```
#####
# R #
#####
# install.packages("<package name>")
# library(<package name>)
# print(<something>)
# Assignment statement: x <- <something>
# Manipulating objects in the workspace:
                            # list all objects in memory
\# rm(<o1>, <o2>, <o3>, ...) \# remove one or more objects from memory by their names
                            # remove all objects from memory (usually not recommended)
# rm(list = ls())
# Operators:
# + Add, 2 + 3 = 5
# - Subtract, 5 - 2 = 3
# * Multiply, 2 * 3 = 6
\# / Divide, 6 / 2 = 3
# ^{2} Exponent, 2 ^{3} = 8
# %% Modulus operator, 9%%2 = 1
# %/% Integer division, 9 %/% 2 = 4
# < Less than
# > Greater than
# = Equal to
# <= Less than or equal to
# >= Greater than or equal to
# != Not equal to
#! Not
# |
     OR
# & And
# Expressions:
\# <x > / <y > - <z >^2 ...
# Absolute value:
# abs(<value>)
```

```
# Vectors:
# <y> <- c(<something1>, <something2>, <something3>, ...)
# <y> <- rep(<something>, <times>)
# <y> <- <int1>:<int2>
\# <y> <- seq(from = <value1>, to = <value2>, by = <step>)
# Matrices:
\# < m > < - matrix(c(3, 5, 7, 1, 9, 4), nrow = 3, ncol = 2, byrow = TRUE)
# <m>.nrow <- nrow(<m>) # number of rows
# <m>.ncol <- ncol(<m>) # number of columns
# <m> <- t(<m>)
                        # transpose <m>
\# < m > [3,2]
\# < m > [2, ]
# Lists: ordered collections of elements of different types
# <list> <- list(<e1.name> = <e1>, <e2.name> = <e2>, <e3.name> = <e3>, ...)
# <list>[[<index>]]
                        # accessing list element by index, showing value only (returns a vector)
# <list>[<index>]
                         # accessing list element by index, showing both name and value (returns a list)
# <list>$<element.name> # accessing list element by its name
# is.list(<something>)
                                                           # Is <something> a list?
# <combined.list> <- c(<list1>, <list2>, <list3>, ...) # list concatenation
# names(<list>)
                                            # names of list elements
\# <list>[names(<list>) == <element.name>] \# all elements of a list having the same name
                                            # convert list into a named vector
# unlist(<list>)
# unlist(<list>, use.names = FALSE)
                                           # convert list into a character vector
# append(<list>,
                                            # insert new element into an existing list, after index <n>
         list(\langle e1.name \rangle = \langle e \rangle),
                                            # new element must be a list itself, that's why list(<e1.name> =
<e>)
                                            # <n> is optional; if omitted, new element is appended at the end
              \langle n \rangle
# <list>[[<n>]] <- NULL
                                            # remove <n>th element from <list>
# class(<something>)
                                          # data type
# mode(something), typeof(<something>) # how a data item is internally stored in memory
# Factors:
\# b <- c(1, 2, 2, 2, 3, 1, 1, 4, 5, 4)
# b.as.factor <- as.factor(b)</pre>
# levels(b.as.factor)
\# f \leftarrow factor(c(1, 2, 3))
```

```
# Dataframes:
# e.g., <dataframe> <- as.data.frame(<matrix>)
# str(<dataframe>)
# Reading a dataset:
# <dataframe> <- read.csv("<filename>", stringsAsFactors = FALSE)
# Saving a dataset (modified or newly created dataset):
\# write.csv(x = <dataframe>, file = "<filename>", row.names = F) \# do not include the row names (row
numbers) column
# saveRDS(object = <dataframe or another R object>, file = "<filename>") # save R object for the next
# <dataframe or another R object> <- readRDS(file = "<filename>")
                                                                         # restore R object in the next
session
# Examining a dataframe:
# str(<dataframe>)
                               # structure of <dataframe>, all variables/columns
# dim(<dataframe>)
                              # showing dimensions (numbers of rows and columns) of a dataframe
# names(<dataframe>)
                              # showing column names
# head(<dataframe>)
                               # the first few rows
# tail(<dataframe>)
                              # the last few rows
# <dataframe>[ , ]
                              # the entire dataframe
# <dataframe>
                              # the entire dataframe
# <dataframe>[<m>, ]
                              # m-th row
# <dataframe>[ ,<n>]
                              # n-th column
# summary(<dataframe>$<column>) # summarizing a variable/column values
# fix(<dataframe>)
                               # editing a dataframe
# new.df <- edit(<dataframe>)  # editing a dataframe and assigning the modified dataframe to another
datavrame
# Adding/Removing columns to/from a dataframe:
# <dataframe>$<new column name> <- <default value> # adding a new column (default values)
# <dataframe>$<column name> <- NULL</pre>
                                                    # removing a column
# Adding a new row to a dataframe - the row must be a 1-line dataframe with the same column names:
\# <new row> <- data.frame(<column name 1> = <value 1>, <column name 2> = <value 2>,...)
