with ridge regression, the lasso shrinks the coefficient estimates towards zero.

- 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.



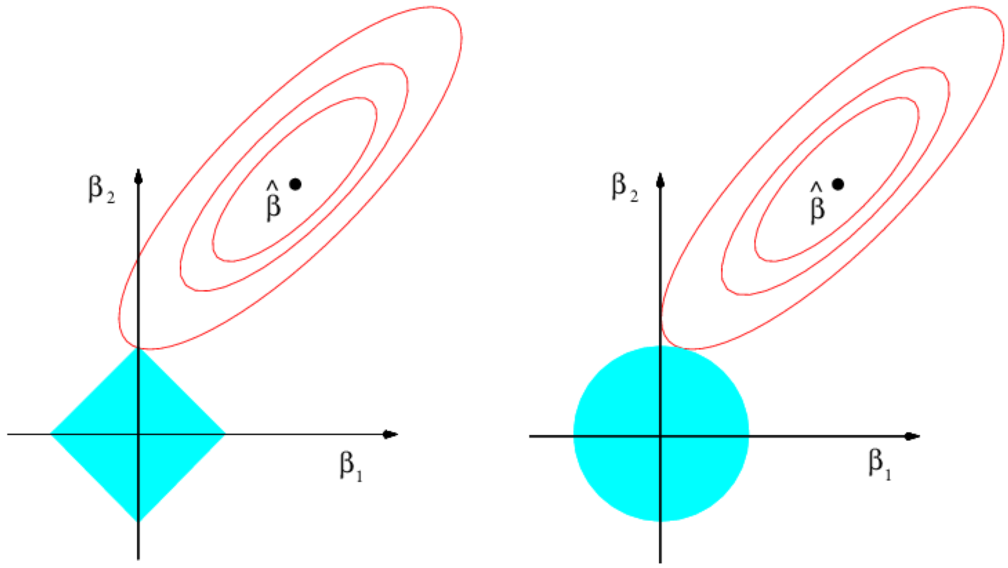
- The Variable Selection Property of the Lasso
  - Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero ?
  - One can show that the lasso and ridge regression coefficient estimates solve the problems

$$\min_{\beta} \text{RSS} \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s$$

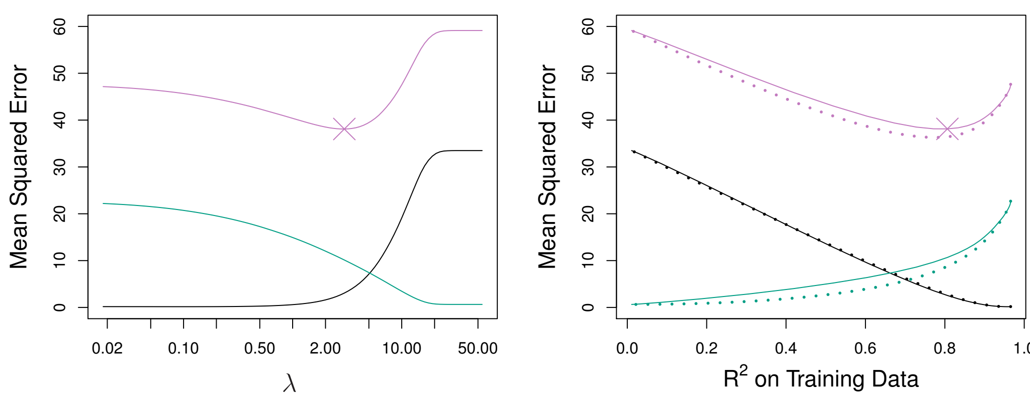
and

$$\min_{\beta} \text{RSS} \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s,$$

