

FIGURE 3.20. Test MSE for linear regression (black dashed lines) and KNN (green curves) as the number of variables p increases. The true function is non-linear in the first variable, as in the lower panel in Figure 3.19, and does not depend on the additional variables. The performance of linear regression deteriorates slowly in the presence of these additional noise variables, whereas KNN's performance degrades much more quickly as p increases.

very poor prediction of $f(x_0)$ and hence a poor KNN fit. As a general rule, parametric methods will tend to outperform non-parametric approaches when there is a small number of observations per predictor.

Even in problems in which the dimension is small, we might prefer linear regression to KNN from an interpretability standpoint. If the test MSE of KNN is only slightly lower than that of linear regression, we might be willing to forego a little bit of prediction accuracy for the sake of a simple model that can be described in terms of just a few coefficients, and for which p-values are available.

3.6 Lab: Linear Regression

3.6.1 Libraries

The library() function is used to load *libraries*, or groups of functions and data sets that are not included in the base R distribution. Basic functions that perform least squares linear regression and other simple analyses come standard with the base distribution, but more exotic functions require additional libraries. Here we load the MASS package, which is a very large collection of data sets and functions. We also load the ISLR package, which includes the data sets associated with this book.

library()

```
> library(MASS)
> library(ISLR)
```

If you receive an error message when loading any of these libraries, it likely indicates that the corresponding library has not yet been installed on your system. Some libraries, such as ${\tt MASS}$, come with ${\tt R}$ and do not need to be separately installed on your computer. However, other packages, such as

ISLR, must be downloaded the first time they are used. This can be done directly from within R. For example, on a Windows system, select the Install package option under the Packages tab. After you select any mirror site, a list of available packages will appear. Simply select the package you wish to install and R will automatically download the package. Alternatively, this can be done at the R command line via install.packages("ISLR"). This installation only needs to be done the first time you use a package. However, the library() function must be called each time you wish to use a given package.

3.6.2 Simple Linear Regression

The MASS library contains the Boston data set, which records medv (median house value) for 506 neighborhoods around Boston. We will seek to predict medv using 13 predictors such as rm (average number of rooms per house), age (average age of houses), and lstat (percent of households with low socioeconomic status).

```
> fix(Boston)
> names(Boston)
[1] "crim"  "zn"  "indus"  "chas"  "nox"  "rm"  "age"
[8] "dis"  "rad"  "tax"  "ptratio"  "black"  "lstat"  "medy"
```

To find out more about the data set, we can type ?Boston.

We will start by using the lm() function to fit a simple linear regression model, with medv as the response and lstat as the predictor. The basic syntax is $lm(y\sim x,data)$, where y is the response, x is the predictor, and data is the data set in which these two variables are kept.

```
> lm.fit=lm(medv~lstat)
Error in eval(expr, envir, enclos) : Object "medv" not found
```

The command causes an error because R does not know where to find the variables medv and lstat. The next line tells R that the variables are in Boston. If we attach Boston, the first line works fine because R now recognizes the variables.

```
> lm.fit=lm(medv~lstat,data=Boston)
> attach(Boston)
> lm.fit=lm(medv~lstat)
```

If we type lm.fit, some basic information about the model is output. For more detailed information, we use summary(lm.fit). This gives us p-values and standard errors for the coefficients, as well as the R^2 statistic and F-statistic for the model.

lm()

```
Coefficients:
(Intercept)
                   lstat
     34.55
                   -0.95
> summary(lm.fit)
Call:
lm(formula = medv \sim lstat)
Residuals:
  Min 1Q Median
                       3 Q
                               Max
-15.17 -3.99 -1.32 2.03 24.50
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 34.5538 0.5626 61.4 <2e-16 ***
lstat -0.9500 0.0387 -24.5 <2e-16 ***
lstat
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 6.22 on 504 degrees of freedom
Multiple R-squared: 0.544, Adjusted R-squared: 0.543
F-statistic: 602 on 1 and 504 DF, p-value: <2e-16
```

We can use the names() function in order to find out what other pieces of information are stored in lm.fit. Although we can extract these quantities by name—e.g. lm.fit\$coefficients—it is safer to use the extractor functions like coef() to access them.

