final seven-component model PCR fit, 46.69%. This is because PCR only attempts to maximize the amount of variance explained in the predictors, while PLS searches for directions that explain variance in both the predictors and the response.

6.8 Exercises

Conceptual

- 1. We perform best subset, forward stepwise, and backward stepwise selection on a single data set. For each approach, we obtain p + 1 models, containing $0, 1, 2, \ldots, p$ predictors. Explain your answers:
 - (a) Which of the three models with k predictors has the smallest training RSS?
 - (b) Which of the three models with k predictors has the smallest test RSS?
 - (c) True or False:
 - i. The predictors in the k-variable model identified by forward stepwise are a subset of the predictors in the (k+1)-variable model identified by forward stepwise selection.
 - ii. The predictors in the k-variable model identified by backward stepwise are a subset of the predictors in the (k+1)-variable model identified by backward stepwise selection.
 - iii. The predictors in the k-variable model identified by backward stepwise are a subset of the predictors in the (k+1)-variable model identified by forward stepwise selection.
 - iv. The predictors in the k-variable model identified by forward stepwise are a subset of the predictors in the (k+1)-variable model identified by backward stepwise selection.
 - v. The predictors in the k-variable model identified by best subset are a subset of the predictors in the (k+1)-variable model identified by best subset selection.
- 2. For parts (a) through (c), indicate which of i. through iv. is correct. Justify your answer.
 - (a) The lasso, relative to least squares, is:
 - More flexible and hence will give improved prediction accuracy when its increase in bias is less than its decrease in variance.
 - More flexible and hence will give improved prediction accuracy when its increase in variance is less than its decrease in bias.

- iii. Less flexible and hence will give improved prediction accuracy when its increase in bias is less than its decrease in variance.
- iv. Less flexible and hence will give improved prediction accuracy when its increase in variance is less than its decrease in bias.
- (b) Repeat (a) for ridge regression relative to least squares.
- (c) Repeat (a) for non-linear methods relative to least squares.
- 3. Suppose we estimate the regression coefficients in a linear regression model by minimizing

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \le s$$

for a particular value of s. For parts (a) through (e), indicate which of i. through v. is correct. Justify your answer.

- (a) As we increase s from 0, the training RSS will:
 - i. Increase initially, and then eventually start decreasing in an inverted U shape.
 - ii. Decrease initially, and then eventually start increasing in a U shape.
 - iii. Steadily increase.
 - iv. Steadily decrease.
 - v. Remain constant.
- (b) Repeat (a) for test RSS.
- (c) Repeat (a) for variance.
- (d) Repeat (a) for (squared) bias.
- (e) Repeat (a) for the irreducible error.
- 4. Suppose we estimate the regression coefficients in a linear regression model by minimizing

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

for a particular value of λ . For parts (a) through (e), indicate which of i. through v. is correct. Justify your answer.

- (a) As we increase λ from 0, the training RSS will:
 - Increase initially, and then eventually start decreasing in an inverted U shape.
 - ii. Decrease initially, and then eventually start increasing in a U shape.
 - iii. Steadily increase.
 - iv. Steadily decrease.
 - v. Remain constant.
- (b) Repeat (a) for test RSS.
- (c) Repeat (a) for variance.
- (d) Repeat (a) for (squared) bias.
- (e) Repeat (a) for the irreducible error.
- 5. It is well-known that ridge regression tends to give similar coefficient values to correlated variables, whereas the lasso may give quite different coefficient values to correlated variables. We will now explore this property in a very simple setting.



Suppose that n=2, p=2, $x_{11}=x_{12}$, $x_{21}=x_{22}$. Furthermore, suppose that $y_1+y_2=0$ and $x_{11}+x_{21}=0$ and $x_{12}+x_{22}=0$, so that the estimate for the intercept in a least squares, ridge regression, or lasso model is zero: $\hat{\beta}_0=0$.

- (a) Write out the ridge regression optimization problem in this setting.
- (b) Argue that in this setting, the ridge coefficient estimates satisfy $\hat{\beta}_1 = \hat{\beta}_2$.
- (c) Write out the lasso optimization problem in this setting.
- (d) Argue that in this setting, the lasso coefficients $\hat{\beta}_1$ and $\hat{\beta}_2$ are not unique—in other words, there are many possible solutions to the optimization problem in (c). Describe these solutions.
- 6. We will now explore (6.12) and (6.13) further.
 - (a) Consider (6.12) with p = 1. For some choice of y_1 and $\lambda > 0$, plot (6.12) as a function of β_1 . Your plot should confirm that (6.12) is solved by (6.14).
 - (b) Consider (6.13) with p = 1. For some choice of y_1 and $\lambda > 0$, plot (6.13) as a function of β_1 . Your plot should confirm that (6.13) is solved by (6.15).