# <new data frame> <- rbind(<dataframe>, <new row>) # append new row to the end of the existing dataframe
# <new data frame> <- rbind(<dataframe>[1:i, ], # insert new row in the middle
```

```
<new row>.
                            <dataframe>[(i + 1):nrow(<dataframe>), ])
# Removing rows from a dataframe
# <dataframe>[-i, ]
                                                    # show dataframe without i-th row
# <dataframe>[-c(i, j, k), ]
                                                    # show dataframe without rows i, j, k
# <dataframe> <- <dataframe>[-i, ]
                                                    # remove i-th row from dataframe
# <dataframe> <- <dataframe>[-c(i, j, k), ]
                                                   # remove rows i, j, k from dataframe
# <dataframe> <- <dataframe>[-(i:k), ]
                                                    # remove rows i to k from dataframe
# Changing column names:
# colnames(<dataframe>)[i] <- "<new name>"
# Changing row names:
# rownames(<dataframe>)[i] <- "<new name>"
# rownames(<dataframe>) <- c("<new name 1>", "<new name 2>",...)
\# rownames (<dataframe>) <- c(1, 2,...)
# rownames(<dataframe>) <- list("<new name 1>", <numeric 2>,...)
# Slicing and dicing dataframes:
# <selection> <- <dataframe>[<some rows>, <some columns>]
# <selection> <- <dataframe>[i:k, c("<column 1>", "<column 2>",...)]
# <selection> <- <dataframe>[<indexes>, ]
# <selection> <- subset(<dataframe>,
                                                                      # subset() is much like SELECT...
FROM... WHERE
                        <logical condition for the rows to return>,
                        <select statement for the columns to return>) # can be omitted; column names not
prefixed by <dataframe>$
# <new dataframe> <- <dataframe>[, c("<col1 name>", "<col2 name>")]
# <new dataframe> <- <dataframe>[, <col1 index>:<col2 index>)]
# Shuffling rows/columns:
# <dataframe> <- <dataframe>[sample(nrow(<dataframe>)), ] # shuffle row-wise
# <dataframe> <- <dataframe>[, sample(ncol(<dataframe>))] # shuffle column-wise
# Replacing selected values in a column:
# <selected var name> <- <dataframe>$<column> == <selected value>
# <dataframe>$<column>[<selected var name>] <- <new value>
```

```
# Applying functions to all elements in rows/columns of a dataframe:
# apply(\langle dataframe \rangle, \langle 1 \mid 2 \rangle, \langle function(x) \{ ... \} \rangle) # 1 | 2: apply function(x) by row | column
# IMPORTANT: use drop = FALSE in apply(...) when subsetting <dataframe> with [],
# i.e. <dataframe>[i, j, drop = FALSE]
# sapply(\langle vector \rangle, FUN = function(x) {...}) # function(x): function to be applied to each element of
<vector>
# Partitioning a dataframe:
# install.packages('caret')
# library(caret)
# set.seed(<any specific int>) # allows for repeating the randomization process exactly
# <indexes> <- createDataPartition(<dataframe>$<column>, p = 0.8, list = FALSE)
# <partition 1> <- <dataframe>[<indexes>, ]
# <partition 2> <- <dataframe>[-<indexes>, ]
# for, if, break, next:
# for (<i> in <int vector>) {
# <line 1>
# <line 2>
# ...
# if (<logical condition>) {
# <line i1>
# <line i2>
# ...
# break
                  # break: exit the loop; next: skip the remaining lines in this iteration
# }
# ...
# <line n>
# }
# while, if-else, break, next:
# <i> <- <initial value>
# while (logical condition involving <i>) {
# <line 1>
# <line 2>
# ...
# if (<logical condition>) {
  e i1>
# <line i2>
```

```
. . .
