Machine Learning - the basics in R

Jan-Philipp Kolb

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Content of this section

- The first section is about laying the foundations in R. We will need all things covered later on.

Topics section:

- Why R is a good choice
- Constraints of R-usage
- R is modular
- Import and export of data

Why R is a good choice . . .

- . . . because it is an **open source language**
- . . . outstanding graphs - **graphics**, **graphics**, **graphics**
- . . . relates to other languages - **R can be used in combination with other programs** - e.g. **data linking**
- . . . R can be used **for automation**
- . . . Vast Community - **you can use the intelligence of other people ;-)** and new statistical methodologies are implemented quite fast
- Because R can be combined with other programs like `PostgreSQL` or `Python`

Constraints

Newer modules in Python

- Machine learning is a field that changes rapidly.
- Some new tools are first developed in Python.
- The package `reticulate` offers the possibility to use these modules from an R environment.
- Good news - Python is also Open Source

Big Data

- Especially if you work with web data, you quickly have to deal with large amounts of data.
- Therefore one must fall back on databases and parallelization strategies, which can be used in R.

R is modular

Install packages from CRAN Server

```
install.packages("lme4")
```

Install packages from Bioconductor Server

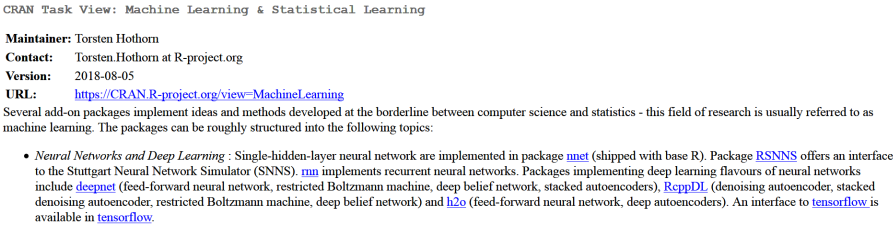
```
source("https://bioconductor.org/biocLite.R")
biocLite(c("GenomicFeatures", "AnnotationDbi"))
```

Install packages from Github

```
install.packages("devtools")
library(devtools)

devtools::install_github("koalaverse/vip")
```

Task View Machine Learning



CRAN Task View: Machine Learning & Statistical Learning

Maintainer:	Torsten Hothorn
Contact:	Torsten.Hothorn at R-project.org
Version:	2018-08-05
URL:	https://CRAN.R-project.org/view=MachineLearning

Several add-on packages implement ideas and methods developed at the borderline between computer science and statistics - this field of research is usually referred to as machine learning. The packages can be roughly structured into the following topics:

- *Neural Networks and Deep Learning* : Single-hidden-layer neural network are implemented in package nnet (shipped with base R). Package RSNNS offers an interface to the Stuttgart Neural Network Simulator (SNNS). rnn implements recurrent neural networks. Packages implementing deep learning flavours of neural networks include deepnet (feed-forward neural network, restricted Boltzmann machine, deep belief network, stacked autoencoders), RcppDL (denoising autoencoder, stacked denoising autoencoder, restricted Boltzmann machine, deep belief network) and h2o (feed-forward neural network, deep autoencoders). An interface to tensorflow is available in tensorflow.

Install all packages of a task view

```
install.packages("ctv")
ctv::install.views("MachineLearning")
```

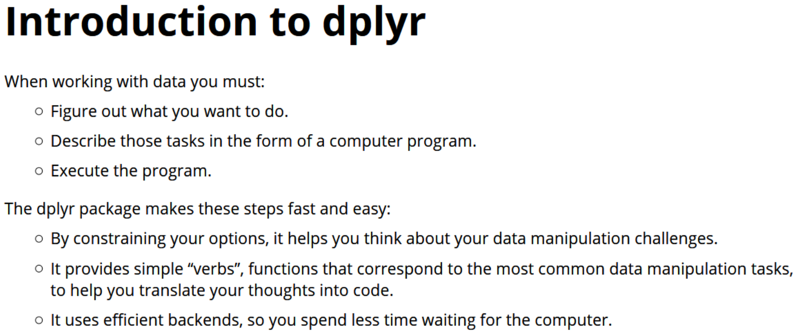
Exercise: Find R-packages

Go to https://cran.r-project.org/ and search for packages that can be used:

1) to reduce overfitting
2) for regression trees
3) for gradient boosting
4) for neural networks
5) for clustering

Preparation - packages

```r
library(dplyr)
```



Introduction to dplyr

When working with data you must:

- Figure out what you want to do.
- Describe those tasks in the form of a computer program.
- Execute the program.

The dplyr package makes these steps fast and easy:

- By constraining your options, it helps you think about your data manipulation challenges.
- It provides simple “verbs”, functions that correspond to the most common data manipulation tasks, to help you translate your thoughts into code.
- It uses efficient backends, so you spend less time waiting for the computer.

