Linear Regression

Loading the required R packages

```
library(MASS)
#install.packages('corrplot')
library(corrplot)
library(ggplot2)
```

We use the Boston dataset that is a part of the MASS R package. Let's start by examining the dataset:

```
str(Boston)
```

```
## 'data.frame':    506 obs. of  14 variables:
##  $ crim   : num  0.00632 0.02731 0.02729 0.03237 0.06905 ...
##  $ zn     : num  18 0 0 0 0 0 12.5 12.5 12.5 12.5 ...
##  $ indus  : num  2.31 7.07 7.07 2.18 2.18 2.18 7.87 7.87 7.87 7.87 ...
##  $ chas   : int  0 0 0 0 0 0 0 0 0 0 ...
##  $ nox    : num  0.538 0.469 0.469 0.458 0.458 0.458 0.524 0.524 0.524
0.524 ...
##  $ rm     : num  6.58 6.42 7.18 7 7.15 ...
##  $ age    : num  65.2 78.9 61.1 45.8 54.2 58.7 66.6 96.1 100 85.9 ...
##  $ dis    : num  4.09 4.97 4.97 6.06 6.06 ...
##  $ rad    : int  1 2 2 3 3 3 5 5 5 5 ...
##  $ tax    : num  296 242 242 222 222 222 311 311 311 311 ...
##  $ ptratio: num  15.3 17.8 17.8 18.7 18.7 18.7 15.2 15.2 15.2 15.2 ...
##  $ black  : num  397 397 393 395 397 ...
##  $ lstat  : num  4.98 9.14 4.03 2.94 5.33 ...
##  $ medv   : num  24 21.6 34.7 33.4 36.2 28.7 22.9 27.1 16.5 18.9 ...
```

We will seek to predict medv (median house value) using (some of) the other 13 variables.

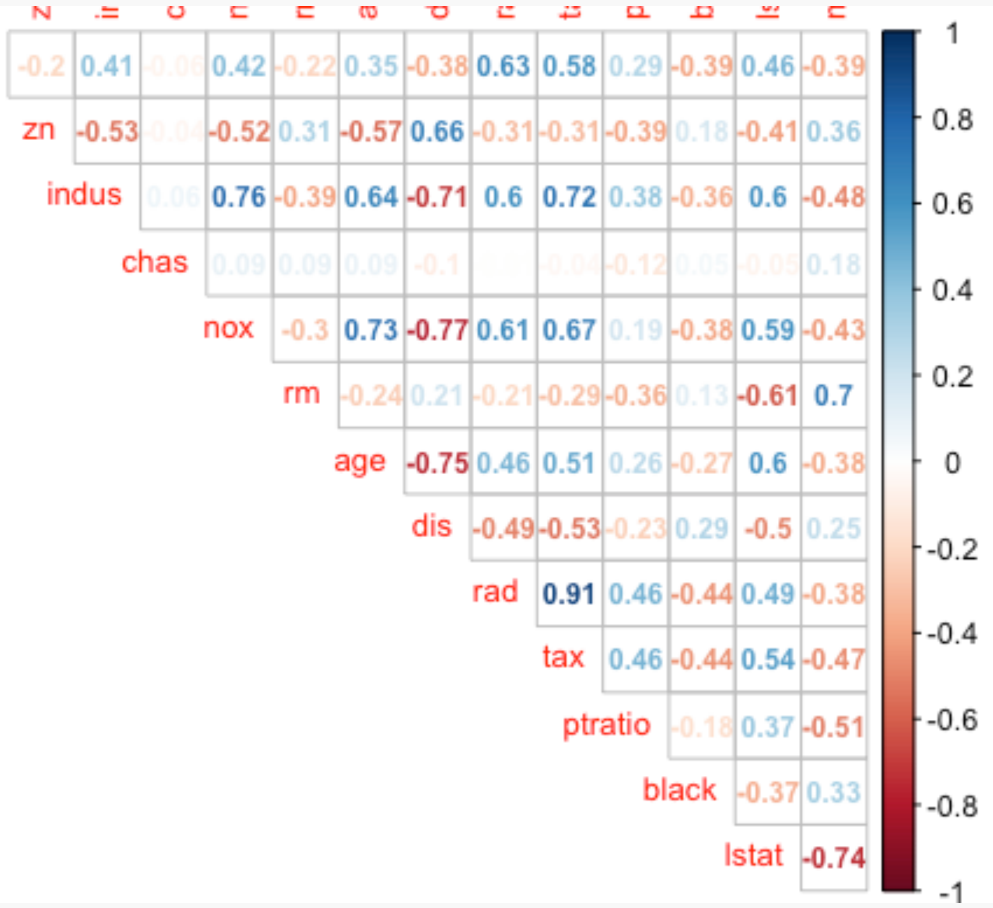
To find out more about the data set, type ?Boston

```
?Boston
```

Let's start by examining which of the 13 predictors might be relevant for predicting the response valiable (medv). One way to do that is to examine correlation between the predictors and the response variable.