                  # break: exit the loop; next: skip the remaining lines in this iteration
     break
  } else {
   <line j1>
  12>
   . . .
 }
 . . .
# <line n>
# <i> <- <modify <i>>>
# }
# ifelse(<condition>, v1, v2) # can return a vector
# Data type conversion
\# b <- c(1, 2, 2, 2, 3, 1, 1, 4, 5, 4)
# b.as.factor <- as.factor(b)</pre>
# levels(b.as.factor)
# e.g., <dataframe> <- as.data.frame(<matrix>)
# str(<dataframe>)
# ...
# Convert numeric to factor:
# <dataframe>$<numeric column with few different values> <-
     factor(<dataframe>$<numeric column with few different values>,
              levels = c(0, 1, ..., k), labels = c("<11>", "<12>", ..., "<1k>"))
# Attributes of R objects (dataframes, matrices, factors, lists, tables...)
# attributes(<dataframe> | <matrix> | <factor> | <list> | table | ...)
# Tables
# The table() function:
# table(<var>) # typically a factor or an integer var
# The prop.table() function:
# prop.table(table(<var>))
# round(prop.table(table(<var>)), digits = <n>)
# Row and column margins:
# table(<var1>, <var2>)
                                                          # <var1>, <var2>: usually factors or integers
# table(<rows title> = <var1>, <columns title> = <var2>) # add common titles for rows/columns
# prop.table(table(<var1>, <var2>), margin = 1)
                                                          # all row margins (sums of values by row) are 1.0
```

```
# prop.table(table(<var1>, <var2>), margin = 2)  # all column margins (sums of values by column)
are 1.0
# Vectors
# Differences in initializing vectors and dataframe columns:
# <vector> <- rep(<value>, <times>)
# <vector> <- <value>
# <dataframe>$<column> <- rep(<value>, <times>)
# <dataframe>$<column> <- <value>
# Length of a vector:
# length(<vector>)
\# Counting the number of elements with the values of \langle x \rangle in a vector:
# 1.  <- table(<vector>)
      \langle table \rangle ["\langle x \rangle"], or \langle table \rangle [names(\langle table \rangle)] == \langle x \rangle [
\# 2. sum(<vector> == <x>)
# 3. length(which(\langle vector \rangle == \langle x \rangle)
                                          # which() is like WHERE in SQL
# Appending an element to a vector:
# <vector> <- c(<vector>, <element>)
                                               # type conversion occurs if <element> is of different type than
v[i]
# <vector> <- append(<vector>, <element>)
                                               # type conversion occurs if <element> is of different type than
v[i]
# <vector> <- append(<vector>, <element>,
                                               # insert <=> append at a desired location
                             after = \langle n \rangle
# <vector> <- append(<vector>, NA)
# Removing NAs from a vector in NA-sensitive functions:
# <function>(<vector>, na.rm = TRUE)
# Selecting items matching criteria from a numeric vector (added check for NAs and NaNs):
# <numeric vector> <- c(<n1>, <n2>, <n3>, ..., NA, ...NaN)
# <selected> <- <numeric vector>[<logical criterion> & !is.na(<numeric vector>)] # is.na() is TRUE for both
NA and NaN
# is.na() is the only way to test if <something> is NA (<something> == NA does not work)
# Range of a numeric vector:
# range(<vector>)
# Create numeric vector with <length> elements:
# <vector> <- vector(mode = "numeric", length = <length>)
# Check if numeric variables follow normal distribution:
```

```
# summary(<numeric variable>)
                                           # the mean and the median values similar: probably normal
distribution
# plot(density((<numeric variable>))
                                           # visual inspection
# hist(<numeric variable>, breaks = <n>) # visual inspection; <n>: number of bins in the histogram
# ggnorm(<numeric variable>)
                                           # values lie more or less along the diagonal (straight line)
# shapiro.test(<numeric variable>)
                                           # good for small sample sizes, e.g. n < ~2000; H0: normal
distribution
# Discretizing numeric variables (using bnlearn::discretize()):
# librarv(bnlearn)
# ?discretize()
# <new dataframe with discretized variables> <-
# discretize(<numeric dataframe>,
                                                   # <original dataframe>[, c(<num. col. 1>, <num. col. 1>,
. . . 1
              method = "quantile" |
                                                   # use equal-frequency intervals (default)
             method = "interval",
                                                   # use equal-length intervals
