Resampling Methods

Are tools, involve repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model. ***For example, in order to estimate the variability of a linear regression fit.***

The process of evaluating a model's performance is known as ***model assessment*** whereas the process of selecting the proper level of flexibility for a model is known as ***model selection*** .

Cross-Validation:

The Validation Set Approach: It involves randomly dividing the available set of observations into two parts, ***a training set and a validation set or hold-out set*** . The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set. The resulting validation set error rate—typically assessed using MSE in the case of a quantitative response—provides an estimate of the test error rate.

We can assess the model using p-values, but we could also assess it using the validation method. We randomly split the available set of observations into trainings set and validation set. We can fit the model on training set and can get validation set error rates and can compare this error rate for different model. For example, the validation set MSE for the quadratic fit is considerably smaller than for the linear fit. However, the validation set MSE for the cubic fit is actually slightly larger than for the quadratic fit. This implies that including a cubic term in the regression does not lead to better prediction than simply using a quadratic term.

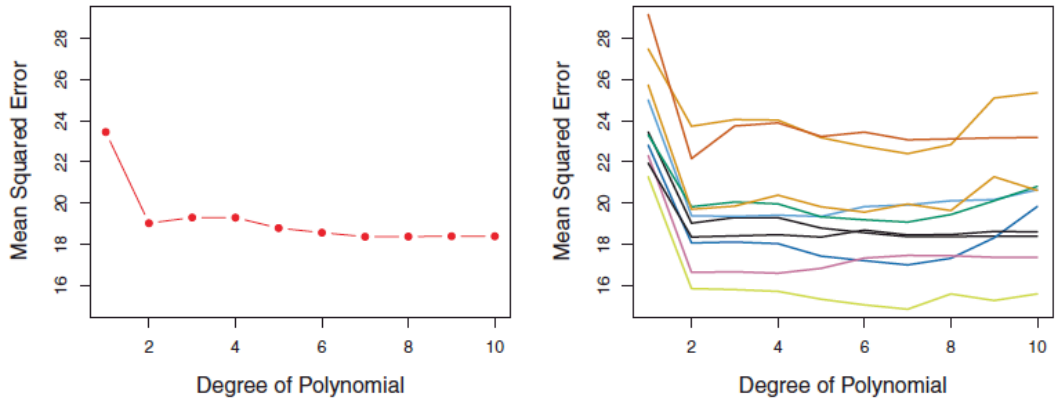


FIGURE 5.2. *The validation set approach was used on the* `Auto` *data set in order to estimate the test error that results from predicting* `mpg` *using polynomial functions of* `horsepower`. Left: *Validation error estimates for a single split into training and validation data sets.* Right: *The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability in the estimated test MSE that results from this approach.*

it has two potential drawbacks:
1. As is shown in the right-hand panel of Figure 5.2, the validation estimate of the test error rate can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
2. Since statistical methods tend to perform worse when trained on fewer observations, this suggests that the validation set error rate may tend to overestimate the test error rate for the model fit on the entire data set

Leave-One-Out Cross-Validation:

Instead of creating two subsets of comparable size, a single observation (x_1, y_1) is used for the validation set, and the remaining observations $\{(x_2, y_2), \ldots, (x_n, y_n)\}$ make up the training set.

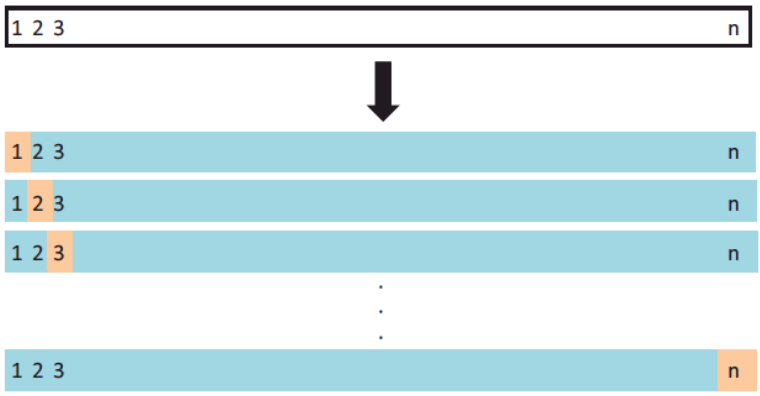


FIGURE 5.3. *A schematic display of LOOCV. A set of n data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in beige). The test error is then estimated by averaging the n resulting MSE's. The first training set contains all but observation 1, the second training set contains all but observation 2, and so forth.*

The LOOCV estimate for the test MSE is the average of these n test error estimates:

$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\mathrm{MSE}_i. \qquad (5.1)$$

A schematic of the LOOCV approach is illustrated in Figure 5.3.

