Lecture 8: Fitting Data

Statistical Computing, 36-350

Wednesday October 7, 2015

In previous episodes

- Loading and saving data sets in R format
- Loading and saving data sets in other structured formats
- Intro to regression modeling

Today

- Using data frames for statistical purposes
- Basics of regression modeling

So you've got a data frame

Recall prostate cancer data set from last time:

```
pros = read.table("http://statweb.stanford.edu/~tibs/ElemStatLearn/datasets/prostate.data")
nrow(pros)
```

```
## [1] 97
```

```
head(pros)
```

```
##       lcavol  lweight age      lbph svi       lcp gleason pgg45       lpsa
## 1 -0.5798185 2.769459  50 -1.386294   0 -1.386294       6     0 -0.4307829
## 2 -0.9942523 3.319626  58 -1.386294   0 -1.386294       6     0 -0.1625189
## 3 -0.5108256 2.691243  74 -1.386294   0 -1.386294       7    20 -0.1625189
## 4 -1.2039728 3.282789  58 -1.386294   0 -1.386294       6     0 -0.1625189
## 5  0.7514161 3.432373  62 -1.386294   0 -1.386294       6     0  0.3715636
## 6 -1.0498221 3.228826  50 -1.386294   0 -1.386294       6     0  0.7654678
##   train
## 1  TRUE
## 2  TRUE
## 3  TRUE
## 4  TRUE
## 5  TRUE
## 6  TRUE
```

What can we do with it?

- Plot it: examine multiple variables and distributions
- Test it: compare groups of individuals to each other

- Model it: try to predict, say, one variable from the others

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Recall the variables that we have measured over 97 men:

- `lpsa`: log PSA score
- `lcavol`: log cancer volume
- `lweight`: log prostate weight
- `age`: age of patient
- `lbph`: log of the amount of benign prostatic hyperplasia
- `svi`: seminal vesicle invasion
- `lcp`: log of capsular penetration
- `gleason`: Gleason score
- `pgg45`: percent of Gleason scores 4 or 5

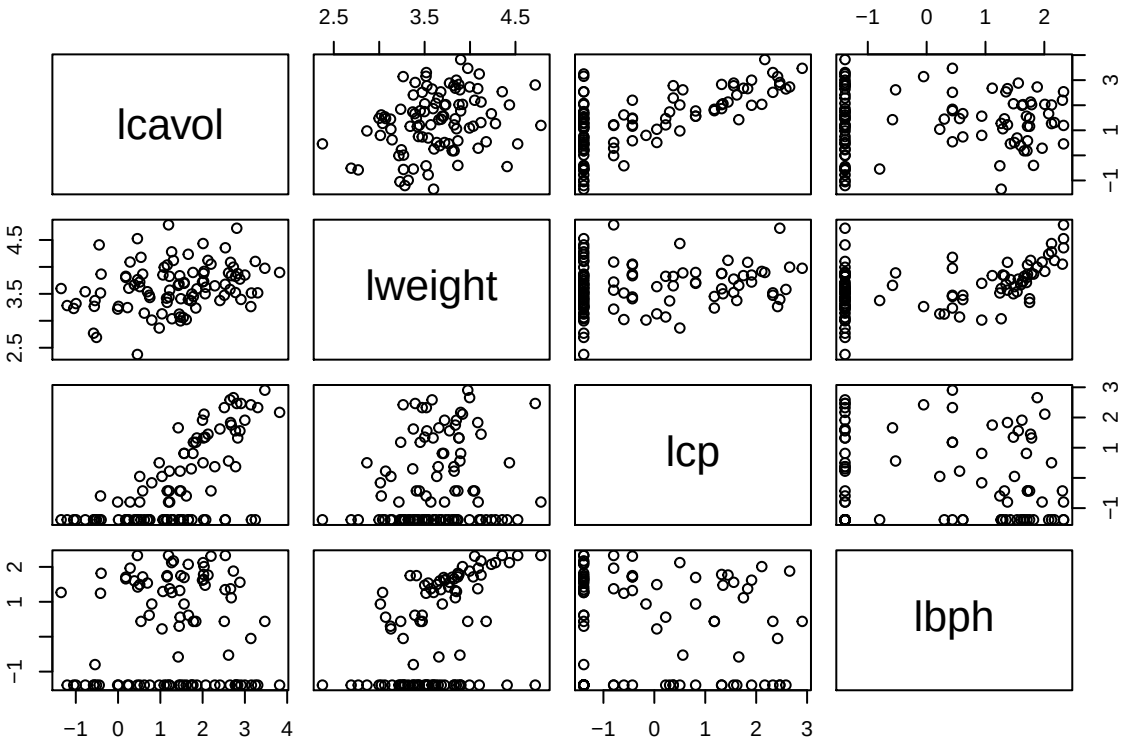
Last time we plotted the distribution of each varaible individually; and computed the correlations between variables; we learned that

