## Data Analysis in Software Engineering using R

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## Welcome

This **Data Analysis in Software Engineering (DASE)** book/notes will try teach you how to do data science with R in Software Engineering.

It is a work in progress.

#### Acknowledgments

#### Projects:

- PRESI: TIN2013-46928-C3
  - amuSE TIN2013-46928-C3-2-R
  - PERTEST TIN2013-46928-C3-1-R
- QARE: TIN2016-76956-C3
  - -Badge People: TIN<br/>2016-76956-C3-3-R
  - TESTEAMOS: TIN2016-76956-C3-1-R
- Network SBSE (SEBASENet): TIN2015-71841-REDT

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8 CONTENTS

# $$\operatorname{Part} \ I$$ Introduction to the R Language

## Chapter 1

### Introduction to R

The goal of the first part of this book is to get you up to speed with the basics of **R** as quickly as possible.

#### 1.1 Installation

Follow the procedures according to your operating system.

- Linux: You need to have blas and gfortran installed on your Linux, for installing the coin package.
- Rgraphviz requires installation from source("http://bioconductor.org/biocLite.R"), then biocLite("Rgraphviz").
- Uncomment the following lines for installing all missing packages (this will take some time):

```
# listofpackages <- c("arules", "arulesViz", "bookdown", "qqplot2", "vioplot", "UsinqR", "fpc", "reshape
# newpackages <- listofpackages[!(listofpackages %in% installed.packages()[,"Package"])]
# if(length(newpackages)>0) install.packages(newpackages,dependencies = TRUE)
# # install from archive
# if (!is.element("rqp", installed.packages()[,1]))
# { install.packages("https://cran.r-project.org/src/contrib/Archive/rgp/rgp_0.4-1.tar.gz",
                                                      repos = NULL)
# }
## end of installing packages
# in Linux you may need to run several commands (in the terminal) and install additional libraries, e.g
# sudo R CMD javareconf
# sudo apt-qet install build-essential
# sudo apt-get install libxml2-dev
# sudo apt-get install libpq
# sudo apt-qet install libpq-dev
# sudo apt-get install -y libmariadb-client-lgpl-dev
# sudo apt-qet install texlive-xetex
```

#### 1.2 R and RStudio

• R is a programming language for statistical computing and data analysis that supports a variety of programming styles. See R in Wikipedia

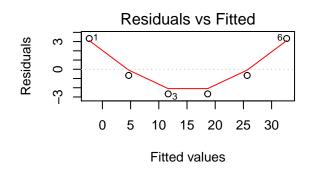
• R has multiple online resources and books. • R coding style • R-Bloggers • Getting help in R - RStudio cheat sheet - Base R cheat sheet Advanced R cheat sheet - Data Visualization cheat sheet - R Markdown cheatsheet - [R Markdown Basics] (http://rmarkdown.rstudio.com/authoring\_basics.html) - help(" ") command • R as a calculator. Console: It uses the command-line interface. Examples: # Create ordered collection (vector)  $x \leftarrow c(1,2,3,4,5,6)$  $y < - x^2$ # Square the elements of x print(y) # print (vector) y ## [1] 1 4 9 16 25 36 # Calculate average (arithmetic mean) of (vector) y; result is scalar mean(y) ## [1] 15.16667 # Calculate sample variance var(y) ## [1] 178.9667  $lm_1 \leftarrow lm(y \sim x)$ # Fit a linear regression model "y = f(x)" or "y = B0 + (B1 \* x)" # store the results as lm\_1 # Print the model from the (linear model object) lm\_1 print(lm\_1) ## ## Call: ## lm(formula = y ~ x)## ## Coefficients: ## (Intercept) Х -9.333 7.000 summary(lm\_1) # Compute and print statistics for the fit

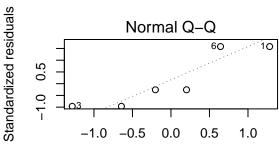
```
##
## Call:
## lm(formula = y \sim x)
##
## Residuals:
                 2
##
                        3
   3.3333 -0.6667 -2.6667 -2.6667 -0.6667 3.3333
##
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -9.3333
                           2.8441 -3.282 0.030453 *
## x
                 7.0000
                            0.7303
                                     9.585 0.000662 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
```

1.2. R AND RSTUDIO

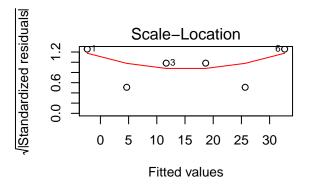
```
## Residual standard error: 3.055 on 4 degrees of freedom
## Multiple R-squared: 0.9583, Adjusted R-squared: 0.9478
## F-statistic: 91.88 on 1 and 4 DF, p-value: 0.000662

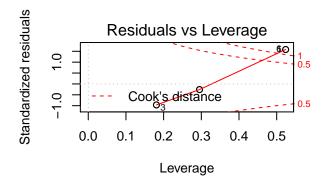
# of the (linear model object) lm_1
par(mfrow=c(2, 2)) # Request 2x2 plot layout
plot(lm_1) # Diagnostic plot of regression model
```





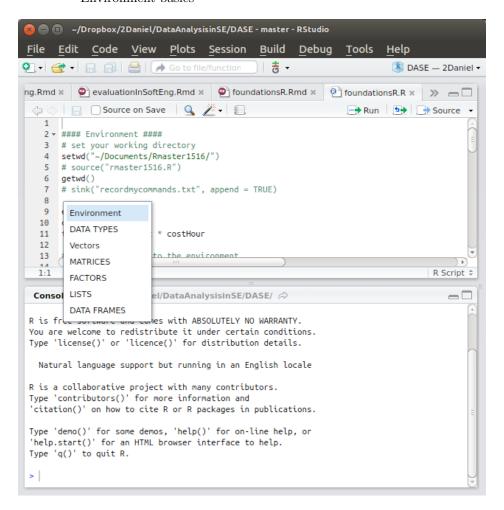
Theoretical Quantiles





- R script. # A file with R commands # comments source("filewithcommands.R") sink("recordmycommands.lis") savehistory()
- From command line:
  - Rscript
  - Rscript file with -e (e.g. Rscript -e 2+2)
  - To exit R: quit()
- Variables
- Operators
  - assign operator <-</li>
  - sequence operator, for example: mynums <- 0:20
  - arithmetic operators:  $+ = /^{\infty} / \%$  (integer division) %% (modulus operator)
- The workspace. Objects.
  - ls() objects() ls.str() lists and describes the objects
  - rm(x) delete a variable. E.g., rm(totalCost)

- s.str()
- objects()
- str() The structure function provides information about the variable
- RStudio, RCommander and RKWard are the well-known IDEs for R (more later).
- Four # ('####') create an *environment* in RStudio. An environment binds a set of names to a set of values. You can think of an environment as a bag of names.
  - Environment basics



#### Working directories:

```
# set your working directory
# setwd("~/workingDir/")
getwd()
```

#### ## [1] "/home/javier/DocProjects/DASE"

```
# record R commands:
# sink("recordmycommands.txt", append = TRUE)
```

#### 1.3 Basic Data Types

```
• class( )
  • logical: TRUE, FALSE
  • numeric, integer:
      - is.numeric( )
      - is.integer( )
  • character
Examples:
TRUE
## [1] TRUE
class(TRUE)
## [1] "logical"
FALSE
## [1] FALSE
NA # missing
## [1] NA
class(NA)
## [1] "logical"
## [1] TRUE
## [1] FALSE
# numeric data type
## [1] 2
class(2)
## [1] "numeric"
2.5
## [1] 2.5
2L # integer
## [1] 2
class(2L)
## [1] "integer"
is.numeric(2)
## [1] TRUE
```

```
is.numeric(2L)
## [1] TRUE
is.integer(2)
## [1] FALSE
is.integer(2L)
## [1] TRUE
   • data type coercion:
       - as.numeric( )
       - as.character( )
       - as.integer( )
Examples:
truenum <- as.numeric(TRUE)</pre>
truenum
## [1] 1
class(truenum)
## [1] "numeric"
falsenum <- as.numeric(FALSE)</pre>
falsenum
## [1] 0
num2char <- as.character(55)</pre>
num2char
## [1] "55"
char2num <- as.numeric("55.3")</pre>
char2int <- as.integer("55.3")</pre>
```

#### 1.3.1 Mising values

- NA stands for Not Available, which is not a number as well. It applies to missing values.
- NaN means 'Not a Number'

Examples:

```
NA + 1
## [1] NA
mean(c(5,NA,7))
## [1] NA
mean(c(5,NA,7), na.rm=TRUE) # some functions allow to remove NAs
## [1] 6
```

1.4. VECTORS

#### 1.4 Vectors

```
Examples:
phases <- c("reqs", "dev", "test1", "test2", "maint")</pre>
str(phases)
## chr [1:5] "reqs" "dev" "test1" "test2" "maint"
is.vector(phases)
## [1] TRUE
thevalues <-c(15, 60, 30, 35, 22)
names(thevalues) <- phases</pre>
str(thevalues)
## Named num [1:5] 15 60 30 35 22
## - attr(*, "names")= chr [1:5] "reqs" "dev" "test1" "test2" ...
thevalues
## reqs
           dev test1 test2 maint
##
     15
           60
                 30 35
# a single value is a vector
aphase <- 44
is.vector(aphase)
## [1] TRUE
A single value is a vector! Example:
aphase <- 44
is.vector(aphase)
## [1] TRUE
length(aphase)
## [1] 1
length(thevalues)
## [1] 5
```

#### 1.4.1 Coercion for vectors

```
thevalues1 <- c(15, 60, "30", 35, 22)
class(thevalues1)

## [1] "character"
thevalues1

## [1] "15" "60" "30" "35" "22"

# <- is equivalent to assign ()

assign("costs", c(50, 100, 30))</pre>
```

#### 1.4.2 Vector arithmetic

```
It is done in all elements. For example:
assign("costs", c(50, 100, 30))
costs/3
## [1] 16.66667 33.33333 10.00000
costs - 5
## [1] 45 95 25
costs <- costs - 5
incomes <-c(200, 800, 10)
earnings <- incomes - costs
sum(earnings)
## [1] 845
# R recycles values in vectors!
Subsetting vectors
### Subsetting vectors
phase1 <- phases[1]</pre>
phase1
## [1] "reqs"
phase3 <- phases[3]</pre>
phase3
## [1] "test1"
thevalues[phase1]
## reqs
## 15
thevalues["reqs"]
## reqs
testphases <- phases[c(3,4)]</pre>
thevalues[testphases]
## test1 test2
      30
### Negative indexes
phases1 <- phases[-5]</pre>
phases
## [1] "reqs" "dev"
                        "test1" "test2" "maint"
phases1
## [1] "reqs" "dev"
                        "test1" "test2"
```

1.4. VECTORS 19

```
#phases2 <- phases[-testphases] ## error in argument</pre>
phases2 <- phases[-c(3,4)]
phases2
                       "maint"
## [1] "reqs" "dev"
### subset using logical vector
phases3 <- phases[c(FALSE, TRUE, TRUE, FALSE)] #recicled first value</pre>
phases3
## [1] "dev"
               "test1"
selectionv <- c(FALSE, TRUE, TRUE, FALSE)
phases3 <- phases[selectionv]</pre>
phases3
## [1] "dev"
               "test1"
selectionvec2 <- c(TRUE, FALSE)</pre>
thevalues2 <- thevalues[selectionvec2]</pre>
thevalues2
## reqs test1 maint
     15
           30
                  22
### Generating regular sequenceswith : and seq
aseqofvalues <- 1:20
aseqofvalues2 <- seq(from=-3, to=3, by=0.5)
aseqofvalues2
## [1] -3.0 -2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0
aseqofvalues3 \leftarrow seq(0, 100, by=10)
aseqofvalues4 <- aseqofvalues3[c(2, 4, 6, 8)]
aseqofvalues4
## [1] 10 30 50 70
aseqofvalues4 <- aseqofvalues3[-c(2, 4, 6, 8)]
aseqofvalues4
       0 20 40 60 80 90 100
aseqofvalues3[c(1,2)] <- c(666,888)
aseqofvalues3
## [1] 666 888 20 30 40 50 60 70 80 90 100
### Logical values in vectors TRUE/FALSE
aseqofvalues3 > 50
## [1] TRUE TRUE FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE
aseqofvalues5 <- aseqofvalues3[aseqofvalues3 > 50]
aseqofvalues5
```

```
## [1] 666 888 60 70 80 90 100
aseqofvalues6 <- aseqofvalues3[!(aseqofvalues3 > 50)]
aseqofvalues6
## [1] 20 30 40 50
### Comparison functions
aseqofvalues7 <- aseqofvalues3[aseqofvalues3 == 50]</pre>
aseqofvalues7
## [1] 50
aseqofvalues8 <- aseqofvalues3[aseqofvalues3 == 22]</pre>
aseqofvalues8
## numeric(0)
aseqofvalues9 <- aseqofvalues3[aseqofvalues3 != 50]</pre>
aseqofvalues9
## [1] 666 888 20 30 40 60 70 80 90 100
logicalcond <- aseqofvalues3 >= 50
aseqofvalues10 <- aseqofvalues3[logicalcond]</pre>
aseqofvalues10
## [1] 666 888 50 60 70 80 90 100
### Remove Missing Values (NAs)
aseqofvalues3[c(1,2)] <- c(NA,NA)
aseqofvalues3
## [1] NA NA 20 30 40 50 60 70 80 90 100
aseqofvalues3 <- aseqofvalues3[!is.na(aseqofvalues3)]</pre>
aseqofvalues3
## [1] 20 30 40 50 60 70 80 90 100
```

#### 1.5 Arrays and Matrices

```
mymat <- matrix(1:12, nrow =2)</pre>
mymat
       [,1] [,2] [,3] [,4] [,5] [,6]
## [1,]
                        7
                             9
                                 11
       1 3
                   5
## [2,]
          2
               4
                    6
                            10
                                 12
mymat <- matrix(1:12, ncol =3)</pre>
mymat
       [,1] [,2] [,3]
## [1,] 1 5
          2 6
## [2,]
                  10
```

```
## [3,]
        3
              7 11
## [4,]
         4
              8
                  12
mymat <- matrix(1:12, nrow=2, byrow = TRUE)</pre>
mymat
##
       [,1] [,2] [,3] [,4] [,5] [,6]
## [1,] 1 2 3 4 5 6
## [2,]
        7 8
                   9 10
                          11
mymat <- matrix(1:12, nrow=3, ncol=4)</pre>
mymat
       [,1] [,2] [,3] [,4]
## [1,]
       1 4 7 10
## [2,]
          2
              5
                   8
                       11
## [3,]
       3
            6
                   9
                      12
mymat <- matrix(1:12, nrow=3, ncol=4, byrow=TRUE)</pre>
mymat
##
     [,1] [,2] [,3] [,4]
## [1,] 1 2 3 4
## [2,]
          5 6 7
## [3,]
       9 10 11 12
### recycling
mymat <- matrix(1:5, nrow=3, ncol=4, byrow=TRUE)</pre>
## Warning in matrix(1:5, nrow = 3, ncol = 4, byrow = TRUE): data length [5]
## is not a sub-multiple or multiple of the number of rows [3]
mymat
##
       [,1] [,2] [,3] [,4]
## [1,]
       1 2 3 4
## [2,]
          5 1 2
                        3
## [3,]
          4
             5
                   1
### rbind cbind
cbind(1:3, 1:3)
     [,1] [,2]
## [1,]
         1 1
## [2,]
          2
## [3,]
          3
rbind(1:3, 1:3)
       [,1] [,2] [,3]
##
## [1,] 1 2
## [2,]
         1
                   3
mymat <- matrix(1)</pre>
mymat <- matrix(1:8, nrow=2, ncol=4, byrow=TRUE)</pre>
mymat
       [,1] [,2] [,3] [,4]
##
```

```
## [1,] 1 2 3 4
## [2,] 5 6 7 8
rbind(mymat, 9:12)
## [,1] [,2] [,3] [,4]
## [1,]
      1 2 3 4
## [2,]
        5 6
               7
## [3,]
       9 10 11 12
mymat <- cbind(mymat, c(5,9))</pre>
mymat
## [,1] [,2] [,3] [,4] [,5]
## [1,] 1 2 3 4 5
## [2,] 5 6 7 8
                          9
mymat <- matrix(1:8, byrow = TRUE, nrow=2)</pre>
mymat
##
     [,1] [,2] [,3] [,4]
## [1,] 1 2 3 4
       5 6 7 8
## [2,]
rownames(mymat) <- c("row1", "row2")</pre>
mymat
      [,1] [,2] [,3] [,4]
## row1 1 2 3 4
## row2
       5 6 7 8
colnames(mymat) <- c("col1", "col2", "col3", "col4")</pre>
mymat
      col1 col2 col3 col4
## row1 1 2 3 4
       5 6 7
## row2
mymat2 <- matrix(1:12, byrow=TRUE, nrow=3, dimnames=list(c("row1", "row2", "row3"),
                                               c("col1", "col2", "col3", "col4")))
mymat2
      col1 col2 col3 col4
##
## row1 1 2 3 4
           6 7
## row2
         5
## row3
       9 10 11 12
### Coercion in Arrays
matnum <- matrix(1:8, ncol = 2)</pre>
matnum
## [,1] [,2]
## [1,] 1 5
## [2,] 2 6
## [3,] 3 7
## [4,]
        4 8
matchar <- matrix(LETTERS[1:6], nrow = 4, ncol = 3)</pre>
matchar
```

```
[,1] [,2] [,3]
##
## [1,] "A" "E" "C"
## [2,] "B" "F" "D"
## [3,] "C" "A" "E"
## [4,] "D" "B" "F"
matchars <- cbind(matnum, matchar)</pre>
matchars
       [,1] [,2] [,3] [,4] [,5]
##
## [1,] "1" "5" "A" "E" "C"
## [2,] "2" "6" "B" "F" "D"
## [3,] "3" "7" "C" "A" "E"
## [4,] "4" "8" "D" "B" "F"
### Subsetting
mymat3 <- matrix(sample(-8:15, 12), nrow=3)</pre>
mymat3
       [,1] [,2] [,3] [,4]
##
## [1,] 2
## [2,] -2 13 1 -1
             12 7 4
## [3,]
       11
mymat3[2,3]
## [1] 1
mymat3[1,4]
## [1] -8
mymat3[3,]
## [1] 11 12 7 4
mymat3[,4]
## [1] -8 -1 4
mymat3[5] # counts elements by column
## [1] 13
mymat3[9]
## [1] 7
## Subsetting multiple elements
mymat3[2, c(1,3)]
## [1] -2 1
mymat3[c(2,3), c(1,3,4)]
##
     [,1] [,2] [,3]
## [1,] -2 1 -1
## [2,] 11 7 4
```

```
rownames(mymat3) <- c("r1", "r2", "r3")
colnames(mymat3) <- c("c1", "c2", "c3", "c4")</pre>
mymat3["r2", c("c1", "c3")]
## c1 c3
## -2 1
### Subset by logical vector
mymat3[c(FALSE, TRUE, FALSE),
c(TRUE, FALSE, TRUE, FALSE)]
## c1 c3
## -2 1
mymat3[c(FALSE, TRUE, TRUE),
   c(TRUE, FALSE, TRUE, TRUE)]
     c1 c3 c4
## r2 -2 1 -1
## r3 11 7 4
### matrix arithmetic
row1 <- c(220, 137)
row2 \leftarrow c(345, 987)
row3 \leftarrow c(111, 777)
mymat4 <- rbind(row1, row2, row3)</pre>
rownames(mymat4) <- c("row_1", "row_2", "row_3")</pre>
colnames(mymat4) <- c("col_1", "col_2")</pre>
mymat4
       col 1 col 2
## row_1 220 137
## row_2 345 987
## row_3 111 777
mymat4/10
       col_1 col_2
## row_1 22.0 13.7
## row_2 34.5 98.7
## row_3 11.1 77.7
mymat4 -100
##
         col_1 col_2
## row_1 120
                  37
## row_2
           245
                 887
## row_3 11
                677
mymat5 \leftarrow rbind(c(50,50), c(10,10), c(100,100))
mymat5
##
       [,1] [,2]
## [1,] 50 50
## [2,] 10
             10
## [3,] 100 100
```

1.6. FACTORS 25

```
mymat4 - mymat5
       col_1 col_2
## row 1 170
                 87
                977
## row_2
          335
## row_3
         11
                677
mymat4 * (mymat5/100)
##
        col_1 col_2
## row_1 110.0 68.5
## row_2 34.5 98.7
## row_3 111.0 777.0
### index matrices
m1 \leftarrow array(1:20, dim=c(4,5))
m1
       [,1] [,2] [,3] [,4] [,5]
##
## [1,]
          1
              5
                 9
                       13
## [2,]
          2
               6
                 10
                       14
                            18
## [3,]
          3
             7 11
                       15
                            19
          4
             8 12
                            20
## [4,]
                       16
index <- array(c(1:3, 3:1), dim=c(3,2))
index
##
       [,1] [,2]
## [1,]
          1
## [2,]
          2
               2
## [3,]
m1[index] < -0
m1
       [,1] [,2] [,3] [,4] [,5]
##
## [1,]
       1
             5 0
                       13
## [2,]
          2
               0 10
                            18
                       14
## [3,] 0
             7 11
                       15
                            19
## [4,] 4 8 12
                       16
                            20
```

#### 1.6 Factors

• Factors in R are stored as a vector of integer values with a corresponding set of character values to use when the factor is displayed.

```
personnel <- c("Analyst1", "ManagerL2", "Analyst1", "Analyst2", "Boss", "ManagerL1", "ManagerL2", "Propersonnel_factors <- factor(personnel)
personnel_factors #sorted alphabetically

## [1] Analyst1 ManagerL2 Analyst1 Analyst2 Boss
## [6] ManagerL1 ManagerL2 Programmer1 Programmer2 Programmer3
## [11] Designer1 Designer2 OtherStaff</pre>
```

```
## 11 Levels: Analyst1 Analyst2 Boss Designer1 Designer2 ... Programmer3
str(personnel_factors)
## Factor w/ 11 levels "Analyst1", "Analyst2",..: 1 7 1 2 3 6 7 9 10 11 ...
personnel2 <- factor(personnel,</pre>
                       levels = c("Boss", "ManagerL1", "ManagerL2", "Analyst1", "Analyst2",
                                                                                                "Designer1
personnel2
  [1] Analyst1
                    ManagerL2
                                Analyst1
                                             Analyst2
                                                          Boss
## [6] ManagerL1
                    ManagerL2
                                Programmer1 Programmer2 Programmer3
## [11] Designer1
                                OtherStaff
                    Designer2
## 11 Levels: Boss ManagerL1 ManagerL2 Analyst1 Analyst2 ... OtherStaff
str(personnel2)
## Factor w/ 11 levels "Boss", "ManagerL1", ...: 4 3 4 5 1 2 3 8 9 10 ...
# a factor's levels will always be character values.
levels(personnel2) <- c("B", "M1", "M2", "A1", "A2", "D1", "D2", "P1", "P2", "P3", "OS")</pre>
personnel2
## [1] A1 M2 A1 A2 B M1 M2 P1 P2 P3 D1 D2 OS
## Levels: B M1 M2 A1 A2 D1 D2 P1 P2 P3 OS
personnel3 <- factor(personnel,</pre>
                     levels = c("Boss", "ManagerL1", "ManagerL2", "Analyst1", "Analyst2",
                                                                                              "Designer1",
                     c("B", "M1", "M2", "A1", "A2", "D1", "D2", "P1", "P2", "P3", "OS"))
personnel3
## [1] A1 M2 A1 A2 B M1 M2 P1 P2 P3 D1 D2 OS
## Levels: B M1 M2 A1 A2 D1 D2 P1 P2 P3 OS
### Nominal versus ordinal, ordered factors
personnel3[1] < personnel3[2] # error, factors not ordered</pre>
## Warning in Ops.factor(personnel3[1], personnel3[2]): '<' not meaningful for
## factors
## [1] NA
tshirts <- c("M", "L", "S", "S", "L", "M", "L", "M")
tshirt_factor <- factor(tshirts, ordered = TRUE,</pre>
                        levels = c("S", "M", "L"))
tshirt_factor
## [1] M L S S L M L M
## Levels: S < M < L
tshirt_factor[1] < tshirt_factor[2]</pre>
## [1] TRUE
```

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#### 1.7 Lists

```
• '[' returns a list
  • '[[' returns the list element
  • '$' returns the content of that element in the list
c("R good times", 190, 5)
                                        "5"
## [1] "R good times" "190"
song <- list("R good times", 190, 5)</pre>
is.list(song)
## [1] TRUE
str(song)
## List of 3
## $ : chr "R good times"
## $ : num 190
## $ : num 5
names(song) <- c("title", "duration", "track")</pre>
song
## $title
## [1] "R good times"
##
## $duration
## [1] 190
##
## $track
## [1] 5
song$title
## [1] "R good times"
song2 <- list(title="Good Friends",</pre>
               duration = 125,
               track = 2,
               rank = 6)
song3 <- list(title="Many Friends",</pre>
               duration = 125,
               track= 2,
               rank = 1,
               similar2 = song2)
song[1]
## $title
## [1] "R good times"
song$title
## [1] "R good times"
```

```
str(song[1])
## List of 1
## $ title: chr "R good times"
song[[1]]
## [1] "R good times"
str(song[[1]])
## chr "R good times"
song2[3]
## $track
## [1] 2
song3[5] # a list
## $similar2
## $similar2$title
## [1] "Good Friends"
## $similar2$duration
## [1] 125
## $similar2$track
## [1] 2
##
## $similar2$rank
## [1] 6
str(song3[5])
## List of 1
## $ similar2:List of 4
## ..$ title : chr "Good Friends"
## ..$ duration: num 125
##
   ..$ track : num 2
## ..$ rank : num 6
song3[[5]]
## $title
## [1] "Good Friends"
## $duration
## [1] 125
## $track
## [1] 2
##
## $rank
## [1] 6
song3$similar2
```

## \$title

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```
## [1] "Good Friends"
##
## $duration
## [1] 125
## $track
## [1] 2
##
## $rank
## [1] 6
song[c(1,3)]
## $title
## [1] "R good times"
## $track
## [1] 5
str(song[c(1,3)])
## List of 2
## $ title: chr "R good times"
## $ track: num 5
result <- song[c(1,3)]
result[1]
## $title
## [1] "R good times"
result[[1]]
## [1] "R good times"
str(result)
## List of 2
## $ title: chr "R good times"
## $ track: num 5
result$title
## [1] "R good times"
result$track
## [1] 5
# access with [[ to content
song3[[5]][[1]]
## [1] "Good Friends"
song3\similar2[[1]]
## [1] "Good Friends"
# Subsets
### subset by names
song[c("title", "track")]
```

```
## $title
## [1] "R good times"
## $track
## [1] 5
song3["similar2"]
## $similar2
## $similar2$title
## [1] "Good Friends"
## $similar2$duration
## [1] 125
##
## $similar2$track
## [1] 2
## $similar2$rank
## [1] 6
resultsimilar <- song3["similar2"]</pre>
str(resultsimilar)
## List of 1
## $ similar2:List of 4
   ..$ title : chr "Good Friends"
## ..$ duration: num 125
## ..$ track : num 2
     ..$ rank
                : num 6
resultsimilar1 <-song3[["similar2"]]</pre>
str(resultsimilar1)
## List of 4
## $ title : chr "Good Friends"
## $ duration: num 125
## $ track : num 2
## $ rank : num 6
resultsimilar1$title
## [1] "Good Friends"
# subset by logicals
song[c(TRUE, FALSE, TRUE, FALSE)]
## $title
## [1] "R good times"
##
## $track
## [1] 5
result3 <- song[c(TRUE, FALSE, TRUE, FALSE)] # is a list of two elements
# extending the list
shared <- c("Hillary", "Javi", "Mikel", "Patty")</pre>
```

1.8. DATA FRAMES 31

```
song3$shared <- shared
str(song3)
## List of 6
## $ title
            : chr "Many Friends"
## $ duration: num 125
## $ track : num 2
## $ rank
             : num 1
## $ similar2:List of 4
## ..$ title : chr "Good Friends"
## ..$ duration: num 125
##
    ..$ track : num 2
##
   ..$ rank : num 6
## $ shared : chr [1:4] "Hillary" "Javi" "Mikel" "Patty"
cities <- list("Bilbao", "New York", "Tartu")</pre>
song3[["cities"]] <- cities</pre>
str(song3)
## List of 7
## $ title
            : chr "Many Friends"
## $ duration: num 125
## $ track : num 2
## $ rank
             : num 1
## $ similar2:List of 4
   ..$ title : chr "Good Friends"
##
    ..$ duration: num 125
##
    ..$ track : num 2
##
    ..$ rank : num 6
## $ shared : chr [1:4] "Hillary" "Javi" "Mikel" "Patty"
## $ cities :List of 3
    ..$ : chr "Bilbao"
##
##
   ..$ : chr "New York"
##
    ..$ : chr "Tartu"
```

#### 1.8 Data frames

## 5 Edurne 65 FALSE

```
thenames <- c("Ane", "Mike", "Xabi", "Viktoria", "Edurne")
ages <-c(44, 20, 33, 15, 65)
employee <- c(FALSE, FALSE, TRUE, TRUE, FALSE)</pre>
mydataframe <- data.frame(thenames, ages, employee)</pre>
mydataframe
    thenames ages employee
        Ane 44
## 1
                    FALSE
        Mike 20
## 2
                     FALSE
## 3
        Xabi 33 TRUE
## 4 Viktoria 15
                     TRUE
```

```
names(mydataframe) <- c("FirstName", "Age", "Employee")</pre>
str(mydataframe)
## 'data.frame':
                    5 obs. of 3 variables:
## $ FirstName: Factor w/ 5 levels "Ane", "Edurne", ..: 1 3 5 4 2
          : num 44 20 33 15 65
## $ Employee : logi FALSE FALSE TRUE TRUE FALSE
#strings are not factors!
mydataframe <- data.frame(thenames, ages, employee,</pre>
                          stringsAsFactors=FALSE)
names(mydataframe) <- c("FirstName", "Age", "Employee")</pre>
str(mydataframe)
## 'data.frame':
                    5 obs. of 3 variables:
## $ FirstName: chr "Ane" "Mike" "Xabi" "Viktoria" ...
## $ Age : num 44 20 33 15 65
## $ Employee : logi FALSE FALSE TRUE TRUE FALSE
# subset data frame
mydataframe[4,2]
## [1] 15
mydataframe[4, "Age"]
## [1] 15
mydataframe[, "FirstName"]
## [1] "Ane"
                  "Mike"
                             "Xabi"
                                        "Viktoria" "Edurne"
mydataframe[c(2,5), c("Age", "Employee")]
     Age Employee
## 2 20
           FALSE
## 5 65
            FALSE
matfromframe <- as.matrix(mydataframe[c(2,5), c("Age", "Employee")])</pre>
str(matfromframe)
## num [1:2, 1:2] 20 65 0 0
## - attr(*, "dimnames")=List of 2
   ..$ : chr [1:2] "2" "5"
## ..$ : chr [1:2] "Age" "Employee"
mydataframe[3]
##
    Employee
## 1
      FALSE
## 2
        FALSE
## 3
        TRUE
## 4
        TRUE
## 5
        FALSE.
# convert to vector
mydf0 <- mydataframe[3] #data.frame</pre>
```

1.8. DATA FRAMES 33

```
str(mydf0)
                   5 obs. of 1 variable:
## 'data.frame':
## $ Employee: logi FALSE FALSE TRUE TRUE FALSE
myvec <- mydataframe[[3]] #vector</pre>
str(myvec)
## logi [1:5] FALSE FALSE TRUE TRUE FALSE
mydf0asvec <- as.vector(mydataframe[3]) # but it doesn't work . Use [[]]
str(mydf0asvec)
## 'data.frame':
                   5 obs. of 1 variable:
## $ Employee: logi FALSE FALSE TRUE TRUE FALSE
mydf0asvec <- as.vector(mydataframe[[3]])</pre>
str(mydf0asvec)
## logi [1:5] FALSE FALSE TRUE TRUE FALSE
# add column
height <- c(166, 165, 158, 176, 199)
weight \leftarrow c(66, 77, 99, 88, 109)
mydataframe$height <- height
mydataframe[["weight"]] <- weight</pre>
mydataframe
    FirstName Age Employee height weight
##
## 1
          Ane 44
                   FALSE
                              166
## 2
         Mike 20
                     FALSE
                              165
                                      77
                      TRUE
## 3
         Xabi 33
                              158
                                      99
## 4 Viktoria 15
                     TRUE 176
                                      88
## 5
       Edurne 65
                  FALSE 199
                                    109
# add a column
birthplace <- c("Tallinn", "London", "Donostia", "Paris", "New York")
mydataframe <- cbind(mydataframe, birthplace)</pre>
mydataframe
##
    FirstName Age Employee height weight birthplace
## 1
          Ane 44
                   FALSE
                              166
                                    66
                                           Tallinn
         Mike 20
## 2
                     FALSE
                              165
                                     77
                                            London
## 3
         Xabi 33
                     TRUE 158 99 Donostia
## 4 Viktoria 15
                     TRUE 176 88
                                             Paris
                   FALSE 199
                                  109 New York
## 5
       Edurne 65
# add a row
anton <- data.frame(FirstName = "Anton", Age = 77, Employee=TRUE, height= 170, weight = 65, birthplace
mydataframe <- rbind (mydataframe, anton)
mydataframe
##
    FirstName Age Employee height weight birthplace
## 1
          Ane 44 FALSE
                              166
                                    66
                                           Tallinn
## 2
         Mike 20
                     FALSE
                              165
                                     77
                                            London.
```

```
## 3
          Xabi
               33
                       TRUE
                                158
                                        99
                                             Donostia
## 4
     Viktoria 15
                       TRUE
                                176
                                        88
                                                Paris
        Edurne
## 5
                      FALSE
                                199
                                       109
                                             New York
## 6
         Anton
               77
                       TRUE
                                170
                                        65
                                            Amsterdam
# sorting
mydataframeSorted <- mydataframe[order(mydataframe$Age, decreasing = TRUE), ] #all columns
mydataframeSorted
##
     FirstName Age Employee height weight birthplace
## 6
         Anton
               77
                       TRUE
                                170
                                        65
                                            Amsterdam
## 5
        Edurne 65
                      FALSE
                                199
                                       109
                                             New York
                                              Tallinn
## 1
           Ane 44
                      FALSE
                                166
                                        66
## 3
          Xabi 33
                       TRUE
                                158
                                        99
                                             Donostia
## 2
          Mike
               20
                      FALSE
                                165
                                        77
                                               London
## 4
     Viktoria 15
                       TRUE
                                176
                                        88
                                                Paris
mydataframeSorted2 <- mydataframe[order(mydataframe$Age, decreasing = TRUE), c(1,2,6)]
mydataframeSorted2
##
     FirstName Age birthplace
## 6
         Anton
               77
                    Amsterdam
## 5
        Edurne
                65
                     New York
## 1
           Ane
                44
                      Tallinn
## 3
                33
          Xabi
                     Donostia
## 2
          Mike
                20
                       London
## 4
     Viktoria 15
                        Paris
```

#### 1.9 Reading Data

```
library(foreign)
isbsg <- read.arff("datasets/effortEstimation/isbsg10teaser.arff")

mydataISBSG <- isbsg[, c("FS", "N_effort")]

str(mydataISBSG)

## 'data.frame': 37 obs. of 2 variables:
## $ FS : num 225 599 333 748 158 427 461 257 115 116 ...
## $ N_effort: num 1856 10960 5661 1518 3670 ...</pre>
```

#### 1.10 Plots

There are several graphic packages that are recommended, in particular ggplot. However, there is some basic support in the R base for graphics. The following Figure 1.1 shows a simple plot.