Advantages of LOOCV:

1. It has far less bias. The LOOCV approach tends not to overestimate the test error rate as much as the validation set approach does. As it is using n-1 observations.
2. In contrast to the validation approach which will yield different results when applied repeatedly due to randomness in the training/validation set splits, performing LOOCV multiple times will always yield the same results: there is no randomness in the training/validation set splits.

Disadvantage:

1. LOOCV has the potential to be expensive to implement, since the model has to be fit n times.

k-Fold Cross-Validation:

An alternative to LOOCV is k-fold CV . This approach involves randomly dividing the set of observations into k groups, or folds , of approximately equal size. The first fold is treated as a validation set, and the method is fit on the remaining k − 1 folds. The mean squared error, MSE1 , is then computed on the observations in the held-out fold. This procedure is repeated k times; each time, a different group of observations is treated as a validation set. This process results in k estimates of the test error, MSE1, MSE2, . . . , MSEk . The k -fold CV estimate is computed by averaging these values,

$$\mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k}\mathrm{MSE}_i. \tag{5.3}$$

Purpose of cross validation:

- How well a given statistical learning procedure can be expected to perform on independent data; in this case, the actual estimate of the test MSE isof interest.
- But at other times we are interested only in the location of the minimum point in the estimated test MSE curve . This is because we might be performing cross-validation on a number of statistical learning methods, or on a single method using different levels of flexibility, in order to identify the method that results in the lowest test error. For this purpose,the location of the minimum point in the estimated test MSE curve is important, but the actual value of the estimated test MSE is not.

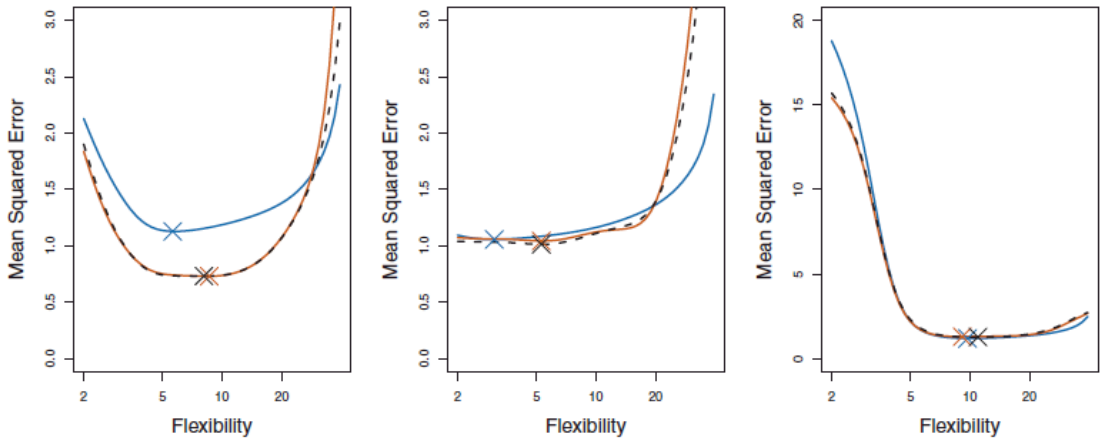


FIGURE 5.6. *True and estimated test MSE for the simulated data sets in Figures 2.9 (*left*), 2.10 (*center*), and 2.11 (*right*). The true test MSE is shown in blue, the LOOCV estimate is shown as a black dashed line, and the* 10*-fold CV estimate is shown in orange. The crosses indicate the minimum of each of the MSE curves.*

Bias-Variance Trade-Off for k-Fold Cross-Validation:

We mentioned in Section 5.1.3 that k -fold CV with k < n has a computational advantage to LOOCV. But putting computational issues aside, ***a less obvious but potentially more important advantage of k -fold CV is that it often gives more accurate estimates of the test error rate than does LOOCV.*** This has to do with a bias-variance trade-off.