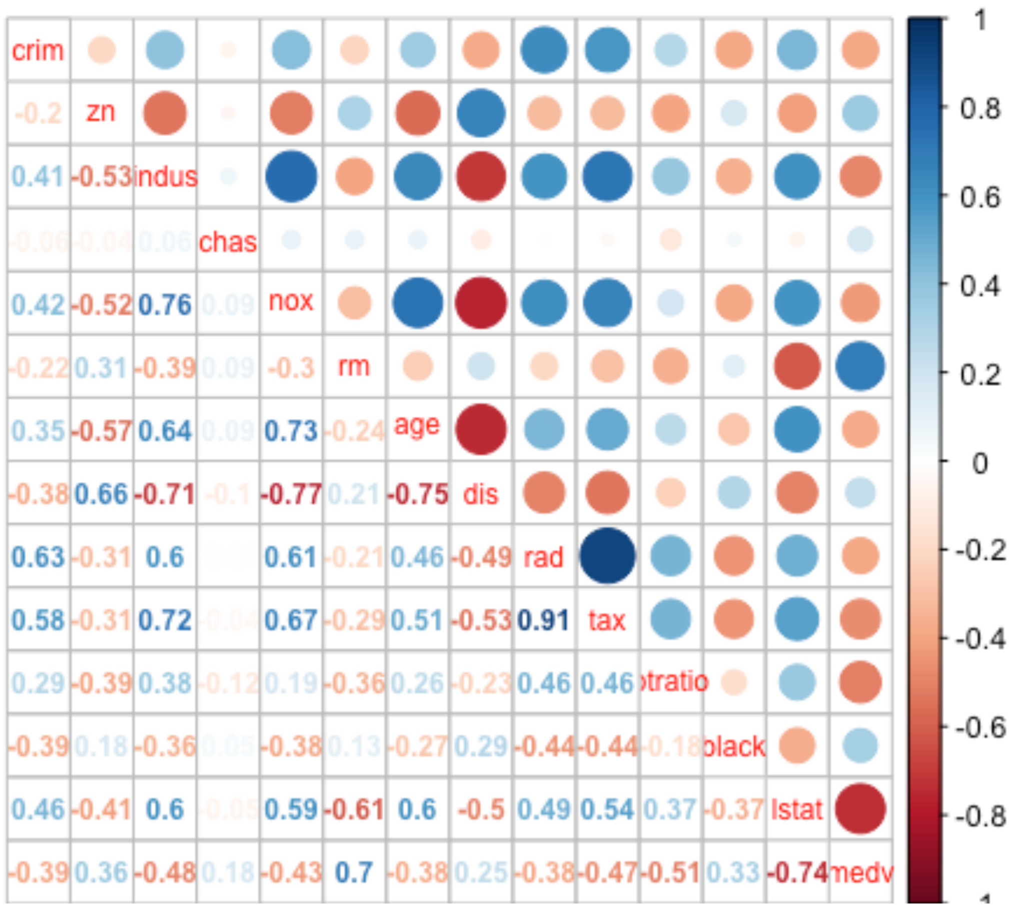
Since we have many variables, examining a correlation matrix will not be that easy, so, it is better to plot the correlations. To that end, we'll use the *corrplot* package. To explore the plotting options offered by this package, check: https://cran.r-project.org/web/packages/corrplot/vignettes/corrplot-intro.html

```r
# compute the correlation matrix
corr.matrix <- cor(Boston)
# one option for plotting correlations: using colors to represent the extent
of correlation
corrplot(corr.matrix, method = "number", type = "upper", diag = FALSE,
         number.cex=0.75, tl.cex = 0.85)
```



crim	-0.2	0.41	-0.06	0.42	-0.22	0.35	-0.38	0.63	0.58	0.29	-0.39	0.46	-0.39
zn		-0.53	-0.04	-0.52	0.31	-0.57	0.66	-0.31	-0.31	-0.39	0.18	-0.41	0.36
indus			0.06	0.76	-0.39	0.64	-0.71	0.6	0.72	0.38	-0.36	0.6	-0.48
chas				0.09	0.09	0.09	-0.1	[illegible]	-0.04	-0.12	0.05	-0.05	0.18
nox					-0.3	0.73	-0.77	0.61	0.67	0.19	-0.38	0.59	-0.43
rm						-0.24	0.21	-0.21	-0.29	-0.36	0.13	-0.61	0.7
age							-0.75	0.46	0.51	0.26	-0.27	0.6	-0.38
dis								-0.49	-0.53	-0.23	0.29	-0.5	0.25
rad									0.91	0.46	-0.44	0.49	-0.38
tax										0.46	-0.44	0.54	-0.47
ptratio											-0.18	0.37	-0.51
black												-0.37	0.33
lstat													-0.74

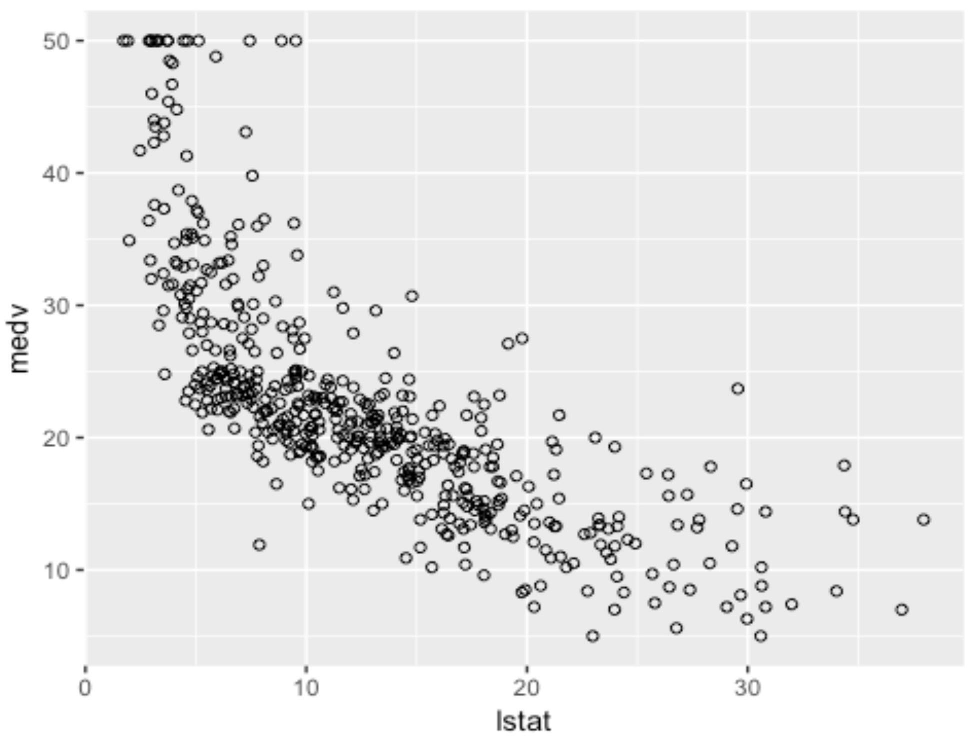
```r
# another option, with both colors and exact correlation scores
corrplot.mixed(corr.matrix, tl.cex=0.75, number.cex=0.75)
```



