Intro to Machine Learning Notes

Introduction to Machine Learning/Statistical Analysis and Learning

R Setup

```r
#Load packages for chapter labs
library("ISLR2") #Introduction to Statistical Learning datasets'
library("tidyverse")
```

Week 1 Notes

Types of machine learning:

- Supervised learning
  - Regression models - quantitative/continous output
  - Classification models - qualitative/discrete output
- Unsupervised learning
  - Clustering models - patterns from input data without specified output

Why study statistical learning?

- Inference - how does a particular input drive an output variable
- Prediction - only the value of the outcome variable is of interest
  - Example: "How much rainfall will California have in 2050?"?

Week 2: Statistical Learning Introduction

Notes

Shared assumptions of linear and non-linear statistical models for estimating f:

- Parametric vs. non-parametric
- Flexibility (complexity) vs. interpretability
  - Flexible models are beneficial for prediction
  - Interpretable models are beneficial for inference
- Supervised vs. unsupervised learning
  - Unsupervised has no specified outcome variable

How to determine the best statistical model for a problem

- Quality of fit
- Variance/Bias tradeoff
  - Variance: the amount by which $\hat{f}$ would change if estimated with a different training set
  - Bias: the error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much simpler model.
  - In general, with more flexible methods, variance increases and bias decreases

Inference vs. Prediction

- Sometimes both are of interest, but often only one is of primary interest. The goals of the analyst here are the primary driver in selecting a model

How do we estimate f?

- Training data used to estimate f
- Parametric approach
  - Step 1: Specify an estimated functional form for f (i.e. a linear function)
  - Step 2: Training data is used to estimate the parameters of the function
  - Disadvantage of parametric methods: not well suited to estimate a function for a complex dataset
- Non-parametric approach

  - Avoids the assumption of a particular functional form for f
  - Disadvantage: they require very large data sets to make an accurate prediction of f

Why would we ever choose to use a more restrictive method instead of a very flexible approach?

- Interpretability, inference, to avoid overfitting

Should we always choose a more complex (flexible) approach when prediction is the objective?

- Only if there is a very large dataset. With a small amount of data, more complexity is not always good

Measuring the Quality of Fit

- Mean Squared Error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

- Training MSE vs. Test MSE
- Why does *training* MSE always decrease with added flexibility?
  - With enough flexibility you can get your model to perfectly fit the training data (but *test* MSE would be much worse)
- highest quality of fit does not equal the best predictive model (overfitting)

Lab: Intro to R

`c()` Create a vector of items

`length()` Returns the length of a vector

`ls()` Lists all objects such as data and functions saved in the environment

`rm()` Remove an object from the environment

`matrix(data = , nrow = , ncol =)` Create a matrix

`sqrt()` calculate the square root

`rnorm(n)` Generates a vector of random normal variables of $_n$ sample size

`cor(x, y)` Calculates the correlation between two sets of numbers `set.seed()` Used to set a consistent seed for a random number function

`mean()` Mean

`var()` Variance

`sd()` Standard Deviation

`plot()` Basic plotting function

`countour()` Creates a countour plot to represent 3D data

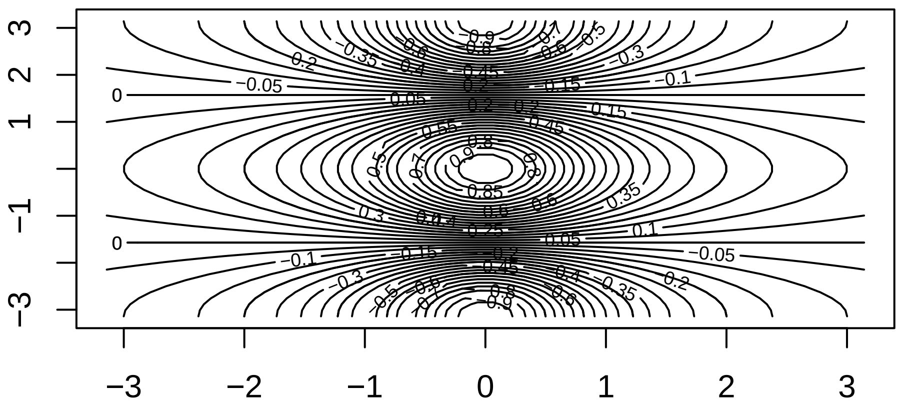
```
x <- seq(1,10)
x
```

```
[1]  1  2  3  4  5  6  7  8  9 10
```