ames(

```
coef()

> names(lm.fit)

[1] "coefficients" "residuals" "effects"

[4] "rank" "fitted.values" "assign"

[7] "qr" "df.residual" "xlevels"

[10] "call" "terms" "model"

> coef(lm.fit)

(Intercept) lstat

34.55 -0.95
```

In order to obtain a confidence interval for the coefficient estimates, we can use the **confint()** command.

confint()

```
> confint(lm.fit)
2.5 % 97.5 %
(Intercept) 33.45 35.659
lstat -1.03 -0.874
```

The predict() function can be used to produce confidence intervals and prediction intervals for the prediction of medv for a given value of lstat.

predict()

For instance, the 95% confidence interval associated with a lstat value of 10 is (24.47, 25.63), and the 95% prediction interval is (12.828, 37.28). As expected, the confidence and prediction intervals are centered around the same point (a predicted value of 25.05 for medv when lstat equals 10), but the latter are substantially wider.

We will now plot medv and lstat along with the least squares regression line using the plot() and abline() functions.

abline()

```
> plot(lstat,medv)
> abline(lm.fit)
```

There is some evidence for non-linearity in the relationship between lstat and medv. We will explore this issue later in this lab.

The abline() function can be used to draw any line, not just the least squares regression line. To draw a line with intercept a and slope b, we type abline(a,b). Below we experiment with some additional settings for plotting lines and points. The lwd=3 command causes the width of the regression line to be increased by a factor of 3; this works for the plot() and lines() functions also. We can also use the pch option to create different plotting symbols.

```
> abline(lm.fit,lwd=3)
> abline(lm.fit,lwd=3,col="red")
> plot(lstat,medv,col="red")
> plot(lstat,medv,pch=20)
> plot(lstat,medv,pch="+")
> plot(1:20,1:20,pch=1:20)
```

Next we examine some diagnostic plots, several of which were discussed in Section 3.3.3. Four diagnostic plots are automatically produced by applying the $\mathtt{plot}()$ function directly to the output from $\mathtt{lm}()$. In general, this command will produce one plot at a time, and hitting Enter will generate the next plot. However, it is often convenient to view all four plots together. We can achieve this by using the $\mathtt{par}()$ function, which tells \mathtt{R} to split the display screen into separate panels so that multiple plots can be viewed simultaneously. For example, $\mathtt{par}(\mathtt{mfrow=c(2,2)})$ divides the plotting region into a 2×2 grid of panels.

par(

```
> par(mfrow=c(2,2))
> plot(lm.fit)
```

Alternatively, we can compute the residuals from a linear regression fit using the residuals() function. The function rstudent() will return the studentized residuals, and we can use this function to plot the residuals against the fitted values.

residuals()
rstudent()

```
> plot(predict(lm.fit), residuals(lm.fit))
> plot(predict(lm.fit), rstudent(lm.fit))
```

On the basis of the residual plots, there is some evidence of non-linearity. Leverage statistics can be computed for any number of predictors using the hatvalues() function.

hatvalues()

```
> plot(hatvalues(lm.fit))
> which.max(hatvalues(lm.fit))
375
```

The which.max() function identifies the index of the largest element of a vector. In this case, it tells us which observation has the largest leverage statistic.

hich.max()

3.6.3 Multiple Linear Regression

In order to fit a multiple linear regression model using least squares, we again use the lm() function. The syntax $lm(y\sim x1+x2+x3)$ is used to fit a model with three predictors, x1, x2, and x3. The summary() function now outputs the regression coefficients for all the predictors.

```
> lm.fit=lm(medv~lstat+age,data=Boston)
> summary(lm.fit)
lm(formula = medv \sim lstat + age, data = Boston)
Residuals:
  Min 1Q Median
                      3 Q
                             Max
-15.98 -3.98 -1.28 1.97 23.16
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 33.2228 0.7308 45.46 <2e-16 ***
lstat
           -1.0321
                       0.0482 -21.42
                                        <2e-16 ***
                                 2.83 0.0049 **
             0.0345
                      0.0122
age
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 6.17 on 503 degrees of freedom
Multiple R-squared: 0.551,
                             Adjusted R-squared: 0.549
F-statistic: 309 on 2 and 503 DF, p-value: <2e-16
```