```
plot(mydataISBSG$FS, mydataISBSG$N_effort)
```

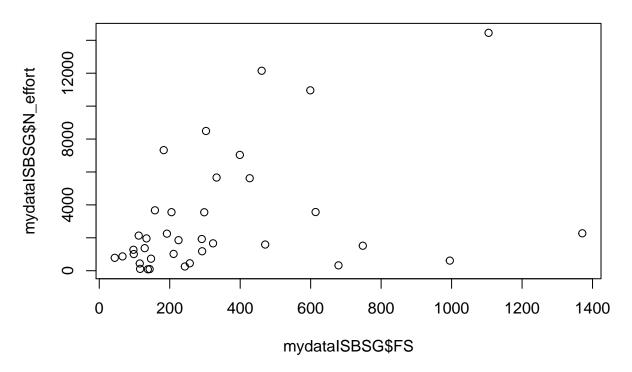


Figure 1.1: Simple plot

#### 1.11 Flow of Control

```
Ifelse:
```

```
library(foreign)
kc1 <- read.arff("datasets/defectPred/D1/KC1.arff")</pre>
kc1$Defective <- ifelse(kc1$Defective == "Y", 1, 0)</pre>
head(kc1, 1)
     LOC BLANK BRANCH COUNT LOC CODE AND COMMENT LOC COMMENTS
##
## 1
             0
     CYCLOMATIC_COMPLEXITY DESIGN_COMPLEXITY ESSENTIAL_COMPLEXITY
##
## 1
                          1
     LOC_EXECUTABLE HALSTEAD_CONTENT HALSTEAD_DIFFICULTY HALSTEAD_EFFORT
##
                                                      2.67
## 1
                                11.58
     HALSTEAD_ERROR_EST HALSTEAD_LENGTH HALSTEAD_LEVEL HALSTEAD_PROG_TIME
##
## 1
                   0.01
                                                    0.38
                                                                        4.57
                                       11
     HALSTEAD_VOLUME NUM_OPERANDS NUM_OPERATORS NUM_UNIQUE_OPERANDS
##
## 1
               30.88
                                 4
##
     NUM_UNIQUE_OPERATORS LOC_TOTAL Defective
                                   5
## 1
                         4
```

#### 1.12 Rattle

There is graphical interface, Rattle, that allow us to perform some data mining tasks with R (Williams, 2011).

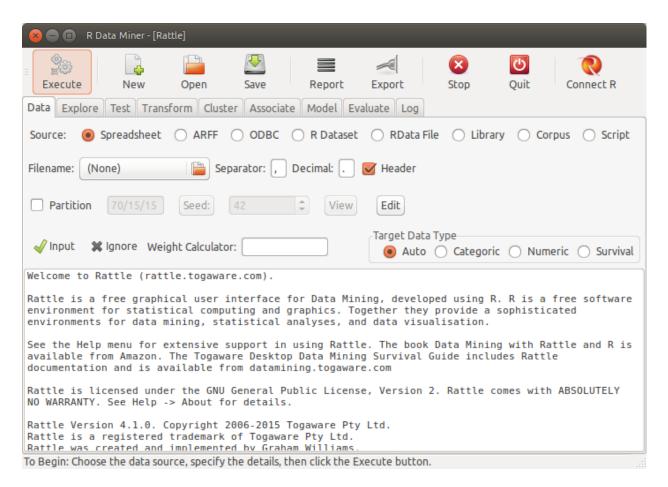


Figure 1.2: Rattle: GUI for Data mining with R

# Part II Introduction to Data Mining

We will deal with extracting information from data, either for estimation, defect prediction, planning, etc. We will provide an overview of data analysis using different techniques.

### Chapter 2

## What is Data Mining / Knowledge Discovery in Databases (KDD)

The non-trivial process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data (Fayyad et al., 1996)

The Cross Industry Process for Data Mining (CRISP-DM) also provides a common and well-developed framework for delivering data mining projects identifying six steps (Shearer, 2000):

- 1. Problem Understanding
- 2. Data Understanding
- 3. Data Preparation
- 4. Modeling
- 5. Evaluation
- 6. Deployment

#### 2.1 The Aim of Data Analysis and Statistical Learning

- The aim of any data analysis is to understand the data
- and to build models for making predictions and estimating future events based on past data
- and to make statistical inferences from our data.
- We may want to test different hypothesis on the data
- We want to generate conclusions about the population where our sample data comes from
- Most probably we are interested in building a model for quality, time, defects or effort prediction
- We want to find a function f(), that given X1, X2, ... computes Y = f(X1, X2, ..., Xn)

#### 2.2 Basic References

Generic books about statistics:

- John Verzani, simpleR Using R for Introductory Statistics
- Peter Dalgaard, Introductory Statistics with R, 2nd Edt., Springer, 2008
- Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani, An Introduction to Statistical Learning with Applications in R, Springer, 2013

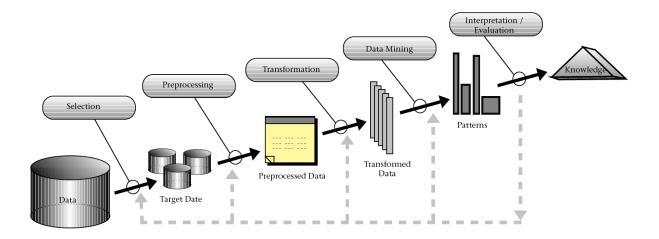


Figure 2.1: KDD Process



Figure 2.2: CRISP-DM (Wikipedia)

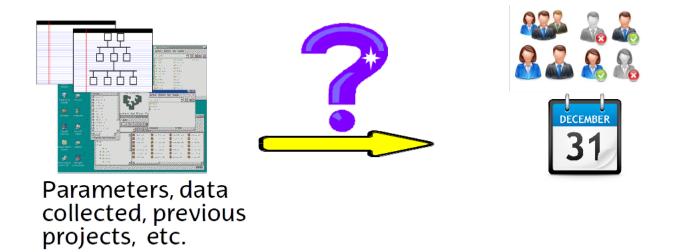


Figure 2.3:

• Geoff Cumming, Understanding the New Statistics: Effect Sizes, Confidence Intervals, and Meta-Analysis, Routledge, New York, 2012

#### 2.3 Data Mining with R

 $\bullet$  Graham Williams, Data Mining with Rattle and R: The Art of Excavating Data for Knowledge Discovery, Springer 2011

Also the author maintains a Web site: http://rattle.togaware.com/

- Luis Torgo, Data Mining with R: Learning with Case Studies, Chapman and Hall/CRC, 2010
- http://www.rdatamining.com/

#### 2.4 Data Mining with Weka

Weka is another popular framework in Java:

• Ian Witten, Eibe Frank, Mark Hall, Christopher J. Pal, Data Mining: Practical Machine Learning Tools and Techniques (4th Edt), Morgan Kaufmann, 2016, ISBN: 978-0128042915

## Part III

## Data Sources and Metrics and Standards in Software Engineering Defect Prediction

### Chapter 3

## Data Sources in Software Engineering

We classify this trail in the following categories:

- Source code can be studied to measure its properties, such as size or complexity.
- Source Code Management Systems (SCM) make it possible to store all the changes that the different source code files undergo during the project. Also, SCM systems allow for work to be done in parallel by different developers over the same source code tree. Every change recorded in the system is accompanied with meta-information (author, date, reason for the change, etc) that can be used for research purposes.
- Issue or Bug tracking systems (ITS). Bugs, defects and user requests are managed in ISTs, where users and developers can fill tickets with a description of a defect found, or a desired new functionality. All the changes to the ticket are recorded in the system, and most of the systems also record the comments and communications among all the users and developers implied in the task.
- Messages between developers and users. In the case of free/open source software, the projects are open
  to the world, and the messages are archived in the form of mailing lists and social networks which can
  also be mined for research purposes. There are also some other open message systems, such as IRC or
  forums.
- Meta-data about the projects. As well as the low level information of the software processes, we can also find meta-data about the software projects which can be useful for research. This meta-data may include intended-audience, programming language, domain of application, license (in the case of open source), etc.
- Usage data. There are statistics about software downloads, logs from servers, software reviews, etc.

Types of information stored in the repositories:

- Meta-information about the project itself and the people that participated.
  - Low-level information
    - \* Mailing Lists (ML)
    - \* Bug Tracking Systems (BTS) or Project Tracker System (PTS)
    - \* Software Configuration Management Systems (SCM)
  - Processed information. For example project management information about the effort estimation and cost of the project.
- Whether the repository is public or not
- Single project vs. multiprojects. Whether the repository contains information of a single project with multiples versions or multiples projects and/or versions.

#### hello.c

```
#include <stdio.h>
int main() {
  printf("Hello world");
  return 0;
}
```

### Artifact Source code file

#### hello.c.diff

```
- printf("Hello world");
+ printf("Hello world\n");
```

Author: rms

Date: 20100618 04:34 UTC

Change: +1 -1

Log: Forgot to add new line

## Repository Change to an artifact Meta-information

Figure 3.1: Metadata (source: Israel Herraiz)

- Type of content, open source or industrial projects
- Format in which the information is stored and formats or technologies for accessing the information:
  - Text. It can be just plain text, CSV (Comma Separated Values) files, Attribute-Relation File Format (ARFF) or its variants
  - Through databases. Downloading dumps of the database.
  - Remote access such as APIs of Web services or REST

## Chapter 4

## Repositories

There is a number of open research repositories in Software Engineering. Among them:

- PROMISE (PRedictOr Models In Software Engineering): http://openscience.us/repo/
- Finding Faults using Ensemble Learners (ELFF) (Shippey et al., 2016) http://www.elff.org.uk/
- FLOSSMole (Howison et al., 2006) http://flossmole.org/
- FLOSSMetrics (Herraiz et al., 2009): http://flossmetrics.org/
- Qualitas Corpus (QC) (Tempero et al., 2010): http://qualitascorpus.com/
- Sourcerer Project (Linstead et al., 2009): http://sourcerer.ics.uci.edu/
- Ultimate Debian Database (UDD) (Nussbaum and Zacchiroli, 2010) http://udd.debian.org/
- SourceForge Research Data Archive (SRDA) (Van Antwerp and Madey, 2008) http://zerlot.cse.nd.edu/
- SECOLD (Source code ECOsystem Linked Data): http://www.secold.org/
- Software-artifact Infrastructure Repository (SIR) [http://sir.unl.edu]
- OpenHub: https://www.openhub.net/

Not openly available (and mainly for effort estimation):

- The International Software Benchmarking Standards Group (ISBSG) http://www.isbsg.org/
- TukuTuku http://www.metrig.biz/tukutuku/

Some papers and publications/theses that have been used in the literature:

- Helix Data Set (Vasa, 2010): http://www.ict.swin.edu.au/research/projects/helix/
- Bug Prediction Dataset (BPD) (D'Ambros et al., 2010, D'Ambros et al. (2011)): http://bug.inf.usi.ch/
- Eclipse Bug Data (EBD) (Zimmermann et al., 2007, Nagappan et al. (2012)): http://www.st.cs. uni-saarland.de/softevo/bug-data/eclipse/

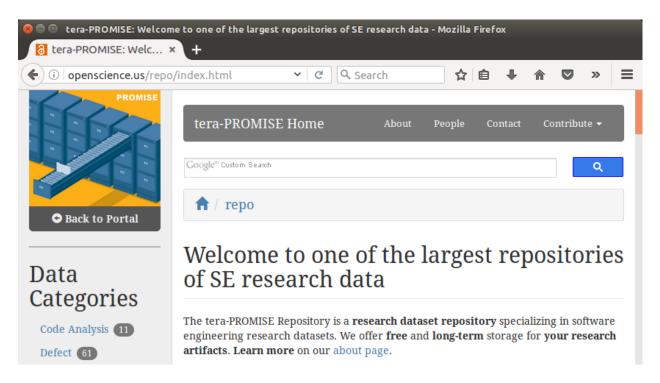


Figure 4.1: Promise Repository

## Chapter 5

## Open Tools/Dashboards to extract data

Process to extract data:

Within the open source community, several toolkits allow us to extract data that can be used to explore projects:

Metrics Grimoire http://metricsgrimoire.github.io/

SonarQube http://www.sonarqube.org/

CKJM (OO Metrics tool) http://gromit.iiar.pwr.wroc.pl/p\_inf/ckjm/

Collects a large number of object-oriented metrics from code.

#### 5.1 Issues

There are problems such as different tools report different values for the same metric (Lincke et al., 2008) It is well-know that the NASA datasets have some problems:

- (Gray et al., 2011) The misuse of the NASA metrics data program data sets for automated software defect prediction
- (Shepperd et al., 2013) Data Quality: Some Comments on the NASA Software Defect Datasets

#### 5.2 Effort Estimation Data in Software Engineering

It is worth highlighting the case of software effort estimation datasets with their peculiarities. First, most effort estimation datasets used in the literature are scattered through research papers with the exception of a few kept in the PROMISE repository. Mair et al (2005) also have analysed available datasets in the field of cost estimation identifying 65 different datasets in 50 papers.



Figure 5.1: Process

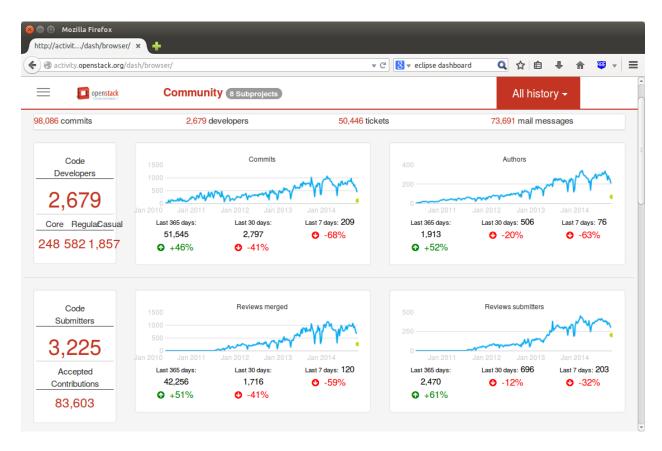


Figure 5.2: Grimoire

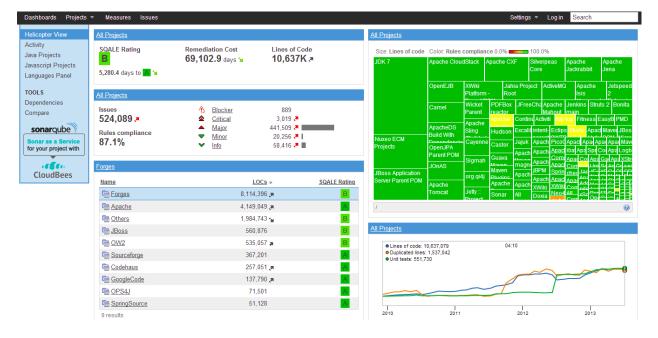


Figure 5.3: SonarQube

Second, their size is very small with the exception of ISBSG repository discussed previously which a small sample is available through PROMISE and the China dataset with 499 instances.

Third, some can be quite old in a context and time that is not applicable to current development environments. The authors noted that the oldest datasets (COCOMO, Desharnais, Kemerer and Albrecht and Gaffney) tend to be the most studied ones and a subset of the most relevant ones. Also, from the artificial intelligence or data mining point of view effort estimation has been mainly tackled with different types of regression techniques and more recently with techniques which are also typically considered under the umbrella of data mining techniques. However, as the number of examples per dataset is increasing, other machine learning techniques are also being studied (e.g.: Dejaeger et al (2012) report on a comparison of several machine learning techniques to effort estimation with only 5 out the 9 used datasets publicly available). From the data mining point of view, the small number of instances hinders the application of machine learning techniques.

However, software effort and cost estimation still remain one of the main challenges in software engineering and have attracted a great deal of interest by many researchers (2007). For example, there are continuous analyses of whether software development follows economies or diseconomies of scale (see (Dolado, 2001, Banker et al. (1994), Kitchenham (2002))).

Next Table 5.1 (following Mair et al (2005) ) shows the most open cost/effort datasets available in the literature with their main reference.

Table 5.1: Effort Estimation Dataset from articles

Reference	Instances	Attributes
Abran and Robillard (1996)	21	31
Albrecht-Gaffney (1983)	24	7
Bailey and Basili (1981)	18	9
Belady and Lehman (1979)	33	
Boehm (aka COCOMO Dataset) (1981)	63	43
China dataset <sup>1</sup>	499	18
Desharnais (1988)	61	10
Dolado (1997)	24	7
Hastings and Sajeev (2001)	8	14
Heiat and Heiat (Heiat and Heiat, 1997)	35	4
Jeffery and Stathis (1996)	17	7
Jorgensen (2004)	47	4
Jorgensen et al. (2003)	20	4
Kemerer (1987)	15	5
Kitchenham (Mermaid 2) (2002)	30	5
Kitchenham et al. (CSC) (2002)	145	9
Kitchenham and Taylor (ICL) (1985)	10	6
Kitchenham and Taylor (BT System X) (1985)	10	3
Kitchenham and Taylor (BT Software Houses)	12	6
(1985)		
Li et al.(USP05) $(2007)^2$	202	16
Mišić and Tevsić (1998)	6	16
Maxwell (Dev Effort) (2002)	63	32
Maxwell (Maintenance Eff) (2002)	67	28
Miyazaki et al. (1994)	47	9
Moser et al. (1999)	37	4
Shepperd and Cartwright (Shepperd and Cartwright, 2001)	39	3

<sup>&</sup>lt;sup>1</sup>Donated through PROMISE.

 $<sup>^2</sup>$ Only a subset of the data in the paper, the complete dataset is donated through PROMISE

Reference	Instances	Attributes
Shepperd and Schofield (Telecom 1) (1997)	18	5
Schofield (real-time 1) (1998, Shepperd and	21	4
Schofield (1997))		
Schofield (Mermaid) (1998)	30	18
Schofield (Finnish) (1998)	39	30
Schofield (Hughes) (1998)	33	14
Woodfield et al. (1981)	63	8

## Part IV

## Exploratory and Descriptive Data analysis

## Chapter 6

## **Exploratory Data Analysis**

#### 6.1 Descriptive statistics

The first task with any dataset is to characterise it in terms of summary statistics and graphics.

Displaying information graphically will help us to identify the main characteristics of the data. To describe a distribution we often want to know where it is centered and and what the spread is (mean, median, quantiles)

#### 6.2 Basic Plots

- *Histogram* defines a sequence of breaks and then counts the number of observations in the bins formed by the breaks.
- Boxplot used to summarize data succinctly, quickly displaying if the data is symmetric or has suspected
  outliers.
- Q-Q plot is used to determine if the data is close to being normally distributed. The quantiles of the standard normal distribution is represented by a straight line. The normality of the data can be evaluated by observing the extent in which the points appear on the line. When the data is normally distributed around the mean, then the mean and the median should be equal.
- Scatterplot provides a graphical view of the relationship between two sets of numbers: one numerical variable against another.
- Kernel Density plot visualizes the underlying distribution of a variable. Kernel density estimation is a non-parametric method of estimating the probability density function of continuous random variable. It helps to identify the distribution of the variable.
- Violin plot is a combination of a boxplot and a kernel density plot.

#### 6.3 Normality

- A normal distribution is an arrangement of a data set in which most values cluster in the middle of the range
- A graphical representation of a normal distribution is sometimes called a *bell curve* because of its shape.
- Many procedures in statistics are based on this property. *Parametric* procedures require the normality property.

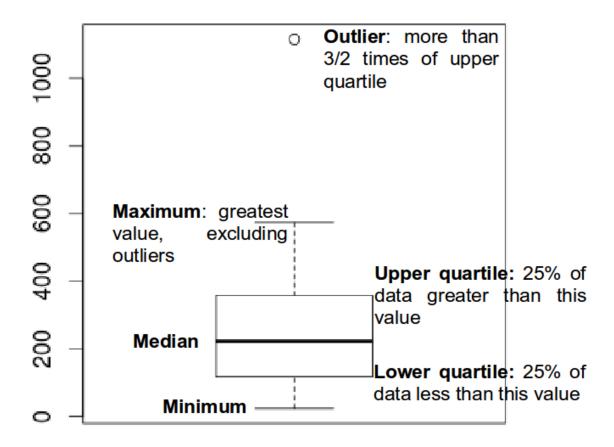


Figure 6.1: Boxplot description

6.3. NORMALITY 59

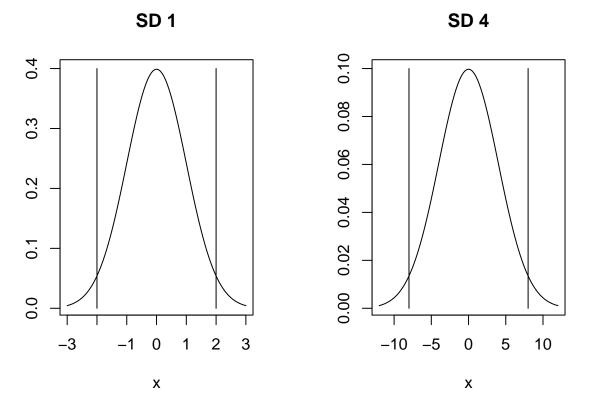


Figure 6.2: Plot exaple of the area within 2 and 4SD of the mean respectively

- In a normal distribution about 95% of the probability lies within 2 Standard Deviations of the mean.
- Two examples: one population with mean 60 and the standard deviation of 1, and the other with mean 60 and sd = 4 (means shifted to 0)

• if we sample from this population we get "another population":

```
sample.means <- rep(NA, 1000)
for (i in 1:1000) {
    sample.40 <- rnorm(40, mean = 60, sd = 4)
    # rnorm generates random numbers from normal distribution
    sample.means[i] <- mean(sample.40)
}
means40 <- mean(sample.means)
sd40 <- sd(sample.means)
means40</pre>
```

#### Histogram of sample.means

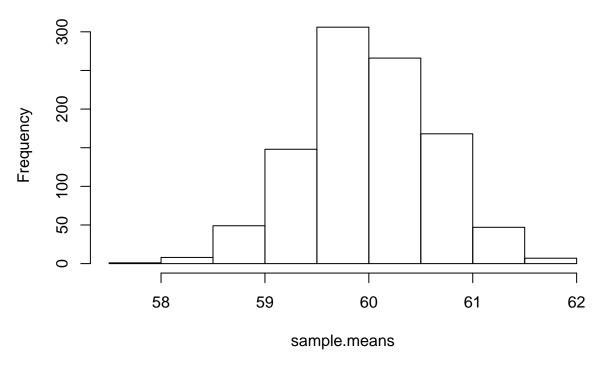


Figure 6.3: Sample means histogram

```
## [1] 60.00575
sd40
```

## [1] 0.6244761

• These sample means are another "population". The sampling distribution of the sample mean is normally distributed meaning that the "mean of a representative sample provides an estimate of the unknown population mean". This is shown in Figure 6.3

hist(sample.means)

#### 6.4 Using a running Example to visualise the different plots

As a running exmple we do next:

- 1. Set the path to to the file
- 2. Read the Telecom1 dataset and print out the summary statistics with the command summary

```
options(digits = 3)
telecom1 <- read.table("./datasets/effortEstimation/Telecom1.csv", sep = ",",
    header = TRUE, stringsAsFactors = FALSE, dec = ".") #read data
summary(telecom1)</pre>
```

```
## size effort EstTotal
## Min. : 3.0 Min. : 24 Min. : 30
## 1st Qu.: 37.2 1st Qu.: 119 1st Qu.: 142
```

```
Median: 68.5
                  Median: 222
                                 Median:289
##
         :100.3
                  Mean : 284
                                 Mean
                                       :320
   Mean
                  3rd Qu.: 352
                                 3rd Qu.:472
   3rd Qu.:164.0
          :284.0
  Max.
                  Max.
                         :1116
                                        :777
                                 Max.
```

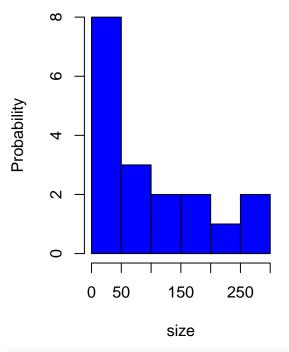
- We see that this dataset has three variables (or parameters) and few data points (18)
  - size: the independent variable
  - effort: the dependent variable
  - EstTotal: the estimates coming from an estimation method
- Basic Plots

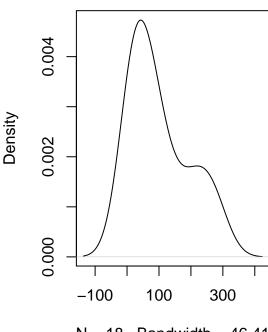
```
par(mfrow = c(1, 2)) #n figures per row
size_telecom1 <- telecom1$size
effort_telecom1 <- telecom1$effort

hist(size_telecom1, col = "blue", xlab = "size", ylab = "Probability", main = "Histogram of project Siz
lines(density(size_telecom1, na.rm = T, from = 0, to = max(size_telecom1)))
plot(density(size_telecom1))</pre>
```

#### **Histogram of project Size**

#### density.default(x = size\_telecom



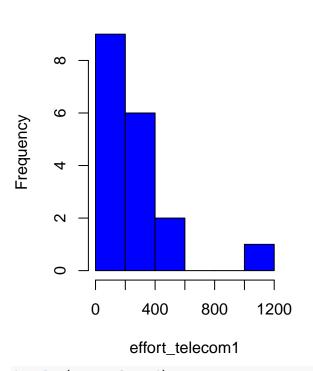


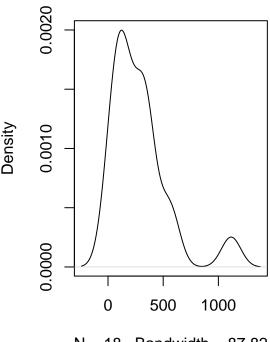
N = 18 Bandwidth = 46.41

```
hist(effort_telecom1, col = "blue")
plot(density(effort_telecom1))
```

#### **Histogram of effort\_telecom1**

#### density.default(x = effort\_telecom

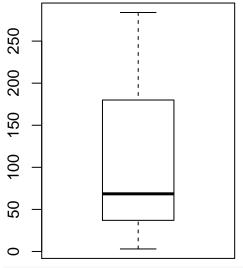


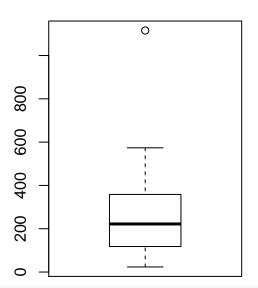


N = 18 Bandwidth = 87.82

boxplot(size\_telecom1) boxplot(effort\_telecom1)

# violin plots for those two variables library(vioplot)

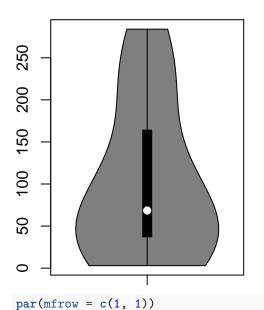


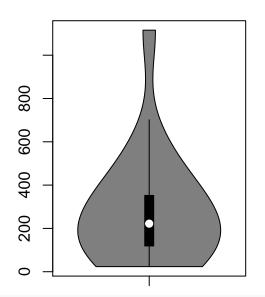


```
vioplot(size_telecom1, names = "")
title("Violin Plot of Project Size")
vioplot(effort_telecom1, names = "")
title("Violin Plot of Project Effort")
```

#### **Violin Plot of Project Size**

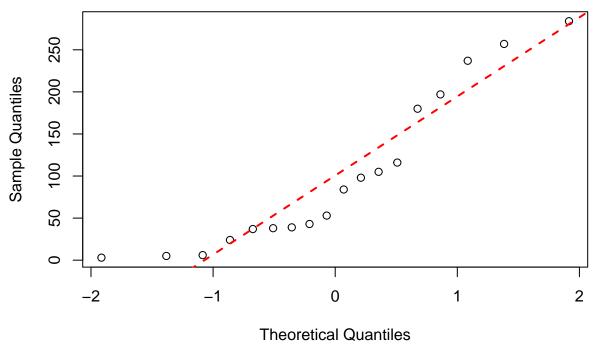
#### **Violin Plot of Project Effort**





```
qqnorm(size_telecom1, main = "Q-Q Plot of 'size'")
qqline(size_telecom1, col = 2, lwd = 2, lty = 2) #draws a line through the first and third quartiles
```

#### Q-Q Plot of 'size'



```
qqnorm(effort_telecom1, main = "Q-Q Plot of 'effort'")
qqline(effort_telecom1)
```

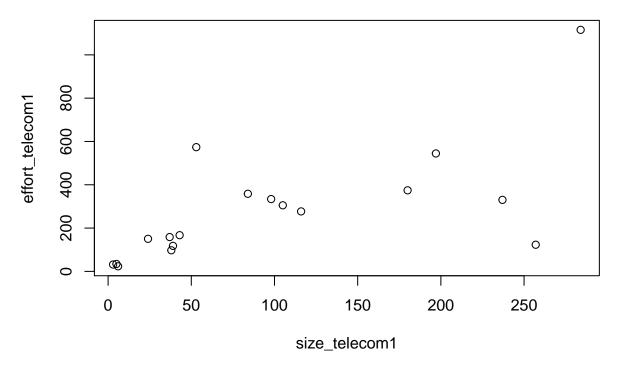
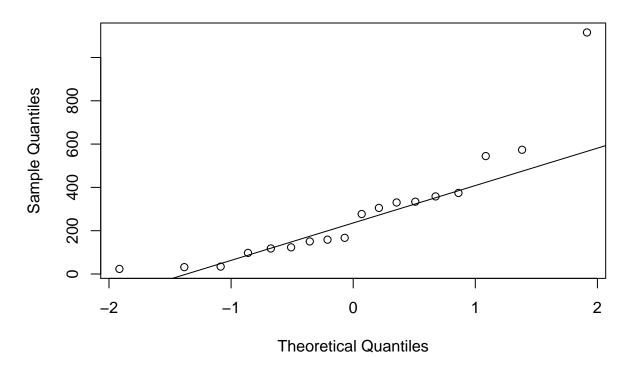


Figure 6.4: Scatterplot. Relationship between size and effort

#### Q-Q Plot of 'effort'



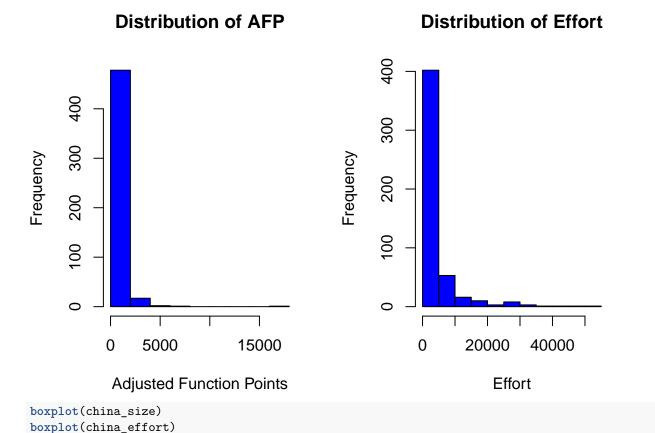
- $\bullet\,$  We can observe the non-normality of the data.
- We may look the posible relationship between size and effort with a scatterplot

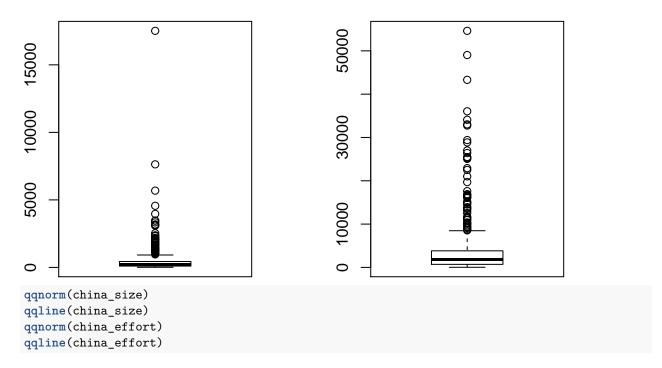
plot(size\_telecom1, effort\_telecom1)

#### 6.4.1 Example with the China dataset (from the tera-Promise Repository)