              breaks = c(<n1>, <n2>, ..., <ncol>))
                                                           # no. of discrete intervals for each column
# Scatterplot matrices (useful for examining the presence of linear relationship between several pairs of
variables):
\# pairs (\sim<x1> + <x2> + ..., data = <dataframe>)
# Data normalization:
# library(clusterSim)
# <dataframe with numeric columns> <-</pre>
                                                             # works with vectors and matrices as well
 data.Normalization(<dataframe with numeric columns>,
                       type = "n4",
                                                             # normalization: (x - min(x)) / (max(x) -
min(x))
                       normalization = "column")
                                                             # normalization by columns
# Alternatively:
\# < \text{norm.f} > = \text{function}(x) \{ (x-\min(x)) / (\max(x) - \min(x)) \}
# <dataframe with numeric columns>[] <-</pre>
                                                             # [] preserves the "data.frame" class
# lapply(<dataframe with numeric columns>, <norm.f>)
# Alternatively:
# install.packages("scales")
# librarv(scales)
# <dataframe with numeric columns> <-
# lapply(<dataframe with numeric columns>, rescale) # normalization: (x - min(x)) / (max(x) - min(x))
min(x))
```

```
# Alternatively:
# install.packages("caret")
# library(caret)
# processed object> <-</pre>
# preProcess(<dataframe with numeric columns>,
             method = 'range')
                                                          # normalization: (x - min(x)) / (max(x) -
min(x))
# <dataframe with numeric columns> <-</pre>
 predict(<pre-processed object>,
           <dataframe with numeric columns>)
# Correlation plots:
                                               # correlations between numeric variables in the dataset
# <numeric dataframe> <-</pre>
                                                              # create all-numeric dataframe,
# data.frame(<num col 1 name> = <dataframe>$<num col 1>, # leave out all non-numeric columns
              # <correlation matrix> <- cor(<numeric dataframe>)
                                                            # all-numeric dataframe
# library(corrplot)
# corrplot.mixed(<correlation matrix>, tl.cex = <text font size>, number.cex = <number font size>)
# Ouantiles/Percentiles:
# <quantiles> <- quantile(<dataset>$<column name>, # examine the 0th, 2.5th, ..., percentile
                         probs = seq(from = 0.0, to = 0.1, by = 0.025))
# Sorting:
                               # sort <numeric vector>
# sort(<numeric vector>)
# install.packages("knitr")
                                                           # pretty-printing tables etc. in the console
# library(knitr)
                                                          # (a set of "fancy" reporting tools)
\# kable(x = <stats>, format = "rst")
#### aaplot2
# Bar graphs:
# ggplot(data = <dataframe>,
        aes(x = \langle column 1 \rangle, y = \langle column 2 \rangle, fill = \langle column 1 \rangle)) + # fill = \langle column 1 \rangle is optional; no y
for counts
```

```
# geom bar(stat = "identity") +
                                                                      # "identity" for values, "count" for
counts
# xlab("<x-axis label>") + ylab("<y-axis label>") +
# ggtitle("<graph title>")
# Render a bar chart that shows mean values on the y axis (not sums of y values):
# ggplot(data = <dataframe>,
         aes(x = \langle column 1 \rangle, y = \langle column 2 \rangle, fill = \langle column 1 \rangle)) + # fill = \langle column 1 \rangle is optional; no y
for counts
# geom bar(stat = "summary", fun = "mean")
                                                                      # use both stat = "summary" and fun =
"mean"
\# qqplot(<dataframe>, aes(x = <column 1>, fill = <column 2>)) +
# geom bar(position = "dodge", width = <bin width>) +
                                                                      # "dodge": bar grouping, <bin width>:
0.2-0.6
\# labs(x = "<x-label>", y = "<y-label>", title = "<title>") +
# theme bw()
# Line graphs:
# ggplot(data = <dataframe>,
         aes(x = \langle column 1 \rangle, y = \langle column 2 \rangle, group = 1)) + # group = 1: one line, all points connected
  geom line(colour = "<colour>", linetype = "<linetype>", size = <line thickness>) +
  geom point(colour="<colour>", size = <point size>, shape = <point shape>, fill = "<point fill colour>")