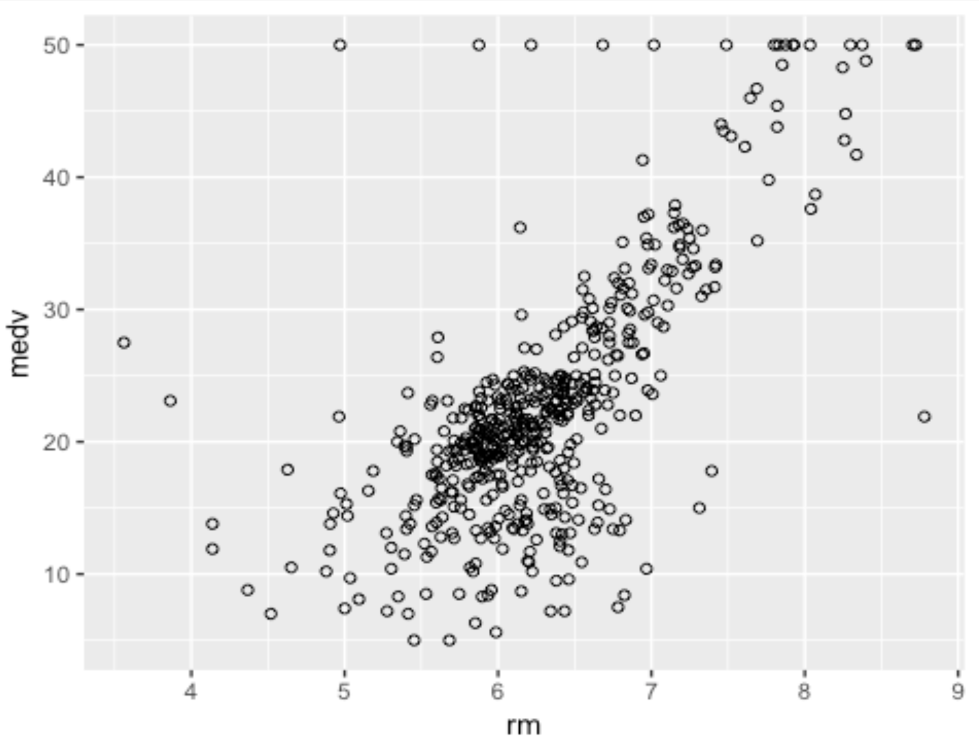
Predictors *lstat* (percent of households with low socioeconomic status) and *rm* (average number of rooms per house) have the highest correlation with the outcome variable.

To examine this further, we can plot *lstat* and *rm* against the response variable.

```r
p1 <- ggplot(data = Boston, mapping = aes(x = lstat, y = medv)) +
  geom_point(shape = 1)
p1
```



```
p2 <- ggplot(data = Boston, mapping = aes(x = rm, y = medv)) +
  geom_point(shape = 1)
p2
```



Simple Linear Regression

Let's start by building a simple linear regression model, with *medv* as the response and *lstat* as the predictor.

```
lm1 <- lm(medv ~ lstat, data = Boston)
summary(lm1)

##
## Call:
## lm(formula = medv ~ lstat, data = Boston)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -15.168  -3.990  -1.318   2.034  24.500
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 34.55384    0.56263   61.41   <2e-16 ***
## lstat       -0.95005    0.03873  -24.53   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.216 on 504 degrees of freedom
## Multiple R-squared:  0.5441, Adjusted R-squared:  0.5432
## F-statistic: 601.6 on 1 and 504 DF,  p-value: < 2.2e-16
```

As we see, the summary() function gives us:

- p-values and standard errors for the coefficients,
- R-squared (R2) statistic
- F-statistic for the model

In particular, we can conclude the following:

- based on the coefficient of the lstat variable, with each unit increase in lstat, that is, with a percentage increase in the households with low socioeconomic status, median house value decreases by 0.95005 units.
- based on the R2 value, this model explains 54.4% of variability in the median house value.
- based on the F statistic and the associated p-value, there is a significant linear relation between the predictor and the response variable.

To find out what other pieces of information are stored in the fitted model (that is, the lm1 object), we can use the names() f.

```
names(lm1)
```

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

So, for instance, to get the coefficients of the model:

```
lm1$coefficients

## (Intercept)       lstat
##  34.5538409  -0.9500494
```

Note, there is also the coef() f. that returns the coefficients:

```
coef(lm1)

## (Intercept)       lstat
##  34.5538409  -0.9500494
```

Or, if we want to compute the residual sum of squares (RSS):

```
lm1_rss <- sum(lm1$residuals^2)
lm1_rss

## [1] 19472.38
```

Recall that the obtained coefficent values are just estimates (of the real coefficient values) obtained using one particular sample from the target population. If some other sample was taken, these estimates might have been somewhat different. So, we usually compute the **95 confidence interval** for the coefficients to get an interval of values within which we can expect, in 95% of cases (i.e. 95% of examined samples), that the 'true' value for the coefficents will be.

```
confint(lm1, level = 0.95)

##                 2.5 %     97.5 %
## (Intercept) 33.448457 35.6592247
## lstat       -1.026148 -0.8739505
```

Now that we have a model, we can predict the value of *medv* based on the given *lstat* values. To do that, we will create a tiny test data frame.

```
df.test <- data.frame(lstat=c(5, 10, 15))
predict(lm1, newdata = df.test)

##        1        2        3
## 29.80359 25.05335 20.30310
```