```
library(foreign)
china <- read.arff("./datasets/effortEstimation/china.arff")</pre>
china_size <- china$AFP</pre>
summary(china_size)
##
      Min. 1st Qu. Median
                                Mean 3rd Qu.
                                                 Max.
##
                100
                        215
                                 487
                                          438
                                                17518
china_effort <- china$Effort</pre>
summary(china_effort)
##
      Min. 1st Qu. Median
                                Mean 3rd Qu.
                                                 Max.
##
        26
               704
                       1829
                                3921
                                         3826
                                                54620
par(mfrow=c(1,2))
hist(china_size, col="blue", xlab="Adjusted Function Points", main="Distribution of AFP")
```

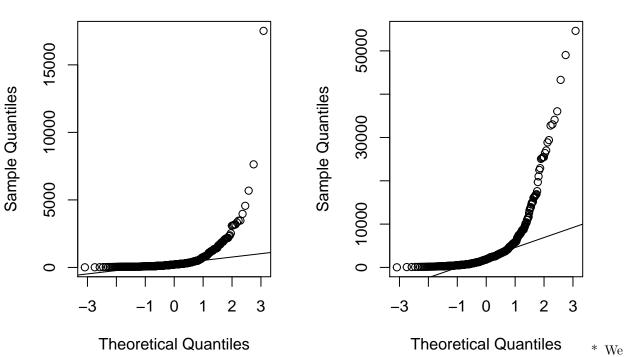
hist(china\_effort, col="blue",xlab="Effort", main="Distribution of Effort")







## Normal Q-Q Plot



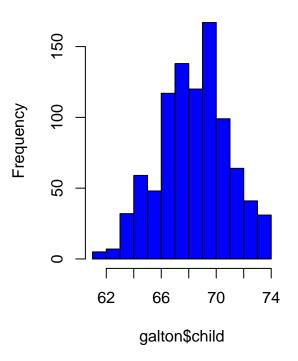
observe the non-normality of the data.

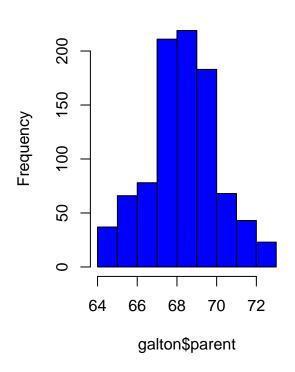
#### 6.4.1.1 Normality. Galton data

It is the data based on the famous 1885 Francis Galton's study about the relationship between the heights of adult children and the heights of their parents.



#### **Histogram of galton\$parent**



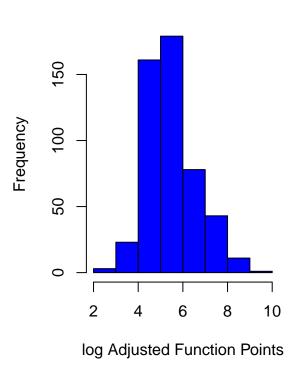


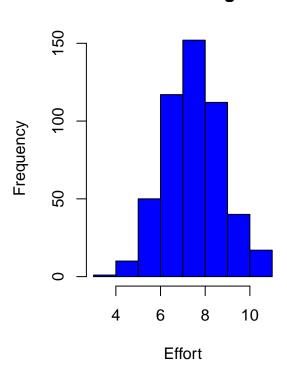
#### 6.4.1.2 Normalization

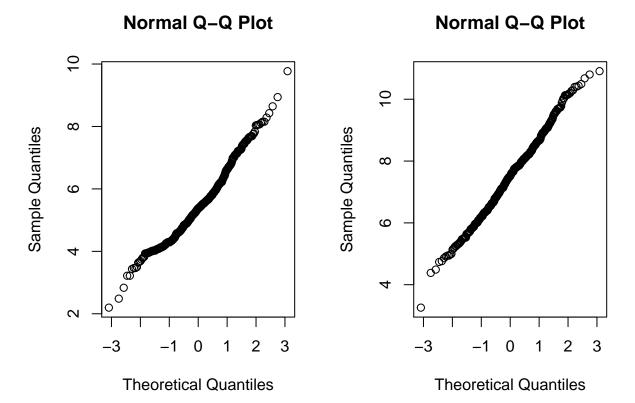
Take logs in both independent variables. For example, with the China dataset.

#### **Distribution of log AFP**

#### **Distribution of log Effort**







- If the  $\log$  transformation is used, then the estimation equation is:

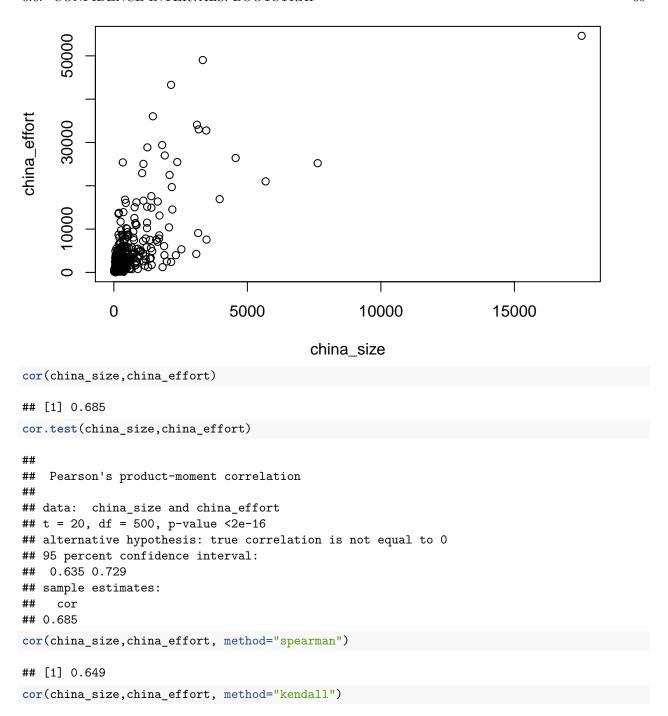
$$y = e^{b_0 + b_1 \log(x)}$$

#### 6.5 Correlation

Correlation is a statistical relationship between two sets of data. With the whole dataset we may check for the linear Correlation of the variables we are interested in.

As an example with the China dataset

```
par(mfrow=c(1,1))
plot(china_size,china_effort)
```



#### 6.6 Confidence Intervals. Bootstrap

• Until now we have generated point estimates

## [1] 0.468

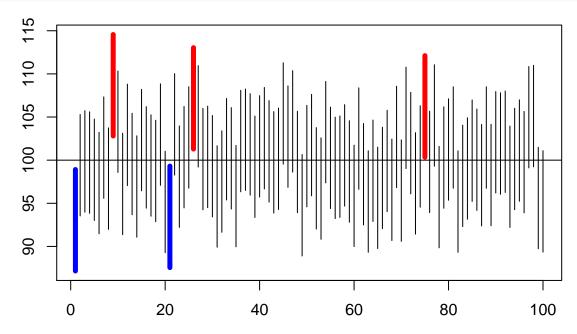
• A confidence interval (CI) is an interval estimate of a population parameter. The parameter can be the mean, the median or other. The frequentist CI is an observed interval that is different from sample to sample. It frequently includes the value of the unobservable parameter of interes if the experiment is repeated. The confidence level is the value that measures the frequency that the constructed intervals

contain the true value of the parameter.

- The construction of a confidence interval with an exact value of confidence level for a distribution requires some statistical properties. Usually, *normality* is one of the properties required for computing confidence intervals.
  - Not all confidence intervals contain the true value of the parameter.
  - Simulation of confidence intervals

An example from Ugarte et al. (Ugarte et al., 2015)

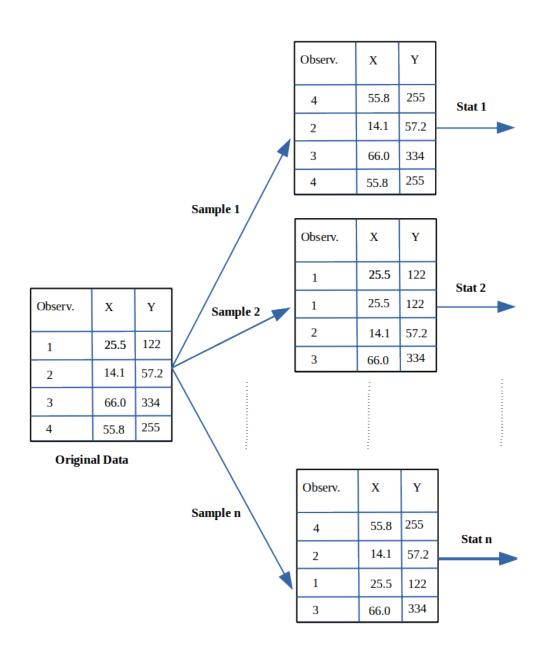
```
set.seed(10)
norsim(sims = 100, n = 36, mu = 100, sigma = 18, conf.level = 0.95)
```



- The range defined by the confidence interval will vary with each sample, because the sample size will vary each time and the standard deviation will vary too.
- 95% confidence interval: it is the probability that the hypothetical confidence intervals (that would be computed from the hypothetical repeated samples) will contain the population mean.
- the particular interval that we compute on one sample does not mean that the population mean lies within that interval with a probability of 95%.
- Recommended reading: (Hoekstra et al., 2014) Robust misinterpretation of confidence intervals

#### 6.7 Nonparametric Bootstrap

- For computing CIs the important thing is to know the assumptions that are made to "know" the distribution of the statistic.
- There is a way to compute confidence intervals without meeting the requirements of parametric methods.
- **Resampling** or **bootstraping** is a method to calculate estimates of a parameter taking samples from the original data and using those *resamples* to calculate statistics. Using the resamples usually gives more accurate results than using the original single sample to calculate an estimate of a parameter.



-

An example of bootstrap CI can be found in Chapter 13, "Evaluation in Software Engineering"

## Chapter 7

# Classical Hypothesis Testing

- By "classical" we mean the standard "frequentist" approach to hypothesis testing. The "frequentist" approach to probability sees it as the frequency of events in the long run. We repeat experiments over and over and we count the times that our object of interest appears in the sequence.
- The classical approach is usually called **null hypothesis significance testing** (NHST) because the process starts by setting a null hypothesis  $H_0$  which is the opposite about what we think is true.
- The rationale of the process is that the statistical hypothesis should be *falsifiable*, that is, we can find evidence that the hypothesis is not true. We try to find evidence against the null hypothesis in order to support our alternative hypothesis  $H_A$
- Usually, the null hypothesis is described as the situation of "no effect" and the alternative hypothesis describes the effect that we are looking for.
- After collecting data, taking an actual sample, we measure the distance of our parameter of interest from the hypothesized population parameter, and use the facts of the sampling distribution to determine the probability of obtaining such a sample assuming the hypothesis is true. This is amounts to a test of the hypothesis.
- If the probability of our sample, given the null hypothesis is high, this provides evidence that the null hypothesis is true. Conversely, if the probability of the sample is low (given the hypothesis), this is evidence against the null hypothesis. The hypothesis being tested in this way is named the null hypothesis.
- The goal of the test is to determine if the null hypothesis can be rejected. A statistical test can either reject or fail to reject a null hypothesis, but never prove it true.
- We can make two types of errors: false positive (Type I) and false negative (Type II)
- Type I and Type II errors
- Two-tailed NHST
- One-tailed NHST
- elementary example

```
data = c(52.7, 53.9, 41.7, 71.5, 47.6, 55.1, 62.2, 56.5, 33.4, 61.8, 54.3, 50.0, 45.3, 63.4, 53.9, 65.5 t.test(data, mu=50, alternative = 'greater')
```

```
##
## One Sample t-test
##
## data: data
```

		Null hypothesis ( $H_0$ ) is	
		Valid/True	Invalid/False
Judgement of Null Hypothesis ( $H_0$ )	Reject	Type I error False Positive	Correct inference True Positive
	Fail to reject	Correct inference True Negative	Type II error False negative

Figure 7.1:

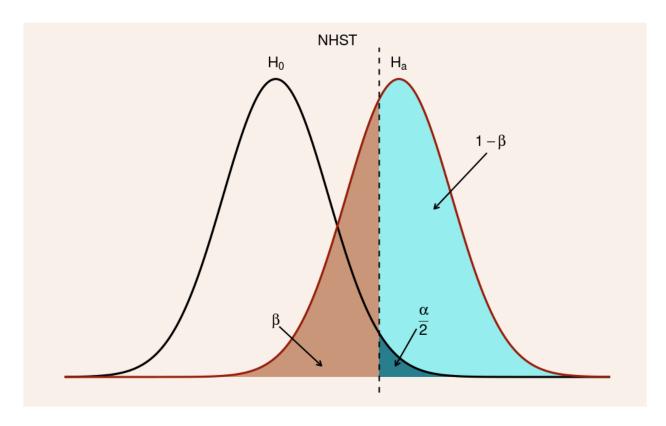
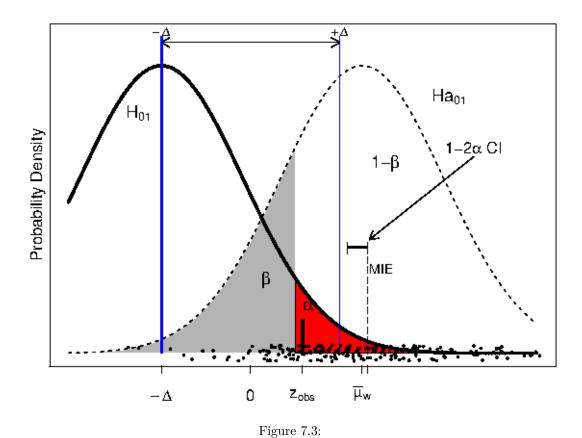


Figure 7.2:



```
## t = 2, df = 20, p-value = 0.02
## alternative hypothesis: true mean is greater than 50
## 95 percent confidence interval:
## 50.9 Inf
## sample estimates:
## mean of x
##
        54.3
```

- Keeping this simple, we could start hypothesis testing about one sample median with the wilcoxon test for non-normal distributions.
- "ae" is the absolute error in the China Test data

```
median(ae)
## [1] 867
mean(ae)
## [1] 1867
wilcox.test(ae, mu=800, alternative = 'greater') #change the values of mu and see the results
##
   Wilcoxon signed rank test with continuity correction
##
##
## data: ae
## V = 9000, p-value = 8e-04
## alternative hypothesis: true location is greater than 800
```

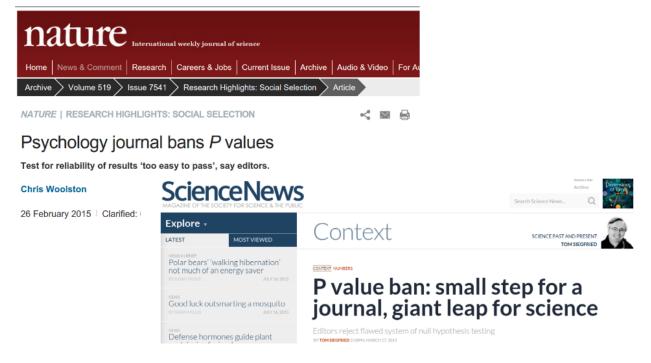


Figure 7.4:

• Quick introduction at https://psychstatsworkshop.wordpress.com/2014/08/06/lesson-9-hypothesis-testing/

## 7.1 p-values

- p-value: the p-value of a statistical test is the probability, computed assuming that  $H_0$  is true, that the test statistic would take a value as extreme or more extreme than that actually observed.
- http://www.nature.com/news/psychology-journal-bans-p-values-1.17001
- https://www.sciencenews.org/blog/context/p-value-ban-small-step-journal-giant-leap-science

# $\begin{array}{c} {\rm Part} \; {\rm V} \\ \\ {\rm Preprocessing} \end{array}$

## Chapter 8

# Preprocessing

Following the data mining process, we describe what is meant by preprocessing, classical supervised models, unsupervised models and evaluation in the context of software engineering with examples

This task is probably the hardest and where most of effort is spend in the data mining process. It is quite typical to transform the data, for example, finding inconsistencies, normalising, imputing missing values, transforming input data, merging variables, etc.

Typically, preprocessing consist of the following tasks (subprocesses):

- Data cleaning (consistency, noise detection, outliers)
- Data integration
- Data transformation (normalisation, discretisation) and derivation of new attributes from existing ones (e.g., population density from population and area)
- Missing data imputation
- Data reduction (feature selection and instace selection)

#### 8.1 Data

Consistent data are semantically correct based on real-world knowledge of the problem, i.e., no constrains are violated and data that can be used for inducing models and analysis. For example, the LoC or effort is constrained to non-negative values. We can also consider that to multiple attributes are consistent among them, and even datasets (e.g., same metrics but collected by different tools)

## 8.2 Missing values

Missing values will have a negative effect when analysing the data or learning models. The results can be biased when compared with the models induced from the complete data, the results can be harder to analyse, it may be needed to discard records with missing values depending on the algorithm and this can be an important problems with small datasets such as the effort estimation ones.

Missing data is typically classified into: \* MCAR (Missing Completely at Random) or MAR (Missing At Random) where there is no reason for those missing values and we can assume that the distribution could follow the attribute's distribution. \* MNAR (Missing Not At Random) where there is a pattern for those missing values and it may may be advisable to check the data gathering process to try to understand why such information is missing.

*Imputation* consists in replacing missing values for estimates of those missing values. Many algorithms do cannot handle missing values and therefore, imputation methods are needed. We can use simple approaches such as the replacing the missing values with the mean or mode of the attribute. More elaborated approaches include:

- EM (Expectation-Maximisation)
- Distance-based
  - kNN (k Nearest Neighbours)
  - Clustering

In R, a missing value is represented with NA and the analyst must decide what to do with missing data. The simplest approach is to leave out instances (ignore missing -IM-) with with missing data. This functionality is supported by many base functions through the na.rm option.

The mice R package. MICE (Multivariate Imputation via Chained Equations) assumes that data are missing at random. Other packages include Amelia, missForest, Hmisc and mi.

#### 8.3 Noise

Imperfections of the real-world data that influences negatively in the induced machine learning models. Approaches to deal with noisy data include: \* Robust learners capable of handling noisy data (e.g., C4.5 through pruning strategies) \* Data polishing methods which aim to correct noisy instances prior training \* Noise filters which are used to identify and eliminate noisy instances from the training data.

Types of noise data: \* Class Noise (aka label noise). + There can be contradictory cases (all attributes have the same value except the class) + Misclassifications. The class attribute is not labeled with the true label (golden truth) \* Attribute Noise. Values of attributes that are noise, missing or unknown.

## 8.4 Outliers

There is a large amount of literature related to outlier detection, and furthermore several definitions of outlier exist.

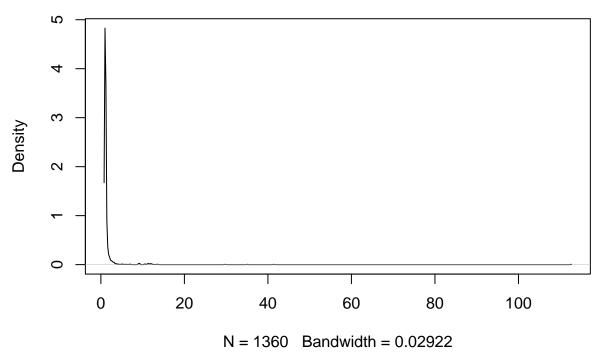
```
library(DMwR)
library(foreign)

kc1 <- read.arff("./datasets/defectPred/D1/KC1.arff")</pre>
```

The LOF algorithm (lofactor), given a data set it produces a vector of local outlier factors for each case.

```
kc1num <- kc1[,1:21]
outlier.scores <- lofactor(kc1num, k=5)
plot(density(na.omit(outlier.scores)))</pre>
```

## density.default(x = na.omit(outlier.scores))



outliers <- order(outlier.scores, decreasing=T)[1:5]
print(outliers)</pre>

## [1] 1 6 14 31 33

Another simple method of Hiridoglou and Berthelot for positive observations.

#### 8.5 Feature selection

Feature Selection (FS) aims at identifying the most relevant attributes from a dataset. It is important in different ways:

- A reduced volume of data allows different data mining or searching techniques to be applied.
- Irrelevant and redundant attributes can generate less accurate and more complex models. Furthermore, data mining algorithms can be executed faster.
- It avoids the collection of data for those irrelevant and redundant attributes in the future.

The problem of FS received a thorough treatment in pattern recognition and machine learning. Most of the FS algorithms tackle the task as a *search* problem, where each state in the search specifies a distinct subset of the possible attributes (Blum and Langley, 1997). The search procedure is combined with a criterion to evaluate the merit of each candidate subset of attributes. There are a multiple possible combinations between each procedure search and each attribute measure (Liu and Yu, 2005).

There are two major approaches in FS from the method's output point of view:

- Feature subset selection (FSS)
- Feature ranking in which attributes are ranked as a list of features which are ordered according to evaluation measures (a subset of features is often selected from the top of the ranking list).

FFS algorithms designed with different evaluation criteria broadly fall into two categories:

- The *filter* model relies on general characteristics of the data to evaluate and select feature subsets without involving any data mining algorithm.
- The *wrapper* model requires one predetermined mining algorithm and uses its performance as the evaluation criterion. It searches for features better suited to the mining algorithm aiming to improve mining performance, but it also tends to be more computationally expensive than filter model (Kohavi and John, 1997, Langley (1994)).

Feature subset algorithms search through candidate feature subsets guide by a certain evaluation measure (Liu and Motoda, 1998) which captures the goodness of each subset. An optimal (or near optimal) subset is selected when the search stops.

Some existing evaluation measures that have been shown effective in removing both irrelevant and redundant features include the consistency measure (Dash et al., 2000), the correlation measure (Hall, 1999) and the estimated accuracy of a learning algorithm (Kohavi and John, 1997).

- Consistency measure attempts to find a minimum number of features that separate classes as consistently as the full set of features can. An inconsistency is defined as to instances having the same feature values but different class labels.
- Correlation measure evaluates the goodness of feature subsets based on the hypothesis that good feature subsets contain features highly correlated to the class, yet uncorrelated to each other.
- Wrapper-based attribute selection uses the target learning algorithm to estimate the worth of attribute subsets. The feature subset selection algorithm conducts a search for a good subset using the induction algorithm itself as part of the evaluation function.

Langley (1994) notes that feature selection algorithms that search through the space of feature subsets must address four main issues: (i) the starting point of the search, (ii) the organization of the search, (iii) the evaluation of features subsets and (iv) the criterion used to terminate the search. Different algorithms address these issues differently.

It is impractical to look at all possible feature subsets, even with a small number of attributes. Feature selection algorithms usually proceed greedily and are be classified into those that add features to an initially empty set (forward selection) and those that remove features from an initially complete set (backwards elimination). Hybrids both add and remove features as the algorithm progresses. Forward selection is much faster than backward elimination and therefore scales better to large data sets. A wide range of search strategies can be used: best-first, branch-and-bound, simulated annealing, genetic algorithms (see Kohavi and John (1997) for a review).

#### 8.5.1 FSelector package in R

The FSelector package in R implements many algorithms available in Weka

```
library(FSelector)
library(foreign)

cm1 <- read.arff("./datasets/defectPred/D1/CM1.arff")

cm1RFWeigths <- random.forest.importance(Defective ~ ., cm1)
cutoff.biggest.diff(cm1RFWeigths)</pre>
```

```
## [1] "LOC_COMMENTS" "NUM_UNIQUE_OPERATORS"
```

Using the Information Gain meaure as ranking:

```
cm1GRWeights <- gain.ratio(Defective ~ ., cm1)
cm1GRWeights</pre>
```

## [10] "HALSTEAD\_CONTENT"

```
##
                                    attr_importance
## LOC_BLANK
                                             0.0000
## BRANCH_COUNT
                                             0.0000
## CALL_PAIRS
                                             0.0000
## LOC_CODE_AND_COMMENT
                                             0.0000
## LOC COMMENTS
                                             0.0754
## CONDITION COUNT
                                             0.0000
## CYCLOMATIC_COMPLEXITY
                                             0.0000
## CYCLOMATIC_DENSITY
                                             0.0000
## DECISION_COUNT
                                             0.0000
## DECISION_DENSITY
                                             0.0000
## DESIGN_COMPLEXITY
                                             0.0000
## DESIGN_DENSITY
                                             0.0000
## EDGE_COUNT
                                             0.0000
## ESSENTIAL_COMPLEXITY
                                             0.0000
## ESSENTIAL_DENSITY
                                             0.0000
## LOC_EXECUTABLE
                                             0.0888
## PARAMETER COUNT
                                             0.0000
## HALSTEAD_CONTENT
                                             0.0701
## HALSTEAD_DIFFICULTY
                                             0.0000
## HALSTEAD_EFFORT
                                             0.0375
## HALSTEAD_ERROR_EST
                                             0.0448
## HALSTEAD_LENGTH
                                             0.0425
## HALSTEAD LEVEL
                                             0.0000
## HALSTEAD_PROG_TIME
                                             0.0375
## HALSTEAD_VOLUME
                                             0.0471
## MAINTENANCE_SEVERITY
                                             0.0000
## MODIFIED_CONDITION_COUNT
                                             0.0000
## MULTIPLE_CONDITION_COUNT
                                             0.0000
## NODE_COUNT
                                             0.0000
## NORMALIZED_CYLOMATIC_COMPLEXITY
                                             0.0000
## NUM_OPERANDS
                                             0.0000
## NUM_OPERATORS
                                             0.0471
## NUM_UNIQUE_OPERANDS
                                             0.0589
## NUM_UNIQUE_OPERATORS
                                             0.0616
## NUMBER_OF_LINES
                                             0.0573
## PERCENT COMMENTS
                                             0.0663
## LOC_TOTAL
                                             0.0763
cutoff.biggest.diff(cm1GRWeights)
## [1] "LOC_EXECUTABLE"
                                "LOC_TOTAL"
                                                       "LOC_COMMENTS"
  [4] "HALSTEAD_CONTENT"
                                "PERCENT_COMMENTS"
                                                       "NUM_UNIQUE_OPERATORS"
  [7] "NUM_UNIQUE_OPERANDS"
                                "NUMBER_OF_LINES"
                                                       "HALSTEAD_VOLUME"
                                "HALSTEAD_ERROR_EST"
## [10] "NUM OPERATORS"
                                                       "HALSTEAD LENGTH"
## [13] "HALSTEAD_EFFORT"
                               "HALSTEAD_PROG_TIME"
# After assigning weights, we can select the statistaclly significant ones
cm1X2Weights <- chi.squared(Defective ~ ., cm1)</pre>
cutoff.biggest.diff(cm1X2Weights)
    [1] "LOC_EXECUTABLE"
                                "LOC COMMENTS"
                                                       "LOC TOTAL"
##
  [4] "NUM_UNIQUE_OPERATORS" "NUM_UNIQUE_OPERANDS" "NUMBER_OF_LINES"
##
  [7] "HALSTEAD_VOLUME"
                                "NUM_OPERATORS"
                                                       "HALSTEAD_ERROR_EST"
```

"HALSTEAD\_EFFORT"

"HALSTEAD\_PROG\_TIME"

```
## [13] "HALSTEAD_LENGTH" "PERCENT_COMMENTS"
```

Using CFS attribute selection

```
library(FSelector)
library(foreign)

cm1 <- read.arff("./datasets/defectPred/D1/CM1.arff")

result <- cfs(Defective ~ ., cm1)
f <- as.simple.formula(result, "Defective")
f

## Defective ~ LOC_COMMENTS + LOC_EXECUTABLE + HALSTEAD_CONTENT +
## NUM_UNIQUE_OPERATORS + PERCENT_COMMENTS
## <environment: Ox56441b203ea0>
```

Other packages for Feature selection in R include FSelectorRccp which re-implments the FSlector without WEKA dependencies.

Another popular package is Boruta, which is based on selection based on Random Forest.

## 8.6 Instance selection

Removal of samples (complementary to the removal of attributes) in order to scale down the dataset prior to learning a model so that there is (almost) no performance loss.

There are two types of processes:

- Prototype Selection (PS) (Garcia et al., 2012) when the subset is used with a distance based method (kNN)
- Training Set Selection (TSS) (Cano et al., 2007) in which an actual model is learned.

It is also a search problem as with *feature selection*. Garcia et al. (2012) provide a comprehensive overview of the topic.

#### 8.7 Discretization

This process transforms continuous attributes into discrete ones, by associating categorical values to intervals and thus transforming quantitative data into qualitative data.

## 8.8 Correlation Coefficient and Covariance for Numeric Data

Two random variables x and y are called independent if the probability distribution of one variable is not affected by the presence of another.

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```
## X-squared = 20000, df = 2000, p-value <2e-16
chisq.test(kc1$DESIGN_COMPLEXITY,kc1$CYCLOMATIC_COMPLEXITY)

##
## Pearson's Chi-squared test
##
## data: kc1$DESIGN_COMPLEXITY and kc1$CYCLOMATIC_COMPLEXITY
## X-squared = 30000, df = 700, p-value <2e-16</pre>
```

## 8.9 Normalization

#### 8.9.1 Min-Max Normalization

```
\begin{split} z_i &= \frac{x_i - \min(x)}{\max(x) - \min(x)} \\ \text{library(caret)} \\ \text{preObj } &\leftarrow \text{preProcess(kc1[, -22], method=c("center", "scale"))} \end{split}
```

#### 8.9.2 Z-score normalization

TBD

## 8.10 Transformations

## 8.10.1 Linear Transformations and Quadratic Trans formations

TBD

## 8.10.2 Box-cox transformation

TBD

#### 8.10.3 Nominal to Binary tranformations

TBD

## 8.11 Preprocessing in R

## 8.11.1 The dplyr package

The *dplyr* package created by Hadley Wickham. Some functions are similar to SQL syntax and it key functions in dplyr include:

- select: select columns from a dataframe
- filter: select rows from a dataframe
- summarize: allows us to do summary stats based upon the grouped variable

- group by: group by a factor variable
- arrange: order the dataset
- joins: as in sql left join

Tutorial: https://github.com/justmarkham/dplyr-tutorial

Examples

```
library(dplyr)
```

Describe the dataframe:

```
str(kc1)
```

```
## 'data.frame':
                   2096 obs. of
                                 22 variables:
##
   $ LOC BLANK
                          : num 0000200002...
  $ BRANCH COUNT
                          : num 1 1 1 1 1 1 1 1 1 1 ...
  $ LOC_CODE_AND_COMMENT : num 0 0 0 0 0 0 0 0 0 ...
   $ LOC_COMMENTS
                          : num
                                0 0 0 0 0 0 0 0 0 0 ...
##
  $ CYCLOMATIC_COMPLEXITY: num
                                1 1 1 1 1 1 1 1 1 1 ...
  $ DESIGN COMPLEXITY
                          : num
                                1 1 1 1 1 1 1 1 1 1 ...
   $ ESSENTIAL_COMPLEXITY : num
##
                                1 1 1 1 1 1 1 1 1 1 ...
##
   $ LOC_EXECUTABLE
                          : num
                                3 1 1 1 8 3 1 1 1 9 ...
##
   $ HALSTEAD_CONTENT
                          : num 11.6 0 0 0 18 ...
  $ HALSTEAD_DIFFICULTY : num 2.67 0 0 0 3.5 2.67 0 0 0 3.75 ...
   $ HALSTEAD_EFFORT
##
                          : num 82.3 0 0 0 220.9 ...
## $ HALSTEAD_ERROR_EST
                          : num 0.01 0 0 0 0.02 0.01 0 0 0 0.04 ...
## $ HALSTEAD LENGTH
                         : num 11 1 1 1 19 11 1 1 1 29 ...
  $ HALSTEAD_LEVEL
                          : num 0.38 0 0 0 0.29 0.38 0 0 0 0.27 ...
   $ HALSTEAD_PROG_TIME
                         : num 4.57 0 0 0 12.27 ...
##
##
   $ HALSTEAD_VOLUME
                          : num 30.9 0 0 0 63.1 ...
## $ NUM OPERANDS
                          : num 4 0 0 0 7 4 0 0 0 10 ...
## $ NUM_OPERATORS
                          : num 7 1 1 1 12 7 1 1 1 19 ...
## $ NUM_UNIQUE_OPERANDS : num
                                3 0 0 0 5 3 0 0 0 8 ...
##
  $ NUM_UNIQUE_OPERATORS : num 4 1 1 1 5 4 1 1 1 6 ...
## $ LOC_TOTAL
                                 5 3 3 3 12 5 3 3 3 13 ...
                          : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
   $ Defective
```

tbl\_df creates a "local data frame" as a wrapper for better printing

```
kc1_tbl <- tbl_df(kc1)</pre>
```

Filter:

```
# Filter rows: use comma or & to represent AND condition filter(kc1_tbl, Defective == "Y" & LOC_BLANK != 0)
```

```
## # A tibble: 251 x 22
      LOC_BLANK BRANCH_COUNT LOC_CODE_AND_CO~ LOC_COMMENTS CYCLOMATIC_COMP~
##
           <dbl>
                                            <dbl>
                                                          <dbl>
##
                         <dbl>
                                                                             <dbl>
##
               6
                            21
   1
                                                0
                                                             10
                                                                                11
##
    2
               5
                            15
                                                0
                                                              2
                                                                                 8
               2
                                                              0
                                                                                 3
##
    3
                             5
                                                0
##
   4
               4
                             5
                                                              2
                                                                                 3
               2
                                                              2
##
   5
                            11
                                                0
                                                                                 6
##
    6
               2
                            23
                                                0
                                                              3
                                                                                12
                                                0
                                                              2
##
   7
               1
                            11
                                                                                 6
##
   8
               1
                            13
                                                0
                                                              2
                                                                                 7
                                                              2
               2
                            17
                                                0
                                                                                 9
##
    9
```

Another operator is %in%.