LOOCV has low bias and high variance, But k-fold CV has high bias and low variance.

To summarize, there is a bias-variance trade-off associated with the choice of k in k -fold cross validation.

Cross-Validation on Classification Problems

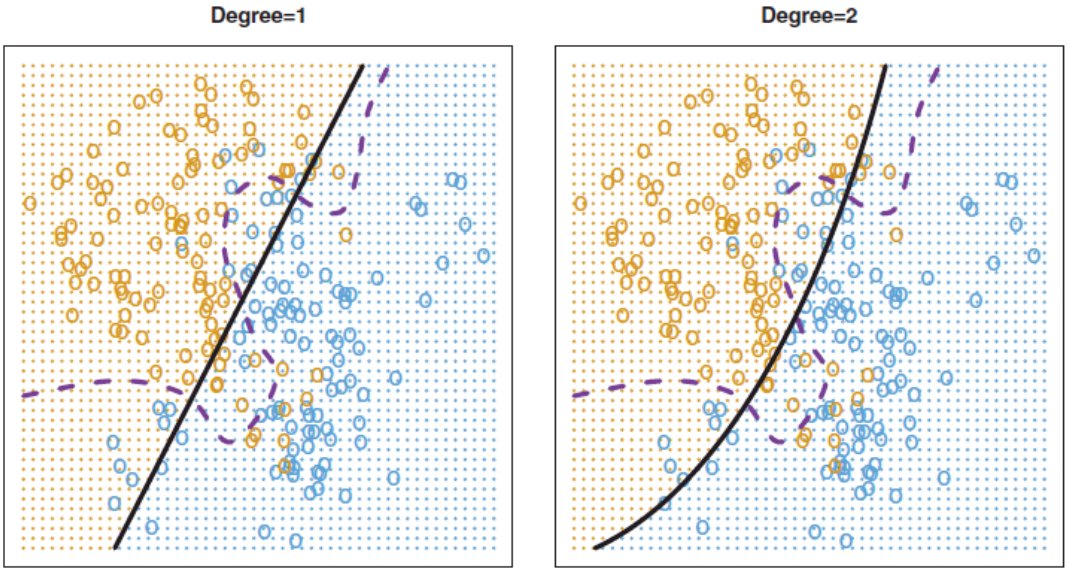
For instance, in the classification setting, the LOOCV error rate takes the form

$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{Err}_i, \tag{5.4}$$

where $\mathrm{Err}_i = I(y_i \neq \hat{y}_i)$. The k-fold CV error rate and validation set error rates are defined analogously.

As an example, we fit various logistic regression models on the two dimensional classification data displayed in Figure 2.13. we can fit a quadratic logistic regression model, given by

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2 + \beta_4 X_2^2. \tag{5.5}$$