We can also include the confidence interval for the predictions:

```
predict(lm1, newdata = df.test, interval = "confidence")

##        fit      lwr      upr
## 1 29.80359 29.00741 30.59978
## 2 25.05335 24.47413 25.63256
## 3 20.30310 19.73159 20.87461
```

Or, we can examine prediction intervals:

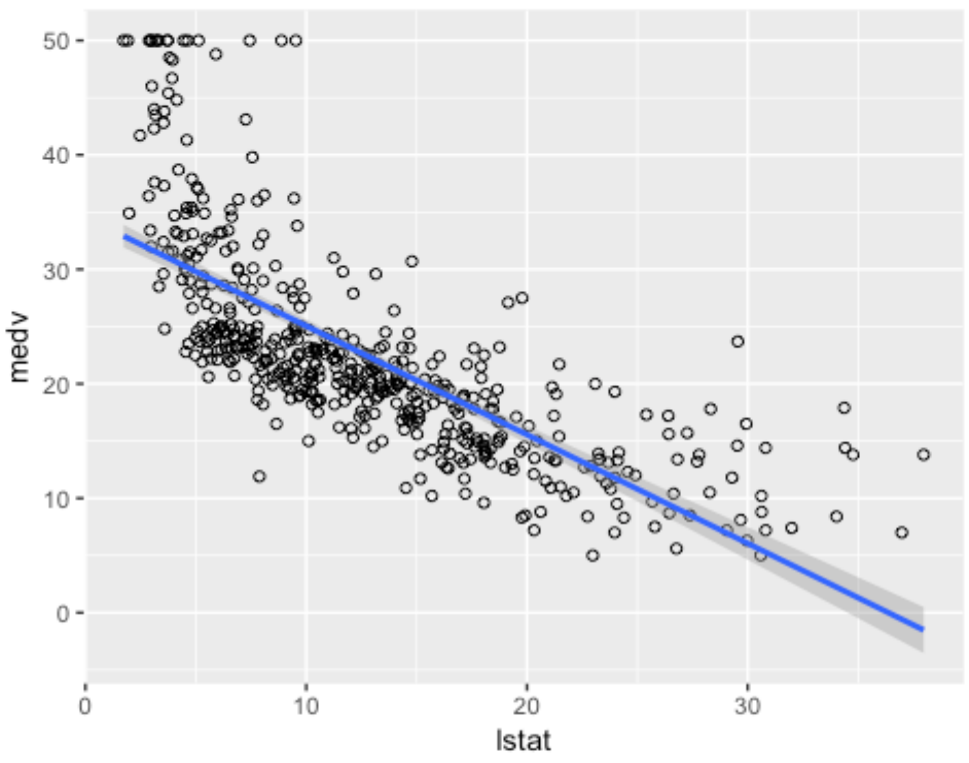
```
predict(lm1, newdata = df.test, interval = "predict")
```

```
##        fit       lwr      upr
## 1 29.80359 17.565675 42.04151
## 2 25.05335 12.827626 37.27907
## 3 20.30310  8.077742 32.52846
```

Notice the difference between the confidence and prediction intervals - the latter are much wider, reflecting far more uncertainty in the predicted value. Hint: recall the difference between the prediction and confidence intervals.

Now, we have to examine how well our model 'fits the data'. To do that, we will first plot the regression line, and observe how well the regression line fits the data

```
ggplot(data = Boston, mapping = aes(x = lstat, y = medv)) +
  geom_point(shape = 1) +
  geom_smooth(method = "lm")
```