#### Select:

```
select(kc1_tbl, contains("LOC"), Defective)
```

```
## # A tibble: 2,096 x 6
     LOC BLANK LOC CODE AND CO~ LOC COMMENTS LOC EXECUTABLE LOC TOTAL
##
##
         <dbl>
                          <dbl>
                                       <dbl>
                                                       <dbl>
                                                                 <dbl>
## 1
                               0
                                                          3
                                                                     5
## 2
             0
                               0
                                           0
                                                          1
                                                                     3
## 3
             0
                              0
                                                                     3
                                           0
                                                          1
## 4
             0
                                           0
                                                          1
                                                                    3
## 5
             2
                              0
                                           0
                                                          8
                                                                   12
                                                          3
## 6
             0
                              0
                                           0
                                                                    5
## 7
             0
                              0
                                           0
                                                          1
                                                                     3
## 8
             0
                              0
                                           0
                                                          1
                                                                     3
## 9
             0
                              0
                                                                     3
                                           0
                                                          1
## 10
                                           0
## # ... with 2,086 more rows, and 1 more variable: Defective <fct>
```

Now, kc1\_tbl contains("LOC"), Defective

Filter and Select together:

```
# nesting method
filter(select(kc1_tbl, contains("LOC"), Defective), Defective !=0)
```

```
## # A tibble: 2,096 x 6
     LOC_BLANK LOC_CODE_AND_CO~ LOC_COMMENTS LOC_EXECUTABLE LOC_TOTAL
##
##
          <dbl>
                           <dbl>
                                       <dbl>
                                                       <dbl>
                                                                 <dbl>
                              0
## 1
             0
                                                           3
                                                                     5
                                           0
## 2
              0
                               0
                                            0
## 3
              0
                               0
                                            0
                                                           1
                                                                     3
## 4
             0
                               0
                                            0
                                                           1
                                                                     3
## 5
              2
                               0
                                                           8
                                            0
                                                                    12
              0
                                                           3
## 6
                                            0
                                                                     5
## 7
                              0
              0
                                            0
                                                           1
                                                                     3
## 8
              0
                               0
                                            0
                                                           1
                                                                     3
## 9
              0
                                                                     3
## 10
              2
                               0
                                            0
                                                                    13
## # ... with 2,086 more rows, and 1 more variable: Defective <fct>
```

It is easier usign the chaining method:

```
# chaining method
kc1_tbl %>%
    select(contains("LOC"), Defective) %>%
```

```
filter(Defective !=0)
## # A tibble: 2,096 x 6
     LOC_BLANK LOC_CODE_AND_CO~ LOC_COMMENTS LOC_EXECUTABLE LOC_TOTAL
##
          <dbl>
                           <dbl>
                                        <dbl>
                                                       <dbl>
                                                                 <dbl>
## 1
                                                           3
                                                                     5
## 2
              0
                               0
                                            0
                                                           1
                                                                     3
              0
                                                                     3
## 3
                               0
                                            0
                                                           1
## 4
              0
                               0
                                            0
                                                                     3
                                                           1
## 5
              2
                               0
                                            0
                                                           8
                                                                    12
## 6
              0
                               0
                                            0
                                                           3
                                                                     5
## 7
              0
                                            0
                                                           1
                                                                     3
              0
                               0
                                            0
## 8
                                                           1
                                                                     3
## 9
              0
                               0
                                            0
                                                                     3
                                                           1
## 10
              2
                                                                    13
                               0
                                            0
                                                           9
## # ... with 2,086 more rows, and 1 more variable: Defective <fct>
Arrange ascending
#
kc1_tbl %>%
    select(LOC_TOTAL, Defective) %>%
    arrange(LOC_TOTAL)
## # A tibble: 2,096 x 2
##
    LOC_TOTAL Defective
##
         <dbl> <fct>
## 1
             1 N
              1 N
## 2
## 3
              1 N
## 4
              1 N
## 5
              1 N
## 6
              1 N
##
   7
             1 N
## 8
             1 N
## 9
             1 N
              1 N
## 10
## # ... with 2,086 more rows
Arrange descending:
kc1_tbl %>%
    select(LOC_TOTAL, Defective) %>%
    arrange(desc(LOC_TOTAL))
## # A tibble: 2,096 x 2
##
     LOC_TOTAL Defective
##
          <dbl> <fct>
## 1
            288 Y
## 2
           286 Y
## 3
           283 N
## 4
           220 Y
## 5
           217 Y
## 6
           210 N
## 7
           205 Y
           184 Y
## 8
```

```
## 9
            179 Y
## 10
            176 Y
## # ... with 2,086 more rows
Mutate:
kc1 tbl %>%
    filter(Defective == "Y") %>%
    select(NUM_OPERANDS, NUM_OPERATORS, Defective) %>%
    mutate(HalsteadLength = NUM_OPERANDS + NUM_OPERATORS)
## # A tibble: 325 x 4
##
      NUM_OPERANDS NUM_OPERATORS Defective HalsteadLength
##
             <dbl>
                           <dbl> <fct>
                                                     <db1>
                             107 Y
## 1
                64
                                                       171
## 2
                52
                              89 Y
                                                       141
## 3
                17
                              41 Y
                                                        58
## 4
                41
                              74 Y
                                                       115
## 5
                              95 Y
                54
                                                       149
## 6
                75
                              156 Y
                                                       231
## 7
                54
                              95 Y
                                                       149
## 8
                56
                              99 Y
                                                       155
## 9
                69
                              124 Y
                                                       193
## 10
                44
                              60 Y
                                                       104
## # ... with 315 more rows
summarise: Reduce variables to values
# Create a table grouped by Defective, and then summarise each group by taking the mean of loc
kc1_tbl %>%
    group_by(Defective) %>%
    summarise(avg_loc = mean(LOC_TOTAL, na.rm=TRUE))
## # A tibble: 2 x 2
    Defective avg_loc
##
     <fct>
                 <db1>
## 1 N
                  15.9
                  44.7
## 2 Y
# Create a table grouped by Defective, and then summarise each group by taking the mean of loc
kc1 tbl %>%
    group_by(Defective) %>%
    summarise_each(funs(mean, min, max), BRANCH_COUNT, LOC_TOTAL)
## `summarise_each()` is deprecated.
## Use `summarise_all()`, `summarise_at()` or `summarise_if()` instead.
## To map `funs` over a selection of variables, use `summarise_at()`
## # A tibble: 2 x 7
     Defective BRANCH_COUNT_me~ LOC_TOTAL_mean BRANCH_COUNT_min LOC_TOTAL_min
##
     <fct>
                          <dbl>
                                          <dbl>
                                                           <dbl>
                                                                          <dbl>
## 1 N
                           3.68
                                           15.9
                                                               1
                                                                              1
                                           44.7
                          10.1
## # ... with 2 more variables: BRANCH_COUNT_max <dbl>, LOC_TOTAL_max <dbl>
```

It seems than the number of Defective modules is larger than the Non-Defective ones. We can count them with:

```
# n() or tally
kc1_tbl %>%
   group_by(Defective) %>%
   tally()
## # A tibble: 2 x 2
## Defective n
   <fct>
              <int>
## 1 N
               1771
## 2 Y
                325
It seems that it's an imbalanced dataset...
# randomly sample a fixed number of rows, without replacement
kc1_tbl %>% sample_n(2)
## # A tibble: 2 x 22
    LOC_BLANK BRANCH_COUNT LOC_CODE_AND_CO~ LOC_COMMENTS CYCLOMATIC_COMP~
##
         <dbl>
                    <dbl>
                                      <dbl>
                                             <dbl>
                                                                    <dbl>
## 1
          0
                                        0
                                                   0
                                                                     1
            2
                         7
                                          0
                                                                        4
## 2
## # ... with 17 more variables: DESIGN_COMPLEXITY <dbl>,
## # ESSENTIAL_COMPLEXITY <dbl>, LOC_EXECUTABLE <dbl>,
      HALSTEAD CONTENT <dbl>, HALSTEAD DIFFICULTY <dbl>,
      HALSTEAD_EFFORT <dbl>, HALSTEAD_ERROR_EST <dbl>,
## #
      HALSTEAD_LENGTH <dbl>, HALSTEAD_LEVEL <dbl>, HALSTEAD_PROG_TIME <dbl>,
## # HALSTEAD VOLUME <dbl>, NUM OPERANDS <dbl>, NUM OPERATORS <dbl>,
      NUM UNIQUE OPERANDS <dbl>, NUM UNIQUE OPERATORS <dbl>,
      LOC_TOTAL <dbl>, Defective <fct>
## #
# randomly sample a fraction of rows, with replacement
kc1_tbl %>% sample_frac(0.05, replace=TRUE)
## # A tibble: 105 x 22
     LOC_BLANK BRANCH_COUNT LOC_CODE_AND_CO~ LOC_COMMENTS CYCLOMATIC_COMP~
##
##
         <dbl>
                <dbl>
                                     <dbl>
                                                  <dbl>
                                                                     <dbl>
## 1
             1
                          1
                                                        0
                                                                         1
## 2
             0
                                           0
                                                        0
                          1
                                                                         1
## 3
             5
                          7
                                           0
                                                        0
                                                                         4
            0
## 4
                          1
                                                        0
            0
                                           0
                                                        0
## 5
                          1
                                                                         1
            2
                          3
                                           0
                                                        0
                                                                         2
## 6
## 7
                                                                         2
            1
                          3
                                           1
                                                        1
## 8
             1
                          3
                                           0
                                                        0
                                                                         2
## 9
             0
                          3
                                           0
                                                        0
                                                                         2
## 10
                                           0
                                                        0
## # ... with 95 more rows, and 17 more variables: DESIGN_COMPLEXITY <dbl>,
      ESSENTIAL_COMPLEXITY <dbl>, LOC_EXECUTABLE <dbl>,
      HALSTEAD_CONTENT <dbl>, HALSTEAD_DIFFICULTY <dbl>,
## #
## #
      HALSTEAD_EFFORT <dbl>, HALSTEAD_ERROR_EST <dbl>,
      HALSTEAD LENGTH <dbl>, HALSTEAD LEVEL <dbl>, HALSTEAD PROG TIME <dbl>,
## #
## #
      HALSTEAD_VOLUME <dbl>, NUM_OPERANDS <dbl>, NUM_OPERATORS <dbl>,
## #
      NUM_UNIQUE_OPERANDS <dbl>, NUM_UNIQUE_OPERATORS <dbl>,
## #
      LOC_TOTAL <dbl>, Defective <fct>
```

# # Better formatting adapted to the screen width glimpse(kc1\_tbl)

```
## Observations: 2,096
## Variables: 22
## $ LOC_BLANK
                     <dbl> 0, 0, 0, 0, 2, 0, 0, 0, 0, 2, 2, 0, 2, 1...
## $ BRANCH COUNT
                     ## $ LOC_CODE_AND_COMMENT
                     <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0...
## $ LOC COMMENTS
                     ## $ DESIGN COMPLEXITY
                     ## $ ESSENTIAL COMPLEXITY
                     ## $ LOC EXECUTABLE
                     <dbl> 3, 1, 1, 1, 8, 3, 1, 1, 1, 9, 8, 1, 8, 1...
                     <dbl> 11.6, 0.0, 0.0, 0.0, 18.0, 11.6, 0.0, 0....
## $ HALSTEAD_CONTENT
## $ HALSTEAD_DIFFICULTY
                     <dbl> 2.67, 0.00, 0.00, 0.00, 3.50, 2.67, 0.00...
## $ HALSTEAD_EFFORT
                     <dbl> 82.3, 0.0, 0.0, 0.0, 220.9, 82.3, 0.0, 0...
## $ HALSTEAD_ERROR_EST
                     <dbl> 0.01, 0.00, 0.00, 0.00, 0.02, 0.01, 0.00...
## $ HALSTEAD_LENGTH
                     <dbl> 11, 1, 1, 1, 19, 11, 1, 1, 1, 29, 19, 1,...
## $ HALSTEAD_LEVEL
                     <dbl> 0.38, 0.00, 0.00, 0.00, 0.29, 0.38, 0.00...
## $ HALSTEAD_PROG_TIME
                     <dbl> 4.57, 0.00, 0.00, 0.00, 12.27, 4.57, 0.0...
## $ HALSTEAD_VOLUME
                     <dbl> 30.9, 0.0, 0.0, 0.0, 63.1, 30.9, 0.0, 0....
                     <dbl> 4, 0, 0, 0, 7, 4, 0, 0, 0, 10, 7, 0, 7, ...
## $ NUM OPERANDS
                     <dbl> 7, 1, 1, 1, 12, 7, 1, 1, 1, 19, 12, 1, 1...
## $ NUM_OPERATORS
## $ NUM UNIQUE OPERANDS
                     <dbl> 3, 0, 0, 0, 5, 3, 0, 0, 0, 8, 5, 0, 5, 0...
## $ NUM_UNIQUE_OPERATORS
                     <dbl> 4, 1, 1, 1, 5, 4, 1, 1, 1, 6, 5, 1, 5, 1...
                     <dbl> 5, 3, 3, 3, 12, 5, 3, 3, 13, 12, 3, 1...
## $ LOC_TOTAL
                     ## $ Defective
```

## 8.12 Other libraries and tricks

The lubridate package contains a number of functions facilitating the conversion of text to POSIX dates. As an example, consider the following code. We may use this, for example, with time series.

 $For example https://cran.r-project.org/doc/contrib/de\_Jonge+van\_der\_Loo-Introduction\_to\_data\_cleaning\_with\_R.pdf$ 

```
library(lubridate)
dates <- c("15/02/2013", "15 Feb 13", "It happened on 15 02 '13")
dmy(dates)
```

```
## [1] "2013-02-15" "2013-02-15" "2013-02-15"
```

# Part VI Supervised Models

## Chapter 9

# **Supervised Classification**

A classification problem can be defined as the induction, from a dataset  $\mathcal{D}$ , of a classification function  $\psi$  that, given the attribute vector of an instance/example, returns a class c. A regression problem, on the other hand, returns an numeric value.

Dataset,  $\mathcal{D}$ , is typically composed of n attributes and a class attribute C.

$\overline{Att_1}$	 $Att_n$	Class
$\overline{a_{11}}$	 $a_{1n}$	$c_1$
$a_{21}$	 $a_{2n}$	$c_2$
$a_{m1}$	 $a_{mn}$	$c_m$

Columns are usually called *attributes* or *features*. Typically, there is a *class* attribute, which can be numeric or discrete. When the class is numeric, it is a regression problem. With discrete values, we can talk about binary classification or multiclass (multinomial classification) when we have more than three values. There are variants such *multi-label* classification (we will cover these in the advanced models section).

Once we learn a model, new instances are classified. As shown in the next figure.

We have multiple types of models such as *classification trees*, rules, neural networks, and probabilistic classifiers that can be used to classify instances.

Fernandez et al provide an extensive comparison of 176 classifiers using the UCI dataset (Fernández-Delgado et al., 2014).

We will show the use of different classification techniques in the problem of defect prediction as running example. In this example, the different datasets are composed of classical metrics (*Halstead* or *McCabe* metrics) based on counts of operators/operands and like or object-oriented metrics (e.g. Chidamber and Kemerer) and the class attribute indicating whether the module or class was defective.

## 9.1 Classification Trees

There are several packages for inducing classification trees, for example with the party package (recursive partitioning):

```
library(foreign) # To load arff file
library(party) # Build a decision tree
library(caret)
```

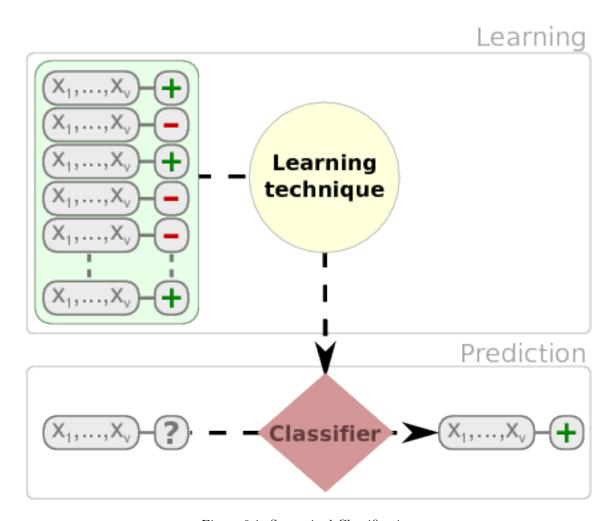
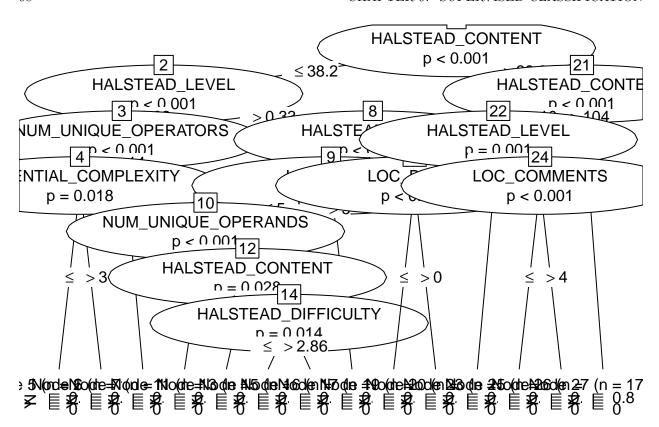


Figure 9.1: Supervised Classification

```
jm1 <- read.arff("./datasets/defectPred/D1/JM1.arff")
str(jm1)</pre>
```

```
## 'data.frame':
                   9593 obs. of 22 variables:
## $ LOC_BLANK
                        : num 447 37 11 106 101 67 105 18 39 143 ...
## $ BRANCH COUNT
                        : num 826 29 405 240 464 187 344 47 163 67 ...
## $ LOC CODE AND COMMENT : num 12 8 0 7 11 4 9 0 1 7 ...
## $ LOC COMMENTS
                         : num 157 42 17 344 75 1 40 10 6 49 ...
## $ CYCLOMATIC_COMPLEXITY: num 470 19 404 127 263 94 207 24 94 34 ...
## $ DESIGN_COMPLEXITY : num 385 19 2 105 256 63 171 13 67 25 ...
## $ ESSENTIAL_COMPLEXITY : num 113 6 1 33 140 27 58 1 3 1 ...
## $ LOC_EXECUTABLE
                     : num 2824 133 814 952 1339 ...
## $ HALSTEAD_CONTENT : num 210 108 101 218 106 ...
## $ HALSTEAD_DIFFICULTY : num 384.4 46.3 206 215.2 337.4 ...
## $ HALSTEAD_EFFORT
                         : num 31079782 232044 4294926 10100867 12120796 ...
## $ HALSTEAD_ERROR_EST : num 26.95 1.67 6.95 15.65 11.98 ...
## $ HALSTEAD_LENGTH : num 8441 685 2033 5669 4308 ...
## $ HALSTEAD_LEVEL
                        : num 0 0.02 0 0 0 0.02 0 0.03 0.01 0.02 ...
## $ HALSTEAD PROG TIME : num 1726655 12891 238607 561159 673378 ...
## $ HALSTEAD_VOLUME
                        : num 80843 5009 20848 46944 35928 ...
## $ NUM OPERANDS
                         : num 3021 295 813 2301 1556 ...
## $ NUM_OPERATORS
                         : num 5420 390 1220 3368 2752 ...
## $ NUM_UNIQUE_OPERANDS : num 609 121 811 262 226 167 279 47 117 355 ...
## $ NUM UNIQUE OPERATORS : num 155 38 411 49 98 27 105 18 52 23 ...
                         : num 3442 222 844 1411 1532 ...
## $ LOC TOTAL
                          : Factor w/ 2 levels "N", "Y": 2 2 2 2 2 2 2 1 2 ...
## $ Defective
# Stratified partition (training and test sets)
set.seed(1234)
inTrain <- createDataPartition(y=jm1$Defective,p=.60,list=FALSE)</pre>
jm1.train <- jm1[inTrain,]</pre>
jm1.test <- jm1[-inTrain,]</pre>
jm1.formula <- jm1$Defective ~ . # formula approach: defect as dependent variable and the rest as indep
jm1.ctree <- ctree(jm1.formula, data = jm1.train)</pre>
# predict on test data
pred <- predict(jm1.ctree, newdata = jm1.test)</pre>
# check prediction result
table(pred, jm1.test$Defective)
```

```
##
## pred N Y
## N 82 3
## Y 3051 700
plot(jm1.ctree)
```



Using the C50 package, there are two ways, specifying train and testing

```
library(C50)
require(utils)
# c50t <- C5.0(jm1.train[,-ncol(jm1.train)], jm1.train[,ncol(jm1.train)])
c50t2 <- C5.0(Defective ~ ., jm1.train)
summary(c50t)
plot(c50t)
c50tPred <- predict(c50t, jm1.train)
# table(c50tPred, jm1.train$Defective)</pre>
```

Using the 'rpart' package

```
# Using the 'rpart' package
library(rpart)
jm1.rpart <- rpart(Defective ~ ., data=jm1.train, parms = list(prior = c(.65,.35), split = "information
# par(mfrow = c(1,2), xpd = NA)
plot(jm1.rpart)
text(jm1.rpart, use.n = TRUE)</pre>
```

9.2. RULES 99

```
NUM_UNIQUE_OPERANDS< 59.5
                          LOC_BLANK< 7.5
03/5e+02
    LOC_CODE_AND_COMMENAL&355AD_DIFFICULT
jm1.rpart
## n= 5757
##
## node), split, n, loss, yval, (yprob)
##
        * denotes terminal node
##
   1) root 5757 2010.0 N (0.650 0.350)
##
      2) LOC_TOTAL< 42.5 4309 1030.0 N (0.744 0.256) *
##
##
     3) LOC_TOTAL>=42.5 1448 743.0 Y (0.430 0.570)
##
       6) NUM UNIQUE OPERANDS < 59.5 1206 655.0 Y (0.473 0.527)
        12) LOC_BLANK< 7.5 449 210.0 N (0.562 0.438)
##
##
          24) LOC_CODE_AND_COMMENT< 3.5 412 172.0 N (0.599 0.401) *
##
          25) LOC_CODE_AND_COMMENT>=3.5 37
                                             13.5 Y (0.262 0.738) *
##
        13) LOC_BLANK>=7.5 757 385.0 Y (0.425 0.575)
          26) HALSTEAD_DIFFICULTY>=64.5 55
##
                                             13.4 N (0.741 0.259) *
##
          27) HALSTEAD_DIFFICULTY< 64.5 702 347.0 Y (0.406 0.594) *
##
       7) NUM_UNIQUE_OPERANDS>=59.5 242
                                         87.6 Y (0.258 0.742) *
library(rpart.plot)
# asRules(jm1.rpart)
```

#### 9.2 Rules

# fancyRpartPlot(jm1.rpart)

```
C5 Rules
```

```
library(C50)
c50r <- C5.0(jm1.train[,-ncol(jm1.train)], jm1.train[,ncol(jm1.train)], rules = TRUE)
summary(c50r)

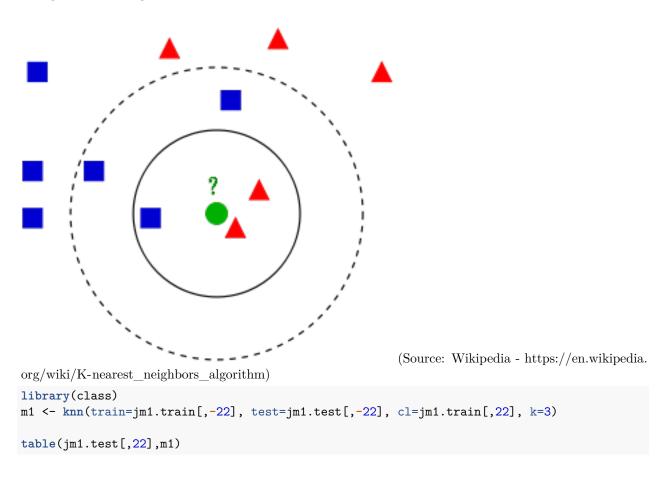
##
## Call:
## C5.0.default(x = jm1.train[, -ncol(jm1.train)], y =
## jm1.train[, ncol(jm1.train)], rules = TRUE)
##
##</pre>
```

```
## C5.0 [Release 2.07 GPL Edition]
                                      Thu Jan 31 16:59:30 2019
## Class specified by attribute `outcome'
## Read 5757 cases (22 attributes) from undefined.data
## Rules:
##
## Rule 1: (5512/923, lift 1.0)
## CYCLOMATIC_COMPLEXITY <= 67
## NUM_UNIQUE_OPERANDS <= 59
## -> class N [0.832]
##
## Rule 2: (11/1, lift 4.6)
## LOC_BLANK > 3
## DESIGN_COMPLEXITY > 3
## LOC EXECUTABLE > 31
## LOC_EXECUTABLE <= 33
## LOC_TOTAL <= 42
## -> class Y [0.846]
##
## Rule 3: (25/5, lift 4.2)
## CYCLOMATIC COMPLEXITY > 67
## -> class Y [0.778]
## Rule 4: (242/110, lift 3.0)
## NUM_UNIQUE_OPERANDS > 59
## LOC_TOTAL > 42
## -> class Y [0.545]
##
## Default class: N
##
##
## Evaluation on training data (5757 cases):
##
##
          Rules
##
      No Errors
##
##
##
       4 1025(17.8%) <<
##
##
##
      (a) (b) <-classified as
##
     4589 112 (a): class N
##
      913 143 (b): class Y
##
##
##
##
   Attribute usage:
##
   99.95% NUM UNIQUE OPERANDS
##
##
   96.18% CYCLOMATIC_COMPLEXITY
    4.39% LOC_TOTAL
##
```

```
## 0.19% LOC_BLANK
## 0.19% DESIGN_COMPLEXITY
## 0.19% LOC_EXECUTABLE
##
##
##
##
Time: 0.1 secs
# c50rPred <- predict(c50r, jm1.train)
# table(c50rPred, jm1.train$Defective)</pre>
```

## 9.3 Distanced-based Methods

In this case, there is no model as such. Given a new instance to classify, this approach finds the closest k-neighbours to the given instance.



```
## m1
## N Y
## N 2827 306
## Y 553 150
```

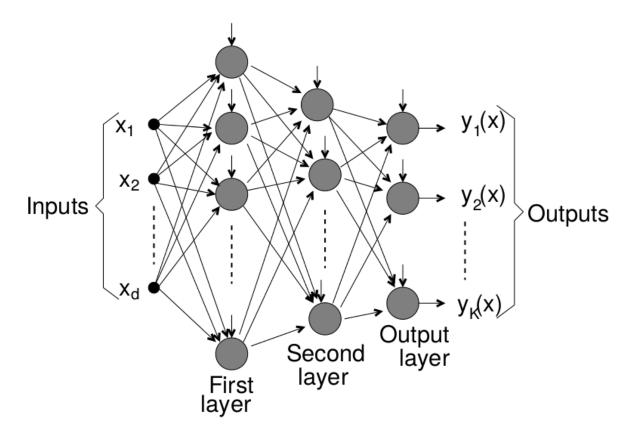


Figure 9.2: Neural Networks

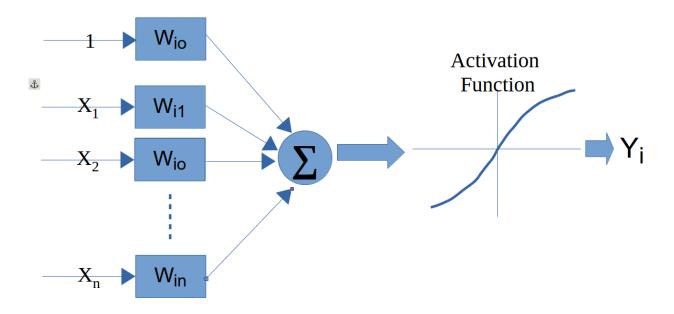


Figure 9.3: Neural Networks

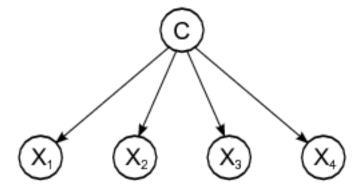
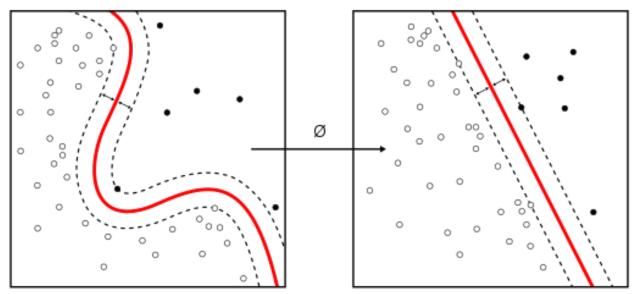


Figure 9.4: Naive Bayes

## 9.4 Neural Networks

## 9.5 Support Vector Machine



 $(Source:\ wikipedia\ https://en.wikipedia.org/wiki/Support\_vector\_machine)$ 

## 9.6 Probabilistic Methods

## 9.6.1 Naive Bayes

Probabilistic graphical model assigning a probability to each possible outcome  $p(C_k, x_1, \ldots, x_n)$ 

Using the klaR package with caret:

library(caret)
library(klaR)

```
## Loading required package: MASS
##
## Attaching package: 'MASS'
## The following object is masked from 'package:dplyr':
##
##
       select
## The following object is masked from 'package:sm':
##
##
       muscle
model <- NaiveBayes(Defective ~ ., data = jm1.train)</pre>
predictions <- predict(model, jm1.test[,-22])</pre>
confusionMatrix(predictions$class, jm1.test$Defective)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction N
##
            N 2990 548
##
            Y 143 155
##
##
                  Accuracy: 0.82
##
                    95% CI: (0.807, 0.832)
##
       No Information Rate: 0.817
##
       P-Value [Acc > NIR] : 0.317
##
##
                     Kappa: 0.225
   Mcnemar's Test P-Value : <2e-16
##
##
##
               Sensitivity: 0.954
##
               Specificity: 0.220
            Pos Pred Value: 0.845
##
##
            Neg Pred Value: 0.520
                Prevalence: 0.817
##
##
            Detection Rate: 0.779
##
      Detection Prevalence: 0.922
##
         Balanced Accuracy: 0.587
##
          'Positive' Class : N
##
##
Using the e1071 package:
library (e1071)
n1 <-naiveBayes(jm1.train$Defective ~ ., data=jm1.train)
# Show first 3 results using 'class'
head(predict(n1,jm1.test, type = c("class")),3) # class by default
## [1] N Y Y
## Levels: N Y
# Show first 3 results using 'raw'
head(predict(n1,jm1.test, type = c("raw")),3)
```

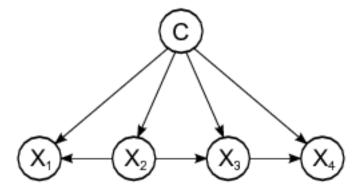


Figure 9.5: Naive Bayes

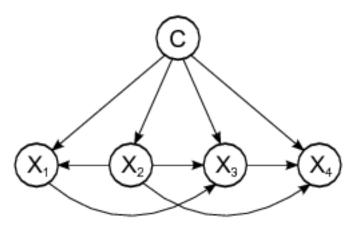


Figure 9.6: Naive Bayes

```
## N Y
## [1,] 1.000000 0.000
## [2,] 0.000000 1.000
## [3,] 0.000754 0.999
```

There are other variants such as TAN and KDB that do not assume the independece condition allowin us more complex structures.

A comprehensice comparison of

## 9.7 Linear Discriminant Analysis (LDA)

One classical approach to classification is Linear Discriminant Analysis (LDA), a generalization of Fisher's linear discriminant, as a method used to find a linear combination of features to separate two or more classes.

```
ldaModel <- train (Defective ~ ., data=jm1.train, method="lda", preProc=c("center","scale"))
ldaModel</pre>
```

```
## Linear Discriminant Analysis
##
## 5757 samples
## 21 predictor
```

```
## 2 classes: 'N', 'Y'
##
## Pre-processing: centered (21), scaled (21)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 5757, 5757, 5757, 5757, 5757, 5757, ...
## Resampling results:
##
## Accuracy Kappa
## 0.817 0.135
We can observe that we are training our model using Defective ~ . as a formula class pariable separate by a and the first pariables. Also, we are the rest of the pariables.
```

We can observe that we are training our model using <code>Defective ~</code>. as a formula were <code>Defective</code> is the class variable separed by <code>~</code> and the <code>'.'</code> means the rest of the variables. Also, we are using a filter for the training data to (preProc) to center and scale.