- 7. We will now derive the Bayesian connection to the lasso and ridge regression discussed in Section 6.2.2.
 - (a) Suppose that $y_i = \beta_0 + \sum_{j=1}^p x_{ij}\beta_j + \epsilon_i$ where $\epsilon_1, \dots, \epsilon_n$ are independent and identically distributed from a $N(0, \sigma^2)$ distribution. Write out the likelihood for the data.
 - (b) Assume the following prior for β : β_1, \ldots, β_p are independent and identically distributed according to a double-exponential distribution with mean 0 and common scale parameter b: i.e. $p(\beta) = \frac{1}{2b} \exp(-|\beta|/b)$. Write out the posterior for β in this setting.
 - (c) Argue that the lasso estimate is the *mode* for β under this posterior distribution.
 - (d) Now assume the following prior for β : β_1, \ldots, β_p are independent and identically distributed according to a normal distribution with mean zero and variance c. Write out the posterior for β in this setting.
 - (e) Argue that the ridge regression estimate is both the *mode* and the *mean* for β under this posterior distribution.

Applied

- 8. In this exercise, we will generate simulated data, and will then use this data to perform best subset selection.
 - (a) Use the rnorm() function to generate a predictor X of length n = 100, as well as a noise vector ϵ of length n = 100.
 - (b) Generate a response vector Y of length n=100 according to the model

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon,$$

where β_0 , β_1 , β_2 , and β_3 are constants of your choice.

(c) Use the regsubsets() function to perform best subset selection in order to choose the best model containing the predictors X, X^2, \ldots, X^{10} . What is the best model obtained according to C_p , BIC, and adjusted R^2 ? Show some plots to provide evidence for your answer, and report the coefficients of the best model obtained. Note you will need to use the data.frame() function to create a single data set containing both X and Y.

- (d) Repeat (c), using forward stepwise selection and also using backwards stepwise selection. How does your answer compare to the results in (c)?
- (e) Now fit a lasso model to the simulated data, again using X, X^2 , ..., X^{10} as predictors. Use cross-validation to select the optimal value of λ . Create plots of the cross-validation error as a function of λ . Report the resulting coefficient estimates, and discuss the results obtained.
- (f) Now generate a response vector Y according to the model

$$Y = \beta_0 + \beta_7 X^7 + \epsilon,$$

and perform best subset selection and the lasso. Discuss the results obtained.

- 9. In this exercise, we will predict the number of applications received using the other variables in the College data set.
 - (a) Split the data set into a training set and a test set.
 - (b) Fit a linear model using least squares on the training set, and report the test error obtained.
 - (c) Fit a ridge regression model on the training set, with λ chosen by cross-validation. Report the test error obtained.
 - (d) Fit a lasso model on the training set, with λ chosen by cross-validation. Report the test error obtained, along with the number of non-zero coefficient estimates.
 - (e) Fit a PCR model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.
 - (f) Fit a PLS model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.
 - (g) Comment on the results obtained. How accurately can we predict the number of college applications received? Is there much difference among the test errors resulting from these five approaches?
- 10. We have seen that as the number of features used in a model increases, the training error will necessarily decrease, but the test error may not. We will now explore this in a simulated data set.
 - (a) Generate a data set with p=20 features, n=1,000 observations, and an associated quantitative response vector generated according to the model

$$Y = X\beta + \epsilon$$
,

where β has some elements that are exactly equal to zero.

- (b) Split your data set into a training set containing 100 observations and a test set containing 900 observations.
- (c) Perform best subset selection on the training set, and plot the training set MSE associated with the best model of each size.
- (d) Plot the test set MSE associated with the best model of each size.
- (e) For which model size does the test set MSE take on its minimum value? Comment on your results. If it takes on its minimum value for a model containing only an intercept or a model containing all of the features, then play around with the way that you are generating the data in (a) until you come up with a scenario in which the test set MSE is minimized for an intermediate model size.
- (f) How does the model at which the test set MSE is minimized compare to the true model used to generate the data? Comment on the coefficient values.
- (g) Create a plot displaying $\sqrt{\sum_{j=1}^{p} (\beta_j \hat{\beta}_j^r)^2}$ for a range of values of r, where $\hat{\beta}_j^r$ is the jth coefficient estimate for the best model containing r coefficients. Comment on what you observe. How does this compare to the test MSE plot from (d)?
- 11. We will now try to predict per capita crime rate in the Boston data set.
 - (a) Try out some of the regression methods explored in this chapter, such as best subset selection, the lasso, ridge regression, and PCR. Present and discuss results for the approaches that you consider.
 - (b) Propose a model (or set of models) that seem to perform well on this data set, and justify your answer. Make sure that you are evaluating model performance using validation set error, crossvalidation, or some other reasonable alternative, as opposed to using training error.
 - (c) Does your chosen model involve all of the features in the data set? Why or why not?