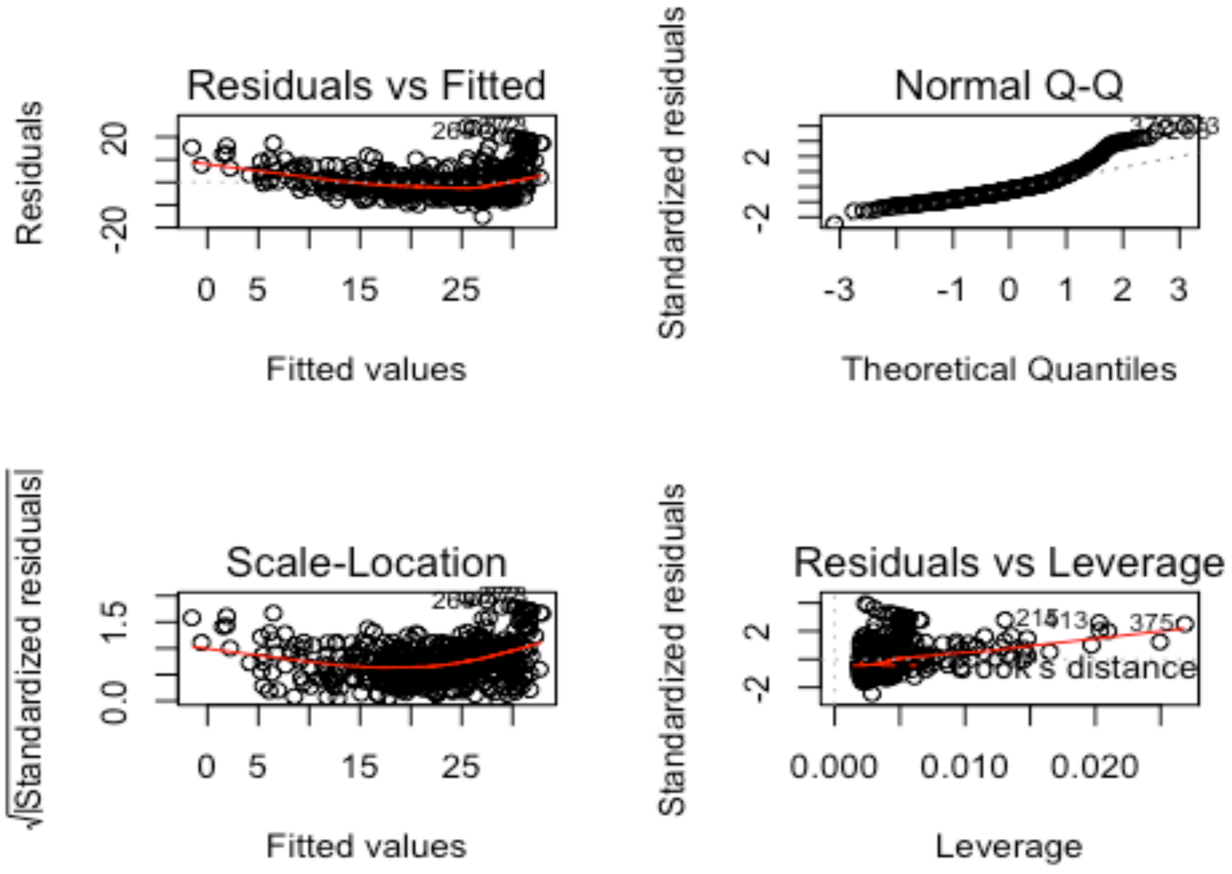


The plot indicates that there is some non-linearity in the relationship between lstat and medv.

Next, we will use *diagnostic plots* to examine the model fittness in more detail. Four diagnostic plots are automatically produced by passing the output from lm() function (e.g.

lm1) to the plot() function. This 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 par() function, which tells R to split the display screen into separate panels so that multiple plots can be viewed simultaneously.

```
par(mfrow=c(2,2)) # splitting the plotting area into 4 cells
plot(lm1)
```



```
par(mfrow=c(1,1)) # reseting the plotting area
```

Interpretation of the plots:

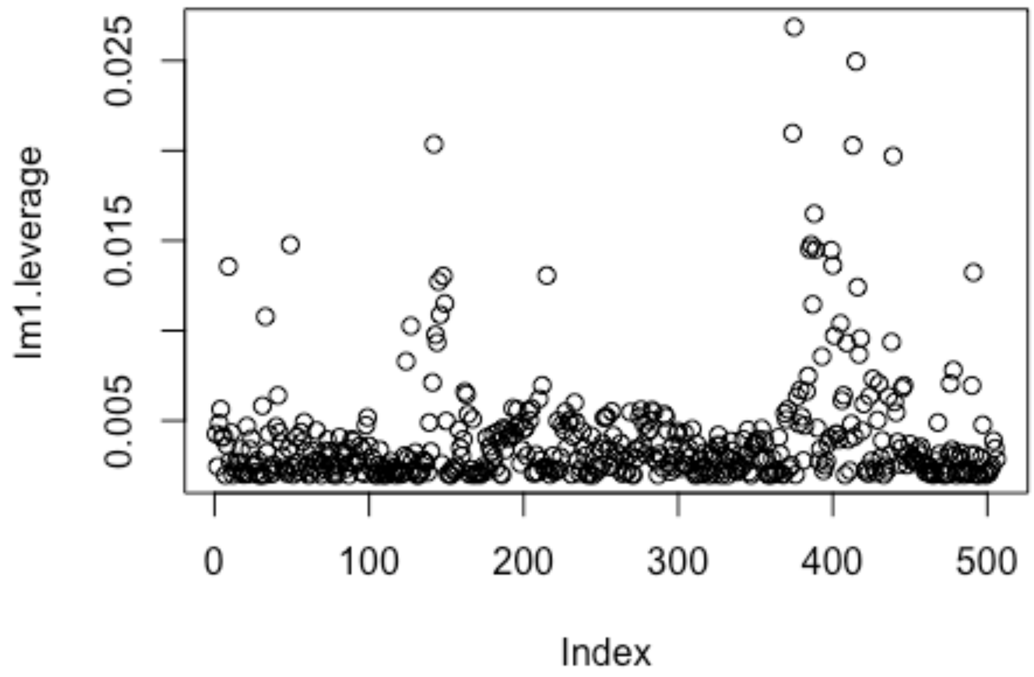
- the 1st plot, Residual vs Fitted value, is used for checking if the linearity assumption is satisfied. The plot shows that there is some indication of non-linear relationship between the predictor and the response variable
- the 2nd plot, Q-Q plot, tells us if residuals are normally distributed; in this case we see a considerable deviation from the diagonal, and therefore, from normal distribution
- the 3rd plot is used for checking the assumption of equal variance of residuals (homoscedasticity); in this case, the variance of the residuals tends to differ, so, the assumption is not fulfiled
- the 4th plot is used for spotting the presence of high leverage points; those would be the observations that have unusually high value of the predictor variable(s); their

presence can seriously affect the estimation of the coefficients; they can be spotted as being outside of the Cook's distance (meaning they have high Cook's distance scores); in this case there are several such observations

For a nice explanation of the diagnostic plots, check this article:
http://data.library.virginia.edu/diagnostic-plots/

If we want to examine leverage points in more detail, we can compute the leverage statistic using the hatvalues() function:

```
lm1.leverage <- hatvalues(lm1)
plot(lm1.leverage)
```



The plot suggests that there are several observations with high leverage values. We can check this further by examining the value of leverage statistic for the observations. Leverage statistics is always between 1/n and 1 (n is the number of observations); observations with leverage statistic considerably above 2*(p+1)/n (p is the number of predictors) are often considered as high leverage points. Let's check this for our data:

```
n <- nrow(Boston)
p <- 1
cutoff <- 2*(p+1)/n
length(which(lm1.leverage > cutoff))

## [1] 34
```