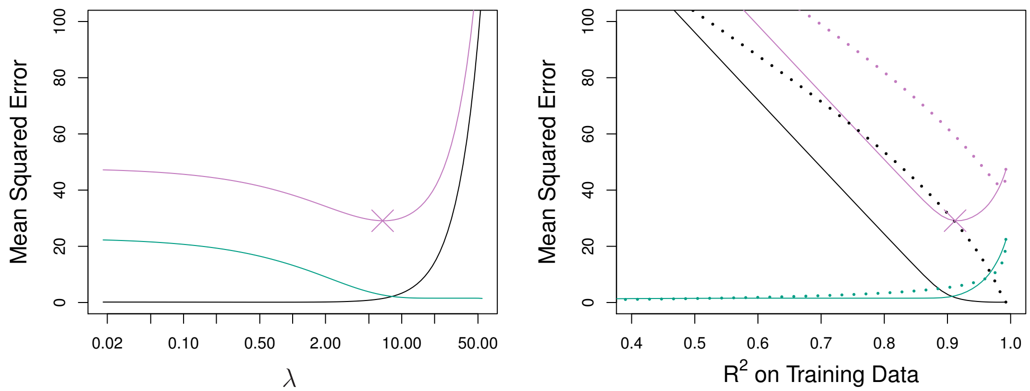
respectively.



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.



Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data set of page 9. 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.



Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso. The simulated data is similar to that in the above figure, except that now only two predictors are related to the response. 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.

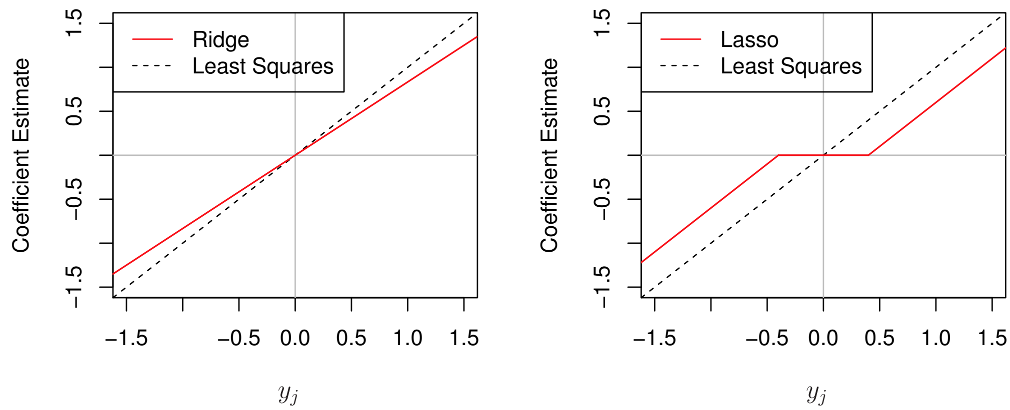
- Consider the problem

$$\min_{\beta} \text{RSS} \quad \text{subject to} \quad \sum_{j=1}^{p} I(\beta_j \neq 0) \leq s.$$

The above optimization amounts to finding a set of coefficient estimates such that RSS is as small as possible, subject to the constraint that no more than s coefficients can be nonzero. The problem is equivalent to best subset selection.

- Ridge regression vs. Lasso
  - 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.

- A Simple Special Case for Ridge Regression and the Lasso
  - For a better intuition, we consider a simple special case with $n = p$, and X a diagonal matrix with 1's on the diagonal and 0's in all off-diagonal elements. Assume also that we are performing regression without an intercept.
  - With these assumptions, the usual least squares problem simplifies to finding $\beta_1, \ldots, \beta_p$ that minimize
$$\sum_{j=1}^{p}(y_j - \beta_j)^2.$$
Then the least squares solution is given by $\hat{\beta}_j = y_j$.
  - The problem for the ridge regression becomes
$$\sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2,$$
and the problem for the lasso is
$$\sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|.$$
  - In this setting, the ridge regression estimates take the form
$$\hat{\beta}_j^R = y_i/(1+\lambda,)$$
and the lasso ones are
$$\hat{\beta}_j^L = \begin{cases} y_j - \lambda/2 & \text{if } y_j > \lambda/2, \\ y_j + \lambda/2 & \text{if } y_j < -\lambda/2, \\ 0 & \text{otherwise} \end{cases}$$