Also, as stated in the documentation about the train method : > http://topepo.github.io/caret/training.html

```
ctrl <- trainControl(method = "repeatedcv",repeats=3)
ldaModel <- train (Defective ~ ., data=jm1.train, method="lda", trControl=ctrl, preProc=c("center","sca
ldaModel

## Linear Discriminant Analysis</pre>
```

```
##
## 5757 samples
##
    21 predictor
##
      2 classes: 'N', 'Y'
##
## Pre-processing: centered (21), scaled (21)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 5182, 5181, 5182, 5182, 5180, 5181, ...
## Resampling results:
##
##
     Accuracy Kappa
##
     0.816
               0.129
```

Instead of accuracy we can activate other metrics using summaryFunction=twoClassSummary such as ROC, sensitivity and specificity. To do so, we also need to speficy classProbs=TRUE.

```
ctrl <- trainControl(method = "repeatedcv",repeats=3, classProbs=TRUE, summaryFunction=twoClassSummary)
ldaModel3xcv10 <- train (Defective ~ ., data=jm1.train, method="lda", trControl=ctrl, preProc=c("center")
ldaModel3xcv10</pre>
```

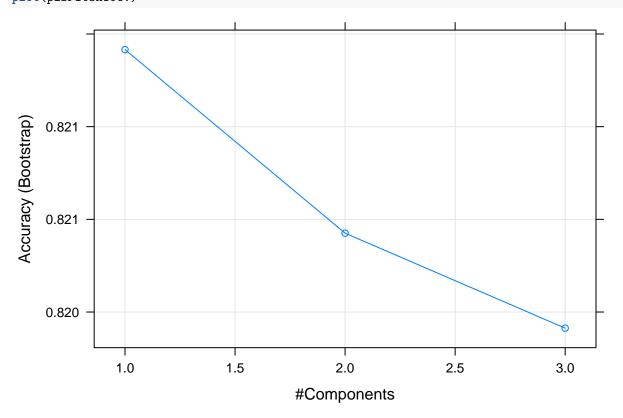
```
## Linear Discriminant Analysis
##
## 5757 samples
##
     21 predictor
      2 classes: 'N', 'Y'
##
## Pre-processing: centered (21), scaled (21)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 5181, 5181, 5181, 5181, 5182, 5182, ...
## Resampling results:
##
##
     ROC
            Sens
                   Spec
     0.706 0.974 0.121
##
```

Most methods have parameters that need to be optimised and that is one of the

```
plsFit3x10cv <- train (Defective ~ ., data=jm1.train, method="pls", trControl=trainControl(classProbs=T
plsFit3x10cv
```

```
## Partial Least Squares
##
## 5757 samples
##
     21 predictor
      2 classes: 'N', 'Y'
##
##
## Pre-processing: centered (21), scaled (21)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 5757, 5757, 5757, 5757, 5757, 5757, ...
## Resampling results across tuning parameters:
##
##
     ncomp Accuracy
                      Kappa
##
     1
            0.821
                      0.0548
            0.820
                      0.0768
##
     2
##
     3
            0.820
                      0.0762
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was ncomp = 1.
```

#### plot(plsFit3x10cv)



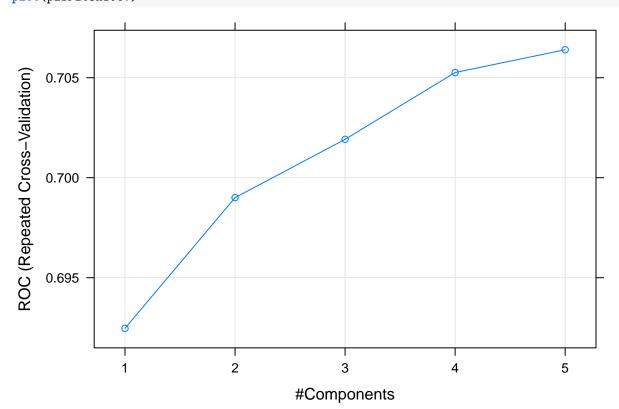
The parameter tuneLength allow us to specify the number values per parameter to consider.

```
plsFit3x10cv <- train (Defective ~ ., data=jm1.train, method="pls", trControl=ctrl, metric="ROC", tuneL
```

#### plsFit3x10cv

```
## Partial Least Squares
##
## 5757 samples
##
     21 predictor
      2 classes: 'N', 'Y'
##
##
## Pre-processing: centered (21), scaled (21)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 5181, 5181, 5181, 5182, 5181, 5181, ...
## Resampling results across tuning parameters:
##
##
    ncomp ROC
                   Sens
                          Spec
##
            0.692 0.995 0.0454
     1
##
            0.699
                  0.991
                         0.0634
##
            0.702 0.990 0.0641
     3
##
            0.705 0.989 0.0656
##
     5
            0.706 0.989 0.0663
## ROC was used to select the optimal model using the largest value.
## The final value used for the model was ncomp = 5.
```

#### plot(plsFit3x10cv)



Finally to predict new cases, caret will use the best classfier obtained for prediction.

```
plsProbs <- predict(plsFit3x10cv, newdata = jm1.test, type = "prob")
plsClasses <- predict(plsFit3x10cv, newdata = jm1.test, type = "raw")</pre>
```

#### confusionMatrix(data=plsClasses,jm1.test\$Defective)

```
## Confusion Matrix and Statistics
##
##
             Reference
                      Y
## Prediction
                 N
##
            N 3108
                    643
            Y
##
                25
                     60
##
##
                  Accuracy: 0.826
                    95% CI: (0.813, 0.838)
##
##
       No Information Rate: 0.817
       P-Value [Acc > NIR] : 0.0743
##
##
##
                     Kappa : 0.117
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.9920
##
               Specificity: 0.0853
##
            Pos Pred Value: 0.8286
##
            Neg Pred Value: 0.7059
##
                Prevalence: 0.8167
##
            Detection Rate: 0.8102
##
      Detection Prevalence: 0.9778
##
         Balanced Accuracy: 0.5387
##
          'Positive' Class : N
##
##
```

#### 9.7.1 Predicting the number of defects (numerical class)

From the Bug Prediction Repository (BPR) http://bug.inf.usi.ch/download.php

Some datasets contain CK and other 11 object-oriented metrics for the last version of the system plus categorized (with severity and priority) post-release defects. Using such dataset:

```
jdt <- read.csv("./datasets/defectPred/BPD/single-version-ck-oo-EclipseJDTCore.csv", sep=";")

# We just use the number of bugs, so we removed others
jdt$classname <- NULL
jdt$nonTrivialBugs <- NULL
jdt$majorBugs <- NULL
jdt$minorBugs <- NULL
jdt$criticalBugs <- NULL
jdt$highPriorityBugs <- NULL
jdt$highPriorityBugs <- NULL
jdt$X <- NULL
# Caret
library(caret)

# Split data into training and test datasets
set.seed(1)
inTrain <- createDataPartition(y=jdt$bugs,p=.8,list=FALSE)</pre>
```

```
jdt.train <- jdt[inTrain,]</pre>
jdt.test <- jdt[-inTrain,]</pre>
ctrl <- trainControl(method = "repeatedcv",repeats=3)</pre>
glmModel <- train (bugs ~ ., data=jdt.train, method="glm", trControl=ctrl, preProc=c("center", "scale"))</pre>
glmModel
## Generalized Linear Model
##
## 798 samples
  17 predictor
##
##
## Pre-processing: centered (17), scaled (17)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 719, 718, 719, 718, 718, 718, ...
## Resampling results:
##
##
     RMSE
            Rsquared MAE
     0.786 0.397
##
                      0.417
Others such as Elasticnet:
glmnetModel <- train (bugs ~ ., data=jdt.train, method="glmnet", trControl=ctrl, preProc=c("center", "sc</pre>
glmnetModel
## glmnet
##
## 798 samples
## 17 predictor
##
## Pre-processing: centered (17), scaled (17)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 718, 718, 719, 718, 718, 718, ...
## Resampling results across tuning parameters:
##
##
     alpha lambda RMSE
                           Rsquared MAE
##
     0.10
           0.0012 0.774
                           0.397
                                      0.417
           0.0120 0.788 0.384
                                      0.421
##
     0.10
##
     0.10
           0.1202 0.794 0.369
                                      0.424
           0.0012 0.773 0.397
##
     0.55
                                     0.416
##
     0.55
           0.0120 0.794 0.375
                                     0.422
##
     0.55
            0.1202 0.805 0.371
                                      0.435
##
     1.00
            0.0012 0.773 0.397
                                      0.416
##
     1.00
            0.0120 0.794 0.373
                                      0.423
##
     1.00
            0.1202 0.812 0.365
                                      0.449
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were alpha = 1 and lambda = 0.0012.
```

# 9.8 Binary Logistic Regression (BLR)

Binary Logistic Regression (BLR) can models fault-proneness as follows

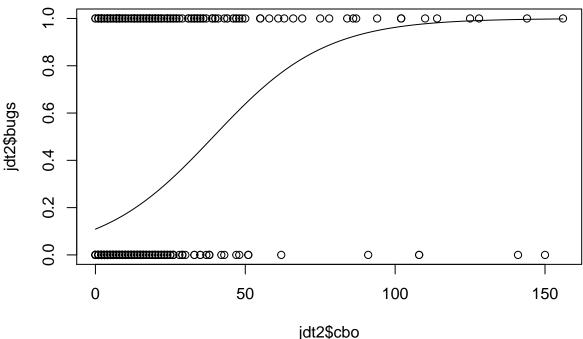
## Number of Fisher Scoring iterations: 5

$$fp(X) = \frac{e^{logit()}}{1 + e^{logit(X)}}$$

where the simplest form for logit is:

```
logit(X) = c_0 + c_1 X
jdt <- read.csv("./datasets/defectPred/BPD/single-version-ck-oo-EclipseJDTCore.csv", sep=";")</pre>
# Caret
library(caret)
# Convert the response variable into a boolean variable (0/1)
jdt$bugs[jdt$bugs>=1]<-1
cbo <- jdt$cbo
bugs <- jdt$bugs
# Split data into training and test datasets
jdt2 = data.frame(cbo, bugs)
inTrain <- createDataPartition(y=jdt2$bugs,p=.8,list=FALSE)</pre>
jdtTrain <- jdt2[inTrain,]</pre>
jdtTest <- jdt2[-inTrain,]</pre>
BLR models fault-proneness are as follows fp(X) = \frac{e^{logit()}}{1 + e^{logit(X)}}
where the simplest form for logit is logit(X) = c_0 + c_1 X
# logit regression
# glmLogit <- train (bugs ~ ., data=jdt.train, method="glm", family=binomial(link = logit))
glmLogit <- glm (bugs ~ ., data=jdtTrain, family=binomial(link = logit))</pre>
summary(glmLogit)
##
## Call:
## glm(formula = bugs ~ ., family = binomial(link = logit), data = jdtTrain)
## Deviance Residuals:
   Min 1Q Median
                               30
                                      Max
## -3.439 -0.601 -0.531 -0.492
                                    2.106
##
## Coefficients:
              Estimate Std. Error z value Pr(>|z|)
0.05342
                           0.00721 7.41 1.3e-13 ***
## cbo
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
       Null deviance: 796.98 on 797 degrees of freedom
## Residual deviance: 711.81 on 796 degrees of freedom
## AIC: 715.8
```

```
Predict a single point:
```

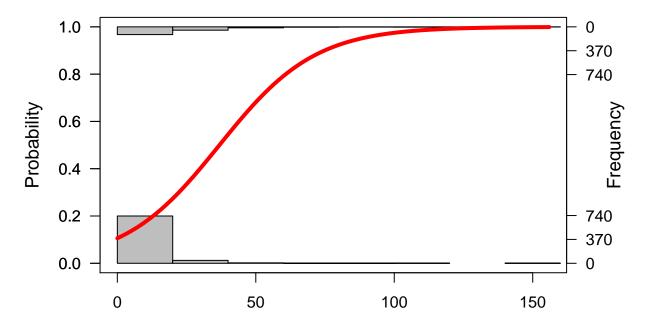


#### # points(jdtTrain\$cbo, fitted(glmLogit))

Another type of graph:

library(popbio)

```
##
##
## Attaching package: 'popbio'
## The following object is masked from 'package:caret':
##
## sensitivity
logi.hist.plot(jdt2$cbo,jdt2$bugs,boxp=FALSE,type="hist",col="gray")
```



# 9.9 The caret package

There are hundreds of packages to perform classification task in R, but many of those can be used throught the 'caret' package which helps with many of the data mining process task as described next.

The caret packagehttp://topepo.github.io/caret/ provides a unified interface for modeling and prediction with around 150 different models with tools for:

- data splitting
- pre-processing
- feature selection
- model tuning using resampling
- variable importance estimation, etc.

Website: http://caret.r-forge.r-project.org JSS Paper: www.jstatsoft.org/v28/i05/paper

Book: Applied Predictive Modeling

# Chapter 10

# Regression

# 10.1 Linear Regression modeling

- Linear Regression is one of the oldest and most known predictive methods. As its name says, the idea is to try to fit a linear equation between a dependent variable and an independent, or explanatory, variable. The idea is that the independent variable x is something the experimenter controls and the dependent variable y is something that the experimenter measures. The line is used to predict the value of y for a known value of x. The variable x is the predictor variable and y the response variable.
- Multiple linear regression uses 2 or more independent variables for building a model. See https://www.wikipedia.org/wiki/Linear\_regression.
- First proposed many years ago but still very useful...
- The equation takes the form  $\hat{y} = b_0 + b_1 * x$
- The method used to choose the values  $b_0$  and  $b_1$  is to minimize the sum of the squares of the residual errors.

#### 10.1.1 Regression: Galton Data

Not related to Software Engineering but ...

```
library(UsingR)
data(galton)
par(mfrow=c(1,2))
hist(galton$child,col="blue",breaks=100)
hist(galton$parent,col="blue",breaks=100)
```

## **Article**

European Journal of Human Genetics (2009) 17, 1070–1075; doi:10.1038/ejhg.2009.5; published online 18 February 2009

Sir Francis Galton, 1886

Predicting human height by Victorian and

genomic methods

RATE OF REGRESSION IN HEREDITARY STATURE.

HEIGHT

DETAILS

REGRESSION IN HEREDITARY STATURE.

HEIGHT

DETAILS

REGRESSION IN HEREDITARY STATURE.

Yurii S Aulchenko<sup>1</sup>,<sup>2</sup>,<sup>7</sup>, Maksim V Struchalir M Belonogova<sup>2</sup>,<sup>4</sup>, Tatiana I Axenovich<sup>2</sup>, Mic Albert Hofman<sup>1</sup>, Andre G Uitterlinden<sup>6</sup>, Mai Ben A Oostra<sup>1</sup>, Cornelia M van Duijn<sup>1</sup>, A Co W Janssens<sup>1</sup> and Pavel M Borodin<sup>2</sup>,<sup>4</sup>

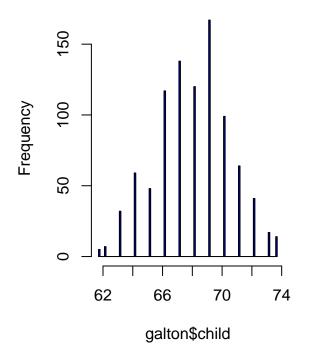
genomic profile should explain to reach certain AUC values. For highly heritable traits such as height, we conclude that in applications in which parental phenotypic information is available (eg, medicine), the Victorian Galton's method will long stay unsurpassed, in terms of both discriminative accuracy and costs. For less neritable traits, and in

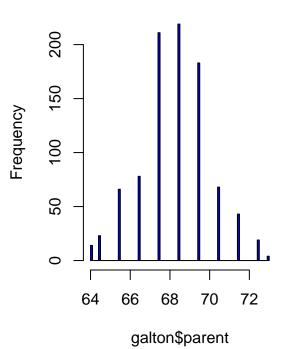
situations in which parental information is not available (eg, forensics), genomic methods may provide an alternative, given that

Figure 10.1: Galton Data

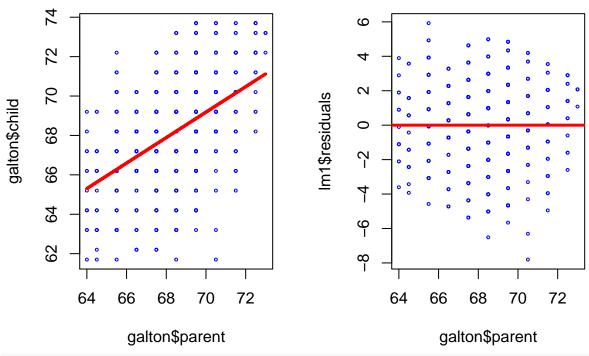
# Histogram of galton\$child

# Histogram of galton\$parent



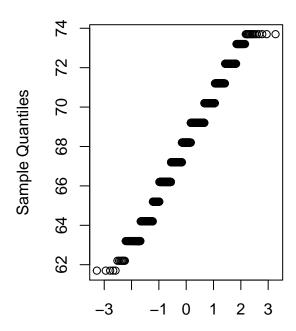


```
plot(galton$parent,galton$child,pch=1,col="blue", cex=0.4)
lm1 <- lm(galton$child ~ galton$parent)
lines(galton$parent,lm1$fitted,col="red",lwd=3)
plot(galton$parent,lm1$residuals,col="blue",pch=1, cex=0.4)
abline(c(0,0),col="red",lwd=3)</pre>
```



qqnorm(galton\$child)

# Normal Q-Q Plot



**Theoretical Quantiles** 

#### 10.1.2 Simple Linear Regression

- Given two variables Y (response) and X (predictor), the assumption is that there is an approximate  $(\approx)$  linear relation between those variables.
- The mathematical model of the observed data is described as (for the case of simple linear regression):

$$Y \approx \beta_0 + \beta_1 X$$

- the parameter  $\beta_0$  is named the *intercept* and  $\beta_1$  is the *slope*
- Each observation can be modeled as

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i; \epsilon_i \sim N(0, \sigma^2)$$

-  $\epsilon_i$  is the error - This means that the variable y is normally distributed:

$$y_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$$

• The predictions or estimations of this model are obtained by a linear equation of the form  $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$ , that is, each new prediction is computed with

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- The actual parameters  $\beta_{0}$  and  $\beta_{1}$  are unknown
- The parameters  $\hat{\beta}_0$  and  $\hat{\beta}_1$  of the linear equation can be estimated with different methods.

#### 10.1.3 Least Squares

- One of the most used methods for computing  $\hat{\beta}_0$  and  $\hat{\beta}_1$  is the criterion of "least squares" minimization.
- The data is composed of n pairs of observations  $(x_i, y_i)$
- Given an observation  $y_i$  and its corresponding estimation  $\hat{y_i}$ ) the residual  $e_i$  is defined as

$$e_i = y_i - \hat{y_i}$$

• the Residual Sum of Squares is defined as

$$RSS = e_1^2 + \dots + e_i^2 + \dots + e_n^2$$

- the Least Squares Approach minimizes the RSS
- as result of that minimizitation, it can be obtained, by means of calculus, the estimation of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  as

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

and

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

where  $\bar{y}$  and  $\bar{x}$  are the sample means.

the variance  $\sigma^2$  is estimated by

$$\hat{\sigma}^2 = RSS/(n-2)$$

where n is the number of observations

• The Residual Standard Error is defined as

$$RSE = \sqrt{RSS/(n-2)}$$

• The equation

$$Y = \beta_0 + \beta_1 X + \epsilon$$

defines the linear model, i.e., the population regression line

- The least squares line is  $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$
- Confidence intervals are computed using the standard errors of the intercept and the slope.
- The 95% confidence interval for the slope is computed as

$$[\hat{\beta}_1 - 2 \cdot SE(\hat{\beta}_1), \hat{\beta}_1 + SE(\hat{\beta}_1)]$$

• where

$$SE(\hat{\beta}_1) = \sqrt{\frac{\sigma^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2}}$$

#### 10.1.4 Linear regression in R

The following are the basic commands in R:

- The basic function is lm(), that returns an object with the model.
- Other commands: summary prints out information about the regression, coef gives the coefficients for the linear model, fitted gives the predictd value of y for each value of x, residuals contains the differences between observed and fitted values.
- predict will generate predicted values of the response for the values of the explanatory variable.

## 10.2 Linear Regression Diagnostics

- Several plots help to evaluate the suitability of the linear regression
  - Residuals vs fitted: The residuals should be randomly distributed around the horizontal line representing a residual error of zero; that is, there should not be a distinct trend in the distribution of points.
  - Standard Q-Q plot: residual errors are normally distributed
  - Square root of the standardized residuals vs the fitted values: there should be no obvious trend. This plot is similar to the residuals versus fitted values plot, but it uses the square root of the standardized residuals.
  - Leverage: measures the importance of each point in determining the regression result. Smaller
    values means that removing the observation has little effect on the regression result.

#### 10.2.1 Simulation example

#### 10.2.1.1 Simulate a dataset

```
set.seed(3456)
# equation is y = -6.6 + 0.13 x +e
# range x 100,400
a <- -6.6
b <- 0.13
num_obs <- 60
xmin <- 100
xmax <- 400
x <- sample(seq(from=xmin, to = xmax, by =1), size= num_obs, replace=FALSE)</pre>
```

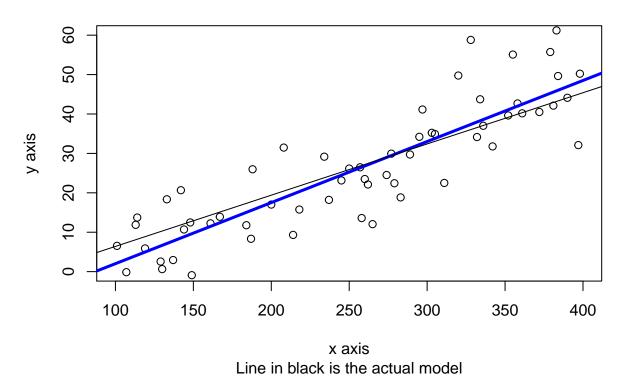
```
sderror <- 9 # sigma for the error term in the model
e <- rnorm(num_obs, 0, sderror)

y <- a + b * x + e

newlm <- lm(y~x)
summary(newlm)</pre>
```

```
##
## Call:
## lm(formula = y ~ x)
## Residuals:
      Min
             1Q Median 3Q
                                     Max
## -15.937 -4.617 -0.923 3.797 21.442
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -13.4765 3.0320 -4.44 4e-05 ***
                          0.0113 13.75 <2e-16 ***
## x
                0.1550
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 7.99 on 58 degrees of freedom
## Multiple R-squared: 0.765, Adjusted R-squared: 0.761
## F-statistic: 189 on 1 and 58 DF, p-value: <2e-16
cfa1 <- coef(newlm)[1]
cfb2 <- coef(newlm)[2]
plot(x,y, xlab="x axis", ylab= "y axis", xlim = c(xmin, xmax), ylim = c(0,60), sub = "Line in black is
title(main = paste("Line in blue is the Regression Line for ", num_obs, " points."))
abline(a = cfa1, b = cfb2, col= "blue", lwd=3)
abline(a = a, b = b, col= "black", lwd=1) #original line
```

## Line in blue is the Regression Line for 60 points.



#### 10.2.1.1.1 Subset a set of points from the same sample

```
\# sample from the same x
                                to compare least squares lines
# change the denominator in newsample to see how the least square lines changes accordingly.
newsample <- as.integer(num_obs/8) # number of pairs x,y</pre>
idxs_x1 <- sample(1:num_obs, size = newsample, replace = FALSE) #sample indexes
x1 \leftarrow x[idxs_x1]
e1 <- e[idxs_x1]
y1 <- a + b * x1 + e1
xy_obs <- data.frame(x1, y1)</pre>
names(xy_obs) <- c("x_obs", "y_obs")</pre>
newlm1 <- lm(y1~x1)
summary(newlm1)
##
## Call:
## lm(formula = y1 ~ x1)
##
## Residuals:
               2
##
                       3
                              4
                                      5
    3.722 -5.067 4.683 -4.716 3.095 -0.813 -0.904
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -14.5356
                             7.0962
                                       -2.05
                                               0.0958 .
                 0.1494
                             0.0272
                                        5.48
                                               0.0027 **
## x1
```

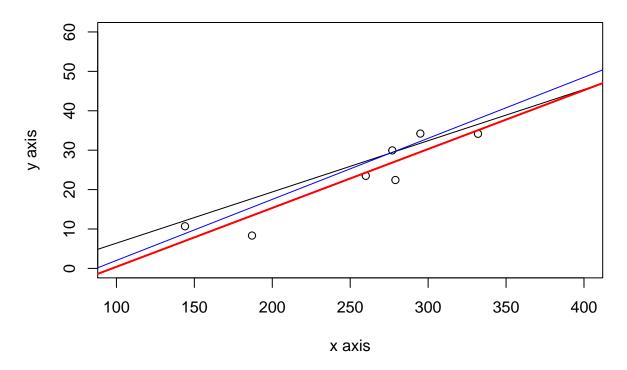
```
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.35 on 5 degrees of freedom
## Multiple R-squared: 0.857, Adjusted R-squared: 0.829
## F-statistic: 30.1 on 1 and 5 DF, p-value: 0.00275

cfa21 <- coef(newlm1)[1]
cfb22 <- coef(newlm1)[2]

plot(x1,y1, xlab="x axis", ylab= "y axis", xlim = c(xmin, xmax), ylim = c(0,60))
title(main = paste("New line in red with ", newsample, " points in sample"))

abline(a = a, b = b, col= "black", lwd=1) # True line
abline(a = cfa1, b = cfb2, col= "blue", lwd=1) #sample
abline(a = cfa21, b = cfb22, col= "red", lwd=2) #new line</pre>
```

# New line in red with 7 points in sample

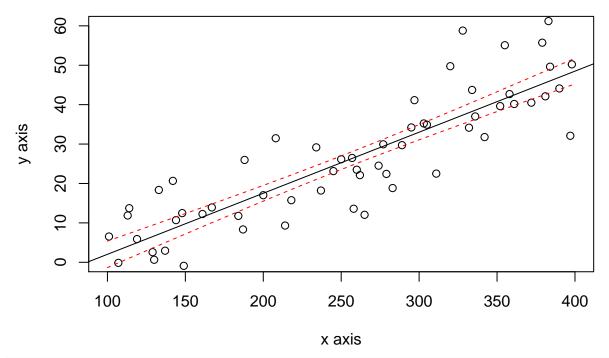


10.2.1.1.2 Compute a confidence interval on the original sample regression line

```
newx <- seq(xmin, xmax)
ypredicted <- predict(newlm, newdata=data.frame(x=newx), interval= "confidence", level= 0.90, se = TRUE

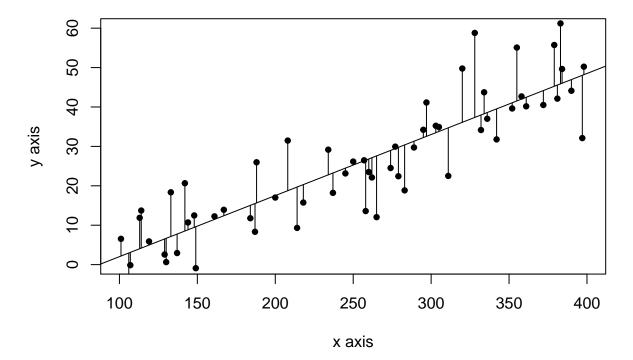
plot(x,y, xlab="x axis", ylab= "y axis", xlim = c(xmin, xmax), ylim = c(0,60))
# points(x1, fitted(newlm1))
abline(newlm)

lines(newx,ypredicted$fit[,2],col="red",lty=2)
lines(newx,ypredicted$fit[,3],col="red",lty=2)</pre>
```



```
# Plot the residuals or errors
ypredicted_x <- predict(newlm, newdata=data.frame(x=x))
plot(x,y, xlab="x axis", ylab= "y axis", xlim = c(xmin, xmax), ylim = c(0,60), sub = "", pch=19, cex=0."
title(main = paste("Residuals or errors", num_obs, " points."))
abline(newlm)
segments(x, y, x, ypredicted_x)</pre>
```

# Residuals or errors 60 points.



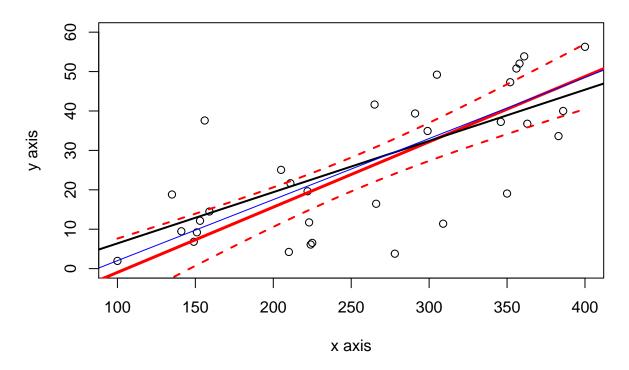
#### 10.2.1.1.3 Take another sample from the model and explore

```
# equation is y = -6.6 + 0.13 x +e
# range x 100,400
num_obs <- 35
xmin <- 100
xmax <- 400
x3 <- sample(seq(from=xmin, to = xmax, by =1), size= num_obs, replace=FALSE)
sderror <- 14 # sigma for the error term in the model
e3 <- rnorm(num_obs, 0, sderror)

y3 <- a + b * x3 + e3
newlm3 <- lm(y3~x3)
summary(newlm3)</pre>
```

```
##
## Call:
## lm(formula = y3 ~ x3)
##
## Residuals:
   Min
          1Q Median
                         3Q
                                Max
## -25.59 -11.19 2.92 8.65 39.16
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -17.5335 7.6813 -2.28 0.029 *
               0.1657
                           0.0285
                                  5.80 1.7e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 15 on 33 degrees of freedom
## Multiple R-squared: 0.505, Adjusted R-squared: 0.49
## F-statistic: 33.7 on 1 and 33 DF, p-value: 1.72e-06
cfa31 <- coef(newlm3)[1]
cfb32 <- coef(newlm3)[2]
plot(x3,y3, xlab="x axis", ylab= "y axis", xlim = c(xmin, xmax), ylim = c(0,60))
title(main = paste("Line in red is the Regression Line for ", num_obs, " points."))
abline(a = cfa31, b = cfb32, col= "red", lwd=3)
abline(a = a, b = b, col= "black", lwd=2) #original line
abline(a = cfa1, b = cfb2, col= "blue", lwd=1) #first sample
# confidence intervals for the new sample
newx <- seq(xmin, xmax)</pre>
ypredicted <- predict(newlm3, newdata=data.frame(x3=newx), interval= "confidence", level= 0.90, se = TR
lines(newx,ypredicted$fit[,2],col="red",lty=2, lwd=2)
lines(newx,ypredicted$fit[,3],col="red",lty=2, lwd=2)
```

# Line in red is the Regression Line for 35 points.



#### 10.2.2 Diagnostics fro assessing the regression line

#### 10.2.2.1 Residual Standard Error

• It gives us an idea of the typical or average error of the model. It is the estimated standard deviation of the residuals.

#### **10.2.2.2** $R^2$ statistic

• This is the proportion of variability in the data that is explained by the model. Best values are those close to 1.

# 10.3 Multiple Linear Regression

#### 10.3.1 Partial Least Squares

- If several predictors are highly correlated, the least squares approach has high variability.
- PLS finds linear combinations of the predictors, that are called *components* or *latent* variables.

# 10.4 Linear regression in Software Effort estimation

Fitting a linear model to log-log - the predictive power equation is  $y = e^{b_0 + b_1 log(x)}$ , ignoring the bias corrections - First, we are fitting the model to the whole dataset. But it is not the right way to do it, because of overfitting.