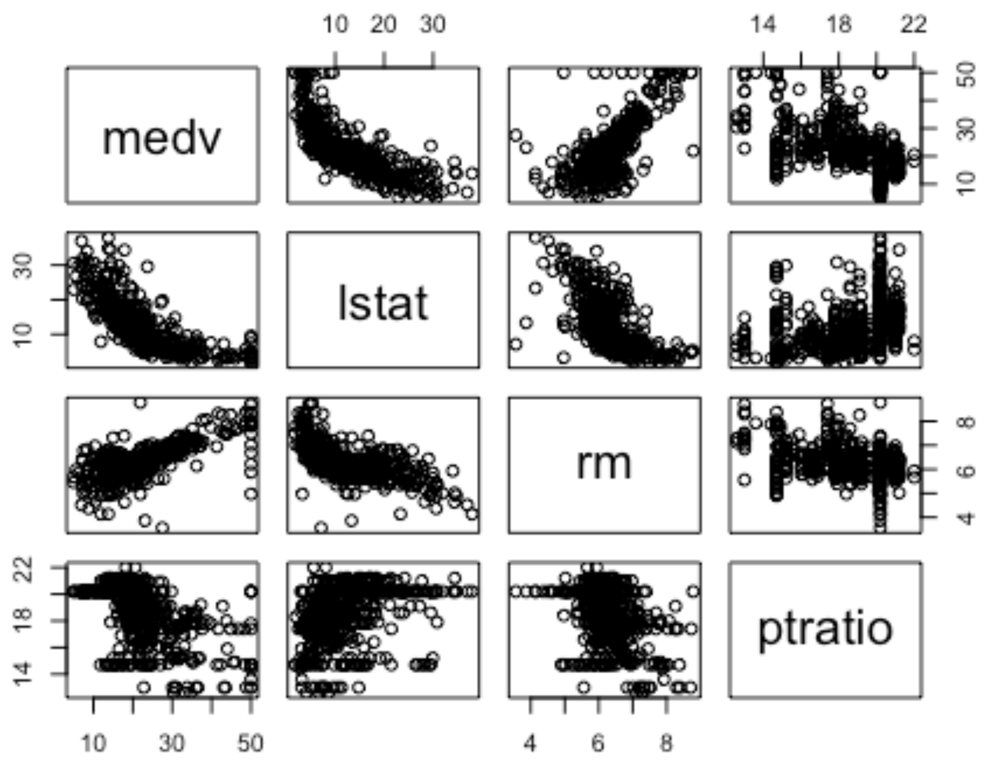
The results confirm that there are several (34) high leverage points.

Multiple Linear Regression

Let's now extend our model by including some other predictor variables that have high correlation with the response variable. Based on the correlation plot, we can include *rm* (average number of rooms per house) and *ptratio* (pupil-teacher ratio by town).

Scatterplot matrices are useful for examining the presence of linear relationship between several pairs of variables

```
pairs(~medv + lstat + rm + ptratio, data = Boston)
```



Far from perfect linear relation, but let's see what the model will look like.

To be able to properly test our model (not use fictitious data points as we did in the case of simple linear regression), we need to split our dataset into:

- *training data* that will be used to build a model
- *test data* to be used to evaluate / test the predictive power of our model.

Typically, 80% of observations are used for training and the rest for testing.

When splitting the dataset, we need to assure that observations are randomly assigned to the training and testing data sets. In addition, we should assure that the outcome variable has the same distribution in the train and test sets. This can be easily done using the createDataPartition() f. from the caret package

```
# install.packages('caret')
library(caret)

## Loading required package: lattice

# assure the replicability of the results by setting the seed
set.seed(123)
# generate indices of the observations to be selected for the training set
train.indices <- createDataPartition(Boston$medv, p = 0.80, list = FALSE)
# select observations at the positions defined by the train.indices vector
train.boston <- Boston[train.indices,]
# select observations at the positions that are NOT in the train.indices
vector
test.boston <- Boston[-train.indices,]
```

Check that the outcome variable (medv) has the same distribution in the training and test sets

```
summary(train.boston$medv)

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##    5.00   16.95   21.20   22.74   25.00   50.00

summary(test.boston$medv)

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##    5.00   17.05   21.00   21.68   24.65   50.00
```

Now, build a model using the training data set

```
lm2 <- lm(medv ~ lstat + rm + ptratio, data = train.boston)
summary(lm2)

## 
## Call:
## lm(formula = medv ~ lstat + rm + ptratio, data = train.boston)
## 
## Residuals:
##      Min       1Q   Median       3Q      Max 
## -14.8219  -3.0757  -0.8036   1.7893  29.7479 
## 
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 18.11824    4.33535   4.179 3.59e-05 ***
## lstat       -0.56496    0.04778 -11.824  < 2e-16 ***
## rm           4.62379    0.45996  10.053  < 2e-16 ***
## ptratio     -0.94082    0.13192  -7.132 4.63e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
##
## Residual standard error: 5.181 on 403 degrees of freedom
## Multiple R-squared:  0.6935, Adjusted R-squared:  0.6912
## F-statistic: 303.9 on 3 and 403 DF,  p-value: < 2.2e-16
```

From the summary, we can see that:

- R-squared has increased considerably, from 0.544 to 0.694 even though we have built it with a smaller dataset (407 observations, instead of 506 observations).
- all 3 predictors are highly significant

TASK 1: Interpret the estimated coefficients (see how it was done for the simple linear regression).

TASK 2: use diagnostic plots to examine how well the model adheres to the assumptions.