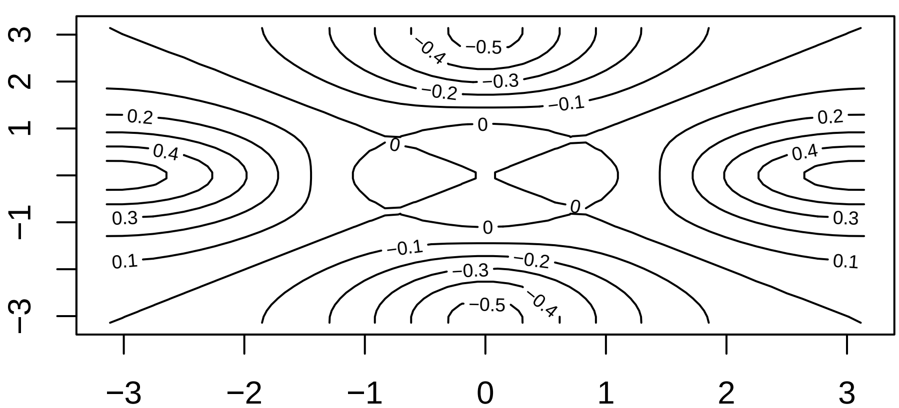
```
x <- 1:10
x
```

```
[1]  1  2  3  4  5  6  7  8  9 10
```

```
x <- seq(-pi, pi, length = 50)

y <- x
f <- outer(x, y, function(x, y) cos(y) / (1 + x^2))

contour(x, y, f)
contour(x, y, f, nlevels = 45, add = T)
```



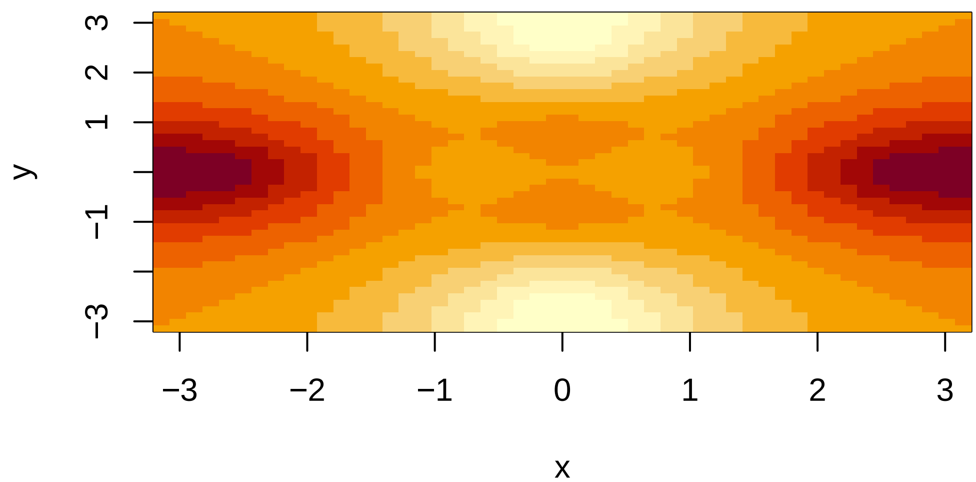
```r
fa <- (f - t(f)) / 2
contour(x, y, fa, nlevels = 15)
```



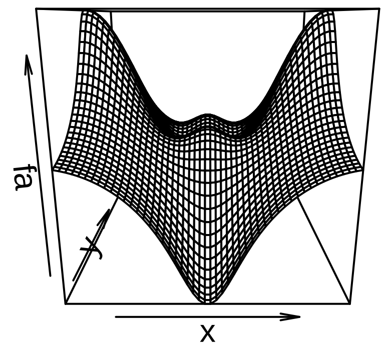
`image()` Produces a heatmap plot

`persp()` Creates a 3D plot, arguments `theta` and `phi` control the viewing angles