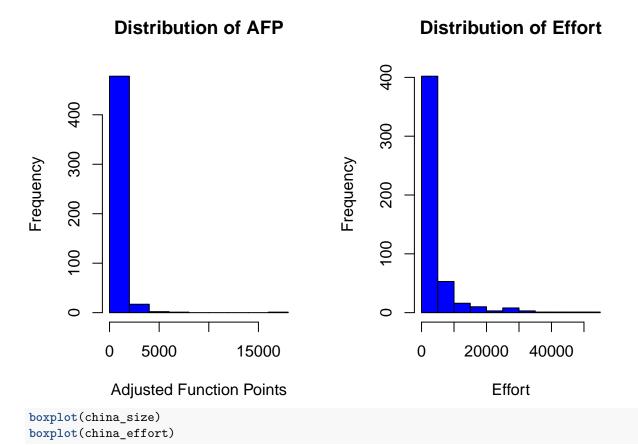
```
library(foreign)
china <- read.arff("./datasets/effortEstimation/china.arff")
china_size <- china$AFP
summary(china_size)</pre>
```

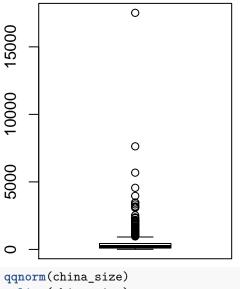
```
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 9 100 215 487 438 17518

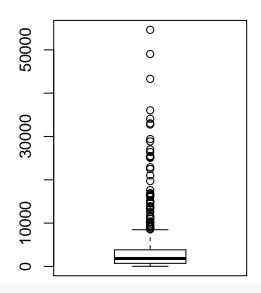
china_effort <- china$Effort
summary(china_effort)</pre>
```

```
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 26 704 1829 3921 3826 54620

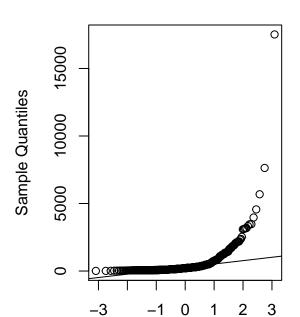
par(mfrow=c(1,2))
hist(china_size, col="blue", xlab="Adjusted Function Points", main="Distribution of AFP")
hist(china_effort, col="blue",xlab="Effort", main="Distribution of Effort")
```





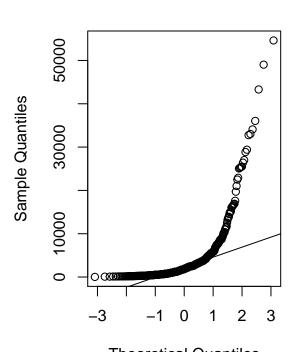


qqnorm(china\_size)
qqline(china\_size)
qqnorm(china\_effort)
qqline(china\_effort)



Normal Q-Q Plot

# Normal Q-Q Plot

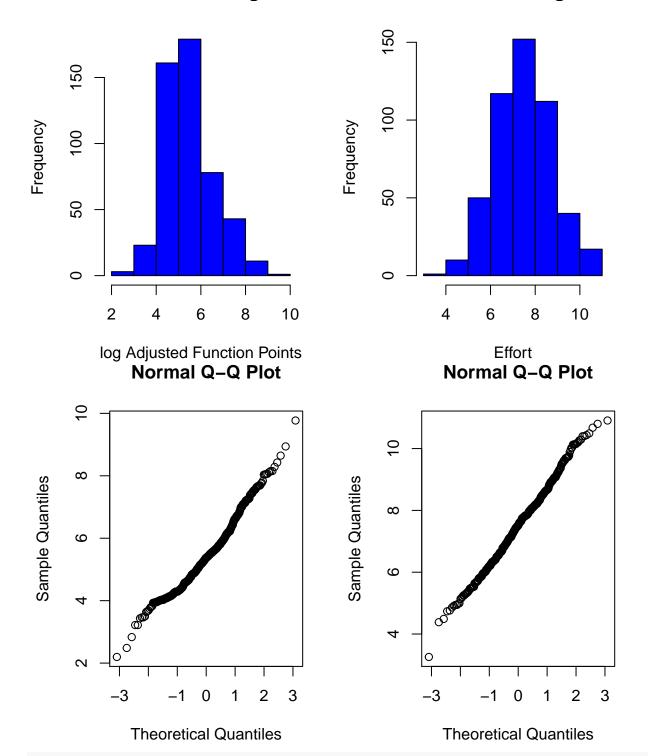


Theoretical Quantiles

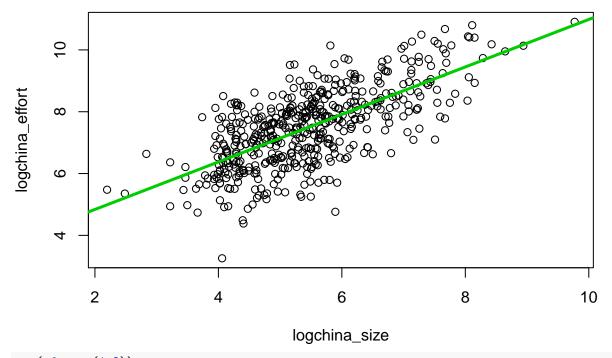
**Theoretical Quantiles** 



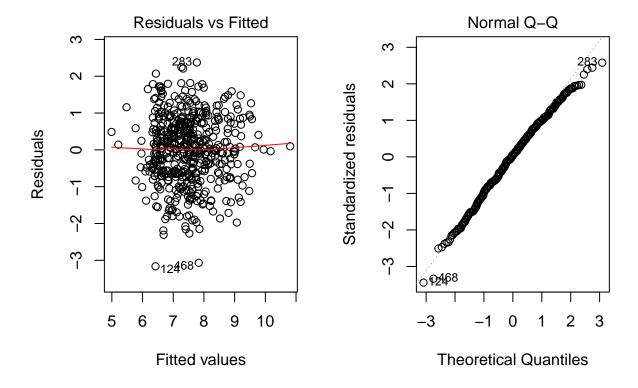
# **Distribution of log Effort**

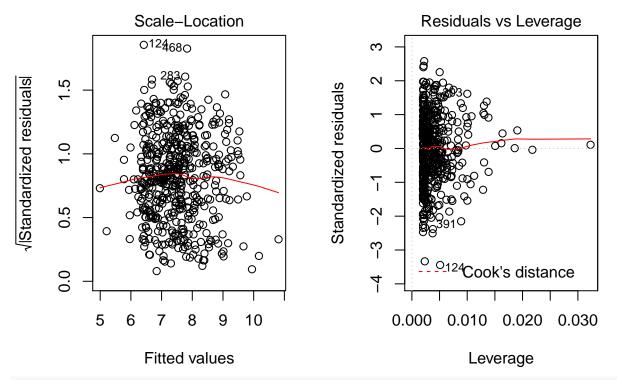


linmodel\_logchina <- lm(logchina\_effort ~ logchina\_size)
par(mfrow=c(1,1))
plot(logchina\_size, logchina\_effort)
abline(linmodel\_logchina, lwd=3, col=3)</pre>



par(mfrow=c(1,2))
plot(linmodel\_logchina, ask = FALSE)





#### linmodel\_logchina

```
##
## Call:
## lm(formula = logchina_effort ~ logchina_size)
##
## Coefficients:
## (Intercept) logchina_size
## 3.301 0.768
```

# 10.5 References

- The New Statistics with R, Andy Hector, 2015
- An Introduction to R, W.N. Venables and D.M. Smith and the R Development Core Team
- Practical Data Science with R, Nina Zumel and John Mount
- G. James et al, An Introduction to Statistical Learning with Applications in R, Springer, 2013

# Part VII Unsupervised Models

# Chapter 11

# Unsupervised or Descriptive modeling

From the descriptive (unsupervised) point of view, patterns are found to predict future behaviour or estimate. This include association rules, clustering, or tree clustering which aim at grouping together objects (e.g., animals) into successively larger clusters, using some measure of similarity or distance. The dataset will be as the previous table without the C class attribute

$\overline{\mathrm{Att}_1}$		$\mathrm{Att}_{\mathrm{n}}$
$a_{11}$		$a_{1n}$
$a_{21}$		$a_{2n}$
$a_{m1}$	•••	$a_{mn}$

# 11.1 Clustering

```
library(foreign)
library(fpc)

kc1 <- read.arff("./datasets/defectPred/D1/KC1.arff")

# Split into training and test datasets
set.seed(1)
ind <- sample(2, nrow(kc1), replace = TRUE, prob = c(0.7, 0.3))
kc1.train <- kc1[ind==1, ]
kc1.test <- kc1[ind==2, ]

# No class
kc1.train$Defective <- NULL
ds <- dbscan(kc1.train, eps = 0.42, MinPts = 5)
kc1.kmeans <- kmeans(kc1.train, 2)</pre>
```

#### 11.1.1 k-Means

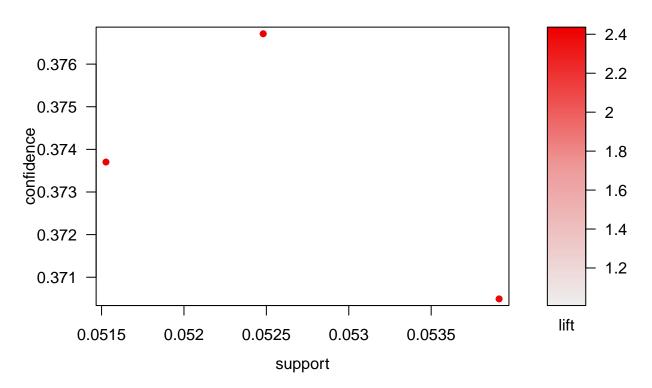
```
library(reshape, quietly=TRUE)
library(graphics)
kc1kmeans <- kmeans(sapply(na.omit(kc1.train), rescaler, "range"), 10)
#plot(kc1kmeans, col = kc1kmeans$cluster)
#points(kc1kmeans$centers, col = 1:5, pch = 8)</pre>
```

#### 11.2 Association rules

```
library(arules)
# x <- as.numeric(kc1$LOC_TOTAL)</pre>
# str(x)
# summary(x)
# hist(x, breaks=30, main="LoC Total")
# xDisc <- discretize(x, categories=5)</pre>
# table(xDisc)
for(i in 1:21) kc1[,i] <- discretize(kc1[,i], method = "interval", breaks = 5)</pre>
rules <- apriori(kc1,
   parameter = list(minlen=3, supp=0.05, conf=0.35),
   appearance = list(rhs=c("Defective=Y"),
   default="lhs"),
   control = list(verbose=F))
#rules <- apriori(kc1,</pre>
 # parameter = list(minlen=2, supp=0.05, conf=0.3),
 # appearance = list(rhs=c("Defective=Y", "Defective=N"),
 # default="lhs"))
inspect(rules)
```

```
##
       lhs
                                                       support confidence lift count
                                         rhs
## [1] {HALSTEAD_CONTENT=[38.6,77.2),
       HALSTEAD_LEVEL=[0,0.4)}
                                      => {Defective=Y} 0.0539
                                                                    0.370 2.39
##
                                                                                 113
## [2] {LOC_CODE_AND_COMMENT=[0,2.4),
##
       HALSTEAD_CONTENT=[38.6,77.2)} => {Defective=Y} 0.0525
                                                                    0.377 2.43
                                                                                 110
## [3] {LOC_CODE_AND_COMMENT=[0,2.4),
##
        HALSTEAD_CONTENT=[38.6,77.2),
       HALSTEAD_LEVEL=[0,0.4)}
                                      => {Defective=Y} 0.0515
                                                                    0.374 2.41
                                                                                  108
library(arulesViz)
plot(rules)
```

# Scatter plot for 3 rules



# Part VIII

# **Evaluation**

# Chapter 12

# Evaluation of Models

Once we obtain the model with the training data, we need to evaluate it with some new data (testing data).

No Free Lunch theorem In the absence of any knowledge about the prediction problem, no model can be said to be uniformly better than any other

## 12.1 Building and Validating a Model

We cannot use the same data for training and testing (it is like evaluating a student with the exercises previouly solved in class, the sudent's marks will be "optimistic" and we do not know about student capability to generalise the learned concepts).

Therefore, we should, at a minimun, divide the dataset into *training* and *testing*, learn the model with the training data and test it with the rest of data as explained next.

#### 12.1.1 Holdout approach

**Holdout approach** consists of dividing the dataset into training (typically approx. 2/3 of the data) and testing (approx 1/3 of the data). + Problems: Data can be skewed, missing classes, etc. if randomly divided. Stratification ensures that each class is represented with approximately equal proportions (e.g., if data contains aprox 45% of positive cases, the training and testing datasets should mantain similar proportion of positive cases).

Holdout estimate can be made more reliable by repeating the process with different subsamples (repeated holdout method)

The error rates on the different iterations are averaged (overall error rate)

- Usually, part of the data points are used for building the model and the remaining points are used for validating the model. There are several approaches to this process.
- Validation Set approach: it is the simplest method. It consists of randomly dividing the available set of oservations into two parts, a training set and a validation set or hold-out set. Usually 2/3 of the data points are used for training and 1/3 is used for testing purposes.

#### 12.1.2 Cross Validation (CV)

k-fold Cross-Validation involves randomly dividing the set of observations into k groups, or folds, of approximately equal size. One fold is treated as a validation set and the method is trained on the remaining k-1



# **Validation**

Figure 12.1: Hold out validation

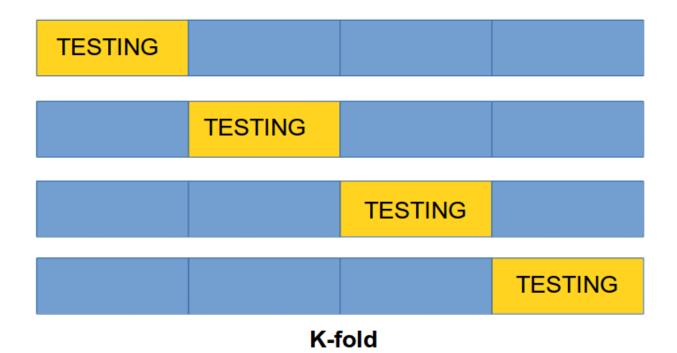


Figure 12.2: k-fold

folds. This procedure is repeated k times. If k is equal to n we are in the previous method.

- 1st step: split dataset  $(\mathcal{D})$  into k subsets of approximately equal size  $C_1, \ldots, C_k$
- 2nd step: we construct a dataset  $D_i = D C_i$  used for training and test the accuracy of the classifier  $D_i$  on  $C_i$  subset for testing

Having done this for all k we estimate the accuracy of the method by averaging the accuracy over the k cross-validation trials

• Leave-One-Out Cross-Validation: This is a special case of CV. Instead of creating two subsets for training and testing, a single observation is used for the validation set, and the remaining observations make up the training set. This approach is repeated n times (the total number of observations) and the estimate for the test mean squared error is the average of the n test estimates.



## Leave one out

Figure 12.3: Leave One Out

#### 12.2 Evaluation of Classification Models

The confusion matrix (which can be extended to multiclass problems) is a table that presents the results of a classification algorithm. The following table shows the possible outcomes for binary classification problems:

	ActPos	ActNeg
$\overline{PredPos}$	TP	$\overline{FP}$
PredNeg	FN	TN

where  $True\ Positives\ (TP)$  and  $True\ Negatives\ (TN)$  are respectively the number of positive and negative instances correctly classified,  $False\ Positives\ (FP)$  is the number of negative instances misclassified as positive (also called Type I errors), and  $False\ Negatives\ (FN)$  is the number of positive instances misclassified as negative (Type II errors).

• Confusion Matrix in Wikipedia

From the confusion matrix, we can calculate:

- True positive rate, or recall  $(TP_r = recall = r = TP/TP + FN)$  is the proportion of positive cases correctly classified as belonging to the positive class.
- False negative rate  $(FN_r = FN/TP + FN)$  is the proportion of positive cases misclassified as belonging to the negative class.
- False positive rate  $(FP_r = FP/FP + TN)$  is the proportion of negative cases misclassified as belonging to the positive class.
- True negative rate  $(TN_r = TN/FP + TN)$  is the proportion of negative cases correctly classified as belonging to the negative class.

There is a tradeoff between  $FP_r$  and  $FN_r$  as the objective is minimize both metrics (or conversely, maximize the true negative and positive rates). It is possible to combine both metrics into a single figure, predictive accuracy:

$$accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

• A suitable and interesting performance metric for binary classification when data are imbalanced is the Matthew's Correlation Coefficient (MCC)~?:

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

MCC can also be calculated from the confusion matrix. Its range goes from -1 to +1; the closer to one the better as it indicates perfect prediction whereas a value of 0 means that classification is not better than random prediction and negative values mean that predictions are worst than random.

#### 12.2.1 Prediction in probabilistic classifiers

A probabilistic classifier estimates the probability of each of the posible class values given the attribute values of the instance P(c|x). Then, given a new instance, x, the class value with the highest a posteriori probability will be assigned to that new instance (the *winner takes all* approach):

$$\psi(x) = argmax_c(P(c|x))$$

# 12.3 Other Metrics used in Software Engineering with Classification

In the domain of defect prediction and when two classes are considered, it is also customary to refer to the probability of detection, (pd) which corresponds to the True Positive rate  $(TP_{rate} \text{ or } Sensitivity)$  as a measure of the goodness of the model, and probability of false alarm (pf) as performance measures~Menzies et al. (2007).

The objective is to find which techniques that maximise pd and minimise pf. As stated by Menzies et al., the balance between these two measures depends on the project characteristics (e.g. real-time systems vs. information management systems) it is formulated as the Euclidean distance from the sweet spot pf = 0 and pd = 1 to a pair of (pf, pd).

$$balance = 1 - \frac{\sqrt{(0 - pf^2) + (1 - pd^2)}}{\sqrt{2}}$$

It is normalized by the maximum possible distance across the ROC square  $(\sqrt{2}, 2)$ , subtracted this value from 1, and expressed it as a percentage.

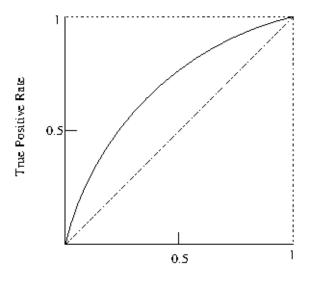
# 12.4 Graphical Evaluation

### 12.4.1 Receiver Operating Characteristic (ROC)

The Receiver Operating Characteristic (ROC)(Fawcett, 2006) curve which provides a graphical visualisation of the results.

The Area Under the ROC Curve (AUC) also provides a quality measure between positive and negative rates with a single value.

A simple way to approximate the AUC is with the following equation:  $AUC = \frac{1+TP_r-FP_r}{2}$ 



False Positive Rate

Figure 12.4: Receiver Operating Characteristic

### 12.4.2 Precision-Recall Curve (PRC)

Similarly to ROC, another widely used evaluation technique is the Precision-Recall Curve (PRC), which depicts a trade off between precision and recall and can also be summarised into a single value as the Area Under the Precision-Recall Curve (AUPRC)~?.

%AUPCR is more accurate than the ROC for testing performances when dealing with imbalanced datasets as well as optimising ROC values does not necessarily optimises AUPR values, i.e., a good classifier in AUC space may not be so good in PRC space. %The weighted average uses weights proportional to class frequencies in the data. %The weighted average is computed by weighting the measure of class (TP rate, precision, recall ...) by the proportion of instances there are in that class. Computing the average can be sometimes be misleading. For instance, if class 1 has 100 instances and you achieve a recall of 30%, and class 2 has 1 instance and you achieve recall of 100% (you predicted the only instance correctly), then when taking the average (65%) you will inflate the recall score because of the one instance you predicted correctly. Taking the weighted average will give you 30.7%, which is much more realistic measure of the performance of the classifier.

#### 12.5 Numeric Prediction Evaluation

RSME

Mean Square Error = 
$$MSE = \frac{(p_1 - a_1)^2 + ... + (p_n - a_n)^2}{n}$$

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

$$RMSD = \sqrt{\frac{\sum_{t=1}^{n} (\hat{y}_t - y)^2}{n}}$$

Mean-absolute error MAE

$$\frac{|p_1-a_1|+\ldots+|p_n-a_n|}{n}$$

Relative absolute error:

$$RAE = \frac{\sum_{i=1}^{N} |\hat{\theta}_i - \theta_i|}{\sum_{i=1}^{N} |\overline{\theta} - \theta_i|}$$

Root relative-squared error:

$$RAE = \sqrt{\frac{\sum_{i=1}^{N} |\hat{\theta}_i - \theta_i|}{\sum_{i=1}^{N} |\overline{\theta} - \theta_i|}}$$

where  $\hat{\theta}$  is a mean value of  $\theta$ .

Relative-squared error  $\frac{(p_1-a_1)^2+\ldots+(p_n-a_n)^2}{(a_1-\hat{a})^2+\ldots+(a_n-\hat{a})^2}$  ( $\hat{a}$  is the mean value over the training data)

Relative Absolut Error

Correlation Coefficient

Correlation coefficient between two random variables X and Y is defined as  $\rho(X,Y) = \frac{\mathbf{Cov}(X,Y)}{\sqrt{\mathbf{Var}(X)\mathbf{Var}(Y)}}$ . The sample correlation coefficient  $\{x_i\}$  between two samples  $x_i$  and  $y_j$  is vydefined as  $r = S_{xy}/\sqrt{S_{xx}S_{yy}}$ 

Example: Is there any linear relationship between the effort estimates  $(p_i)$  and actual effort  $(a_i)$ ?

```
a||39, 43, 21, 64, 57, 47, 28, 75, 34, 52
```

p||65, 78, 52, 82, 92, 89, 73, 98, 56, 75

```
p<-c(39,43,21,64,57,47,28,75,34,52)
a<-c(65,78,52,82,92,89,73,98,56,75)
#
cor(p,a)
```

## [1] 0.84

 $R^2$ 

## Measures of Evaluation in Software Engineering

There are several measures typically used in software engieering. In particular for effort estimation, the following metrics are extensively used in addition or instead of statistical measures.

- Mean of the Absolute Error (MAR): compute the absolute errors and take the mean
- Geometric Mean of the Absolute Error (qMAR): more appropriate when the distribution is skewed
- Mean Magnitude of the Relative Error (MMRE): this measure has been critisized many times as a biased measure  $(\frac{\sum_{i=1}^{n} |\hat{y}_i y_i|/y_i}{n})$
- Median Magnitude of the Relative Error (MdMRE): using the median insted of the mean
- Level of Prediction (Pred(l)) defined as the percentage of estimates that are within the percentage level l of the actual values. The level of prediction is typically set at 25% below and above the actual value and an estimation method is considered good if it gives a result of more than 75%.
- Standardised Accuracy (SA) (proposed by Shepperd&MacDonnell): this measure overcomes all the problems of the MMRE. It is defined as the MAR relative to random guessing ( $SA = 1 \frac{MAR}{\overline{MAR}_{P_0}} \times 100$ )
- Random guessing:  $\overline{MAR}_{P_0}$  is defined as: predict a  $\hat{y}_t$  for the target case t by randomly sampling (with equal probability) over all the remaining n-1 cases and take  $\hat{y}_t = y_r$  where r is drawn randomly from 1 to n and  $r \neq t$ .
- Exact  $\overline{MAR}_{P_0}$ : it is an improvement over  $\overline{MAR}_{P_0}$ . For small datasets the "random guessing" can be computed exactly by iterating over all data points.

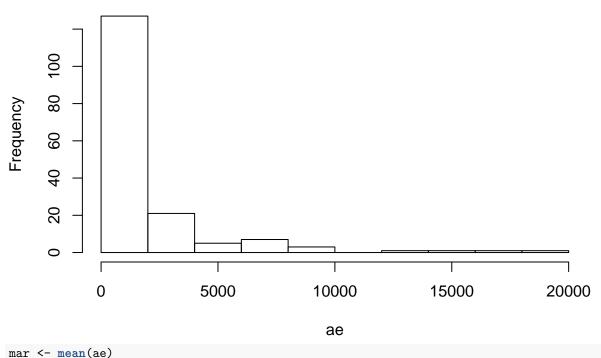
#### 13.1 Evaluation of the model in the Testing data

```
library(foreign)
gm_mean = function(x, na.rm=TRUE){
   exp(sum(log(x[x > 0]), na.rm=na.rm) / length(x))}

chinaTrain <- read.arff("./datasets/effortEstimation/china3AttSelectedAFPTrain.arff")
logchina_size <- log(chinaTrain$AFP)
logchina_effort <- log(chinaTrain$Effort)
linmodel_logchina_train <- lm(logchina_effort ~ logchina_size)</pre>
```

```
chinaTest <- read.arff("./datasets/effortEstimation/china3AttSelectedAFPTest.arff")
b0 <- linmodel_logchina_train$coefficients[1]
b1 <- linmodel_logchina_train$coefficients[2]
china_size_test <- chinaTest$AFP
actualEffort <- chinaTest$Effort
predEffort <- exp(b0+b1*log(china_size_test))
err <- actualEffort - predEffort #error or residual
ae <- abs(err)
hist(ae, main="Absolute Error in the China Test data")</pre>
```

#### **Absolute Error in the China Test data**



```
mar <- mean(ae)
mre <- ae/actualEffort
mmre <- mean(mre)
mdmre <- median(mre)
gmar <- gm_mean(ae)
mar

## [1] 1867
mmre

## [1] 1.15
mdmre

## [1] 0.551
gmar</pre>
```

## [1] 833

```
level_pred <- 0.25 #below and above (both)
lowpred <- actualEffort*(1-level_pred)
uppred <- actualEffort*(1+level_pred)
pred <- predEffort <= uppred & predEffort >= lowpred #pred is a vector with logical values
Lpred <- sum(pred)/length(pred)
Lpred</pre>
```

## [1] 0.186

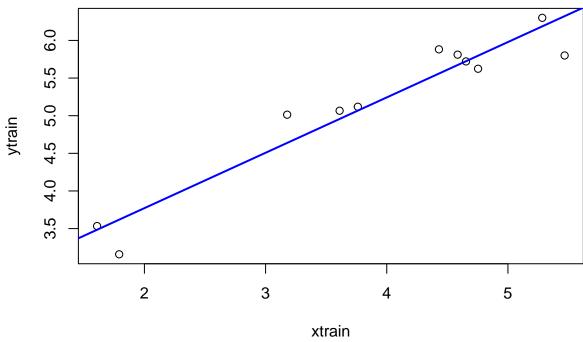
#### 13.2 Building a Linear Model on the Telecom1 dataset

• Although there are few datapoints we split the file into Train (2/3) and Test (1/3)

```
telecom1 <- read.table("./datasets/effortEstimation/Telecom1.csv", sep=",",header=TRUE, stringsAsFactor
samplesize <- floor(0.66*nrow(telecom1))
set.seed(012) # to make the partition reproducible
train_idx <- sample(seq_len(nrow(telecom1)), size = samplesize)
telecom1_train <- telecom1[train_idx, ]
telecom1_test <- telecom1[-train_idx, ]

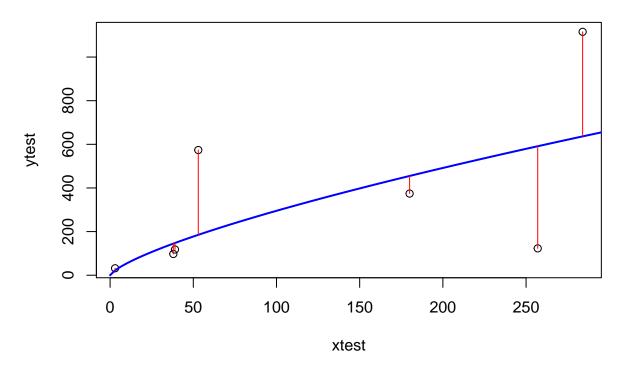
par(mfrow=c(1,1))
# transformation of variables to log-log
xtrain <- log(telecom1_train$size)
ytrain <- log(telecom1_train$effort)

lmtelecom1 <- lm( ytrain ~ xtrain)
plot(xtrain, ytrain)</pre>
abline(lmtelecom1, lwd=2, col="blue")
```



```
b0_tel1 <- lmtelecom1$coefficients[1]
b1_tel1 <- lmtelecom1$coefficients[2]
# calculate residuals and predicted values
res <- signif(residuals(lmtelecom1), 5)

xtest <- telecom1_test$size
ytest <- telecom1_test$effort
pre_tel1 <- exp(b0_tel1+b1_tel1*log(xtest))
# plot distances between points and the regression line
plot(xtest, ytest)
curve(exp(b0_tel1+b1_tel1*log(x)), from=0, to=300, add=TRUE, col="blue", lwd=2)
segments(xtest, ytest, xtest, pre_tel1, col="red")</pre>
```

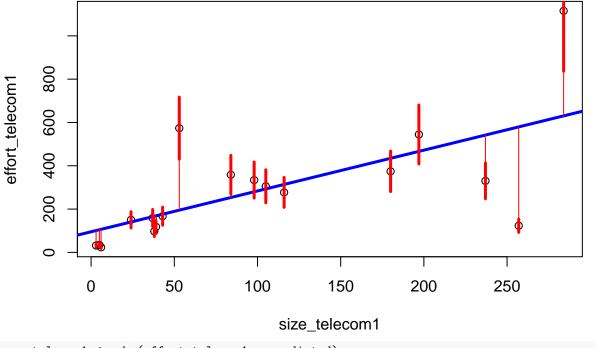


## 13.3 Building a Linear Model on the Telecom1 dataset with all observations

• Just to visualize results

```
par(mfrow=c(1,1))
effort_telecom1 <- telecom1$effort</pre>
size_telecom1 <- telecom1$size</pre>
lmtelecom <- lm(effort_telecom1 ~ size_telecom1)</pre>
plot(size_telecom1, effort_telecom1)
abline(lmtelecom, lwd=3, col="blue")
# calculate residuals and predicted values
res <- signif(residuals(lmtelecom), 5)</pre>
predicted <- predict(lmtelecom)</pre>
# plot distances between points and the regression line
segments(size_telecom1, effort_telecom1, size_telecom1, predicted, col="red")
level_pred <- 0.25 #below and above (both)</pre>
lowpred <- effort_telecom1*(1-level_pred)</pre>
uppred <- effort_telecom1*(1+level_pred)</pre>
predict_inrange <- predicted <= uppred & predicted >= lowpred #pred is a vector with logical values
Lpred <- sum(predict_inrange)/length(predict_inrange)</pre>
Lpred
## [1] 0.444
```

```
#Visually plot lpred
segments(size_telecom1, lowpred, size_telecom1, uppred, col="red", lwd=3)
```



```
err_telecom1 <- abs(effort_telecom1 - predicted)
mar_tel1 <- mean(err_telecom1)
mar_tel1</pre>
```

## [1] 125

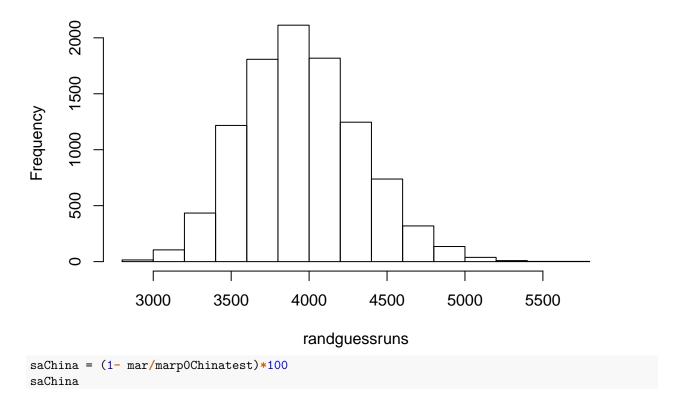
#### 13.4 Standardised Accuracy. MARPO. ChinaTest

• Computing  $MARP_0$  in the China Test data

```
estimEffChinaTest <- predEffort # This will be overwritten, no problem
numruns <- 9999
randguessruns <- rep(0, numruns)
for (i in 1:numruns) {
   for (j in 1:length(estimEffChinaTest)) {
      estimEffChinaTest[j] <- sample(actualEffort[-j],1)}#replacement with random guessingt
   randguessruns[i] <- mean(abs(estimEffChinaTest-actualEffort))
   }
marpOChinatest <- mean(randguessruns)
marpOChinatest</pre>
```

```
## [1] 3956
hist(randguessruns, main="MARPO distribution of the China dataset")
```

#### MARPO distribution of the China dataset

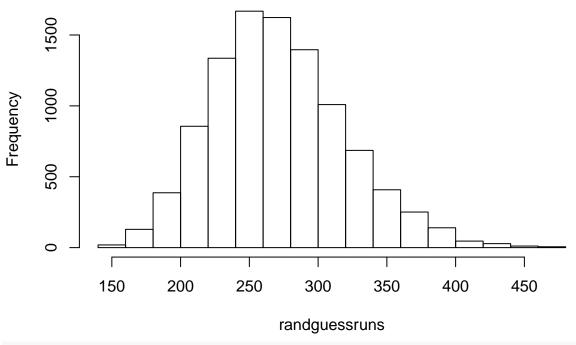


## [1] 52.8

#### 13.5 Standardised Accuracy. MARP0. Telecom1

• Computing  $MARP_0$ 

#### MARP0 distribution of the Telecom1 dataset



saTelecom1 <- (1- mar\_tel1/marp0telecom1)\*100
saTelecom1</pre>

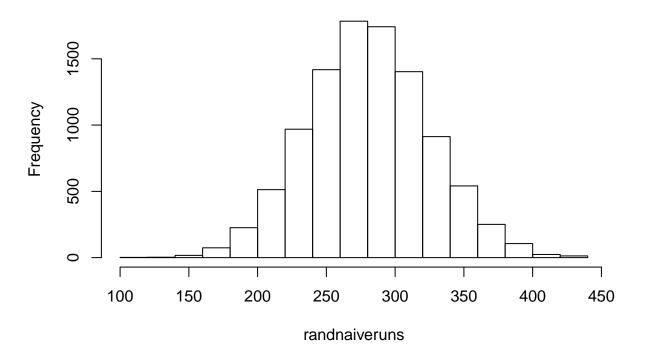
## [1] 54

#### 13.5.1 MARP0 in the Atkinson dataset

- For checking results you may use figure Atkinson in Shepperd&MacDonnell

13.6. EXACT MARPO 153

#### **MARPO** distribution of the Atkinson dataset



#### 13.6 Exact MARP0

#example dataset

## [1] 264

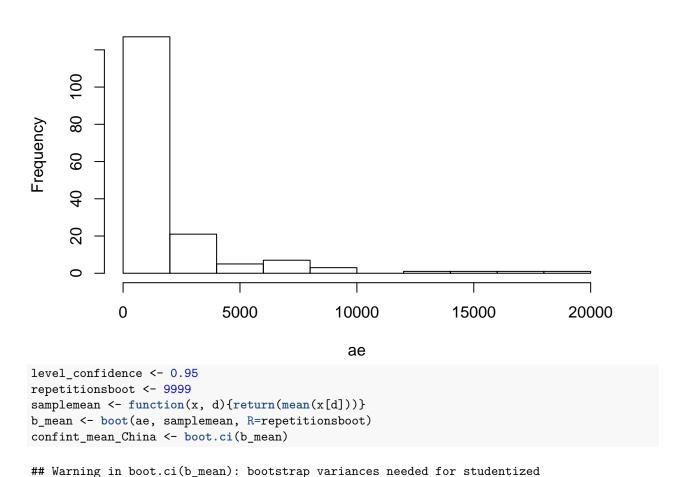
## WBL simple R code to calculate Shepperd and MacDonell's marp0 exactly

```
atkinson_actual_effort <-
  c(670,912,218,595,267,344,229,190,869,109,289,616,557,416,578,438)
myabs <- function(x,y) abs(x-y)</pre>
#diffs is square array whose i,jth element = abs(actual_i - actual_j)
#in practice this is good enough but could be made more efficient by not
#explicitly storing the matrix and only using the values below the diagonal.
diffs <- outer(atkinson_actual_effort,atkinson_actual_effort,myabs)</pre>
marp0 <- mean(diffs)</pre>
marp0
## [1] 264
#### same procedure without using the outer function
act_effort <-
  c(670,912,218,595,267,344,229,190,869,109,289,616,557,416,578,438)
n <- length(act_effort)</pre>
diffs_guess <- matrix(nrow=n, ncol=n)</pre>
colnames(diffs_guess) <- act_effort</pre>
rownames(diffs_guess) <- act_effort</pre>
for (i in 1:n){
  diffs_guess[i,] <- act_effort - act_effort[i]</pre>
diffs_guess <- abs(diffs_guess)</pre>
means_per_point <- apply(diffs_guess, 2, mean)</pre>
marp0 <- mean(means_per_point)</pre>
marp0
```