- Bayesian Interpretation for Ridge Regression and the Lasso
  - A Bayesian viewpoint for regression assumes that the coefficient vector β has some prior distribution, say $p(\beta)$. The likelihood of the data can be written as $f(Y|X,\beta)$. Then the posterior distribution takes the form

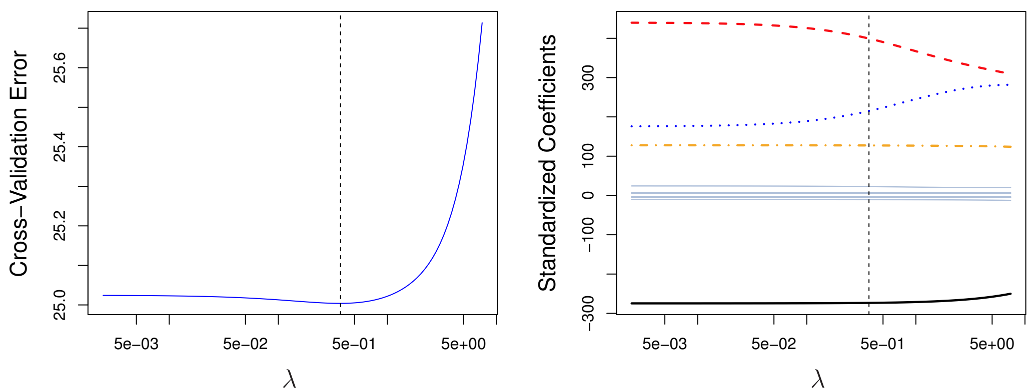
$$p(\beta|X,Y) \propto f(Y|X,\beta)p(\beta).$$

  - We assume the usual linear model with independent Gaussian distributed errors and $p(\beta) = \prod_{j=1}^{p} g(\beta_j)$ for some density function g.
    * If g is a Gaussian distribution with mean zero and standard deviation a function of λ, then it follows that the posterior mean (mode) for β is given by the ridge regression solution.
    * If g is a double-exponential (Laplace) distribution with mean zero and scale parameter a function of λ, then it follows that the posterior mode for β is the lasso solution. However, the lasso solution is not the posterior mean, and in fact, the posterior mean does not yield a sparse coefficient vector.

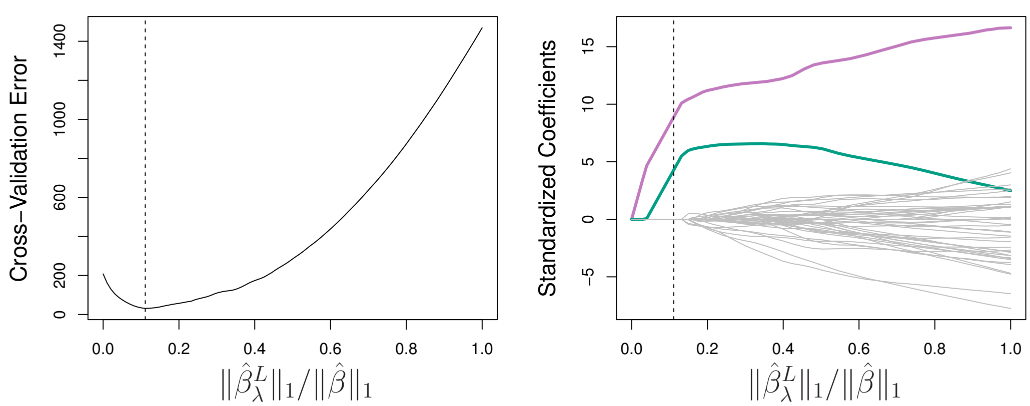
6.2.3 Selecting the Tuning Parameter

- 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 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.