# xlab("<x-axis label>") + ylab("<y-axis label>") +
# ggtitle("<graph title>")
# All parameters in geom line() and in geom point() are optional.
# The defaults are: colour = "black", linetype = "solid", size = 1, shape = 21 (circle), fill = "black"
# See http://www.cookbook-r.com/Graphs/Colors (ggplot2)/
# for more information on colors.
# See http://www.cookbook-r.com/Graphs/Shapes and line types/
# for information on shapes and line types.
# Scatterplots:
\# qqplot(<dataset>, aes(x = <num.var.1>, y = <num.var.2>)) +
# geom point(shape = <n>,
                                   # <n> = 1: hollow circle
               fill = <color 1>, # color of point fill (optional)
               color = <color 2>, # color of point line (optional)
               size = <s>) + # size of point line (optional)
# geom smooth(method = lm, # add regression line (optional); if left out, nonlinear best-fit line is
shown
```

```
se=FALSE)
                                   # do NOT show 95% confidence region as a shaded area (optional)
# <scatterplot> <-</pre>
 qqplot(\langle dataset \rangle, aes(x = \langle num.var.1 \rangle, y = \langle num.var.2 \rangle)) +
   geom point(shape = < n > ,
                                      \# <n> = 1: hollow circle, no fill; <n> = 21: circle that can be filled
                 fill = <color 1>,  # color of point fill (optional)
                 color = <color 2>,  # color of point line (optional)
                 size = \langle s \rangle)
                                      # size of point line (optional)
# <scatterplot> <- <scatterplot> + xlab("<x label>")
                                                                            # label/caption on x-axis
# <scatterplot> <- <scatterplot> + ylab("<y label>")
                                                                            # label/caption on x-axis
# <scatterplot> <- <scatterplot> + ggtitle("<scatterplot title>")
                                                                            # scatterplot title
# Boxplots:
# boxplot(<dataset>$<column name>, xlab = "<column name>")
                                                                 # basic boxplot for <column name>
# boxplot.stats(<dataset>$<column name>)
                                                                 # returns the stats used for drawing a boxplot
# ggplot(<dataset>,
                                                                 # ggplot2 boxplots
         aes(x = "", y = <column name>, fill = "<color>")) + # show boxplot of <column name>
         geom boxplot(width = 0.5) +
                                                                 # boxplot width
         stat boxplot(geom ='errorbar', width = 0.15) +
                                                                 # show whiskers, control their width
         quides(fill = FALSE) +
                                                                 # no legend (it makes no sense here)
         xlab("")
                                                                 # no x-axis label (it makes no sense here)
# Histograms:
\# qqplot(data = <dataset>, mapping = aes(x = <column name>)) +
# geom histogram(bins = <nbins>,
                  fill = "<fill color>",
                   color = "<line color>")
# Density graphs:
# ggplot(data = <dataset>,
         mapping = aes(x = \langle num. var. \rangle, fill = \langle fill var. \rangle)) +
  geom density(alpha = <value>) +
                                                                 # alpha: plot transparency (0-1, optional)
   theme bw()
######
# ML #
######
```

```
# Model building and examination:
\# < model > < - lm(< y > ~ < x1 > + < x2 > + ...,
                                              # build/fit the model over the <dataset>;
            data = <dataset>)
                                                # <x> and <y> are numeric variables from <dataset>
                         # show the model
# <model>
# coef(<model>)
                        # show the coefficients of the linear model (intercept and slope)
# confint(<model>)
                        # show the confidence intervals for the estimated intercept and slope
# summary(<model>)
                        # show the model statistics
# library(rpart)
# <model> <- rpart(<output variable> ~
                                                                         # build the tree
                  data = <train dataset>,
                  method = "class",
                                                                         # build classification tree
                  control = rpart.control(minsplit = <n>, cp = <q>))
                                                                        # decrease both for larger tree