The Boston data set contains 13 variables, and so it would be cumbersome to have to type all of these in order to perform a regression using all of the predictors. Instead, we can use the following short-hand:

```
> lm.fit=lm(medv~.,data=Boston)
> summary(lm.fit)

Call:
lm(formula = medv ~ ., data = Boston)
```

```
Residuals:
            1Q Median
   Min
                          30
                                 Max
-15.594 -2.730 -0.518
                        1.777 26.199
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 3.646e+01 5.103e+00 7.144 3.28e-12 ***
          -1.080e-01 3.286e-02 -3.287 0.001087 **
crim
           4.642e-02
                     1.373e-02 3.382 0.000778 ***
zn.
indus
           2.056e-02
                      6.150e-02
                                 0.334 0.738288
           2.687e+00 8.616e-01 3.118 0.001925 **
chas
           -1.777e+01 3.820e+00 -4.651 4.25e-06 ***
nox
           3.810e+00 4.179e-01 9.116 < 2e-16 ***
                     6.922e-04
age
dis
           -1.476e+00
           3.060e-01 6.635e-02 4.613 5.07e-06 ***
rad
           -1.233e-02 3.761e-03 -3.280 0.001112 **
tax
          -9.527e-01
                     1.308e-01 -7.283 1.31e-12 ***
ptratio
                                3.467 0.000573 ***
           9.312e-03
                      2.686e-03
black
           -5.248e-01 5.072e-02 -10.347 < 2e-16 ***
lstat
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 4.745 on 492 degrees of freedom
Multiple R-Squared: 0.7406, Adjusted R-squared: 0.7338
F-statistic: 108.1 on 13 and 492 DF, p-value: < 2.2e-16
```

We can access the individual components of a summary object by name (type ?summary.lm to see what is available). Hence summary(lm.fit)r.sq gives us the R^2 , and summary(lm.fit)sigma gives us the RSE. The vif() function, part of the car package, can be used to compute variance inflation factors. Most VIF's are low to moderate for this data. The car package is not part of the base R installation so it must be downloaded the first time you use it via the install.packages option in R.

vif(

```
> library(car)
> vif(lm.fit)
  crim
                 indus
                         chas
          zn
                                  nox
                                          rm
                                                  age
  1.79
          2.30
                 3.99
                          1.07
                                 4.39
                                         1.93
                                                 3.10
                  tax ptratio
                                        lstat
   dis
          rad
                                black
       7.48
               9.01 1.80
                               1.35
                                      2.94
```

What if we would like to perform a regression using all of the variables but one? For example, in the above regression output, age has a high p-value. So we may wish to run a regression excluding this predictor. The following syntax results in a regression using all predictors except age.

```
> lm.fit1=lm(medv~.-age,data=Boston)
> summary(lm.fit1)
...
```

Alternatively, the update() function can be used.

```
> lm.fit1=update(lm.fit, ~.-age)
```

3.6.4 Interaction Terms

It is easy to include interaction terms in a linear model using the lm() function. The syntax lstat:black tells R to include an interaction term between lstat and black. The syntax lstat*age simultaneously includes lstat, age, and the interaction term lstat*age as predictors; it is a shorthand for lstat+age+lstat:age.

```
> summary(lm(medv~lstat*age,data=Boston))
lm(formula = medv \sim lstat * age, data = Boston)
Residuals:
                     3 Q
       1Q Median
  Min
                           Max
-15.81 -4.04 -1.33 2.08 27.55
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 36.088536 1.469835 24.55 < 2e-16 ***
lstat
          -1.392117 0.167456 -8.31 8.8e-16 ***
          -0.000721 0.019879 -0.04 0.971
age
lstat:age 0.004156 0.001852 2.24
                                        0.025 *
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 6.15 on 502 degrees of freedom
Multiple R-squared: 0.556, Adjusted R-squared: 0.553
F-statistic: 209 on 3 and 502 DF, p-value: <2e-16
```

3.6.5 Non-linear Transformations of the Predictors

The lm() function can also accommodate non-linear transformations of the predictors. For instance, given a predictor X, we can create a predictor X^2 using $I(X^2)$. The function I() is needed since the $\hat{}$ has a special meaning in a formula; wrapping as we do allows the standard usage in \mathbb{R} , which is to raise \mathbb{X} to the power \mathbb{Z} . We now perform a regression of med v onto lstat and $lstat^2$.