- `lcp`, the log amount of capsular penetration, is very skewed; a bunch of men with little (or none?), then a big spread
- `lcp` and `lcavol`, the log cancer volumne, are highly positive correlated
- `gleason`, which records the current Gleason score, and `pgg45`, which records the historical percentage of Gleason scores 4 or 5, are highly positively correlated

Visualizing multiple relationships, with `pairs()`

Can easily look at multiple relationships at once, using the `pairs()` function:

```
pairs(~ lcavol + lweight + lcp + lbph, data=pros)
```



Numerical correlations:

```
cor(pros[,c("lcavol","lweight","lcp","lbph")])
```

```
##            lcavol   lweight          lcp         lbph
## lcavol  1.0000000 0.2805214  0.675310484  0.027349703
## lweight 0.2805214 1.0000000  0.164537142  0.442264399
## lcp     0.6753105 0.1645371  1.000000000 -0.006999431
## lbph    0.0273497 0.4422644 -0.006999431  1.000000000
```

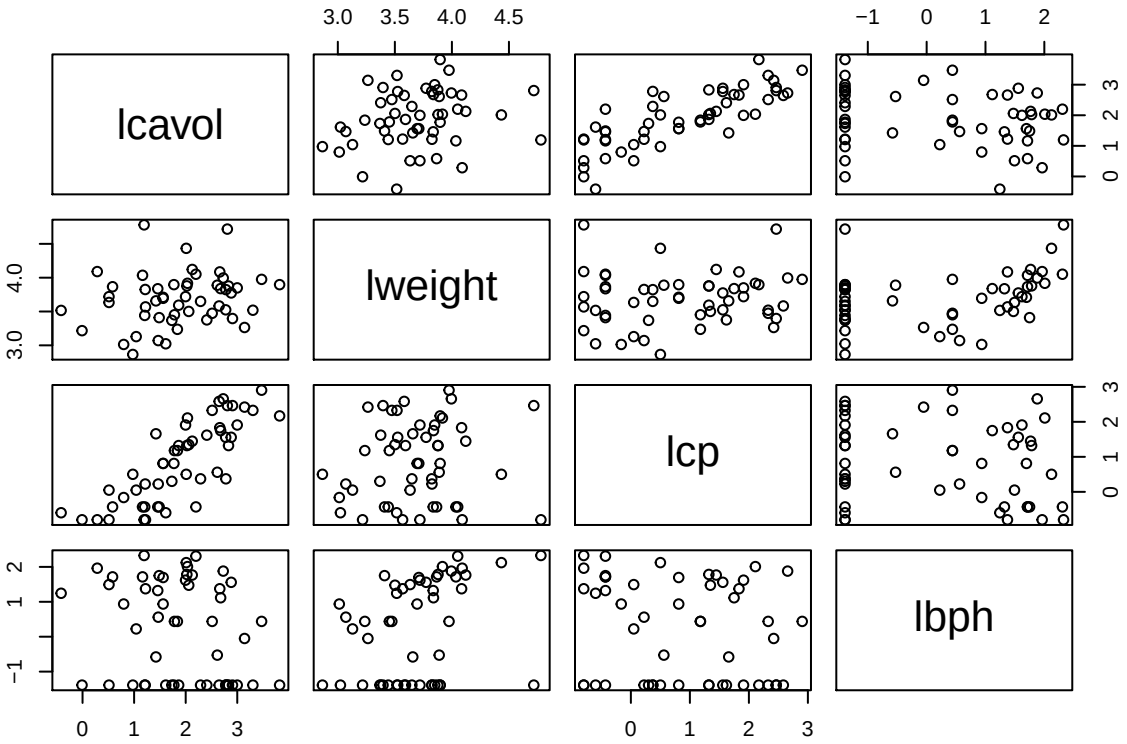
Inspecting relationships over a subset of the observations

We see that `lcp` takes a bunch of really low values, that appear to have little relationship with other variables. For exploratory purposes, let's get rid of them and see what the correlations look like

```
pros.subset = pros[pros$lcp > min(pros$lcp),]
nrow(pros.subset) # Beware, we've lost a half of our data!
```

```
## [1] 52
```

```
pairs(~ lcavol + lweight + lcp + lbph, data=pros.subset)
```



Numerical correlations:

```
cor(pros.subset[,c("lcavol","lweight","lcp","lbph")])
```

```
##             lcavol   lweight        lcp       lbph
## lcavol   1.0000000 0.2209352  0.8049728 -0.2407405
## lweight  0.2209352 1.0000000  0.1134501  0.3381993
## lcp      0.8049728 0.1134501  1.0000000 -0.1794318
## lbph    -0.2407405 0.3381993 -0.1794318  1.0000000
```

(Go back to our doctor friend ... ask if this makes sense ... he tells us that when the recorded capsular penetration value is that small, it basically means that it couldn't be accurately measured at that scale)

Testing means between two different groups

Recall that `svi`, the presence of seminal vesicle invasion, is binary:

```
table(pros$svi)
```

```
##
##  0  1
## 76 21
```