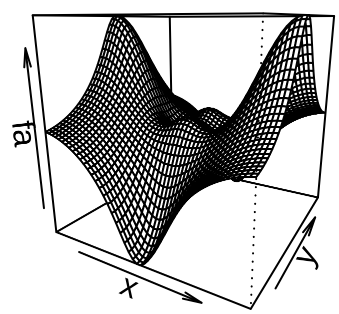
```
image(x, y, fa)
```



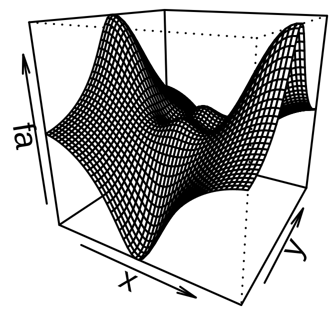

```
persp(x, y, fa)
```



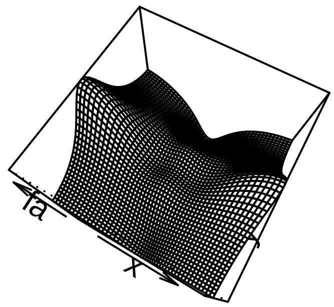

```r
persp(x, y, fa, theta = 30)
```



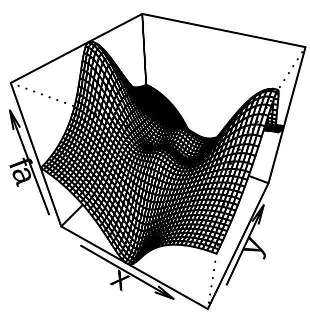
```r
persp(x, y, fa, theta = 30, phi = 20)
```




```r
persp(x, y, fa, theta = 30, phi = 70)
```




```
persp(x, y, fa, theta = 30, phi = 40)
```



`dim()` Dimension function returns the number of rows and columns of a matrix

`read.table()` Import data

`write.table()` Export data

Data Frame functions

`data.frame()` Create a data frame

`str()` Used to view a list of variables and first few observations in a data table

`subset()` Used to filter a data table

`order()` Used to return the order of a vector, can sort a data table

`list()` Create a list

Week 3: Linear Regression

Notes

Inference problem example - which advertising strategy will lead to higher product sales next year?

Simple linear regression is a a method for predicting a quantitatie response Y on the basis of a single predictor variable X. A simple model uses the equation:

$$Y \approx \beta_0 + \beta_1 x_1$$

Residual Sum of Squares (RSS) is the sum of differences between the observed vaues and predicted values

Least squares estimation method minimizes RSS to created an estimation line with the equation above. β_1 and β_0 are computable from the predictors and outcomes in the dataset

Standard Errors for OLS estimates

Hypothesis testing steps - if the regression shows a positive or negative sloped line based on the sample, how can we be sure that it is *not* actually a flat line in the population?

1. estimate parameters and standard errors
2. calculate t-statistic
3. Find the corresponding p value

    - When the t-statistic is large and the p value is low, we can reject the null hypothesis

Accuracy of the model: how well does the model fit the data?

- RSE (Residual Standard Error)
  - How far on average are the actual outcomes from the prediction line?
- R^2 statistic
  - A proportional measure always between 0 and 1 that shows how much variation in the data is explained by the model
  - Can R^2 be negative? Technically yes if the model is very bad
- F-statistic
  - Not about significance but about whether you can reject the null hypothesis for the whole model

Multiple Linear Regression

Lab: Regression in R

Simple Linear Regression

Boston dataset: The outome variable `medv` is median home value by census tract

```r
library(MASS)
```

```

Attaching package: 'MASS'


The following object is masked from 'package:dplyr':

    select


The following object is masked from 'package:ISLR2':

    Boston
```

```r
#view the first 10 observations of the dataset
head(Boston)
```

```
     crim zn indus chas   nox    rm  age    dis rad tax ptratio  black lstat
1 0.00632 18  2.31    0 0.538 6.575 65.2 4.0900   1 296    15.3 396.90  4.98
2 0.02731  0  7.07    0 0.469 6.421 78.9 4.9671   2 242    17.8 396.90  9.14
3 0.02729  0  7.07    0 0.469 7.185 61.1 4.9671   2 242    17.8 392.83  4.03
4 0.03237  0  2.18    0 0.458 6.998 45.8 6.0622   3 222    18.7 394.63  2.94
5 0.06905  0  2.18    0 0.458 7.147 54.2 6.0622   3 222    18.7 396.90  5.33
6 0.02985  0  2.18    0 0.458 6.430 58.7 6.0622   3 222    18.7 394.12  5.21
  medv
1 24.0
2 21.6
3 34.7
4 33.4
5 36.2
6 28.7
```

```r
#Create a regression equation
attach(Boston)
lm.fit <- lm(medv ~ lstat)

#View the regression results
lm.fit
```

```
Call:
lm(formula = medv ~ lstat)

Coefficients:
(Intercept)        lstat
      34.55        -0.95
```

```r
#View details about the regression
summary(lm.fit)
```

```
Call:
lm(formula = medv ~ lstat)

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
```

```r
#See what is stored in the lm.fit list
names(lm.fit)
```