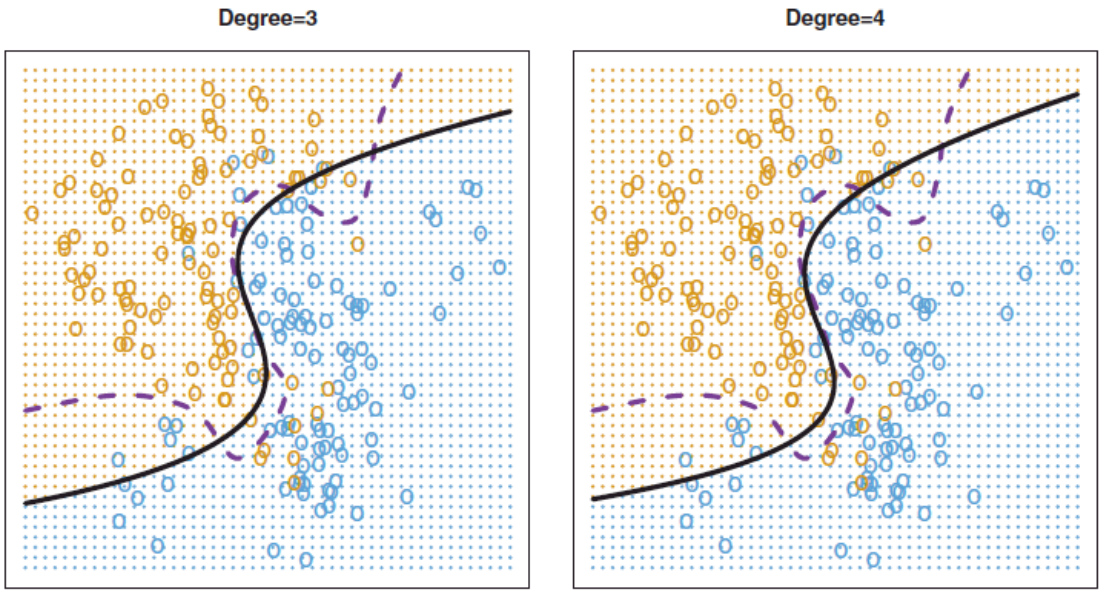


FIGURE 5.7. *Logistic regression fits on the two-dimensional classification data displayed in Figure 2.13. The Bayes decision boundary is represented using a purple dashed line. Estimated decision boundaries from linear, quadratic, cubic and quartic (degrees 1–4) logistic regressions are displayed in black. The test error rates for the four logistic regression fits are respectively* 0.201, 0.197, 0.160, *and* 0.162, *while the Bayes error rate is* 0.133.

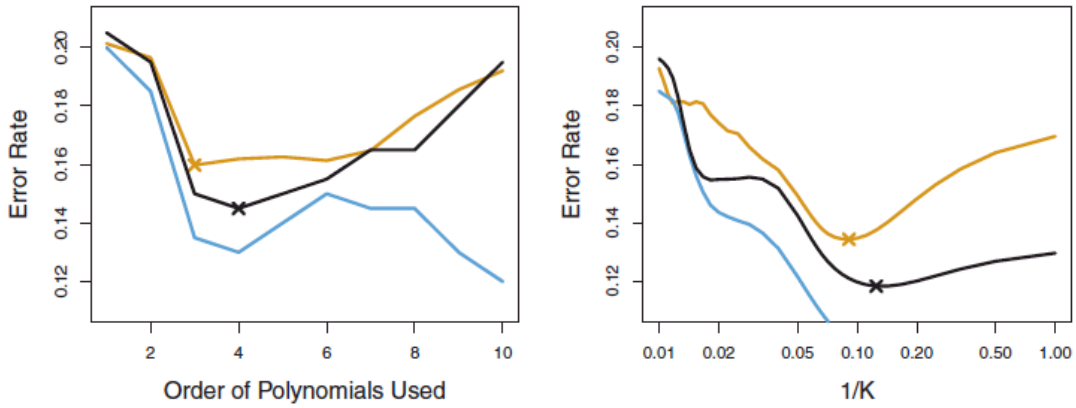


FIGURE 5.8. *Test error (brown), training error (blue), and* 10*-fold CV error (black) on the two-dimensional classification data displayed in Figure 5.7.* Left: *Logistic regression using polynomial functions of the predictors. The order of the polynomials used is displayed on the x-axis.* Right: *The KNN classifier with different values of K, the number of neighbors used in the KNN classifier.*

Above curve for test-error for cross validation, can be used to choose required flexibility for which we will get minimum test error.

The Bootstrap:

The bootstrap is a widely applicable and extremely powerful statistical tool that can be used to ***quantify the uncertainty associated with a given estimator or statistical learning method.*** As a simple example, the bootstrap can be used to estimate the standard errors of the coefficients from a linear regression fit. the power of the bootstrap lies in the fact that it can be easily applied to a wide range of statistical learning methods, including some for which a measure of variability is otherwise difficult to obtain and is not automatically output by statistical software.

For example: **Don't go much into how the things are getting calculated but see how bootstrap is working

Suppose that we wish to invest a fixed sum of money in two financial assets that yield returns of X and Y , respectively, where X and Y are random quantities. We will invest a fraction α of our money in X , and willinvest the remaining 1 − α in Y . Since there is variability associated with the returns on these two assets, we wish to choose α to minimize the total risk, or variance, of our investment. In other words, we want to minimize Var(αX +(1 −α)Y). One can show that the value that minimizes the risk is given by

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}, \tag{5.6}$$

where $\sigma_X^2 = \text{Var}(X), \sigma_Y^2 = \text{Var}(Y)$, and $\sigma_{XY} = \text{Cov}(X, Y)$.