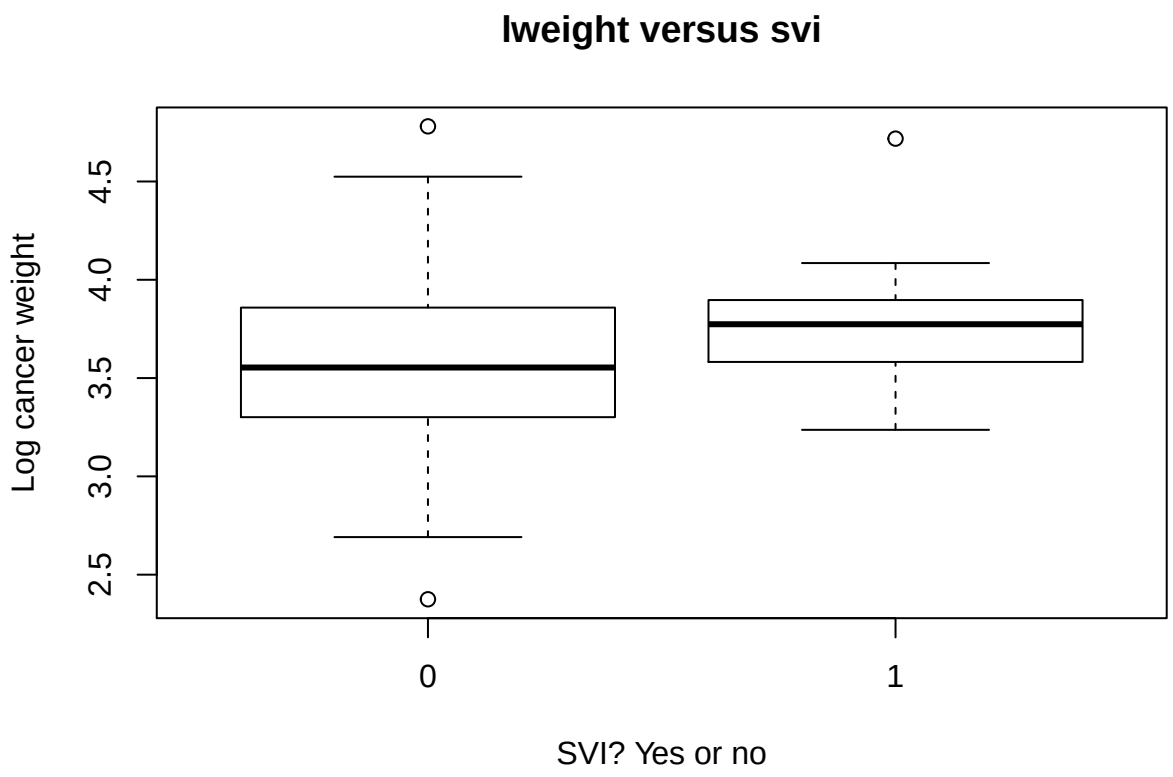
From http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1476128/:

> "When the pathologist's report following radical prostatectomy describes seminal vesicle invasion (SVI) ... prostate cancer in the areolar connective tissue around the seminal vesicles and outside the prostate ... generally the outlook for the patient is poor."

Does seminal vesicle invasion relate to the weight of the cancer?

Plot it first:

```
pros$svi = factor(pros$svi) # Making it a factor helps with plotting
plot(pros$svi, pros$lweight, main="lweight versus svi",
     xlab="SVI? Yes or no", ylab="Log cancer weight")
```



Tough to tell! Let's try a simple two-sample t-test:

```
t.test(pros$lweight[pros$svi==0], pros$lweight[pros$svi==1])
```