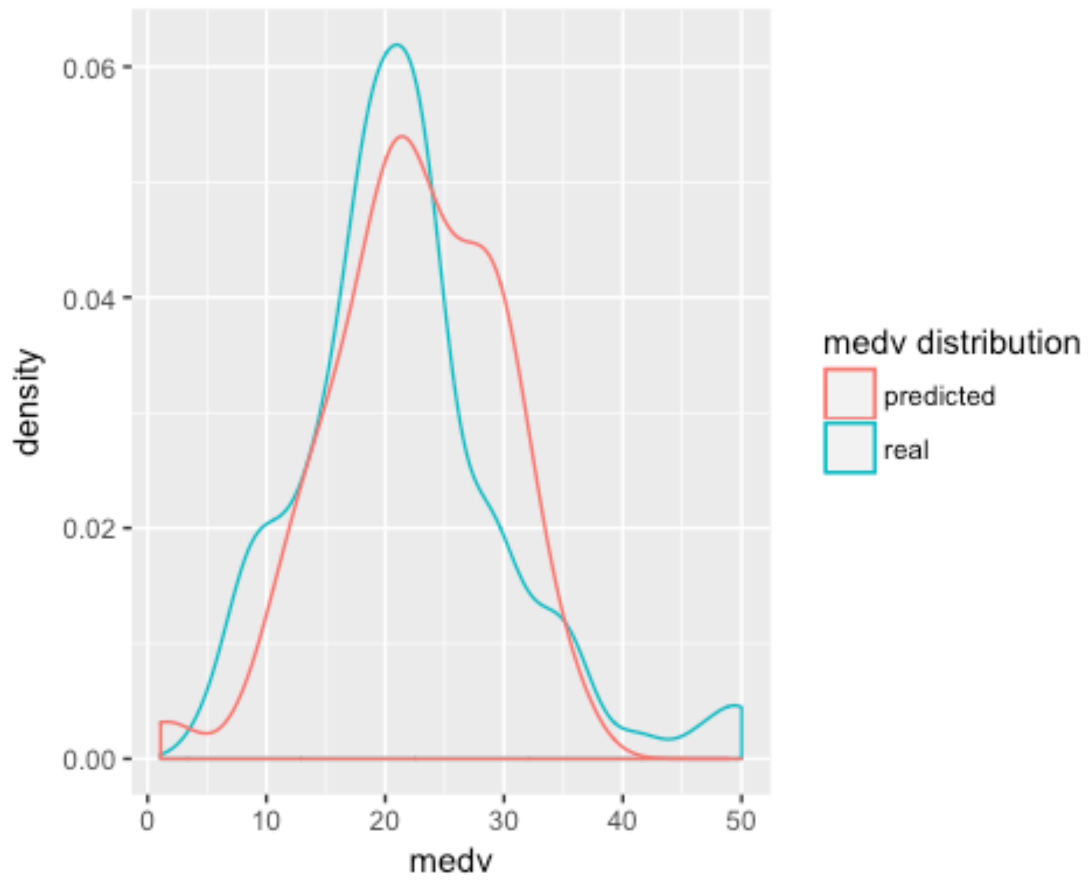
Let's make predictions using this model on the test data set that we have created

```
lm2.predict <- predict(lm2, newdata = test.boston)
head(lm2.predict)

##        3        5       11       12       14       15
## 32.31678 30.55989 21.75026 24.10511 21.20138 20.75116
```

To examine the predicted against the real values of the response variable (medv), we can plot their distributions one against the other

```
test.boston.lm2 <- cbind(test.boston, pred = lm2.predict)
ggplot() +
  geom_density(data = test.boston.lm2, mapping = aes(x=medv, color = 'real'))
+
  geom_density(data = test.boston.lm2, mapping = aes(x=pred, color =
'predicted')) +
  scale_colour_discrete(name ="medv distribution")
```



To evalute the predictive power of the model, we'll compute R-squared on the test data. Recall that R-squared is computed as 1 - RSS/TSS, where TSS is the total sum of squares

```
lm2.test.RSS <- sum((lm2.predict - test.boston$medv)^2)
lm.test.TSS <- sum((mean(train.boston$medv) - test.boston$medv)^2)
lm2.test.R2 <- 1 - lm2.test.RSS/lm.test.TSS
lm2.test.R2

## [1] 0.6076704
```

R2 on the test is lower than the one obtained on the training set, which is expected.

Let's also compute Root Mean Squared Error (RMSE) to see how much error we are making with the predictions. Recall: RMSE = sqrt(RSS/n)

```
lm2.test.RMSE <- sqrt(lm2.test.RSS/nrow(test.boston))
lm2.test.RMSE

## [1] 5.432056
```

To get a perspective of how large this error is, let's check the mean value of the response variable on the test set:

```
mean(test.boston$medv)
```

```
## [1] 21.68384

lm2.test.RMSE/mean(test.boston$medv)

## [1] 0.2505117
```

So, it's not a small error, it's about 25% of the mean value

Let's now build another model using all available predictors:

```
lm3 <- lm(medv ~ ., data = train.boston) # note the use of '.' to mean all
variables
summary(lm3)

##
## Call:
## lm(formula = medv ~ ., data = train.boston)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15.1772  -2.6987  -0.5194   1.7225  26.0486
##
## Coefficients:
##                Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.759e+01  5.609e+00   6.702 7.17e-11 ***
## crim        -9.610e-02  4.024e-02  -2.388  0.01741 *
## zn           4.993e-02  1.521e-02   3.283  0.00112 **
## indus       -5.789e-03  6.745e-02  -0.086  0.93166
## chas         2.292e+00  1.019e+00   2.250  0.02501 *
## nox         -1.723e+01  4.244e+00  -4.059 5.95e-05 ***
## rm           3.784e+00  4.537e-01   8.341 1.26e-15 ***
## age          8.387e-04  1.450e-02   0.058  0.95391
## dis         -1.620e+00  2.217e-01  -7.310 1.50e-12 ***
## rad          3.031e-01  7.434e-02   4.078 5.51e-05 ***
## tax         -1.316e-02  4.144e-03  -3.176  0.00161 **
## ptratio     -9.582e-01  1.473e-01  -6.505 2.37e-10 ***
## black        9.723e-03  2.993e-03   3.249  0.00126 **
## lstat       -5.297e-01  5.691e-02  -9.308  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.692 on 393 degrees of freedom
## Multiple R-squared:  0.7549, Adjusted R-squared:  0.7468
## F-statistic:  93.1 on 13 and 393 DF,  p-value: < 2.2e-16
```

Note that even though we now have 13 predictors, we haven't much improved the R-squared value: in the model with 3 predictors, it was 0.693 and now it is 0.755. In addition, it should be recalled that R2 increases with the increase in the number of predictors, no matter how good/useful they are.