# Alternatively:
# <model> <- rpart(<output variable> ~ .,
                                                                         # use almost all vars,
                  data = subset(<train dataset>,
                                select =
                                 -c(cpredictor variable i> +
                                     cpredictor variable j> + ...)),
                                                                         # excluding some specific ones
                  method = "class")
# Alternatively:
# <model> <- rpart(<output variable> ~ .,
                                                                         # use almost all vars,
                  data = within(<train dataset>,
                                rm(<predictor variable i>,
                                                                         # excluding some specific ones
                                  cpredictor variable j>, ...)
                  method = "class")
# library(rattle)
# library(rpart.plot)
# library(RColorBrewer)
# fancyRpartPlot(<decision tree>)
\# < model > < - kmeans(x = < normalized dataframe >,
                   centers = \langle k \rangle,
                                                      # K = <k>
                  iter.max = \langle i \rangle,
                                                     # max number of iterations allowed, e.g. 20
                  nstart = \langle n \rangle)
                                                     # no. of initial configurations, e.g. 1000 (report
on the best one)
# library(e1071)
# library(caret)
# <folds> = trainControl(method = "cv", number = <k>)# define <k>-fold cross-validation
parameters
```

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# specify the range of the cp values to
# <cpGrid> = expand.grid(.cp =
examine
                         seq(from = <start value>, to = <end value>, by = <step>))
# train(
                                                                  # find the optimal value for cp
       x = \langle train \ dataset \rangle [, \ c(\langle predictor \ variable \ 1 \rangle, \langle predictor \ variable \ 2 \rangle, \ldots)],
        y = <train dataset>$<output variable>,
       method = "rpart",
                                                                  # use rpart() to build multiple
classification trees
        control = rpart.control(minsplit = <n>),
                                                                  # optional; default minsplit is 20
      trControl = <folds>,
                                                                  # <folds> from above
       tuneGrid = <cpGrid>)
                                                                  # <cpGrid> from above
# prunned model> <- prune(<model>, cp = <optimal cp value>)
# library(class)
# <model> <- knn(train = <training dataset>, # training data without the output (class) variable
                                                     # test data without the output (class) variable
                test = <test dataset>,
                cl = <class values for training>, # output (class) variable is specified here
                 k = \langle n \rangle
                                                      # <n>: random guess, or obtained from cross-validation
# library(e1071)
# ?naiveBayes
# <model> <- naiveBayes(<output variable> ~ .,
                                                          # include all predictors from the training set
                        data = <training dataset>)
# <model> <- naiveBayes(<output variable> ~
                        \langle var 1 \rangle + \langle var 2 \rangle + ...,
                                                        # include only selected predictors from the training
set
                        data = <training dataset>)
# Multicolinearity:
# library(car)
# vif(<model>)
                       \# variables with sqrt(vif) > 2 (2.5 - disagreement) are problematic
# sqrt(vif(<model>))
# Making predictions:
# cpredictions> <- predict(<model>,
         <test dataframe>,
         interval = "confidence" |
                                               # include the confidence interval for the predictions
(optional; used only in linear regression)
                     "predict")
                                               # include prediction intervals (optional)
#  #  color = <decision tree>,
                           newdata = <test dataset>,
                           type = "class")  # for classification task
```

```
# cpredictions> <- predict(object = <NB model>,
                          newdata = <test dataset>,
                          type = "raw")  # compute probabilities, not classes