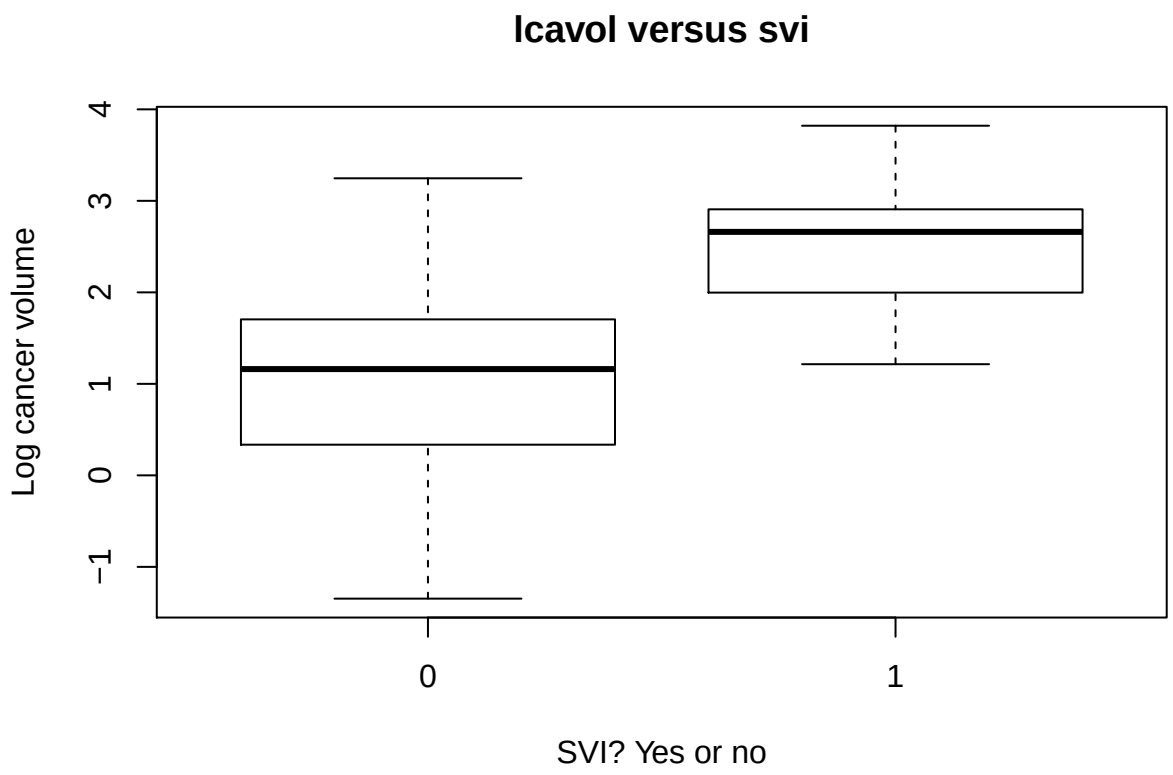
```
##
##  Welch Two Sample t-test
##
## data:  pros$lweight[pros$svi == 0] and pros$lweight[pros$svi == 1]
## t = -1.8266, df = 42.949, p-value = 0.07472
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
```

```
##  -0.33833495  0.01674335
## sample estimates:
## mean of x mean of y
##  3.594131  3.754927
```

Not much significance, it appears ...

What about the relationship to the volume of cancer?

```
plot(pros$svi, pros$lcavol, main="lcavol versus svi",
     xlab="SVI? Yes or no", ylab="Log cancer volume")
```



Try a two-sample t-test again:

```
t.test(pros$lcavol[pros$svi==0], pros$lcavol[pros$svi==1])
```

```
##
##  Welch Two Sample t-test
##
## data:  pros$lcavol[pros$svi == 0] and pros$lcavol[pros$svi == 1]
## t = -8.0351, df = 51.172, p-value = 1.251e-10
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
```

```
##  -1.917326 -1.150810
## sample estimates:
## mean of x mean of y
##  1.017892  2.551959
```

Wow, looks very significant! Should go report this to our doctor friend ...

(Warning: what's wrong with carrying out 5 more t-tests, for the rest of the variables, and taking the significant ones?)

Basic regression modeling

Let's use `lm()` to fit a basic linear model. Recall that this is a model of the form

$$Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \text{noise}$$

for *response* variable Y and *predictor* variables $X_1, \ldots X_p$. Goal is to estimate the coefficients $\beta_0, \beta_1, \ldots \beta_p$

The first argument of `lm()` is a formula, of the form `Y ~ X1 + X2 + ... Xp`. For example:

```
pros.lm.1 = lm(lpsa ~ lcavol + lweight, data=pros)
class(pros.lm.1)
```

```
## [1] "lm"
```

```
names(pros.lm.1)
```

```
##  [1] "coefficients"  "residuals"     "effects"       "rank"
##  [5] "fitted.values" "assign"        "qr"            "df.residual"
##  [9] "xlevels"       "call"          "terms"         "model"
```

```
pros.lm.1
```

```
##
## Call:
## lm(formula = lpsa ~ lcavol + lweight, data = pros)
##
## Coefficients:
## (Intercept)       lcavol      lweight
##     -0.8134       0.6515       0.6647
```

Getting an overview with `summary()`

The function `summary()` gives us a nice summary of the linear model we just fit:

```
summary(pros.lm.1)
```

```
##
## Call:
## lm(formula = lpsa ~ lcavol + lweight, data = pros)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.61051 -0.44135 -0.04666  0.53542  1.90424
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -0.81344    0.65309  -1.246 0.216033
## lcavol       0.65154    0.06693   9.734 6.75e-16 ***
## lweight      0.66472    0.18414   3.610 0.000494 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7419 on 94 degrees of freedom
## Multiple R-squared:  0.5955, Adjusted R-squared:  0.5869
## F-statistic: 69.19 on 2 and 94 DF,  p-value: < 2.2e-16
```

This tells us

- The quantiles of the residuals: ideally, this is a perfect normal dist
- The coefficient estimates
- Their standard errors
- P-values for their individual significance
- (Adjusted) R-squared value: how much variability is explained by the model?
- F-statistic for the overall model significance