The 3 predictors from the previous model are still highly significant, plus, there are a number of other significant variables.

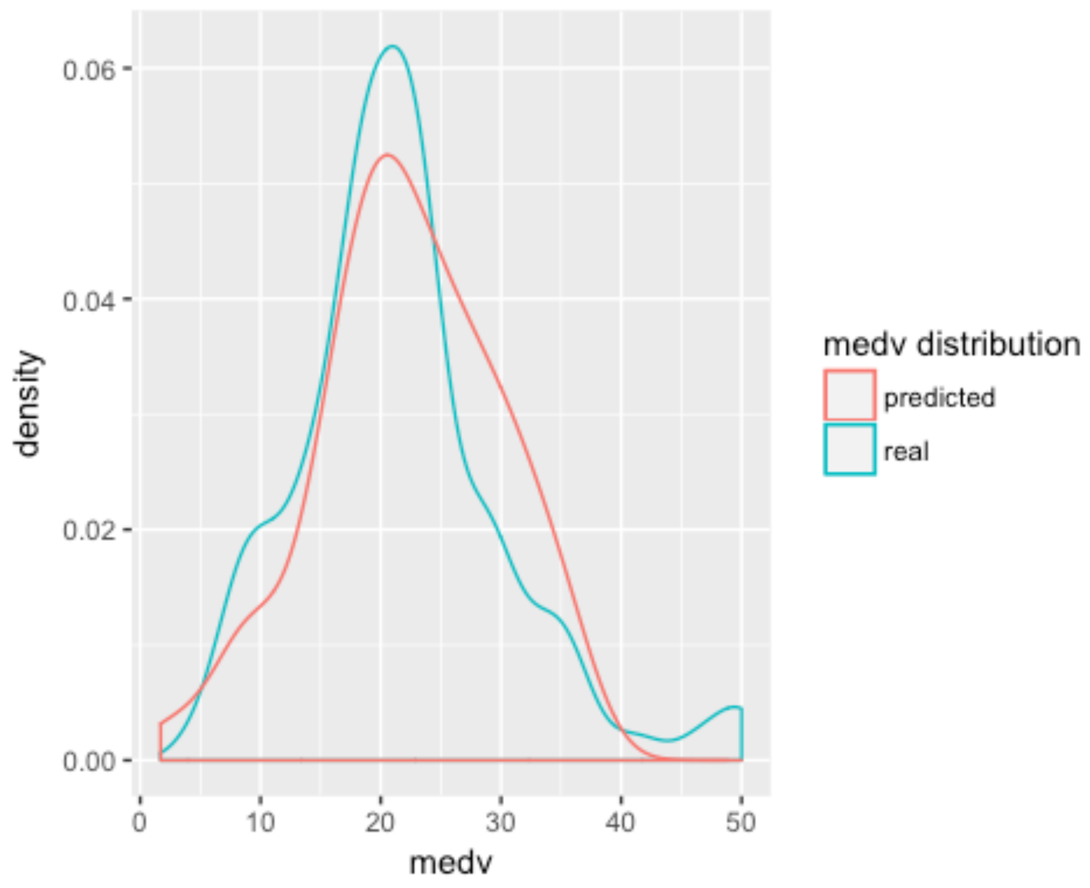
Let's do the prediction using the new model:

```
lm3.predict <- predict(lm3, newdata = test.boston)
head(lm3.predict)
```

```
##        3        5       11       12       14       15
## 30.70615 28.05079 18.88585 21.53429 19.68122 19.43022
```

Plot the distribution of predictions against the real values of the response variable (medv)

```
test.boston.lm3 <- cbind(test.boston, pred = lm3.predict)
ggplot() +
  geom_density(data = test.boston.lm3, mapping = aes(x=medv, color = 'real'))
+
  geom_density(data = test.boston.lm3, mapping = aes(x=pred, color =
'predicted')) +
  scale_colour_discrete(name ="medv distribution")
```



As before, we'll compute R-squared on the test data:

```r
lm3.test.RSS <- sum((lm3.predict - test.boston$medv)^2)
lm3.test.R2 <- 1 - lm3.test.RSS/lm.test.TSS
lm3.test.R2
```

```
## [1] 0.6685588
```

Again, we got lower R2 than on the train set.

We can also compute RMSE:

```r
lm3.test.RMSE <- sqrt(lm3.test.RSS/nrow(test.boston))
lm3.test.RMSE
```

```
## [1] 4.992775
```

It is lower (therefore, better) than with the previous model.

TASK: use diagnostic plots to examine how well the model adheres to the assumptions.

Considering the number of variables in the model, we should check for *multicolinearity*. To do that, we'll compute the variance inflation factor (VIF):

```r
library(car)
vif(lm3)
```

```
##     crim       zn    indus     chas      nox       rm      age      dis 
## 1.865531 2.364859 3.901322 1.064429 4.471619 2.010665 3.018555 3.961686 
##      rad      tax  ptratio    black    lstat 
## 7.799919 9.163102 1.907071 1.311933 2.967784
```

As a rule of thumb, variables having sqrt(vif) > 2 are problematic

```r
sqrt(vif(lm3))
```

```
##     crim       zn    indus     chas      nox       rm      age      dis 
## 1.365844 1.537810 1.975177 1.031712 2.114620 1.417979 1.737399 1.990398 
##      rad      tax  ptratio    black    lstat 
## 2.792833 3.027062 1.380967 1.145396 1.722726
```

So, *tax* and *rad* exhibit multicolinearity - if we go back to the correlation plot, we'll see that they are, indeed, highly correlated (0.91). There are also a few suspicious variables: indus, nox, and dis.

TASK: create a new model (lm4) by excluding either *tax* or *rad* variable. Compare the new model with lm3.