# cpredictions>[<i1>:<ik>]
                                            # examine some of the predictions
# predictions dataframe> <-</pre>
       data.frame(<observation ID> = <test dataset>$<observation ID column>,
                  <another relevant feature> = <test dataset>$<another relevant feature column>,
                  <output feature> = <test dataset>$<output variable>,
                  cpredictions feature> = cpredictions>)
# Diagnostic plots:
\# par(mfrow = c(2,2)) \# set up the plotting panel for 4 graphs \# plot(<model>) \# plot the 4 graphs
\# par(mfrow = c(1,1)) \# reset the plotting panel
# Leverage points:
# plot(<model>, 4, id.n = <k>)
                                               # Cook's distance for points in the <model>,
                                               # highlighting top id.n most extreme values (id.n default:
# <leverge statistic> <- hatvalues(<model>)
                                               # <leverge statistic>: high-leverage points in the model
# plot(<leverge statistic>)
\# <cutoff leverage> <- 2 * (p + 1) / n \# n - no. of observations, p - no. of predictors
# R-squared and RMSE:
# Compute R-squared on the test data for a model:
# R-squared = 1 - RSS/TSS, where RSS is the residual sum of squares, and TSS is the total sum of squares
# # ctions RSS> <-</pre>
# sum((<predictions> - <test dataset>$<output variable>)^2)
# predictions TSS> <-
# sum((mean(<train dataset>$<output variable>) - <test dataset>$<output variable>)^2)
# <R-squared>
# Compute Root Mean Squared Error (RMSE) for a model on the test data
# to see how much error we are making with the predictions:
# RMSE = sqrt(RSS/n)
# cpredictions RMSE> <- sqrt(<predictions RSS> / nrow(<test dataset>))
# # ctions RMSE>
```

```
# ROC curve (Receiver Operating Characteristic)
# library(pROC)
# <ROC curve parameters> <-
                                                           # compute ROC curve parameters
 roc(response = <test dataset>$<output variable>,
        predictor = \langle predicted probabilities \rangle[, \langle 1 \mid 2 \rangle]) # col. no. of the "positive class" (can be the No
class!)
# <ROC curve parameters>$auc
                                                           # extract and show AUC
# plot.roc(<ROC curve parameters>,
                                                 # computed in the previous step
           print.thres = TRUE,
                                                 # show the probability threshold (cut-off point) on the plot
           print.thres.best.method =
              "vouden" |
                                  # maximize the sum of sensitivity and specificity (the distance to the
diag. line)
              "closest.topleft") # minimize the distance to the top-left point of the plot
# <ROC coords> <- coords(<ROC curve parameters>,
                                                                             # computed in the previous step
                         ret = c("accuracy", "spec", "sens", "thr", ...),
                                                                             # ROC curve parameters to return
                                                # the coordinates to look for:
                             "local maximas" | # local maximas of the ROC curve
                             "best" | ...)
                                                # the point with the best sum of sensitivity and
specificity, i.e.
                                                 # the same as the one shown on the ROC curve
# Compare multiple clustering results/schemes:
# install.packages("fpc")
# library(fpc)
# ?cluster.stats
                                        # specify criteria (from cluster.stats()) for comparing
# <comparison criteria> <-</pre>
 c("<criterion 1>",
                                        # different clusterings (e.g., "max.diameter", "min.separation",
   "<criterion 2>", ...)
                                        # "average.between", "average.within", "within.cluster.ss", ...)
# <distance matrix> <-</pre>
 dist(x = <normalized dataset>)
# <comparison> <- sapply(list(<clustering 1 name> = <clustering 1>, # <clustering 1> computed by kmeans()
                              <clustering 1 name> = <clustering 2>, # <clustering 2> computed by kmeans()
                         FUN = function(x)
                          cluster.stats(<distance matrix>, x))[<comparison criteria>, ]
                                                             # pretty-printing tables etc. in the console
# install.packages("knitr")
# library(knitr)
                                                             # (a set of "fancy" reporting tools)
# kable(x = comparison, format = "rst")
```