Getting rid of the intercept

To get rid of the intercept term, we add `+0` to the right-hand side of the formula:

```
pros.lm.2 = lm(lpsa ~ lcavol + lweight+ 0, data=pros)
summary(pros.lm.2)
```

```
##
## Call:
## lm(formula = lpsa ~ lcavol + lweight + 0, data = pros)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.63394 -0.51181  0.00925  0.49705  1.90715
##
## Coefficients:
##         Estimate Std. Error t value Pr(>|t|)
## lcavol   0.66394    0.06638   10.00   <2e-16 ***
## lweight  0.43894    0.03249   13.51   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 0.7441 on 95 degrees of freedom
## Multiple R-squared:  0.9273, Adjusted R-squared:  0.9258
## F-statistic: 606.1 on 2 and 95 DF,  p-value: < 2.2e-16
```

Is the intercept approriate? In general, depends on the variables that make up the linear model

Getting estimated coefficients with `coef()`

How can we access the values of estimated regression coefficients? Well, we could inspect the names of the fitted object:

```
names(pros.lm.1)
```

```
##  [1] "coefficients"  "residuals"     "effects"       "rank"
##  [5] "fitted.values" "assign"        "qr"            "df.residual"
##  [9] "xlevels"       "call"          "terms"         "model"
```

Then grab the appropriate component, as in:

```
pros.lm.1$coefficients
```

```
## (Intercept)      lcavol     lweight
##  -0.8134373   0.6515421   0.6647215
```

But this is not the best strategy. Instead, let's use the `coef()` function:

```
coef(pros.lm.1)
```

```
## (Intercept)      lcavol     lweight
##  -0.8134373   0.6515421   0.6647215
```

Learning to use R's built-in functions like `coef()` to access certain aspects of fitted statistical models is going to pay off in the long run, because most object types (beyond those fit by `lm()`) will allow for this kind of access

Getting the fitted values with `fitted()`

What does our model predict for the log PSA scores of the 97 mean in question? How do these compare to the acutal log PSA scores?

To answer the first question, we could extract the coefficients and then manually multiply and sum the appropriate values:

```
pros.coef = coef(pros.lm.1)
pros.fits.1 = pros.coef[1] + pros.coef[2]*pros$lweight +
  pros.coef[3]*pros$lcavol
```

This is wrong, oops! We mixed up the order of variables; forgot that `lcavol` was supposed to come before `lweight`

Try again:

```
pros.fits.2 = pros.coef[1] + pros.coef[2]*pros$lcavol +
  pros.coef[3]*pros$lweight
```

This strategy is laborious and error-prone; it's better to use `fitted()`, as in:

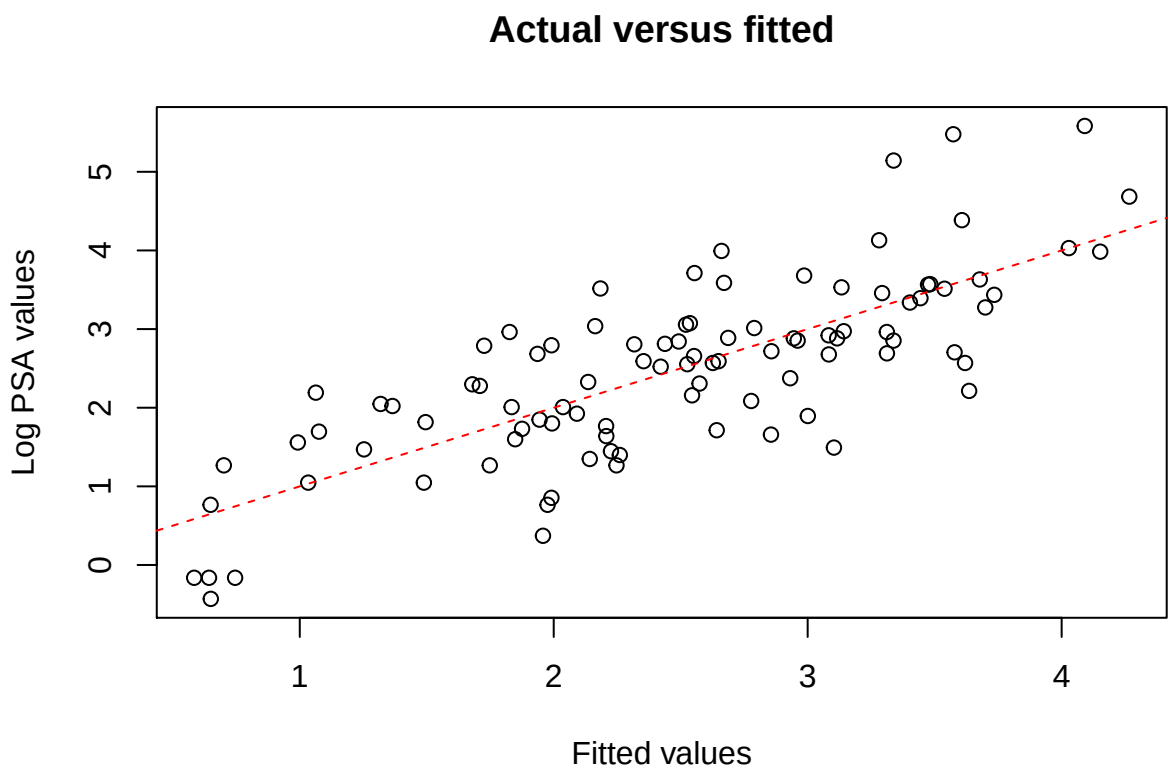
```
pros.fits.3 = fitted(pros.lm.1)
max(abs(pros.fits.3 - pros.fits.2)) # They are the same
```

```
## [1] 1.332268e-15
```