I()

```
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 42.86201 0.87208 49.1 <2e-16 ***
lstat
           -2.33282
                       0.12380
                                -18.8
                                        <2e-16 ***
I(lstat^2) 0.04355
                      0.00375
                                 11.6
                                       <2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 5.52 on 503 degrees of freedom
Multiple R-squared: 0.641, Adjusted R-squared: 0.639
F-statistic: 449 on 2 and 503 DF, p-value: <2e-16
```

The near-zero p-value associated with the quadratic term suggests that it leads to an improved model. We use the <code>anova()</code> function to further quantify the extent to which the quadratic fit is superior to the linear fit.

anova(

```
> lm.fit=lm(medv~lstat)
> anova(lm.fit,lm.fit2)
Analysis of Variance Table

Model 1: medv ~ lstat
Model 2: medv ~ lstat + I(lstat^2)
   Res.Df   RSS Df Sum of Sq   F Pr(>F)
1     504   19472
2     503   15347   1     4125   135   <2e-16 ***
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1</pre>
```

Here Model 1 represents the linear submodel containing only one predictor, <code>lstat</code>, while Model 2 corresponds to the larger quadratic model that has two predictors, <code>lstat</code> and <code>lstat²</code>. The <code>anova()</code> function performs a hypothesis test comparing the two models. The null hypothesis is that the two models fit the data equally well, and the alternative hypothesis is that the full model is superior. Here the F-statistic is 135 and the associated p-value is virtually zero. This provides very clear evidence that the model containing the predictors <code>lstat</code> and <code>lstat²</code> is far superior to the model that only contains the predictor <code>lstat</code>. This is not surprising, since earlier we saw evidence for non-linearity in the relationship between <code>medv</code> and <code>lstat</code>. If we type

```
> par(mfrow=c(2,2))
> plot(lm.fit2)
```

then we see that when the lstat² term is included in the model, there is little discernible pattern in the residuals.

In order to create a cubic fit, we can include a predictor of the form <code>I(X^3)</code>. However, this approach can start to get cumbersome for higher-order polynomials. A better approach involves using the <code>poly()</code> function to create the polynomial within <code>lm()</code>. For example, the following command produces a fifth-order polynomial fit:

poly()

```
> lm.fit5=lm(medv~poly(lstat,5))
 summary(lm.fit5)
lm(formula = medv \sim poly(lstat, 5))
Residuals:
            10 Median
                           30
                                   Max
   Min
-13.543 -3.104 -0.705 2.084 27.115
Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)
               22.533 0.232 97.20 < 2e-16 ***
poly(lstat, 5)1 -152.460
                            5.215 -29.24 < 2e-16 ***
poly(lstat, 5)2 64.227
poly(lstat, 5)3 -27.051
                            5.215
                                    12.32
                                            < 2e-16 ***
                             5.215
                                     -5.19
                                            3.1e-07 ***
poly(lstat, 5)4
                25.452
                            5.215
                                      4.88 1.4e-06 ***
poly(lstat, 5)5 -19.252
                            5.215
                                    -3.69 0.00025 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 5.21 on 500 degrees of freedom
Multiple R-squared: 0.682, Adjusted R-squared: 0.679
F-statistic: 214 on 5 and 500 DF, p-value: <2e-16
```

This suggests that including additional polynomial terms, up to fifth order, leads to an improvement in the model fit! However, further investigation of the data reveals that no polynomial terms beyond fifth order have significant p-values in a regression fit.

Of course, we are in no way restricted to using polynomial transformations of the predictors. Here we try a log transformation.

```
> summary(lm(medv~log(rm),data=Boston))
...
```

3.6.6 Qualitative Predictors

We will now examine the Carseats data, which is part of the ISLR library. We will attempt to predict Sales (child car seat sales) in 400 locations based on a number of predictors.

```
> fix(Carseats)
> names(Carseats)
[1] "Sales" "CompPrice" "Income" "Advertising"
[5] "Population" "Price" "ShelveLoc" "Age"
[9] "Education" "Urban" "US"
```

The Carseats data includes qualitative predictors such as Shelveloc, an indicator of the quality of the shelving location—that is, the space within a store in which the car seat is displayed—at each location. The predictor Shelveloc takes on three possible values, Bad, Medium, and Good.