Left: Cross-validation errors that result from applying ridge regression to the Credit data set with various values of λ. Right: The coefficient estimates as a function of λ. The vertical dashed lines indicates the value of λ selected by cross-validation.



Left: Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data set on page 12. Right: The corresponding lasso coefficient estimates are displayed. The vertical dashed lines indicate the lasso fit for which the cross-validation error is smallest.

6.3 Dimension Reduction Methods

- The methods that we have discussed so far in this chapter have involved fitting linear regression models, via least squares or a shrunken approach, using the original predictors, $X_1, \ldots, X_p$.

- We now explore a class of approaches that transform the predictors and then fit a least squares model using the transformed variables. We will refer to these techniques as dimension reduction methods.

- Let $Z_1, \ldots, Z_M$ represent $M(< p)$ linear combinations of our original p predictors. That is,
$$Z_m = \sum_{j=1}^{p} \phi_{mj} X_j$$
for some constants $\phi_{m1}, \ldots, \phi_{mp}$.

- We can then fit the linear regression model,
$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \epsilon_i, \quad i = 1, \ldots, n.$$
In the above model, if the constants $\phi_{m1}, \ldots, \phi_{mp}$ are chosen wisely, then such dimension reduction approaches can often outperform OLS regression.

- From the above derivation,
$$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{mj} x_{ij} = \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{mj} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij},$$
where
$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}.$$

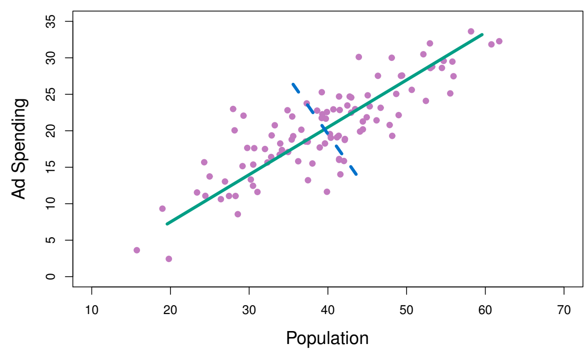
6.3.1 Principal Components Regression

- Here we apply principal components analysis (PCA) (discussed in Chapter 10 of the text) to define the linear combinations of the predictors, for use in our regression.

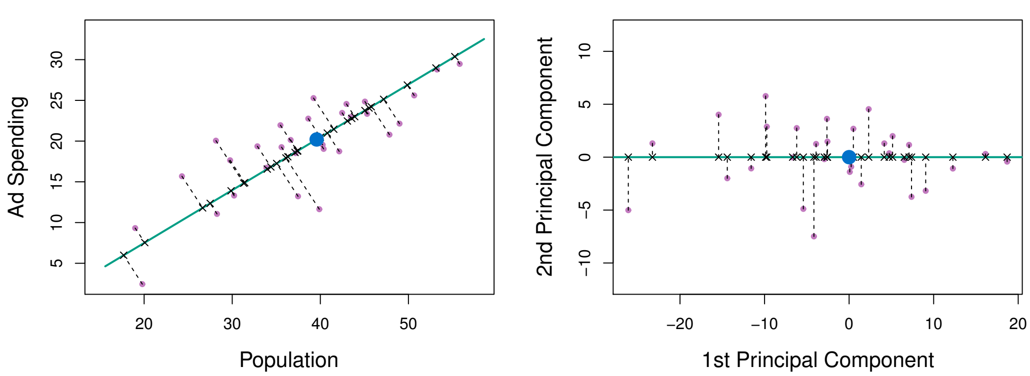
- The first principal component is that (normalized) linear combination of the variables with the largest variance.

- The second principal component has largest variance, subject to being uncorrelated with the first. And so on.