For the same reasons as before, it's good practice to use `fitted()`, a function that works with many common statistical objects in R

Let's plot the actual values versus the fitted ones

```
plot(pros.fits.3, pros$lpsa, main="Actual versus fitted",
     xlab="Fitted values", ylab="Log PSA values")
abline(a=0, b=1, lty=2, col="red")
```

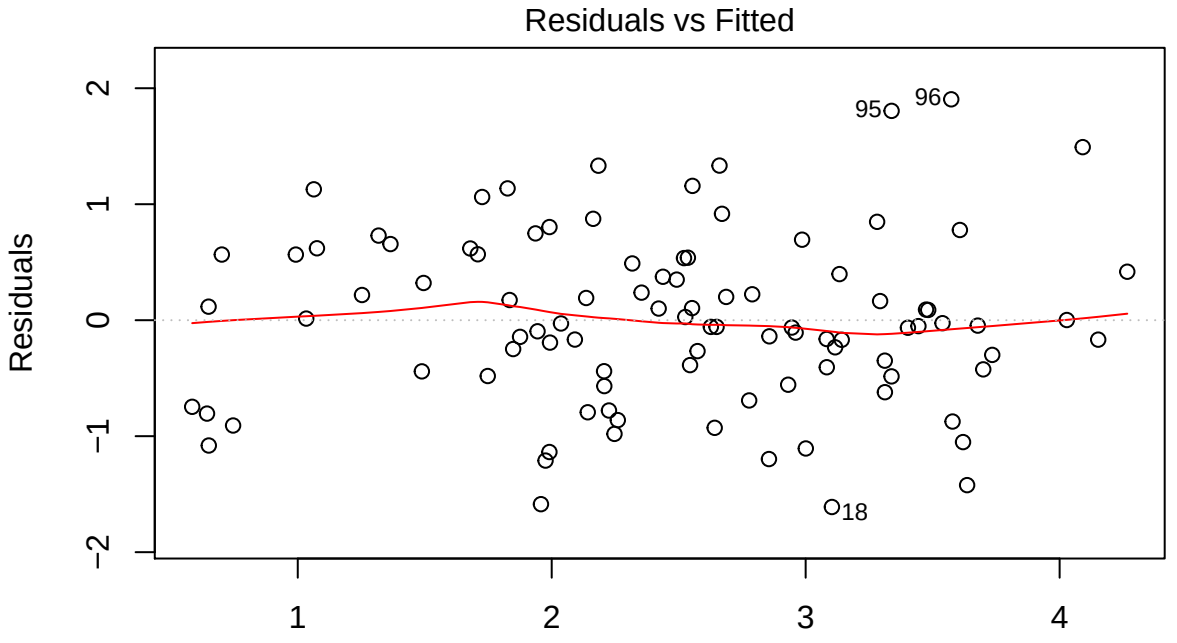


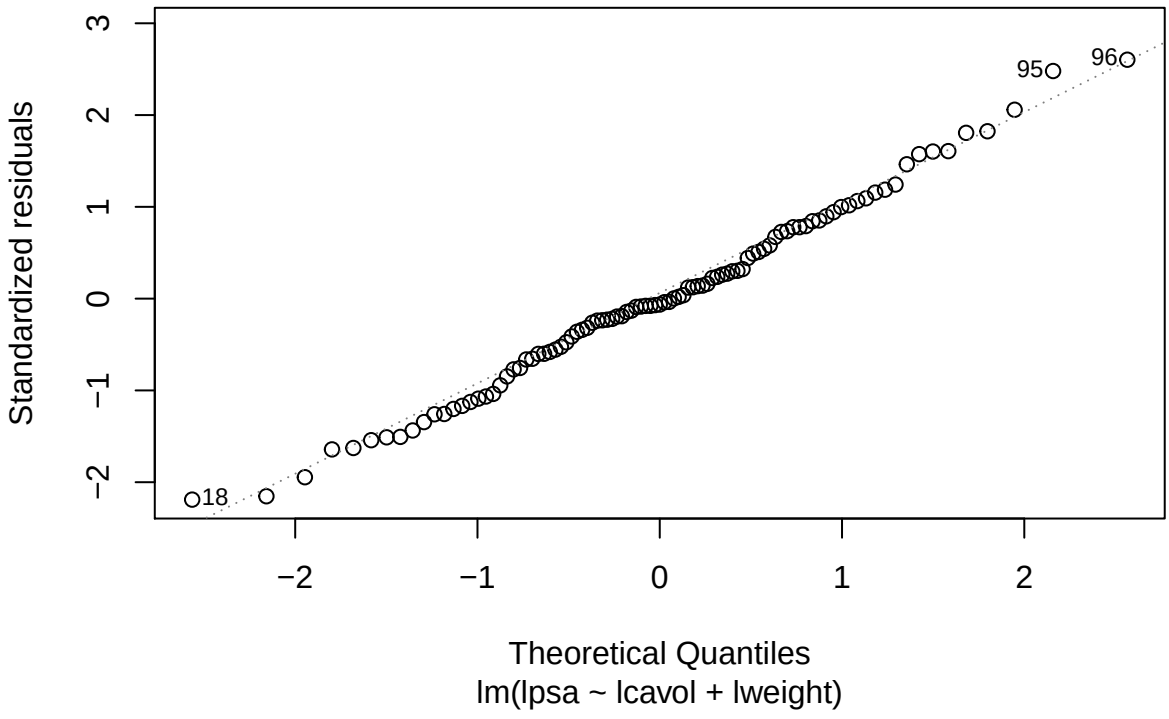
Appears to be a decent fit

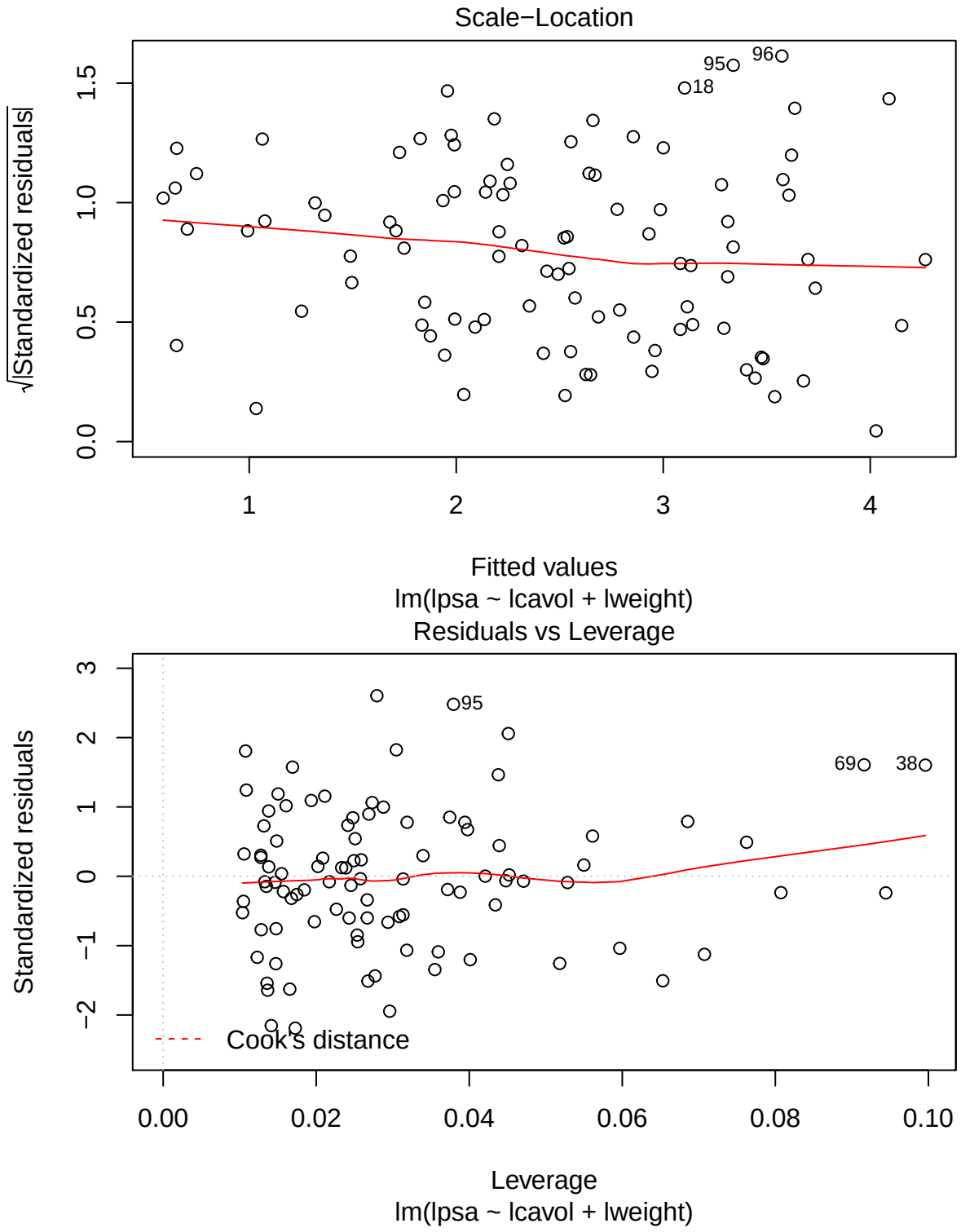
Running diagnostics with `plot()`

We can use the `plot()` function to run a series of diagnostic tests for our regression:

```
plot(pros.lm.1)
```