## 14.1 Computing the bootstraped confidence interval of the mean for the Test observations of the China dataset:

```
library(boot)
##
## Attaching package: 'boot'
## The following object is masked from 'package:survival':
##
##
       aml
## The following object is masked from 'package:lattice':
##
##
       melanoma
## The following object is masked from 'package:sm':
##
##
       dogs
hist(ae, main="Absolute Errors of the China Test data")
```

#### **Absolute Errors of the China Test data**



## intervals

```
confint_mean_China
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
## Based on 9999 bootstrap replicates
##
## CALL :
## boot.ci(boot.out = b_mean)
##
## Intervals :
            Normal
## Level
                                  Basic
## 95% (1412, 2315) (1384, 2283)
##
## Level
           Percentile
                                   BCa
                        (1486, 2419)
## 95%
       (1451, 2350)
## Calculations and Intervals on Original Scale
  • Computing the bootstraped geometric mean
boot geom mean <- function(error vec){</pre>
  log_error <- log(error_vec[error_vec > 0])
  log_error <-log_error[is.finite(log_error)] #remove the -Inf value before calculating the mean, just
  samplemean <- function(x, d){return(mean(x[d]))}</pre>
  b <- boot(log_error, samplemean, R=repetitionsboot) # with package boot
  # this is a boot for the logs
  return(b)
}
# BCAconfidence interval for the geometric mean
BCAciboot4geommean <- function(b){</pre>
  conf_int <- boot.ci(b, conf=level_confidence, type="bca")$bca #following 10.9 of Ugarte et al.'s book
  conf_int[5] <- exp(conf_int[5]) # the boot was computed with log. Now take the measure back to its pr
  conf_int[4] <- exp(conf_int[4])</pre>
  return (conf_int)
}
# this is a boot object
b_gm <- boot_geom_mean(ae) #"ae" is the absolute error in the China Test data
print(paste0("Geometric Mean of the China Test data: ", round(exp(b_gm$t0), digits=3)))
## [1] "Geometric Mean of the China Test data: 832.55"
b ci gm <- BCAciboot4geommean(b gm)</pre>
print(paste0("Confidence Interval: ", round(b_ci_gm[4], digits=3), " - ", round(b_ci_gm[5], digits=3)))
## [1] "Confidence Interval: 673.125 - 1009.427"
# Make a % confidence interval bca
# BCAciboot <- function(b){</pre>
# conf_int <- boot.ci(b, conf=level_confidence, type="bca")$bca #following 10.9 of Ugarte et al.'s bo
  return (conf_int)
```

158CHAPTER 14.	WBL SIMPLE R CODE TO	CALCULATE SHEPPERD A	AND MACDONELL'S MARP0 EXACTLY

# $\begin{array}{c} {\rm Part~IX} \\ {\bf Advanced~Topics} \end{array}$

#### Feature Selection

This technique consists in selecting the most relevant attributes. The need of applying FS includes the following points:

- A reduced volume of data allows different data mining or searching techniques to be applied.
- Irrelevant and redundant attributes can generate less accurate and more complex models. Furthermore, data mining algorithms can be executed faster.
- It is possible to avoid the collection of data for those irrelevant and redundant attributes in the future.

FS algorithms designed with different evaluation criteria broadly fall into two categories [21, 14, 13, 3, 1, 12, 5]:

- The filter model relies on general characteristics of the data to evaluate and select feature subsets without involving any data mining algorithm.
- The wrapper model requires one predetermined mining algorithm and uses its performance as the evaluation criterion. It searches for features better suited to the mining algorithm aiming to improve mining performance, but it also tends to be more computationally expensive than filter model [11, 12].

#### 15.1 Instance Selection

#### 15.2 Missing Data Imputation

### Feature Selection Example

```
Feature Selection in R and Caret
library(caret)
library(doParallel) # parallel processing
## Loading required package: foreach
## Loading required package: iterators
## Loading required package: parallel
library(dplyr) # Used by caret
library(pROC) # plot the ROC curve
## Type 'citation("pROC")' for a citation.
## Attaching package: 'pROC'
## The following objects are masked from 'package:stats':
##
##
       cov, smooth, var
library(foreign)
### Use the segmentationData from caret
# Load the data and construct indices to divided it into training and test data sets.
#set.seed(10)
kc1 <- read.arff("./datasets/defectPred/D1/KC1.arff")</pre>
inTrain <- createDataPartition(y = kc1$Defective,</pre>
 ## the outcome data are needed
 p = .75,
 ## The percentage of data in the
 ## training set
 list = FALSE)
The function createDataPartition does a stratified partitions.
training <- kc1[inTrain,]</pre>
nrow(training)
## [1] 1573
```

```
testing <- kc1[-inTrain, ]
nrow(testing)</pre>
```

```
## [1] 523
```

The train function can be used to + evaluate, using resampling, the effect of model tuning parameters on performance + choose the "optimal" model across these parameters + estimate model performance from a training set

gbmFit1 <- train(Defective  $\sim$  ., data = training, method = "gbm", trControl = fitControl, ## This last option is actually one ## for gbm() that passes through verbose = FALSE) gbmFit1

```
plsFit <- train(Defective ~ .,
    data = training,
    method = "pls",
    ## Center and scale the predictors for the training
    ## set and all future samples.
    preProc = c("center", "scale")
)</pre>
```

To fix {r} testPred <- predict(plsFit, testing) postResample(testPred, testing\$Defective) sensitivity(testPred, testing\$Defective) confusionMatrix(testPred, testing\$Defective)

When there are three or more classes, confusionMatrix will show the confusion matrix and a set of "one-versus-all" results.

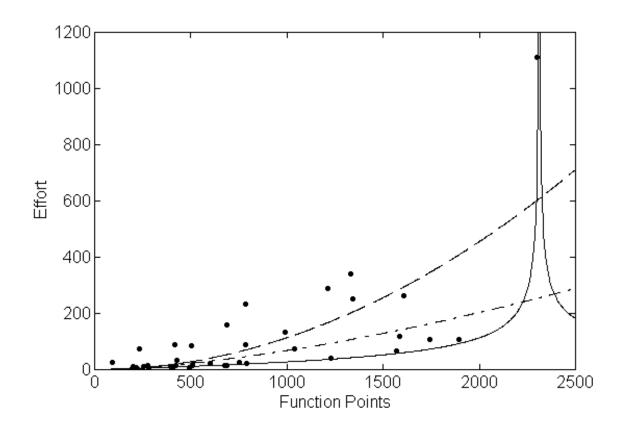
## **Advanced Models**

#### 17.1 Genetic Programming for Symbolic Regression

This technique is inspired by Darwin's evolution theory. + 1960s by I. Rechenberg in his work "Evolution strategies" + 1975 Genetic Algorithms (GAs) invented by J Holland and published in his book" Adaption in Natural and Artificial Systems" + 1992 J. Koza has used genetic algorithm to evolve programs to perform certain tasks. He called his method "genetic programming"

Other reference for GP: Langdon WB, Poli R (2001) Foundations of Genetic Programming. Springer.

• Depending on the function set used and the function to be minimised, GP can generate almost any type of curve



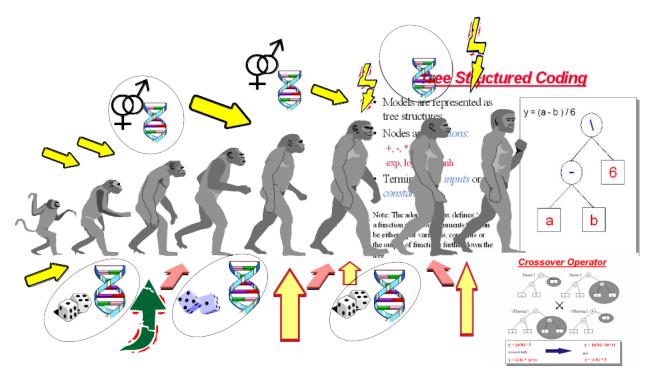
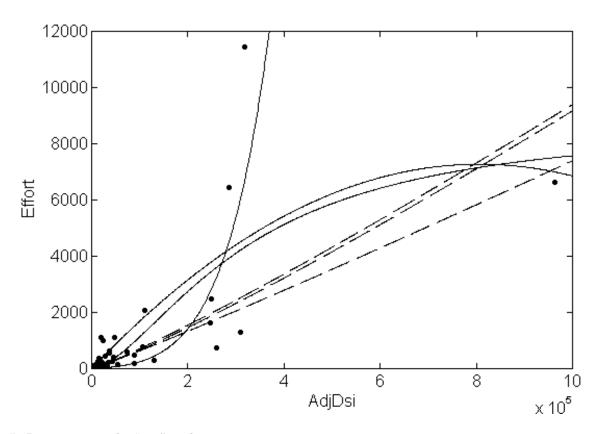


Figure 17.1:



In R, we can use the "rgp" package

```
BEGIN

INITIALISE population with random candidate solutions;

EVALUATE each candidate;

REPEAT UNTIL ( TERMINATION CONDITION is satisfied ) DO

1 SELECT parents;

2 RECOMBINE pairs of parents;

3 MUTATE the resulting offspring;

4 EVALUATE new candidates;

5 SELECT individuals for the next generation;

OD

END
```

Figure 17.2: Evolutionary Algorithms

#### 17.2 Genetic Programming Example

#### 17.2.1 Load Data

```
#read data
telecom1 <- read.table("./datasets/effortEstimation/Telecom1.csv", sep=",",header=TRUE, stringsAsFactor
size_telecom1 <- telecom1$size
effort_telecom1 <- telecom1$effort

chinaTrain <- read.arff("./datasets/effortEstimation/china3AttSelectedAFPTrain.arff")
china_train_size <- chinaTrain$AFP
china_train_effort <- chinaTrain$Effort
chinaTest <- read.arff("./datasets/effortEstimation/china3AttSelectedAFPTest.arff")
china_size_test <- chinaTest$AFP
actualEffort <- chinaTest$AFP</pre>
```

#### 17.2.2 Genetic Programming for Symbolic Regression: China dataset.

```
library("rgp")
options(digits = 5)
stepsGenerations <- 100
initialPopulation <- 100
Steps <- c(10)
y <- china_train_effort #
x <- china_train_size #</pre>
```

```
data2 <- data.frame(y, x) # create a data frame with effort, size
# newFuncSet <- mathFunctionSet</pre>
# alternatives to mathFunctionSet
# newFuncSet <- expLogFunctionSet # sqrt", "exp", and "ln"</pre>
# newFuncSet <- trigonometricFunctionSet</pre>
# newFuncSet <- arithmeticFunctionSet</pre>
newFuncSet <- functionSet("+","-","*", "/","sqrt", "log", "exp") # ,, )</pre>
gpresult <- symbolicRegression(y ~ x,</pre>
                                  data=data2, functionSet=newFuncSet,
                                  populationSize=initialPopulation,
                                  stopCondition=makeStepsStopCondition(stepsGenerations))
bf <- gpresult$population[[which.min(sapply(gpresult$population, gpresult$fitnessFunction))]]
wf <- gpresult$population[[which.max(sapply(gpresult$population, gpresult$fitnessFunction))]]</pre>
bf1 <- gpresult$population[[which.min((gpresult$fitnessValues))]]</pre>
plot(x,y)
lines(x, bf(x), type = "l", col="blue", lwd=3)
lines(x,wf(x), type = "l", col="red", lwd=2)
                          0
                     0
     30000
                          0
                             0
             0
                               5000
                                                    10000
                                                                        15000
                                                 Х
x_test <- china_size_test</pre>
estim_by_gp <- bf(x_test)</pre>
ae_gp <- abs(actualEffort - estim_by_gp)</pre>
mean(ae_gp)
```

Genetic Programming for Symbolic Regression. Telecom1 dataset.

• For illustration purposes only. We use all data points.

## [1] 2135.4

17.2.3

```
# y <- effort_telecom1 # all data points</pre>
# x <- size_telecom1</pre>
\# data2 \leftarrow data.frame(y, x) \# create a data frame with effort, size
# # newFuncSet <- mathFunctionSet
# # alternatives to mathFunctionSet
# newFuncSet <- expLogFunctionSet # sqrt", "exp", and "ln"</pre>
# # newFuncSet <- trigonometricFunctionSet</pre>
# # newFuncSet <- arithmeticFunctionSet</pre>
# # newFuncSet <- functionSet("+","-","*", "/","sqrt", "loq", "exp") # ,, )
# gpresult <- symbolicRegression(y ~ x,</pre>
                                    data=data2, functionSet=newFuncSet,
#
                                    populationSize=initialPopulation,
#
                                    stopCondition=makeStepsStopCondition(stepsGenerations))
\# bf <- gpresult\$population[[which.min(sapply(gpresult\$population, gpresult\$fitnessFunction))]]
\# wf <- gpresult\$population[[which.max(sapply(gpresult\$population, gpresult\$fitnessFunction))]]
# bf1 <- qpresult$population[[which.min((qpresult$fitnessValues))]]</pre>
# plot(x,y)
\# lines(x, bf(x), type = "l", col="blue", lwd=3)
# lines(x, wf(x), type = "l", col="red", lwd=2)
```

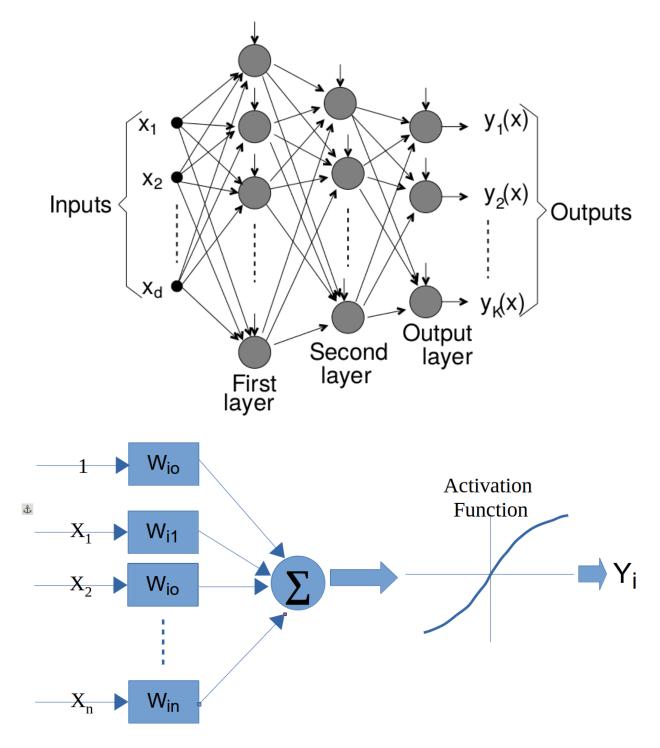
#### 17.3 Neural Networks

A neural network (NN) simulates some of the learning functions of the human brain.

It can recognize patterns and "learn" . Through the use of a trial and error method the system "learns" to become an "expert" in the field.

A NN is composed of a set of nodes (units, neurons, processing elements) + Each node has input and output + Each node performs a simple computation by its node function

Weighted connections between nodes + Connectivity gives the structure/architecture of the net + What can be computed by a NN is primarily determined by the connections and their weights



There are several packages in R to work with NNs + neuralnet + nnet + RSNNS

TO BE FIXED!!!: The following is an example with the neural net package (TO DO, denormalize!). Neural nets need scaling of variables to work properly.

```
library(foreign)
library(neuralnet)

chinaTrain <- read.arff("datasets/effortEstimation/china3AttSelectedAFPTrain.arff")</pre>
```

```
afpsize <- chinaTrain$AFP</pre>
effort_china <- chinaTrain$Effort</pre>
chinaTest <- read.arff("datasets/effortEstimation/china3AttSelectedAFPTest.arff")</pre>
AFPTest <- chinaTest$AFP
actualEffort <- chinaTest$Effort</pre>
trainingdata <- cbind(afpsize,effort china)</pre>
colnames(trainingdata) <- c("Input", "Output")</pre>
testingdata <- cbind(afpsize,effort_china)</pre>
colnames(trainingdata) <- c("Input","Output")</pre>
#Normalize data
norm.fun = function(x)\{(x - min(x))/(max(x) - min(x))\}
data.norm = apply(trainingdata, 2, norm.fun)
#data.norm
testdata.norm <- apply(trainingdata, 2, norm.fun)
#testdata.norm
#Train the neural network
#Going to have 10 hidden layers
#Threshold is a numeric value specifying the threshold for the partial
#derivatives of the error function as stopping criteria.
#net_eff <- neuralnet(Output~Input,trainingdata, hidden=5, threshold=0.25)</pre>
net_eff <- neuralnet(Output~Input, data.norm, hidden=10, threshold=0.01)</pre>
# Print the network
# print(net_eff)
#Plot the neural network
plot(net_eff)
#Test the neural network on some training data
\#testdata.norm < -data.frame((testdata[,1] - min(data[, 'displ']))/(max(data[, 'displ']) - min(data[, 'displ']))/(max(data[, 'displ']))
# Run them through the neural network
# net.results <- compute(net_eff, testdata.norm[,2])</pre>
#net.results <- compute(net_eff, dataTest.norm) # With normalized data</pre>
#Lets see what properties net.sqrt has
#ls(net.results)
#Lets see the results
#print(net.results$net.result)
#Lets display a better version of the results
#cleanoutput <- cbind(testdata.norm[,2],actualEffort,</pre>
                                                  as.data.frame(net.results$net.result))
#colnames(cleanoutput) <- c("Input", "Expected Output", "Neural Net Output")</pre>
```

#print(cleanoutput)

#### 17.4 Support Vector Machines

SVM

#### 17.5 Ensembles

Ensembles or meta-learners combine multiple models to obtain better predictions i.e., this technique consists in combining single classifiers (sometimes are also called weak classifiers).

A problem with ensembles is that their models are difficult to interpret (they behave as blackboxes) in comparison to decision trees or rules which provide an explanation of their decision making process.

They are typically classified as Bagging, Boosting and Stacking (Stacked generalization).

#### 17.5.1 Bagging

Bagging (also known as Bootstrap aggregating) is an ensemble technique in which a base learner is applied to multiple equal size datasets created from the original data using bootstraping. Predictions are based on voting of the individual predictions. An advantage of bagging is that it does not require any modification to the learning algorithm and takes advantage of the instability of the base classifier to create diversity among individual ensembles so that individual members of the ensemble perform well in different regions of the data. Bagging does not perform well with classifiers if their output is robust to perturbation of the data such as nearest-neighbour (NN) classifiers.

#### 17.5.2 Boosting

Boosting techniques generate multiple models that complement each other inducing models that improve regions of the data where previous induced models preformed poorly. This is achieved by increasing the weights of instances wrongly classified, so new learners focus on those instances. Finally, classification is based on a weighted voted among all members of the ensemble.

In particular, AdaBoost.M1 [15] is a popular boosting algorithm for classification. The set of training examples is assigned an equal weight at the beginning and the weight of instances is either increased or decreased depending on whether the learner classified that instance incorrectly or not. The following iterations focus on those instances with higher weights. AdaBoost.M1 can be applied to any base learner.

#### 17.5.3 Rotation Forests

Rotation Forests [40] combine randomly chosen subsets of attributes (random subspaces) and bagging approaches with principal components feature generation to construct an ensemble of decision trees. Principal Component Analysis is used as a feature selection technique combining subsets of attributes which are used with a bootstrapped subset of the training data by the base classifier.

#### 17.5.4 Boosting in R

In R, there are three packages to deal with Boosting: gmb, ada and the mboost packages. An example of gbm using the caret package.

```
# load libraries
library(caret)
library(pROC)
# model it
# Get names of caret supported models (just a few - head)
head(names(getModelInfo()))
## [1] "ada"
                    "AdaBag"
                                 "AdaBoost.M1" "adaboost"
                                                            "amdai"
## [6] "ANFIS"
# Show model info and find out what type of model it is
getModelInfo()$gbm$tags
## [1] "Tree-Based Model"
                                  "Boosting"
## [3] "Ensemble Model"
                                  "Implicit Feature Selection"
## [5] "Accepts Case Weights"
getModelInfo()$gbm$type
## [1] "Regression"
                       "Classification"
library(foreign)
library(caret)
library(pROC)
kc1 <- read.arff("./datasets/defectPred/D1/KC1.arff")</pre>
# Split data into training and test datasets
# TODO: Improve this with createDataParticion from Caret
set.seed(1234)
ind <- sample(2, nrow(kc1), replace = TRUE, prob = c(0.7, 0.3))
kc1.train <- kc1[ind==1, ]</pre>
kc1.test <- kc1[ind==2, ]
# create caret trainControl object to control the number of cross-validations performed
objControl <- trainControl(method='cv', number=3, returnResamp='none', summaryFunction = twoClassSummar
# run model
objModel <- train(Defective ~ .,
                data = kc1.train,
                 method = 'gbm',
                trControl = objControl,
                 metric = "ROC" #,
                 #preProc = c("center", "scale")
```

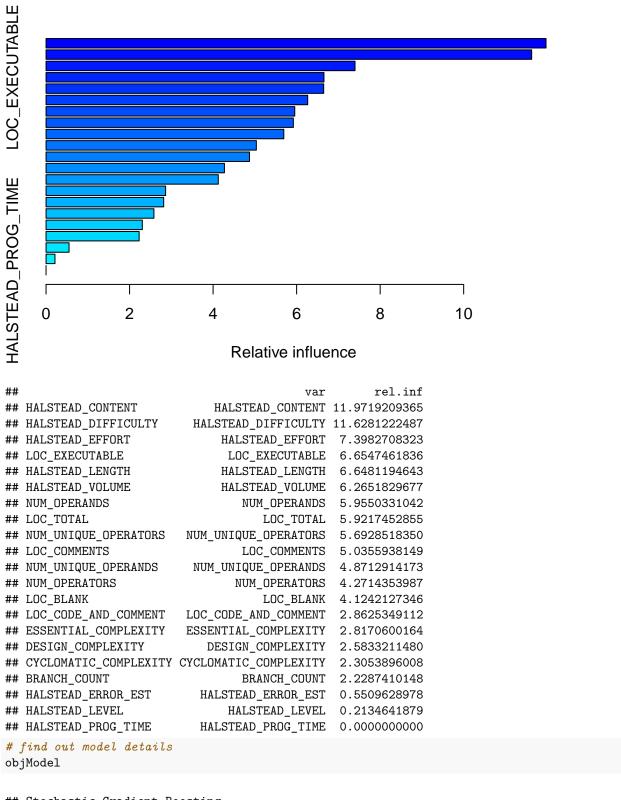
##	Iter	TrainDeviance	ValidDeviance	StepSize	Improve
##	1	0.8424	-nan	0.1000	0.0102
##	2	0.8182	-nan	0.1000	0.0089
##	3	0.7997	-nan	0.1000	0.0067
##	4	0.7873	-nan	0.1000	0.0055
##	5	0.7786	-nan	0.1000	0.0030
##	6	0.7714	-nan	0.1000	0.0020
##	7	0.7640	-nan	0.1000	0.0024
##	8	0.7544	-nan	0.1000	0.0048
##	9	0.7463	-nan	0.1000	0.0032
##	10	0.7410	-nan	0.1000	0.0015
##	20	0.7080	-nan	0.1000	0.0006
##	40	0.6832	-nan	0.1000	-0.0002
##	60	0.6699	-nan	0.1000	-0.0003
##	80	0.6563	-nan	0.1000	-0.0004
##	100	0.6472	-nan	0.1000	0.0001
##	120	0.6391	-nan	0.1000	-0.0003
##	140	0.6308	-nan	0.1000	-0.0010
##	150	0.6260	-nan	0.1000	-0.0003
##					
##	Iter	TrainDeviance	ValidDeviance	${ t StepSize}$	Improve
##	1	0.8310	-nan	0.1000	0.0133
##	2	0.8072	-nan	0.1000	0.0089
##	3	0.7864	-nan	0.1000	0.0081
##	4	0.7689	-nan	0.1000	0.0064
##	5	0.7575	-nan	0.1000	0.0047
##	6	0.7422	-nan	0.1000	0.0042
##	7	0.7320	-nan	0.1000	0.0038
##	8	0.7230	-nan	0.1000	0.0017
##	9	0.7120	-nan	0.1000	0.0029
##	10 20	0.7058	-nan	0.1000	0.0013 0.0015
##	40	0.6618 0.6252	-nan	0.1000	
##	60		-nan	0.1000 0.1000	-0.0012
##	80	0.5999	-nan	0.1000	-0.0010
##	100	0.5761 0.5596	-nan	0.1000	-0.0004 0.0000
##	120	0.5385	-nan	0.1000	-0.0004
##	140	0.5240	-nan -nan	0.1000	-0.0004
##	150	0.5158	-nan	0.1000	-0.0004
##	100	0.0100	nan	0.1000	0.0004
##	Iter	TrainDeviance	ValidDeviance	StepSize	Improve
##	1	0.8345	-nan	0.1000	0.0118
##	2	0.8100	-nan	0.1000	0.0114
##	3	0.7857	-nan	0.1000	0.0083
##	4	0.7714	-nan	0.1000	0.0058
##	5	0.7544	-nan	0.1000	0.0049
##	6	0.7401	-nan	0.1000	0.0067
##	7	0.7312	-nan	0.1000	0.0022
##	8	0.7198	-nan	0.1000	0.0033
##	9	0.7109	-nan	0.1000	0.0014
##	10	0.7021	-nan	0.1000	0.0028
##	20	0.6524	-nan	0.1000	-0.0004
##	40	0.6004	-nan	0.1000	-0.0004
##	60	0.5621	-nan	0.1000	0.0000

##	80	0.5350	-nan	0.1000	-0.0017
##	100	0.5077	-nan	0.1000	-0.0004
##	120	0.4899	-nan	0.1000	-0.0018
##	140	0.4690	-nan	0.1000	-0.0007
##	150	0.4577	-nan	0.1000	-0.0014
##					
##	Iter	TrainDeviance	ValidDeviance	${ t StepSize}$	Improve
##	1	0.8434	-nan	0.1000	0.0111
##	2	0.8213	-nan	0.1000	0.0092
##	3	0.8043	-nan	0.1000	0.0075
##	4	0.7867	-nan	0.1000	0.0050
##	5	0.7735	-nan	0.1000	0.0050
##	6	0.7650	-nan	0.1000	0.0033
##	7	0.7572	-nan	0.1000	0.0022
##	8	0.7500	-nan	0.1000	0.0010
##	9	0.7425	-nan	0.1000	0.0032
##	10	0.7395	-nan	0.1000	0.0007
##	20	0.7068	-nan	0.1000	0.0002
##	40	0.6827	-nan	0.1000	-0.0005
##	60	0.6672	-nan	0.1000	-0.0006
##	80	0.6570	-nan	0.1000	-0.0005
##	100	0.6460	-nan	0.1000	0.0004
##	120	0.6387	-nan	0.1000	-0.0005
##	140	0.6309	-nan	0.1000	-0.0003
##	150	0.6273	-nan	0.1000	-0.0003
## ##	Iter	TrainDeviance	ValidDeviance	StepSize	Tmnrosso
##	1	0.8252	-nan	0.1000	Improve 0.0149
##	2	0.8040	-nan	0.1000	0.0074
##	3	0.7862	-nan	0.1000	0.0052
##	4	0.7709	-nan	0.1000	0.0062
##	5	0.7549	-nan	0.1000	0.0062
##	6	0.7423	-nan	0.1000	0.0033
##	7	0.7322	-nan	0.1000	0.0024
##	8	0.7246	-nan	0.1000	0.0019
##	9	0.7188	-nan	0.1000	0.0006
##	10	0.7103	-nan	0.1000	0.0030
##	20	0.6715	-nan	0.1000	0.0003
##	40	0.6339	-nan	0.1000	-0.0015
##	60	0.6057	-nan	0.1000	-0.0002
##	80	0.5866	-nan	0.1000	-0.0012
##	100	0.5689	-nan	0.1000	-0.0003
##	120	0.5520	-nan	0.1000	-0.0004
##	140	0.5372	-nan	0.1000	-0.0007
##	150	0.5295	-nan	0.1000	-0.0007
##					
##	Iter	TrainDeviance	ValidDeviance	${ t StepSize}$	Improve
##	1	0.8347	-nan	0.1000	0.0162
##	2	0.8090	-nan	0.1000	0.0107
##	3	0.7864	-nan	0.1000	0.0085
##	4	0.7725	-nan	0.1000	0.0028
##	5	0.7588	-nan	0.1000	0.0026
##	6	0.7448	-nan	0.1000	0.0041
##	7	0.7348	-nan	0.1000	0.0024

##	8	0.7237	-nan	0.1000	0.0025
##	9	0.7178	-nan	0.1000	0.0012
##	10	0.7049	-nan	0.1000	0.0041
##	20	0.6472	-nan	0.1000	-0.0004
##	40	0.6046	-nan	0.1000	-0.0008
##	60	0.5684	-nan	0.1000	-0.0014
##	80	0.5432	-nan	0.1000	-0.0011
##	100	0.5152	-nan	0.1000	-0.0010
##	120	0.4900	-nan	0.1000	-0.0009
##	140	0.4707	-nan	0.1000	-0.0008
##	150	0.4625	-nan	0.1000	-0.0013
##					
##	Iter	TrainDeviance	ValidDeviance	${\tt StepSize}$	Improve
##	1	0.8337	-nan	0.1000	0.0127
##	2	0.8137	-nan	0.1000	0.0085
##	3	0.7882	-nan	0.1000	0.0102
##	4	0.7683	-nan	0.1000	0.0089
##	5	0.7520	-nan	0.1000	0.0071
##	6	0.7408	-nan	0.1000	0.0030
##	7	0.7295	-nan	0.1000	0.0052
##	8	0.7242	-nan	0.1000	0.0006
##	9	0.7140	-nan	0.1000	0.0037
##	10	0.7086	-nan	0.1000	0.0016
##	20	0.6677	-nan	0.1000	-0.0001
##	40	0.6394	-nan	0.1000	-0.0009
##	60	0.6252	-nan	0.1000	-0.0002
##	80	0.6171	-nan	0.1000	-0.0003
444	100	0 6072	-non	0.1000	-0.0003
##	100	0.6073	-nan	0.1000	-0.0003
##	120	0.6011	-nan	0.1000	-0.0003
##	120	0.6011	-nan	0.1000	-0.0002
## ##	120 140	0.6011 0.5909	-nan -nan	0.1000 0.1000	-0.0002 -0.0007
## ## ##	120 140	0.6011 0.5909	-nan -nan	0.1000 0.1000	-0.0002 -0.0007
## ## ## ##	120 140 150	0.6011 0.5909 0.5874	-nan -nan -nan	0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006
## ## ## ##	120 140 150 Iter	0.6011 0.5909 0.5874 TrainDeviance	-nan -nan -nan ValidDeviance	0.1000 0.1000 0.1000 StepSize	-0.0002 -0.0007 -0.0006 Improve
## ## ## ## ##	120 140 150 Iter 1	0.6011 0.5909 0.5874 TrainDeviance 0.8310	-nan -nan -nan ValidDeviance -nan	0.1000 0.1000 0.1000 StepSize 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169
## ## ## ## ## ##	120 140 150 Iter 1 2	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017	-nan -nan -nan ValidDeviance -nan -nan	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147
## ## ## ## ## ##	120 140 150 Iter 1 2 3	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752	-nan -nan -nan ValidDeviance -nan -nan -nan	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120
## ## ## ## ## ##	120 140 150 Iter 1 2 3 4	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533	-nan -nan ValidDeviance -nan -nan -nan -nan -nan	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070
## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088
## ## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5 6	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029
## ## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5 6 7	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047
## ## ## ## ## ## ## ## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5 6 7	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045
## ## ## ## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5 6 7 8	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004
## ## ## ## ## ## ## ## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5 6 7 8 9	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004
## ## ## ## ## ## ## ## ## ## ## ## ##	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445	-nan -nan NalidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006
######################################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992	-nan -nan -nan  ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003
######################################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40 60	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740	-nan -nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006 Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003 -0.0007
######################################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40 60 80	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740	-nan -nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006  Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003 -0.0007 -0.0002
#########################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40 60 80 100	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740 0.5518	-nan -nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006  Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003 -0.0007 -0.0002 -0.0005
##########################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40 60 80 100 120	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740 0.5518 0.5276 0.5105	-nan -nan ValidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 StepSize 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006  Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003 -0.0007 -0.0005 -0.0005 -0.0009
##########################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40 60 80 100 120 140	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740 0.5518 0.5276 0.5105 0.4939	-nan -nan NalidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006  Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003 -0.0007 -0.0002 -0.0005 -0.0009 -0.0003
#########################	120 140 150 Iter 1 2 3 4 5 6 7 8 9 10 20 40 60 80 100 120 140	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740 0.5518 0.5276 0.5105 0.4939	-nan -nan NalidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006  Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 0.0005 -0.0006 -0.0003 -0.0007 -0.0002 -0.0005 -0.0009 -0.0003
#########################	120 140 150 Iter  1 2 3 4 5 6 7 8 9 10 20 40 60 80 100 120 140 150	0.6011 0.5909 0.5874 TrainDeviance 0.8310 0.8017 0.7752 0.7533 0.7366 0.7254 0.7137 0.7040 0.6986 0.6945 0.6445 0.5992 0.5740 0.5518 0.5276 0.5105 0.4939 0.4839	-nan -nan NalidDeviance -nan -nan -nan -nan -nan -nan -nan -na	0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000	-0.0002 -0.0007 -0.0006  Improve 0.0169 0.0147 0.0120 0.0070 0.0088 0.0029 0.0047 0.0045 -0.0004 -0.0005 -0.0006 -0.0003 -0.0007 -0.0002 -0.0005 -0.0003 -0.0003 -0.0003