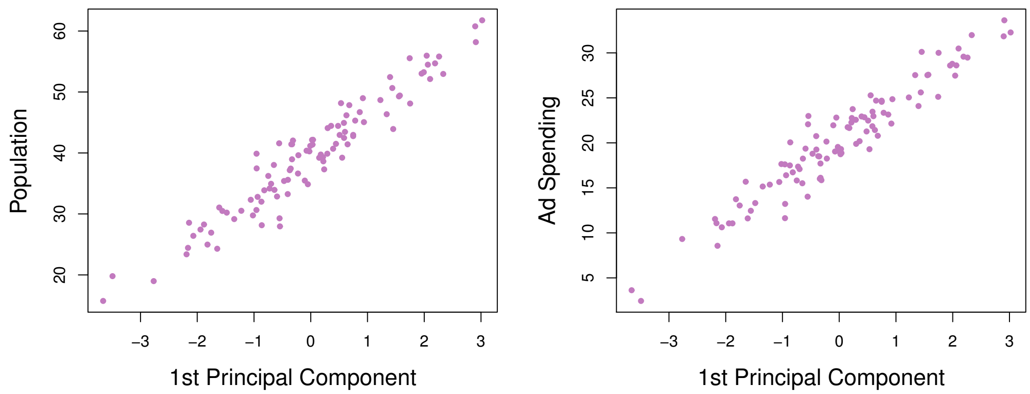
- Hence with many correlated original variables, we replace them with a small set of principal components that capture their joint variation.



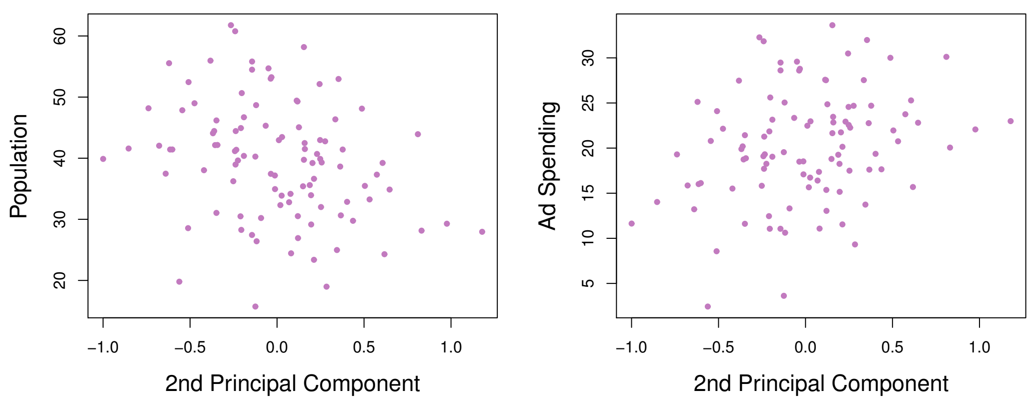
The population size (pop) and ad spending (ad) for 100 different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.



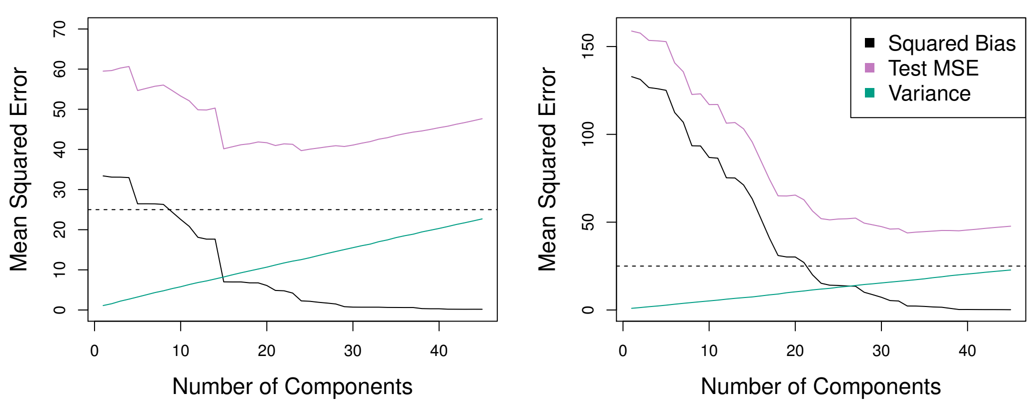
A subset of the advertising data. Left: The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments. Right: The left-hand panel has been rotated so that the first principal component lies on the x-axis.