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

```r
#Function to view the coefficients of lm.fit
coef(lm.fit)
```

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

```r
#View the confidence interval
confint(lm.fit)
```

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

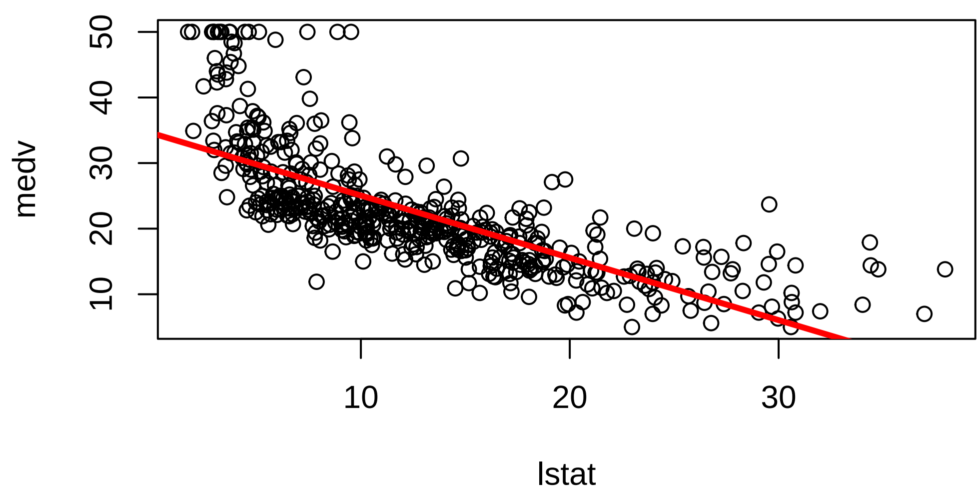
```r
#Generate confidence intervals for given values of lstat
predict(lm.fit, data.frame(lstat = (c(5, 10, 15))), interval = "confidence")
```

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

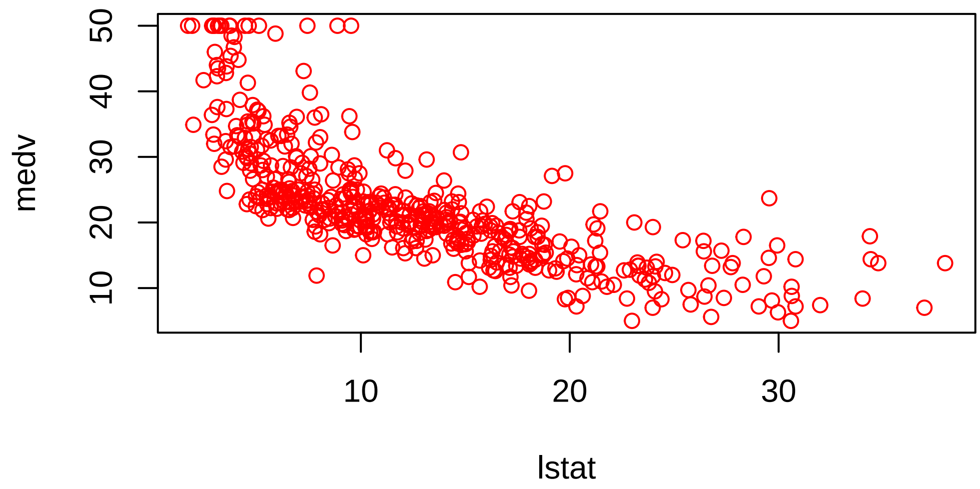
```r
#Generate prediction intervals for given values of lstat
predict(lm.fit, data.frame(lstat = (c(5, 10, 15))), interval = "prediction")
```