In reality, the quantities σ_X^2, σ_Y^2, and σ_{XY} are unknown. We can compute estimates for these quantities, $\hat{\sigma}_X^2$, $\hat{\sigma}_Y^2$, and $\hat{\sigma}_{XY}$, using a data set that contains past measurements for X and Y. We can then estimate the value of α that minimizes the variance of our investment using

$$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}. \tag{5.7}$$

It is natural to wish to quantify the accuracy of our estimate of α . To estimate the standard deviation of ˆα , we repeated the process of simulating 100 paired observations of X and Y , and estimating α using (5.7),

1,000 times. We thereby obtained 1,000 estimates for α, which we can call $\hat{\alpha}_1, \hat{\alpha}_2, \ldots, \hat{\alpha}_{1,000}$. The left-hand panel of Figure 5.10 displays a histogram of the resulting estimates. For these simulations the parameters were set to $\sigma_X^2 = 1, \sigma_Y^2 = 1.25$, and $\sigma_{XY} = 0.5$, and so we know that the true value of α is 0.6. We indicated this value using a solid vertical line on the histogram. The mean over all 1,000 estimates for α is

$$\bar{\alpha} = \frac{1}{1,000} \sum_{r=1}^{1,000} \hat{\alpha}_r = 0.5996,$$

very close to $\alpha = 0.6$, and the standard deviation of the estimates is

$$\sqrt{\frac{1}{1,000 - 1} \sum_{r=1}^{1,000} (\hat{\alpha}_r - \bar{\alpha})^2} = 0.083.$$

This gives us a very good idea of the accuracy of $\hat{\alpha}$: $\mathrm{SE}(\hat{\alpha}) \approx 0.083$. So roughly speaking, for a random sample from the population, we would expect $\hat{\alpha}$ to differ from α by approximately 0.08, on average.

But problem is, for real data we cannot generate new samples from the original population. However, the bootstrap approach allows us to use a computer to emulate the process of obtaining new sample sets,

Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets by repeatedly sampling observations from the original data set .

This approach is illustrated in Figure 5.11 on a simple data set, which we call Z, that contains only $n = 3$ observations. We randomly select n observations from the data set in order to produce a bootstrap data set, Z^{*1}. The sampling is performed with *replacement*, which means that the same observation can occur more than once in the bootstrap data set. In this example, Z^{*1} contains the third observation twice, the first observation once, and no instances of the second observation. Note that if an observation is contained in Z^{*1}, then both its X and Y values are included. We can use Z^{*1} to produce a new bootstrap estimate for α, which we call $\hat{\alpha}^{*1}$. This procedure is repeated B times for some large value of B, in order to produce B different bootstrap data sets, $Z^{*1}, Z^{*2}, \ldots, Z^{*B}$, and B corresponding α estimates, $\hat{\alpha}^{*1}, \hat{\alpha}^{*2}, \ldots, \hat{\alpha}^{*B}$. We can compute the standard error of these bootstrap estimates using the formula

$$\mathrm{SE}_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1} \sum_{r=1}^{B} \left(\hat{\alpha}^{*r} - \frac{1}{B} \sum_{r'=1}^{B} \hat{\alpha}^{*r'} \right)^2}. \tag{5.8}$$

This serves as an estimate of the standard error of $\hat{\alpha}$ estimated from the original data set.

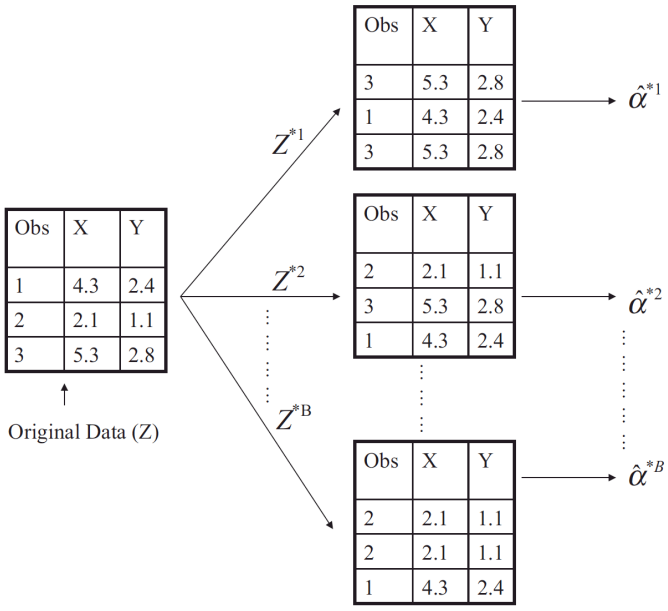


FIGURE 5.11. *A graphical illustration of the bootstrap approach on a small sample containing $n = 3$ observations. Each bootstrap data set contains n observations, sampled with replacement from the original data set. Each bootstrap data set is used to obtain an estimate of α.*