Plots of the first principal component scores z_i^1 versus pop and ad. The relationships are strong.

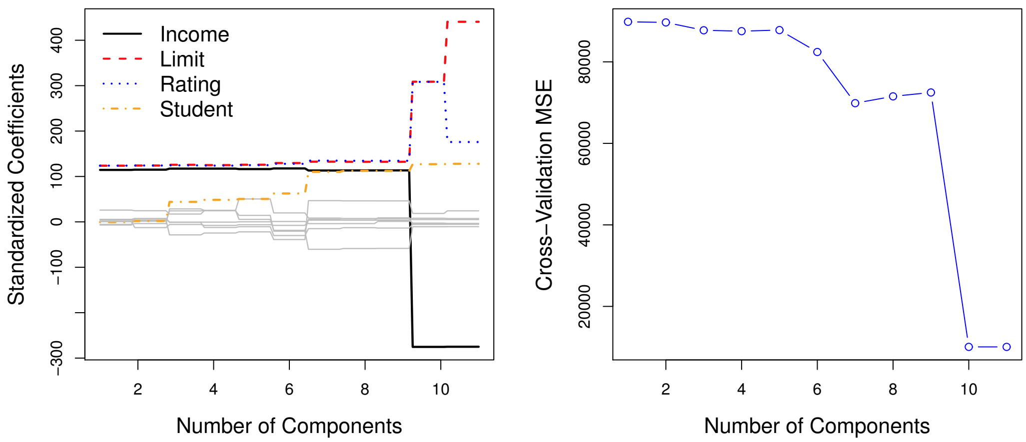


Plots of the second principal component scores z_i^2 versus pop and ad. The relationships are weak.



PCR was applied to two simulated data sets. The black, green, and purple lines correspond to squared bias, variance, and test mean squared error, respectively. Left: Simulated data on page 9. Right: Simulated data on page 12.

Choosing the number of directions M



PCR standardized coefficient estimates on the Credit data set for different values of M. Right: The 10-fold cross validation MSE obtained using PCR, as a function of M.

6.3.2 Partial Least Squares

- PCR identifies linear combinations, or directions, that best represent the predictors $X_1, \ldots, X_p$.
- These directions are identified in an unsupervised way, since the response Y is not used to help determine the principal component directions.
- That is, the response does not supervise the identification of the principal components.
- Consequently, PCR suffers from a potentially serious drawback: there is no guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response.
- Like PCR, PLS is a dimension reduction method, which first identifies a new set of features $Z_1, \ldots, Z_M$ that are linear combinations of the original features, and then fits a linear model via OLS using these M new features.

- But unlike PCR, PLS identifies these new features in a supervised way. That is, it makes use of the response Y in order to identify new features that not only approximate the old features well, but also that are related to the response. Roughly speaking, the PLS approach attempts to find directions that help explain both the response and the predictors.

- After standardizing the p predictors, PLS computes the first direction Z_1 by setting each ϕ_{j1} in $Z_m = \sum_{j=1}^{p} \phi_{mj} X_j$ equal to the coefficient from the simple linear regression of Y onto X_j.

- One can show that this coefficient is proportional to the correlation between Y and X_j.

- Hence, in computing $Z_1 = \sum_{j=1}^{p} \phi_{j1} X_j$, PLS places the highest weight on the variables that are most strongly related to the response.

- Subsequent directions are found by taking residuals and then repeating the above prescription.