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

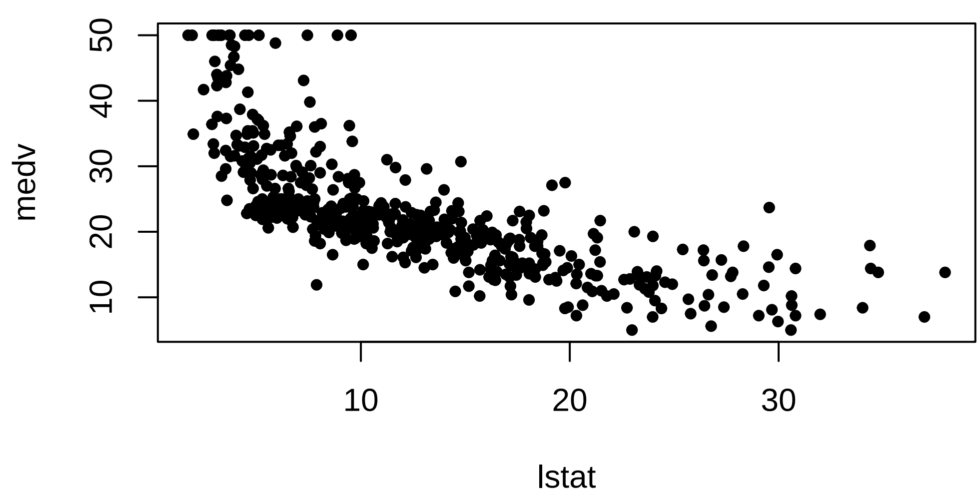
```r
#plot
plot(lstat, medv)

#Add the least squares line to the plot
abline(lm.fit, lwd = 3, col = "red")
```



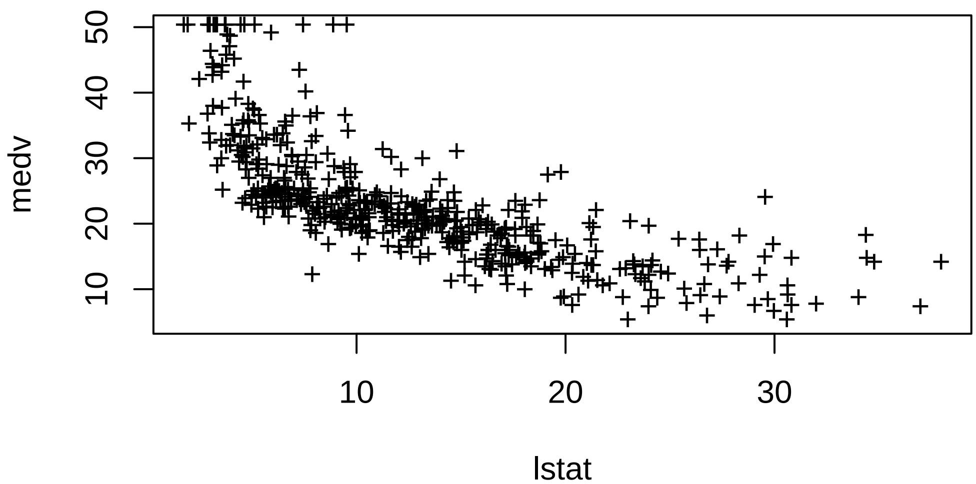

```r
#Use 'col =' to change the color of the points
plot(lstat, medv, col = "red")
```



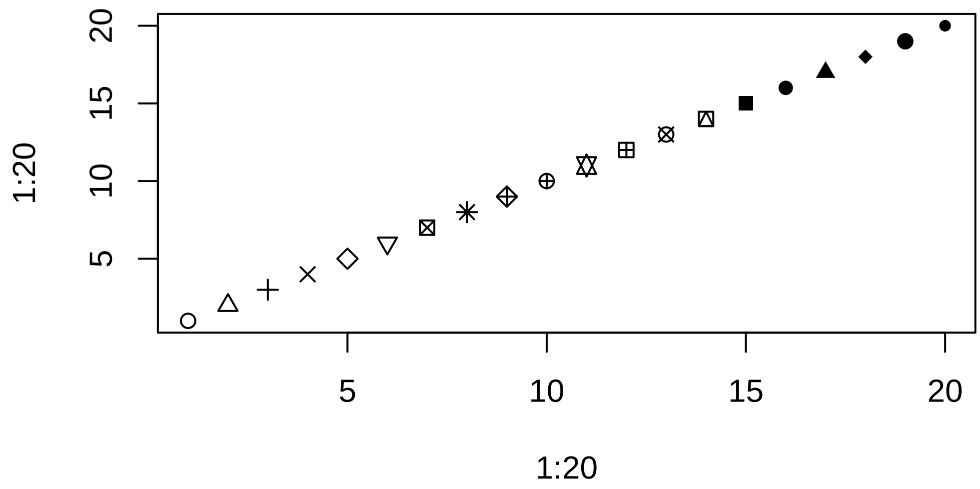

```
#Use 'pch =' to change the shape of the points
plot(lstat, medv, pch = 20)
```