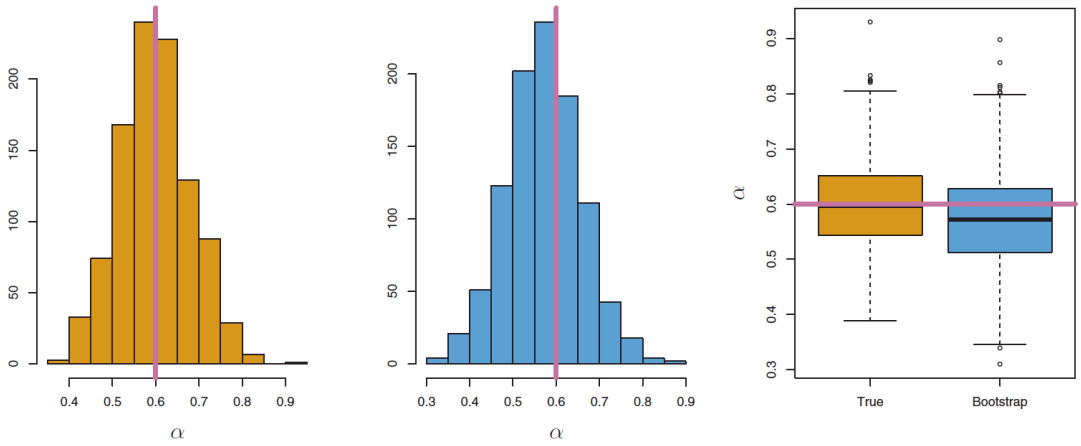


FIGURE 5.10. Left: *A histogram of the estimates of α obtained by generating 1,000 simulated data sets from the true population.* Center: *A histogram of the estimates of α obtained from 1,000 bootstrap samples from a single data set.* Right: *The estimates of α displayed in the left and center panels are shown as boxplots. In each panel, the pink line indicates the true value of α.*

The bootstrap approach is illustrated in the center panel of Figure 5.10, which displays a histogram of 1,000 bootstrap estimates of α , each computed using a distinct bootstrap data set. This panel was constructed on the basis of a single data set, and hence could be created using real data. Note that the histogram looks very similar to the left-hand panel which displays the idealized histogram of the estimates of α obtained by generating

1,000 simulated data sets from the true population. In particular the bootstrap estimate SE(ˆα) from (5.8) is 0. 087, very close to the estimate of 0. 083 obtained using 1,000 simulated data sets. The right-hand panel displays the information in the center and left panels in a different way, via boxplots of the estimates for α obtained by generating 1,000 simulated data sets from the true population and using the bootstrap approach. Again, the boxplots are quite similar to each other, indicating that the bootstrap approach can be used to effectively estimate the variability associated with ˆα .

Estimating the Accuracy of a Linear Regression Model

The bootstrap approach can be used to assess the variability of the coefficient estimates and predictions from a statistical learning method. Here we use the bootstrap approach in order to assess the variability of the estimates for β_0 and β_1, the intercept and slope terms for the linear regression model that uses `horsepower` to predict `mpg` in the `Auto` data set. We will compare the estimates obtained using the bootstrap to those obtained using the formulas for $\mathrm{SE}(\hat{\beta}_0)$ and $\mathrm{SE}(\hat{\beta}_1)$ described in Section 3.1.2.