The results are pretty good

- Residuals versus fitted plot: points appear randomly scattered, no particular pattern

- Normal Q-Q plot: points are more or less along the 45 degree line, so residuals look close to a normal distribution
- Scale-location and residuals versus leverage plots: points appear to be groups, no points are too far from the center

There is a science (and an art?) to interpreting these; you'll learn a lot more in 36-401

Making predictions with `predict()`

Suppose we had a new observation from a man whose log cancer volume was 4.1, and log cancer weight was 4.5. What would our model estimate his log PSA score would be?

Two ways: manual way, and preferred way using `predict()`:

```
pros.pred.1 = pros.coef[1] + pros.coef[2]*4.1 +
  pros.coef[3]*4.5
pros.new = data.frame(lcavol=4.1, lweight=4.5)
pros.pred.2 = predict(pros.lm.1, newdata=pros.new)
abs(pros.pred.2 - pros.pred.1) # They are the same
```

```
## 1
## 0
```

Building a bigger model

We only used two variables in our regression; what happens if we use all 8?

```
pros.lm.3 = lm(lpsa ~ lcavol + lweight + age +
                 lbph + svi + lcp + gleason + pgg45,
               data=pros)
summary(pros.lm.3)
```

```
##
## Call:
## lm(formula = lpsa ~ lcavol + lweight + age + lbph + svi + lcp +
##     gleason + pgg45, data = pros)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.76644 -0.35510 -0.00328  0.38087  1.55770
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.181561   1.320568   0.137  0.89096
## lcavol       0.564341   0.087833   6.425 6.55e-09 ***
## lweight      0.622020   0.200897   3.096  0.00263 **
## age         -0.021248   0.011084  -1.917  0.05848 .
## lbph         0.096713   0.057913   1.670  0.09848 .
## svi1         0.761673   0.241176   3.158  0.00218 **
## lcp         -0.106051   0.089868  -1.180  0.24115
```

```
## gleason      0.049228   0.155341   0.317  0.75207
## pgg45        0.004458   0.004365   1.021  0.31000
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6995 on 88 degrees of freedom
## Multiple R-squared:  0.6634, Adjusted R-squared:  0.6328
## F-statistic: 21.68 on 8 and 88 DF,  p-value: < 2.2e-16
```

It's unclear whether the addition variables added much, based on their p-values

Comparing models based on test data

A very robust a sensible way to pit models against each other is to compare their *test errors*. That is, we hold out some data, and predict the log PSA values of the unseen observations

That last column in `pros`? Looks like the designers of the data set already defined *training* and *test* sets for us

```
head(pros)
```

```
##       lcavol  lweight age      lbph svi       lcp gleason pgg45       lpsa
## 1 -0.5798185 2.769459  50 -1.386294   0 -1.386294       6     0 -0.4307829
## 2 -0.9942523 3.319626  58 -1.386294   0 -1.386294       6     0 -0.1625189
## 3 -0.5108256 2.691243  74 -1.386294   0 -1.386294       7    20 -0.1625189
## 4 -1.2039728 3.282789  58 -1.386294   0 -1.386294       6     0 -0.1625189
## 5  0.7514161 3.432373  62 -1.386294   0 -1.386294       6     0  0.3715636
## 6 -1.0498221 3.228826  50 -1.386294   0 -1.386294       6     0  0.7654678
##   train
## 1  TRUE
## 2  TRUE
## 3  TRUE
## 4  TRUE
## 5  TRUE
## 6  TRUE
```

```
table(pros$train)
```

```
##
## FALSE  TRUE
##    30    67
```

Let's build our two regression models, using only 67 men—our training data:

```
pros.train = pros[pros$train==TRUE,]
pros.test = pros[pros$train==FALSE,]
pros.lm.train.1 = lm(lpsa ~ lcavol + lweight, data=pros.train)
pros.lm.train.2 = lm(lpsa ~ lcavol + lweight + age +
```

```
                      lbph + svi + lcp + gleason + pgg45,
                    data=pros.train)
pros.pred.1 = predict(pros.lm.train.1, newdata=pros.test)
pros.pred.2 = predict(pros.lm.train.2, newdata=pros.test)
test.err.1 = mean((pros.test$lpsa - pros.pred.1)^2)
test.err.2 = mean((pros.test$lpsa - pros.pred.2)^2)
test.err.1
```

```
## [1] 0.4924823
```

```
test.err.2
```

```
## [1] 0.521274
```

We may as well go with the simpler model! Aside from being simpler (which is a plus!) it predicts better, too

Summary

- Plotting, exploring, and performing basic statistical tests in R is easy to do with data frames
- R has powerful regression modeling tools; using them is easy, using them properly requires some training and care (you'll see a lot more in 36-401 and 36-402)