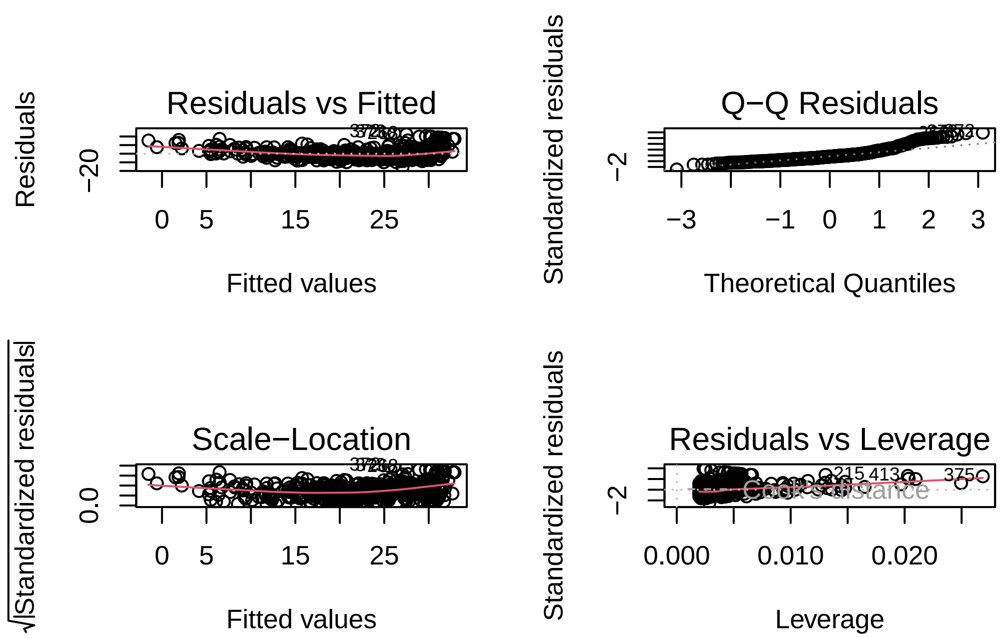
```r
#Define the point shape directly
plot(lstat, medv, pch = "+")
```




```r
#Define the point shape with a number
plot(1:20, 1:20, pch = 1:20)
```

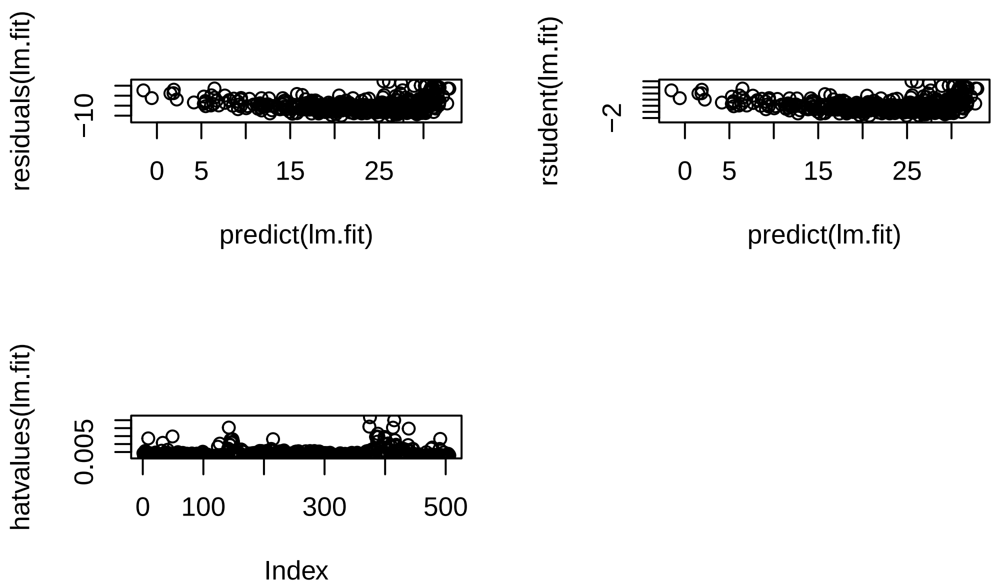



```r
par(mfrow = c(2,2))
plot(lm.fit)
```