We first create a simple function, `boot.fn()`, which takes in the `Auto` data set as well as a set of indices for the observations, and returns the intercept and slope estimates for the linear regression model. We then apply this function to the full set of 392 observations in order to compute the estimates of β_0 and β_1 on the entire data set using the usual linear regression coefficient estimate formulas from Chapter 3. Note that we do not need the { and } at the beginning and end of the function because it is only one line long.

```
> boot.fn=function(data,index)
+ return(coef(lm(mpg~horsepower,data=data,subset=index)))
> boot.fn(Auto,1:392)
(Intercept) horsepower
   39.936   -0.158
```

The `boot.fn()` function can also be used in order to create bootstrap estimates for the intercept and slope terms by randomly sampling from among the observations with replacement. Here we give two examples.

```
> set.seed(1)
> boot.fn(Auto,sample(392,392,replace=T))
(Intercept) horsepower
  38.739     -0.148
> boot.fn(Auto,sample(392,392,replace=T))
(Intercept) horsepower
  40.038     -0.160
```

Next, we use the `boot()` function to compute the standard errors of 1,000 bootstrap estimates for the intercept and slope terms.

```
> boot(Auto,boot.fn,1000)

ORDINARY NONPARAMETRIC BOOTSTRAP

Call:
boot(data = Auto, statistic = boot.fn, R = 1000)

Bootstrap Statistics :
    original     bias    std. error
t1* 39.936       0.0297   0.8600
t2* -0.158      -0.0003   0.0074
```

This indicates that the bootstrap estimate for $\mathrm{SE}(\hat{\beta}_0)$ is 0.86, and that the bootstrap estimate for $\mathrm{SE}(\hat{\beta}_1)$ is 0.0074. As discussed in Section 3.1.2, standard formulas can be used to compute the standard errors for the regression coefficients in a linear model. These can be obtained using the `summary()` function.

```
> summary(lm(mpg~horsepower,data=Auto))$coef
             Estimate Std. Error t value  Pr(>|t|)
(Intercept)    39.936    0.71750    55.7 1.22e-187
horsepower     -0.158    0.00645   -24.5  7.03e-81
```

The standard error estimates for $\hat{\beta}_0$ and $\hat{\beta}_1$ obtained using the formulas from Section 3.1.2 are 0.717 for the intercept and 0.0064 for the slope. Interestingly, these are somewhat different from the estimates obtained using the bootstrap. Does this indicate a problem with the bootstrap? In fact, it suggests the opposite. Recall that the standard formulas given in Equation 3.8 on page 66 rely on certain assumptions. For example, they depend on the unknown parameter σ^2, the noise variance. We then estimate σ^2 using the RSS. Now although the formula for the standard errors do not rely on the linear model being correct, the estimate for σ^2 does. We see in Figure 3.8 on page 91 that there is a non-linear relationship in the data, and so the residuals from a linear fit will be inflated, and so will $\hat{\sigma}^2$. Secondly, the standard formulas assume (somewhat unrealistically) that the x_i are fixed, and all the variability comes from the variation in the errors ϵ_i. The bootstrap approach does not rely on any of these assumptions, and so it is likely giving a more accurate estimate of the standard errors of $\hat{\beta}_0$ and $\hat{\beta}_1$ than is the `summary()` function.

Below we compute the bootstrap standard error estimates and the standard linear regression estimates that result from fitting the quadratic model to the data. Since this model provides a good fit to the data (Figure 3.8), there is now a better correspondence between the bootstrap estimates and the standard estimates of $\mathrm{SE}(\hat{\beta}_0)$, $\mathrm{SE}(\hat{\beta}_1)$ and $\mathrm{SE}(\hat{\beta}_2)$.

```
> boot.fn=function(data,index)
+ coefficients(lm(mpg~horsepower+I(horsepower^2),data=data,
    subset=index))
> set.seed(1)
> boot(Auto,boot.fn,1000)

ORDINARY NONPARAMETRIC BOOTSTRAP

Call:
boot(data = Auto, statistic = boot.fn, R = 1000)

Bootstrap Statistics :
     original     bias    std. error
t1*  56.900    6.098e-03 2.0945
t2* -0.466    -1.777e-04 0.0334
t3*  0.001     1.324e-06 0.0001

> summary(lm(mpg~horsepower+I(horsepower^2),data=Auto))$coef
                Estimate  Std. Error  t value  Pr(>|t|)
(Intercept)      56.9001    1.80043       32 1.7e-109
horsepower       -0.4662    0.03112      -15  2.3e-40
I(horsepower^2)   0.0012    0.00012       10  2.2e-21
```