##	2	0.7959	-nan	0.1000	0.0110
##	3	0.7663	-nan	0.1000	0.0124
##	4	0.7469	-nan	0.1000	0.0052
##	5	0.7293	-nan	0.1000	0.0076
##	6	0.7138	-nan	0.1000	0.0062
##	7	0.7004	-nan	0.1000	0.0052
##	8	0.6883	-nan	0.1000	0.0043
##	9	0.6803	-nan	0.1000	0.0023
##	10	0.6712	-nan	0.1000	0.0005
##	20	0.6192	-nan	0.1000	-0.0007
##	40	0.5594	-nan	0.1000	-0.0000
##	60	0.5264	-nan	0.1000	-0.0015
##	80	0.4934	-nan	0.1000	-0.0003
##	100	0.4707	-nan	0.1000	-0.0009
##	120	0.4484	-nan	0.1000	-0.0007
##	140	0.4306	-nan	0.1000	-0.0006
##	150	0.4218	-nan	0.1000	-0.0004
##					
##	Iter	TrainDeviance	ValidDeviance	${ t StepSize}$	Improve
##	1	0.8323	-nan	0.1000	0.0146
##	2	0.8053	-nan	0.1000	0.0105
##	3	0.7798	-nan	0.1000	0.0119
##	4	0.7633	-nan	0.1000	0.0072
##	5	0.7492	-nan	0.1000	0.0080
##	6	0.7378	-nan	0.1000	0.0033
##	7	0.7258	-nan	0.1000	0.0053
##	8	0.7136	-nan	0.1000	0.0048
##	9	0.7027	-nan	0.1000	0.0040
##	10	0.6940	-nan	0.1000	0.0022
##	20	0.6475	-nan	0.1000	-0.0009
##	40	0.6085	-nan	0.1000	0.0001
##	60	0.5769	-nan	0.1000	-0.0008
##	80	0.5556	-nan	0.1000	-0.0010
##	100	0.5358	-nan	0.1000	0.0001
##	120	0.5147	-nan	0.1000	-0.0010
##	140	0.4989	-nan	0.1000	-0.0005
##	150	0.4924	-nan	0.1000	-0.0006
##					

# Find out variable importance
summary(objModel)



```
## Stochastic Gradient Boosting
##
## 1500 samples
## 21 predictor
## 2 classes: 'N', 'Y'
```

```
##
## No pre-processing
## Resampling: Cross-Validated (3 fold)
## Summary of sample sizes: 1000, 1000, 1000
## Resampling results across tuning parameters:
##
##
    interaction.depth n.trees ROC
                                          Sens
                                                      Spec
##
                      50
                             0.8064922834 0.9826224329 0.1495726496
##
    1
                     100
                             0.8098239964 0.9802527646 0.1923076923
                     150
##
    1
                             0.8110442743 0.9794628752 0.2051282051
##
    2
                      50
                             0.8137379998 0.9731437599 0.1965811966
    2
                     100
                             ##
##
    2
                     150
                             ##
    3
                      50
                             0.8161532385 0.9715639810 0.2136752137
##
    3
                     100
                             ##
    3
                     150
                             0.8164165350 0.9668246445 0.3034188034
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.1
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were n.trees = 150,
   interaction.depth = 3, shrinkage = 0.1 and n.minobsinnode = 10.
# evalutate model
# get predictions on your testing data
# class prediction
predictions <- predict(object=objModel, kc1.test[,-22], type='raw')</pre>
head(predictions)
## [1] N N N N N N
## Levels: N Y
postResample(pred=predictions, obs=as.factor(kc1.test[,22]))
      Accuracy
                    Kappa
## 0.8657718121 0.2891009393
# probabilities
predictions <- predict(object=objModel, kc1.test[,-22], type='prob')</pre>
head(predictions)
##
              N
## 1 0.9185156057 0.08148439428
## 2 0.9797772040 0.02022279595
## 3 0.8470294127 0.15297058732
## 4 0.8799954090 0.12000459096
## 5 0.8298472743 0.17015272568
## 6 0.9578031188 0.04219688123
postResample(pred=predictions[[2]], obs=ifelse(kc1.test[,22]=='yes',1,0))
         RMSE
                 Rsquared
## 0.2165564399
                       NA 0.1347441023
```

```
auc <- roc(ifelse(kc1.test[,22]=="Y",1,0), predictions[[2]])
print(auc$auc)</pre>
```

## Area under the curve: 0.8031553

##

# Further Classification Models

#### 18.1 Multilabel classification

Some datasets, for example, reviews of applications and mobile applications repositories such as App Store or Google play contain reviews that can have several labels at the same time (e.g. bugs, feature requests, etc.)

Self train a model on semi-supervised data http://www.inside-r.org/packages/cran/dmwr/docs/SelfTrain

#### 18.2 Semi-supervised Learning

```
library(DMwR)

## Small example with the Iris classification data set
data(iris)

## Dividing the data set into train and test sets
idx <- sample(150,100)

tr <- iris[idx,]

ts <- iris[-idx,]

## Learn a tree with the full train set and test it
stdTree <- rpartXse(Species~ .,tr,se=0.5)
table(predict(stdTree,ts,type='class'),ts$Species)</pre>
```

```
##
                 setosa versicolor virginica
##
                     14
                                   0
     setosa
                                              2
##
                      0
                                  16
     versicolor
                                             17
     virginica
## Now let us create another training set with most of the target
## variable values unknown
trSelfT <- tr
nas \leftarrow sample(100,70)
trSelfT[nas,'Species'] <- NA</pre>
```

```
## Learn a tree using only the labelled cases and test it
baseTree <- rpartXse(Species~ .,trSelfT[-nas,],se=0.5)</pre>
table(predict(baseTree,ts,type='class'),ts$Species)
##
                setosa versicolor virginica
##
##
     setosa
               14
                                0
##
    versicolor
                   0
                               17
                                          2
     virginica
                     0
                                0
                                          17
## The user-defined function that will be used in the self-training process
f <- function(m,d) {</pre>
      1 <- predict(m,d,type='class')</pre>
      c <- apply(predict(m,d),1,max)</pre>
      data.frame(cl=1,p=c)
}
## Self train the same model using the semi-superside data and test the
## resulting model
treeSelfT <- SelfTrain(Species~ .,trSelfT,learner('rpartXse',list(se=0.5)),'f')</pre>
table(predict(treeSelfT,ts,type='class'),ts$Species)
##
##
                setosa versicolor virginica
##
     setosa
                  14
                               0
                                           0
                                          2
##
     versicolor
                    0
                               17
                     0
                                          17
##
     virginica
                               0
```

# Social Network Analysis in SE

In this example, we will data from the MSR14 challenge. Further information and datasets: http://openscience.us/repo/msr/msr14.html

Similar databases can be obtained using MetricsGrimoire or other tools.

In this simple example, we create a network form the users and following extracted from GitHub and stored in a MySQL database.

We can read a file directly from MySQL dump

```
library(RMySQL)

# Connecting to MySQL

mydb = dbConnect(MySQL(), user='msr14', password='msr14', dbname='msr14', host='localhost')

# Retrieving data from MySQL

sql <- "select user_id, follower_id from followers limit 100;"

rs = dbSendQuery(mydb, sql)
data <- fetch(rs, n=-1)</pre>
```

Alternatively, we can create e CSV file directly from MySQL and load it

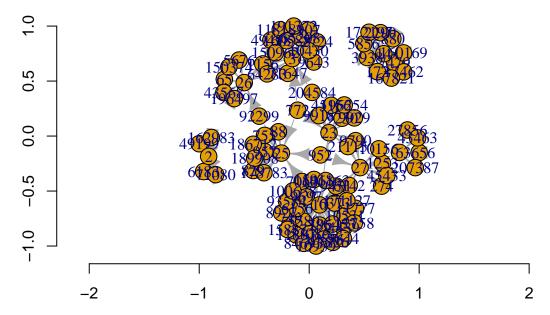
```
$mysql -u msr14 -pmsr14 msr14

> SELECT 'user','follower'
UNION ALL
SELECT user_id,follower_id
   FROM followers
   LIMIT 1000
   INTO OUTFILE "/tmp/followers.csv"
   FIELDS TERMINATED BY ','
   LINES TERMINATED BY '\n';
```

```
# Data already extracted and stored as CSV file (for demo purposes)
dat = read.csv("./datasets/sna/followers.csv", header = FALSE, sep = ",")
dat <- head(dat,100)</pre>
```

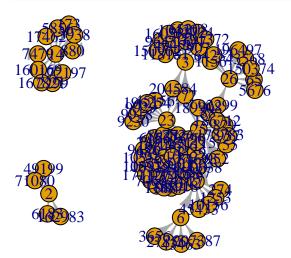
We can now create the graph

```
library(igraph)
##
## Attaching package: 'igraph'
## The following objects are masked from 'package:rgp':
##
##
       %->%, normalize
## The following object is masked from 'package:arules':
##
##
       union
## The following object is masked from 'package:class':
##
##
       knn
## The following object is masked from 'package:modeltools':
##
##
       clusters
## The following objects are masked from 'package:lubridate':
##
       %--%, union
##
## The following objects are masked from 'package:dplyr':
##
##
       as_data_frame, groups, union
## The following objects are masked from 'package:stats':
##
##
       decompose, spectrum
## The following object is masked from 'package:base':
##
##
       union
# Create a graph
g <- graph.data.frame(dat, directed = TRUE)
Some values:
summary(g);
## IGRAPH 692360a DN-- 95 100 --
## + attr: name (v/c)
Plotting the graph:
layout1 <- layout.fruchterman.reingold(g)</pre>
plot(g, layout1)
## Warning in if (axes) {: the condition has length > 1 and only the first
## element will be used
```



Other layout

plot(g, layout=layout.kamada.kawai)



A tk application can launched to show the plot interactively:

```
plot(g, layout = layout.fruchterman.reingold)
```

Some metrics:

```
metrics <- data.frame(
  deg = degree(g),
  bet = betweenness(g),
  clo = closeness(g),
  eig = evcent(g)$vector,
  cor = graph.coreness(g)
)</pre>
```

```
\#\# Warning in closeness(g): At centrality.c:2784 :closeness centrality is not \#\# well-defined for disconnected graphs
```

```
head(metrics)
        deg bet
                          clo
                                        eig cor
## 6183 1 0 0.0001131733816 0.000000000000
## 49199 1 0 0.0001131733816 0.000000000000
## 71080 1 0 0.0001131733816 0.000000000000
                                             1
2
## 907
         1 0 0.0001131733816 0.008141832109
To fix and to do: Explain metrics and better graphs
library(ggplot2)
ggplot(
 metrics,
 aes(x=bet, y=eig,
   label=rownames(metrics),
   colour=res, size=abs(res))
)+
xlab("Betweenness Centrality")+
ylab("Eigenvector Centrality")+
geom_text()
theme(title="Key Actor Analysis")
V(g) $label.cex <- 2.2 * V(g) $degree / max(V(g) $degree) + .2
V(g)$label.color <- rgb(0, 0, .2, .8)
V(g) $frame.color <- NA
egam <- (\log(E(g)\$weight)+.4) / \max(\log(E(g)\$weight)+.4)
E(g)$color <- rgb(.5, .5, 0, egam)
E(g)$width <- egam
# plot the graph in layout1
plot(g, layout=layout1)
```

Further information:

http://sna.stanford.edu/lab.php?l=1

# Text Mining Software Engineering Data

In software engineering, there is a lot of information in plain text such as requirements, bug reports, mails, reviews from applications, etc. Typically that information can be extracted from Software Configuration Management Systems (SCM), Bug Tracking Systems (BTS) such as Bugzilla or application stores such as Google Play or Apple's AppStore, etc. can be mined to extract relevant information. Here we briefly explain the text mining process and how this can be done with R.

The main package for text mining is tm (Feinerer and Hornik, 2015, Feinerer et al. (2008)). Another popular package is wordcloud.

#### 20.1 Terminology

The workflow that we follow for analyzing a set of text documents are:

1. Importing data. A *Corpus* is a collection of text documents, implemented as VCorpus (corpora are R object held in memory). The tm provides several corpus constructors: DirSource, VectorSource, or DataframeSource (getSources()).

There are several parameters that control the creation of a *Corpus*. ((The parameter readerControl of the corpus constructor has to be a list with the named components reader and language))

- 2. Preprocessing: in this step we may remove common words, punctuation and we may perform other operations. We may do this operations after creating the DocumentTermMatrix.
- 3. Inspecting and exploring data: Individual documents can be accessed via [
- 4. Transformations: Transformations are done via the tm\_map() function.
  - tm\_map(\_\_\_\_\_, stripWhitespace)
    tm\_map(\_\_\_\_\_, content\_transformer(tolower))
    tm\_map(\_\_\_\_\_, removeWords, stopwords("english"))
    tm\_map(\_\_\_\_\_, stemDocument)
- 5. Creating Term-Document Matrices: TermDocumentMatrix and DocumentTermMatrix
  - A document term matrix is a matrix with documents as the rows and terms as the columns. Each cell of the matrix contains the count of the frequency of words. We use DocumentTermMatrix() to create the matrix.

- inspect(DocumentTermMatrix( newsreuters, list(dictionary = c("term1", "term2", "term3")))). It displays detailed information on a corpus or a term-document matrix.
- 6. Relationships between terms.
  - findFreqTerms(\_\_\_\_, anumber)
  - findAssocs(Mydtm, "aterm", anumbercorrelation)
  - A dictionary is a (multi-)set of strings. It is often used to denote relevant terms in text mining.
- 7. Clustering and Classification

#### 20.2 Example of classifying bugs from Bugzilla

Bugzilla is Issue Tracking System that allow us to follow the evolution of a project.

The following example shows how to work with entries from Bugzilla. It is assumed that the data has been extracted and we have the records in a flat file (this can be done using Web crawlers or directly using the SQL database).

```
library(foreign)
# path_name <- file.path("C:", "datasets", "textMining")</pre>
# path_name
# dir(path name)
#Import data
options(stringsAsFactors = FALSE)
d <- read.arff("./datasets/textMining/reviewsBugs.arff" )</pre>
str(d) #print out information about d
                    789 obs. of 2 variables:
## 'data.frame':
## $ revContent: chr "Can't see traffic colors now With latest updates I can't see the traffic green/
                : Factor w/ 2 levels "N", "Y": 2 1 1 1 1 1 2 1 2 1 ...
head(d,2) # the first two rows of d.
##
## 1 Can't see traffic colors now With latest updates I can't see the traffic green/red/yellow - I have
## 2
##
   revBug
## 1
## 2
          N
# fifth entry
d$revContent[5]
## [1] "Just deleted No I don't want to sign in or sign up for anything stop asking"
d$revBug[5]
## [1] N
## Levels: N Y
Creating a Document-Term Matrix (DTM)
Now, we can explore things such as "which words are associated with" feature"?"
# which words are associated with "buq"?
findAssocs(dtm, 'bug', .3) # minimum correlation of 0.3. Change accordingly.
```

```
## $bug
##
       it?
              mini
                     major
                             users causing
                                               ipad
##
      1.00
              0.92
                      0.91
                               0.80
                                       0.62
                                               0.57
And find frequent terms.
findFreqTerms(dtm, 15) #terms that appear 15 or more times, in this case
    [1] "google"
                    "map"
                                 "like"
                                             "app"
                                                          "just"
                                                          "get"
##
    [6] "good"
                    "crashes"
                                 "maps"
                                             "time"
                                             "great"
## [11]
       "much"
                    "really"
                                 "update"
                                                          "nice"
## [16] "best"
                    "ever"
                                 "fun"
                                             "review"
                                                          "love"
## [21] "awesome"
                    "cool"
                                                          "clans"
                                 "amazing"
                                             "game"
## [26] "clash"
                    "game."
                                 "game!"
                                             "addicting" "play"
## [31] "playing"
                    "addictive"
Remove some terms
sparseparam <- 0.90 # will make the matrix 90% empty space, maximum. Change this, as you like.
dtm_sprs <- removeSparseTerms(dtm,sparse=sparseparam)</pre>
inspect(dtm_sprs)
## <<DocumentTermMatrix (documents: 789, terms: 9)>>
## Non-/sparse entries: 1233/5868
## Sparsity
                      : 83%
## Maximal term length: 7
## Weighting
                      : term frequency - inverse document frequency (normalized) (tf-idf)
## Sample
                      :
##
        Terms
## Docs app
                 awesome best
                                     clash fun game
                                                            good great
                             0 1.598808368
                                                  0 0.00000000
##
     159
           0 0.000000000
##
     163
           0 3.116086850
                             0 0.000000000
                                                  0 0.000000000
                                                                     0
                                             0
##
     178
           0 3.116086850
                             0 0.000000000
                                             0
                                                  0 0.000000000
                                                                     0
##
     400
           0.000000000
                             0 0.000000000
                                             0
                                                  0 3.100319534
                                                                     0
     421
                                                  0 3.100319534
##
           0 0.000000000
                             0 0.000000000
                                            0
                                                                     0
##
     472
           0 0.00000000
                             0 0.00000000 0
                                                  0 3.100319534
                                                                     0
##
     50
           0 0.00000000
                             0.000000000
                                            0
                                                  0 3.100319534
                                                                     0
##
     525
           0 1.558043425
                             0 0.00000000
                                             0
                                                  0 0.000000000
                                                                     0
##
     527
           0 0.000000000
                             0 0.000000000
                                             0
                                                  0 3.100319534
                                                                     0
           0 0.000000000
##
     532
                             0 1.598808368
                                             0
                                                  0 0.000000000
                                                                     0
##
        Terms
## Docs
##
     159 1.461720886
##
     163 0.000000000
##
     178 0.000000000
##
     400 0.000000000
     421 0.000000000
##
##
     472 0.000000000
##
     50 0.000000000
##
     525 1.461720886
##
     527 0.000000000
     532 1.461720886
maintitle <-paste0("Most frequent terms (sparseness=" ,sparseparam , " )")
barplot(as.matrix(dtm_sprs),xlab="terms",ylab="number of occurrences", main=maintitle)
```

#### Most frequent terms (sparseness=0.9)



```
# organize terms by their frequency

freq_dtm_sprs <- colSums(as.matrix(dtm_sprs))
length(freq_dtm_sprs)

## [1] 9

sorted_freq_dtm_sprs <- sort(freq_dtm_sprs, decreasing = TRUE)
sorted_freq_dtm_sprs

## good great game awesome fun best
## 77.76636458 68.77637155 68.66996351 64.60649534 55.84940440 54.07372345
## love clash app
## 45.36493131 42.48777519 31.29319954</pre>
```

Create a data frame that will be the input to the classifier. Last column will be the label.

As data frame:

```
#dtmdf <- as.data.frame(dtm.90)
#dtmdf <- as.data.frame(inspect(dtm_sprs))
dtmdf <- as.data.frame(as.matrix(dtm_sprs))
# rownames(dtm)<- 1:nrow(dtm)

class <- d$revBug
dtmdf <- cbind(dtmdf,class)
head(dtmdf, 3)</pre>
```

Use any classifier now: - split the data frame into training and testing - Build the classification model using the training subset - apply the model to the testing subset and obtain the Confusion Matrix - Analise the results

```
library(caret)
library(randomForest)
inTraining <- createDataPartition(dtmdf$class, p = .75, list = FALSE)</pre>
training <- dtmdf[ inTraining,]</pre>
testing <- dtmdf[-inTraining,]</pre>
fitControl <- trainControl(## 5-fold CV
                           method = "repeatedcv",
                           number = 5,
                           ## repeated ten times
                           repeats = 5)
gbmFit1 <- train(class ~ ., data = training,</pre>
                 method = "gbm",
                 trControl = fitControl,
                 ## This last option is actually one
                 ## for gbm() that passes through
                 verbose = FALSE)
gbmFit1
## Stochastic Gradient Boosting
##
## 593 samples
   9 predictor
##
     2 classes: 'N', 'Y'
##
## No pre-processing
## Resampling: Cross-Validated (5 fold, repeated 5 times)
## Summary of sample sizes: 475, 474, 475, 474, 474, 474, ...
## Resampling results across tuning parameters:
##
##
     interaction.depth n.trees Accuracy
                                                Kappa
##
                         50
                                 0.7983107819 0.005187831537
                        100
##
                                 0.8030309073 0.100972529170
   1
##
                        150
                                 0.8185586099 0.251719781992
   1
                                 0.8161942743 0.214069621088
##
    2
                        50
##
    2
                        100
                                 0.8162028201 0.281341413948
##
    2
                        150
                                 0.8114798462 0.280302861433
                         50
                                 0.8168636946 0.274826252003
     3
                                 0.8114883920 0.279902522189
##
     3
                        100
##
                        150
                                 0.8087850734 0.282684783972
##
\mbox{\tt \#\#} Tuning parameter 'shrinkage' was held constant at a value of 0.1
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were n.trees = 150,
## interaction.depth = 1, shrinkage = 0.1 and n.minobsinnode = 10.
```

```
# trellis.par.set(caretTheme())
# plot(qbmFit1)
# trellis.par.set(caretTheme())
# plot(gbmFit1, metric = "Kappa")
head(predict(gbmFit1, testing, type = "prob"))
##
## 1 0.6128782934 0.38712170665
## 2 0.5754602498 0.42453975017
## 3 0.6422679898 0.35773201018
## 4 0.6866949197 0.31330508027
## 5 0.9802477705 0.01975222952
## 6 0.9307476992 0.06925230082
conf_mat <- confusionMatrix(testing$class, predict(gbmFit1, testing))</pre>
conf_mat
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction N Y
            N 152
                    5
##
##
            Y 35
                    4
##
                  Accuracy : 0.7959184
##
##
                    95% CI: (0.7326392, 0.8500172)
##
       No Information Rate: 0.9540816
       P-Value [Acc > NIR] : 1
##
##
##
                     Kappa: 0.0994716
   Mcnemar's Test P-Value: 0.000004533294
##
##
##
               Sensitivity: 0.8128342
##
               Specificity : 0.444444
##
            Pos Pred Value : 0.9681529
            Neg Pred Value: 0.1025641
##
##
                Prevalence : 0.9540816
##
            Detection Rate: 0.7755102
##
      Detection Prevalence: 0.8010204
##
         Balanced Accuracy: 0.6286393
##
##
          'Positive' Class : N
```

We may compute manually all derived variables from the Confusion Matrix. See Section – with the description of the Confusion Matrix

```
# str(conf_mat)
TruePositive <- conf_mat$table[1,1]
TruePositive</pre>
```

```
FalsePositive <- conf_mat$table[1,2]
FalsePositive
## [1] 5
FalseNegative <- conf_mat$table[2,1]
FalseNegative
## [1] 35
TrueNegative <- conf_mat$table[2,2]</pre>
TrueNegative
## [1] 4
# Sum columns in the confusion matrix
ConditionPositive <- TruePositive + FalseNegative
ConditionNegative <- FalsePositive + TrueNegative</pre>
TotalPopulation <- ConditionPositive + ConditionNegative
TotalPopulation
## [1] 196
#Sum rows in the confusion matrix
PredictedPositive <- TruePositive + FalsePositive
PredictedNegative <- FalseNegative + TrueNegative</pre>
# Total Predicted must be equal to the total population
PredictedPositive+PredictedNegative
## [1] 196
SensitivityRecall_TPR <- TruePositive / ConditionPositive</pre>
{\tt SensitivityRecall\_TPR}
## [1] 0.8128342246
Specificity_TNR_SPC <- TrueNegative / ConditionNegative</pre>
Specificity_TNR_SPC
## [1] 0.444444444
Precision_PPV <- TruePositive / PredictedPositive</pre>
Precision_PPV
## [1] 0.9681528662
NegativePredictedValue_NPV <- TrueNegative / PredictedNegative
NegativePredictedValue_NPV
## [1] 0.1025641026
Prevalence <- ConditionPositive / TotalPopulation
Prevalence
## [1] 0.9540816327
Accuracy_ACC <- (TruePositive + TrueNegative) / TotalPopulation</pre>
Accuracy_ACC
## [1] 0.7959183673
```

FalseDiscoveryRate\_FDR <- FalsePositive / PredictedPositive FalseDiscoveryRate\_FDR

#### ## [1] 0.03184713376

FalseOmisionRate\_FOR <- FalseNegative / PredictedNegative
FalseOmisionRate\_FOR</pre>

#### ## [1] 0.8974358974

FallOut\_FPR <- FalsePositive / ConditionNegative
FallOut\_FPR</pre>

#### ## [1] 0.555555556

MissRate\_FNR <- FalseNegative / ConditionPositive
MissRate\_FNR</pre>

#### ## [1] 0.1871657754

And finally, a word cloud as an example that appears everywhere these days.

#### library(wordcloud)

# calculate the frequency of words and sort in descending order.
wordFreqs=sort(colSums(as.matrix(dtm\_sprs)),decreasing=TRUE)
wordcloud(words=names(wordFreqs),freq=wordFreqs)

# game great g

### 20.3 Extracting data from Twitter

The hardest bit is to link with Twitter. Using the TwitteR package is explained following this example.

##

##

##

## Attaching package: 'xts'

first, last

## The following objects are masked from 'package:dplyr':

# Time Series

Many sources of information are time related. For example, data from Software Configuration Management (SCM) such as Git, GitHub) systems or Dashboards such as Metrics Grimoire from Bitergia or SonarQube

With MetricsGrimore or SonarQube we can extract datasets or dump of databases. For example, a dashboard for the OpenStack project is located at http://activity.openstack.org/dash/browser/ and provides datasets as MySQL dumps or JSON files.

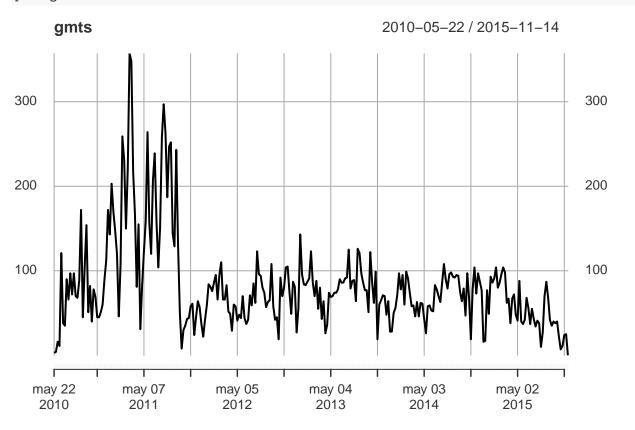
```
With R we can read a JSON file as follows:
library(jsonlite)
# Get the JSON data
\#\ gm < -\ from JSON ("http://activity.openstack.org/dash/browser/data/json/nova.git-scm-rep-evolutionary.js
gm <- fromJSON('./datasets/timeSeries/nova.git-scm-rep-evolutionary.json')</pre>
str(gm)
## List of 13
    $ added_lines : num [1:287] 431874 406 577 697 7283 ...
                   : int [1:287] 1 1 4 2 7 5 4 9 8 11 ...
   $ authors
   $ branches
                   : int [1:287] 1 1 1 1 1 1 1 1 1 1 ...
                   : int [1:287] 3 4 16 11 121 38 35 90 66 97 ...
##
    $ commits
##
    $ committers : int [1:287] 1 1 4 2 7 5 4 9 8 11 ...
##
   $ date
                   : chr [1:287] "May 2010" "May 2010" "Jun 2010" "Jun 2010" ...
##
   $ files
                   : int [1:287] 1878 9 13 7 144 111 28 1900 89 101 ...
                   : int [1:287] 0 1 2 3 4 5 6 7 8 9 ...
##
   $ id
##
                  : int [1:287] 1 1 2 0 4 1 0 4 2 3 ...
   $ newauthors
  $ removed_lines: num [1:287] 864 530 187 326 2619 ...
  $ repositories : int [1:287] 1 1 1 1 1 1 1 1 1 1 ...
                   : chr [1:287] "1274659200" "1275264000" "1275868800" "1276473600" ...
    $ week
                   : int [1:287] 201021 201022 201023 201024 201025 201026 201027 201028 201029 201030
Now we can use time series packages. First, after loading the libraries, we need to create a time series object.
# TS libraries
library(xts)
```

```
library(forecast)
# Library to deal with dates
library(lubridate)
# Ceate a time series object
gmts <-xts(gm$commits,seq(ymd('2010-05-22'),ymd('2015-11-16'), by = '1 week'))
# TS Object
str(gmts)
## An 'xts' object on 2010-05-22/2015-11-14 containing:
    Data: int [1:287, 1] 3 4 16 11 121 38 35 90 66 97 ...
##
     Indexed by objects of class: [Date] TZ: UTC
##
     xts Attributes:
##
##
  NULL
head(gmts, 3)
```

## [,1] ## 2010-05-22 3 ## 2010-05-29 4 ## 2010-06-05 16

Visualise the time series object

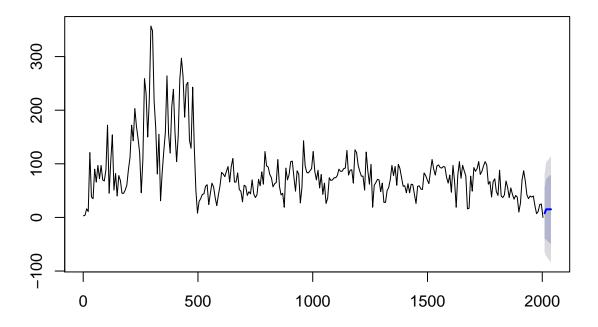
```
plot(gmts)
```



Arima model:

```
fit <- auto.arima(gmts)</pre>
## Series: gmts
## ARIMA(0,1,2)
##
## Coefficients:
##
                ma1
##
         -0.3120662
                     -0.3068537
          0.0580588
                      0.0642417
##
##
## sigma^2 estimated as 1341.396:
                                   log likelihood=-1434.83
## AIC=2875.67
                 AICc=2875.75
                                 BIC=2886.64
forecast(fit, 5)
##
        Point Forecast
                               Lo 80
                                           Hi 80
                                                        Lo 95
                                                                      Hi 95
## 2010
           7.748275458 -39.18864059 54.68519151 -64.03554306
                                                               79.53209398
## 2017
          15.157545088 -41.81337267 72.12846284 -71.97195479 102.28704496
         15.157545088 -44.55527171 74.87036189 -76.16532750 106.48041768
## 2024
## 2031
          15.157545088 -47.17667914 77.49176931 -80.17442420 110.48951438
## 2038
          15.157545088 -49.69220842 80.00729859 -84.02159424 114.33668442
plot(forecast(fit, 5))
```

#### Forecasts from ARIMA(0,1,2)



#### 21.1 Web tutorials about Time Series:

 $http://www.statoek.wiso.uni-goettingen.de/veranstaltungen/zeitreihen/sommer 03/ts\_r\_intro.pdf \\ http://www.statmethods.net/advstats/timeseries.html \\ http://a-little-book-of-r-for-time-series.readthedocs.org/en/latest/$ 

 $https://media.readthedocs.org/pdf/a-little-book-of-r-for-time-series/latest/a-little-book-of-r-for-time-series.\\ pdf$ 

http://www.stat.pitt.edu/stoffer/tsa3/

# $\begin{array}{c} {\rm Part} \ {\rm X} \\ \\ {\rm Bibliography} \end{array}$

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