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

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

375
375



Multiple Linear Regression

```
#Run a regression with specified predictors
lm.fit <- lm(medv ~ lstat + age, data = Boston)
summary(lm.fit)
```

```
Call:
lm(formula = medv ~ lstat + age, data = Boston)

Residuals:
```

```
    Min      1Q  Median      3Q     Max 
-15.981  -3.978  -1.283   1.968  23.158 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 33.22276    0.73085  45.458  < 2e-16 ***
lstat       -1.03207    0.04819 -21.416  < 2e-16 ***
age          0.03454    0.01223   2.826  0.00491 ** 
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 6.173 on 503 degrees of freedom
Multiple R-squared:  0.5513,    Adjusted R-squared:  0.5495 
F-statistic:   309 on 2 and 503 DF,  p-value: < 2.2e-16
```

```r
#Run a regression on all the predictor variables in the dataset
lm.fit <- lm(formula = medv ~ ., data = Boston)
summary(lm.fit)
```

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

Residuals:
    Min      1Q  Median      3Q     Max 
-15.595  -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 ***
crim        -1.080e-01  3.286e-02  -3.287 0.001087 ** 
zn           4.642e-02  1.373e-02   3.382 0.000778 ***
indus        2.056e-02  6.150e-02   0.334 0.738288    
chas         2.687e+00  8.616e-01   3.118 0.001925 ** 
nox         -1.777e+01  3.820e+00  -4.651 4.25e-06 ***
rm           3.810e+00  4.179e-01   9.116  < 2e-16 ***
age          6.922e-04  1.321e-02   0.052 0.958229    
dis         -1.476e+00  1.995e-01  -7.398 6.01e-13 ***
rad          3.060e-01  6.635e-02   4.613 5.07e-06 ***
tax         -1.233e-02  3.760e-03  -3.280 0.001112 ** 
ptratio     -9.527e-01  1.308e-01  -7.283 1.31e-12 ***
```

```
black        9.312e-03  2.686e-03   3.467 0.000573 ***
lstat       -5.248e-01  5.072e-02 -10.347  < 2e-16 ***
---
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
```

```
library(car)
```

```
Loading required package: carData


Attaching package: 'car'


The following object is masked from 'package:dplyr':

    recode


The following object is masked from 'package:purrr':

    some
```

```
#Calculate variance inflation factors
vif(lm.fit)
```

```
    crim       zn    indus     chas      nox       rm      age      dis
1.792192 2.298758 3.991596 1.073995 4.393720 1.933744 3.100826 3.955945
     rad      tax  ptratio    black    lstat
7.484496 9.008554 1.799084 1.348521 2.941491
```

```
#Run the regression all predictors except one (age) using the "-" sign
lm.fit1 <- lm(medv ~ . - age, data = Boston)
summary(lm.fit1)
```

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

Residuals:
     Min       1Q   Median       3Q      Max 
-15.6054  -2.7313  -0.5188   1.7601  26.2243 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)  36.436927   5.080119   7.172 2.72e-12 ***
crim         -0.108006   0.032832  -3.290 0.001075 ** 
zn            0.046334   0.013613   3.404 0.000719 ***
indus         0.020562   0.061433   0.335 0.737989    
chas          2.689026   0.859598   3.128 0.001863 ** 
nox         -17.713540   3.679308  -4.814 1.97e-06 ***
rm            3.814394   0.408480   9.338  < 2e-16 ***
dis          -1.478612   0.190611  -7.757 5.03e-14 ***
rad           0.305786   0.066089   4.627 4.75e-06 ***
tax          -0.012329   0.003755  -3.283 0.001099 ** 
ptratio      -0.952211   0.130294  -7.308 1.10e-12 ***
black         0.009321   0.002678   3.481 0.000544 ***
lstat        -0.523852   0.047625 -10.999  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.74 on 493 degrees of freedom
Multiple R-squared:  0.7406,	Adjusted R-squared:  0.7343 
F-statistic: 117.3 on 12 and 493 DF,  p-value: < 2.2e-16
```

```r
#Another way to change the model using update()
lm.fit1 <- update(lm.fit, ~ . - age)
```

Interaction terms

There are two ways to include interaction terms in the lm() funtion: $x_1 : x_2$ creates an interaction term between the two variables. $x_1 * x_2$ creates an individual variable for each *plus* an interaction term.