Given a qualitative variable such as Shelveloc, R generates dummy variables automatically. Below we fit a multiple regression model that includes some interaction terms.

```
> lm.fit=lm(Sales~.+Income:Advertising+Price:Age,data=Carseats)
> summary(lm.fit)
lm(formula = Sales \sim . + Income:Advertising + Price:Age, data =
Residuals:
         1Q Median
  Min
                       3 Q
                              Max
-2.921 -0.750 0.018 0.675
Coefficients:
                  Estimate Std. Error t value Pr(>|t|)
                                         6.52 2.2e-10 ***
(Intercept)
CompPrice
                                                < 2e-16 ***
                                         4.18 3.6e-05 ***
                  0.010894 0.002604
Income
                 0.070246 0.022609 3.11 0.00203 **
Advertising
                  0.000159 0.000368 0.43 0.66533
-0.100806 0.007440 -13.55 < 2e-16 ***
4.848676 0.152838 31.72 < 2e-16 ***
Population
Price
                  -0.100806
ShelveLocGood
                             0.125768 15.53 < 2e-16 ***
ShelveLocMedium
                  1.953262
                  -0.057947
                             0.015951
                                         -3.63 0.00032 ***
Age
                                       -1.06
                  -0.020852
                             0.019613
Education
                                                0.28836
UrbanYes
                   0.140160
                              0.112402
                                         1.25
                                                0.21317
                  -0.157557 0.148923 -1.06 0.29073
USYes
Income: Advertising 0.000751 0.000278 2.70 0.00729 **
                   0.000107
                              0.000133 0.80 0.42381
Price:Age
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 1.01 on 386 degrees of freedom
Multiple R-squared: 0.876,
                              Adjusted R-squared: 0.872
F-statistic: 210 on 13 and 386 DF, p-value: <2e-16
```

The contrasts() function returns the coding that R uses for the dummy variables.

contrasts()

Use ?contrasts to learn about other contrasts, and how to set them.

R has created a ShelveLocGood dummy variable that takes on a value of 1 if the shelving location is good, and 0 otherwise. It has also created a ShelveLocMedium dummy variable that equals 1 if the shelving location is medium, and 0 otherwise. A bad shelving location corresponds to a zero for each of the two dummy variables. The fact that the coefficient for

ShelveLocGood in the regression output is positive indicates that a good shelving location is associated with high sales (relative to a bad location). And ShelveLocMedium has a smaller positive coefficient, indicating that a medium shelving location leads to higher sales than a bad shelving location but lower sales than a good shelving location.

3.6.7 Writing Functions

As we have seen, R comes with many useful functions, and still more functions are available by way of R libraries. However, we will often be interested in performing an operation for which no function is available. In this setting, we may want to write our own function. For instance, below we provide a simple function that reads in the ISLR and MASS libraries, called LoadLibraries(). Before we have created the function, R returns an error if we try to call it.

```
> LoadLibraries
Error: object 'LoadLibraries' not found
> LoadLibraries()
Error: could not find function "LoadLibraries"
```

We now create the function. Note that the + symbols are printed by R and should not be typed in. The { symbol informs R that multiple commands are about to be input. Hitting *Enter* after typing { will cause R to print the + symbol. We can then input as many commands as we wish, hitting *Enter* after each one. Finally the } symbol informs R that no further commands will be entered.

```
> LoadLibraries=function(){
+ library(ISLR)
+ library(MASS)
+ print("The libraries have been loaded.")
+ }
```

Now if we type in LoadLibraries, R will tell us what is in the function.

```
> LoadLibraries
function(){
library(ISLR)
library(MASS)
print("The libraries have been loaded.")
}
```

If we call the function, the libraries are loaded in and the print statement is output.

```
> LoadLibraries()
[1] "The libraries have been loaded."
```