($x_1 * x_2$ is shorthand for $x_1 + x_2 + x_1 : x_2$)

```r
#Run a regression with a predictor variable
summary(lm(medv ~ lstat*age, data = Boston))
```

```

Call:
lm(formula = medv ~ lstat * age, data = Boston)

Residuals:
    Min      1Q  Median      3Q     Max 
-15.806  -4.045  -1.333   2.085  27.552 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept) 36.0885359  1.4698355  24.553  < 2e-16 ***
lstat       -1.3921168  0.1674555  -8.313 8.78e-16 ***
age         -0.0007209  0.0198792  -0.036   0.9711    
lstat:age    0.0041560  0.0018518   2.244   0.0252 *  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 6.149 on 502 degrees of freedom
Multiple R-squared:  0.5557,	Adjusted R-squared:  0.5531 
F-statistic: 209.3 on 3 and 502 DF,  p-value: < 2.2e-16
```

Non-linear transformations on predictors

To transform a variable in `lm()`, use `I()`. For example, to square a predictor you would use `I(x^2)`.

For higher order variables, use the `poly()` function.

```r
#Run a regression with a squared predictor term
lm.fit2 <- lm(medv ~ lstat + I(lstat^2))
summary(lm.fit2)
```

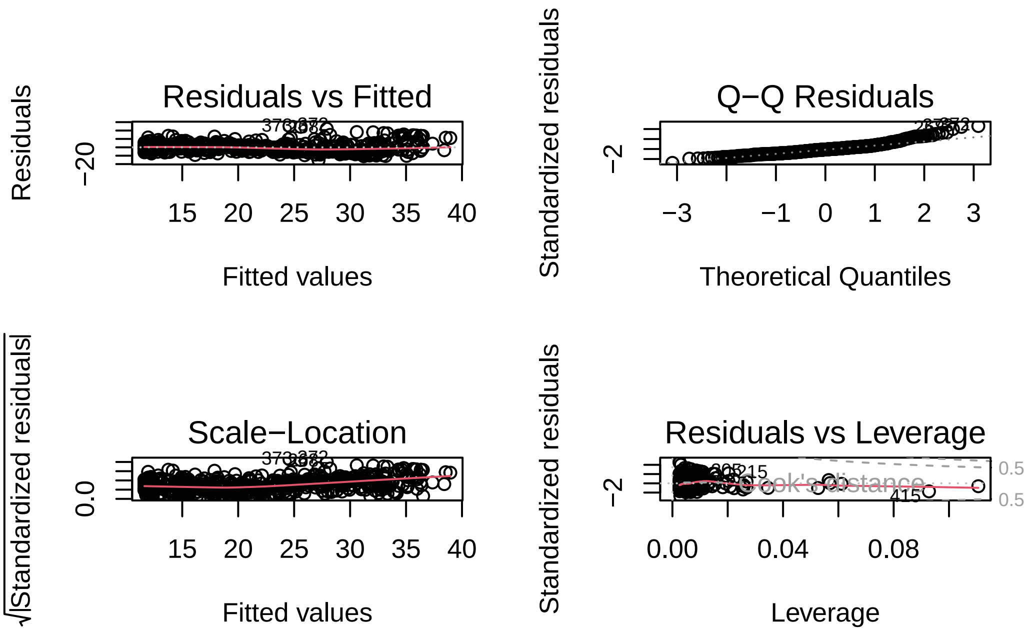
```

Call:
lm(formula = medv ~ lstat + I(lstat^2))

Residuals:
     Min       1Q   Median       3Q      Max 
```

```
-15.2834  -3.8313  -0.5295   2.3095  25.4148

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 42.862007   0.872084   49.15   <2e-16 ***
lstat       -2.332821   0.123803  -18.84   <2e-16 ***
I(lstat^2)   0.043547   0.003745   11.63   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 5.524 on 503 degrees of freedom
Multiple R-squared:  0.6407,    Adjusted R-squared:  0.6393
F-statistic: 448.5 on 2 and 503 DF,  p-value: < 2.2e-16
```

```r
#Use anova() to see if the quadratic fit is better than the original linear fit
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    4125.1 135.2 < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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



Qualitative predictors

Writing functions in R

Week 4: Classification