The package magrittr

```
library(magrittr)
```

Import .csv data

The read.csv command

- Use read.csv2 for German data

```
?read.csv
?read.csv2
```

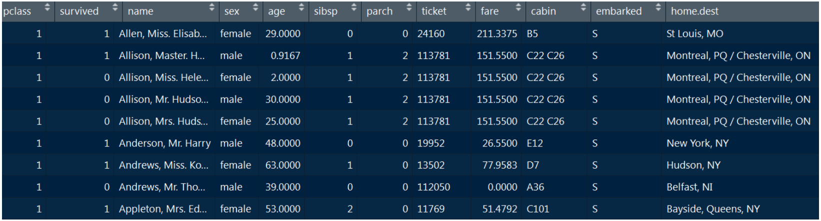
Using a path to import data

```
path1<-"https://raw.githubusercontent.com/"
path2<- "thomaspernet/data_csv_r/master/data/"
dname <- "titanic_csv.csv"
titanic <- read.csv(paste0(path1,path2,dname))
```

Save the dataset

```
save(titanic,file="../data/titanic.RData")
```

The titanic dataset



pclass	survived	name	sex	age	sibsp	parch	ticket	fare	cabin	embarked	home.dest
1	1	Allen, Miss. Elisab...	female	29.0000	0	0	24160	211.3375	B5	S	St Louis, MO
1	1	Allison, Master. H...	male	0.9167	1	2	113781	151.5500	C22 C26	S	Montreal, PQ / Chesterville, ON
1	0	Allison, Miss. Hele...	female	2.0000	1	2	113781	151.5500	C22 C26	S	Montreal, PQ / Chesterville, ON
1	0	Allison, Mr. Hudso...	male	30.0000	1	2	113781	151.5500	C22 C26	S	Montreal, PQ / Chesterville, ON
1	0	Allison, Mrs. Huds...	female	25.0000	1	2	113781	151.5500	C22 C26	S	Montreal, PQ / Chesterville, ON
1	1	Anderson, Mr. Harry	male	48.0000	0	0	19952	26.5500	E12	S	New York, NY
1	1	Andrews, Miss. Ko...	female	63.0000	1	0	13502	77.9583	D7	S	Hudson, NY
1	0	Andrews, Mr. Tho...	male	39.0000	0	0	112050	0.0000	A36	S	Belfast, NI
1	1	Appleton, Mrs. Ed...	female	53.0000	2	0	11769	51.4792	C101	S	Bayside, Queens, NY

The function `scan` to import data

- `scan` has an easy way to distinguish comments from data

```
?scan
```

Example dataset

```
cat("TITLE extra line", "# a comment","2 3 5 7", "11 13 17",
    file = "../data/ex.data", sep = "\n")
```

Import data and skip the first line

```
pp<-scan("../data/ex.data",skip=1,quiet=TRUE)
pp <- scan("../data/ex.data",comment.char="#", skip = 1,
           quiet = TRUE)
```

The download the data from UCI.

```
path1 <- "http://archive.ics.uci.edu/ml/"
path2 <- "machine-learning-databases/00243/"
dname <- 'yacht_hydrodynamics.data'

url<- paste0(path1,path2,dname)
Yacht_Data <- readr::read_table(file = url)
```

Built in datasets

- A sample dataset is often provided to demonstrate the functionality of a package.
- These records can be loaded using the `data` command.

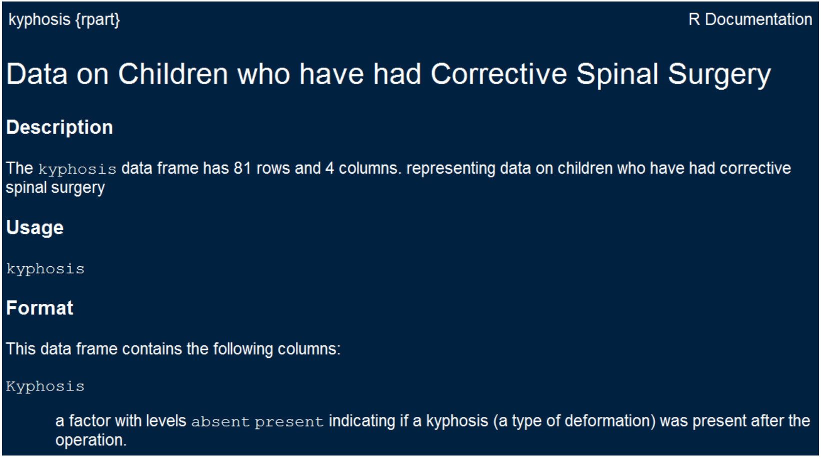
```
data(iris)
```

- There is also a **RStudio Add-In** that helps to find a built-in dataset.

```
install.packages("datasets.load")
```

Help page for built in datasets

```
?kyphosis
```



kyphosis {rpart} R Documentation

Data on Children who have had Corrective Spinal Surgery

Description

The `kyphosis` data frame has 81 rows and 4 columns. representing data on children who have had corrective spinal surgery

Usage

```
kyphosis
```

Format

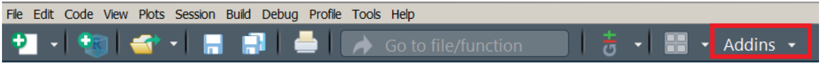
This data frame contains the following columns:

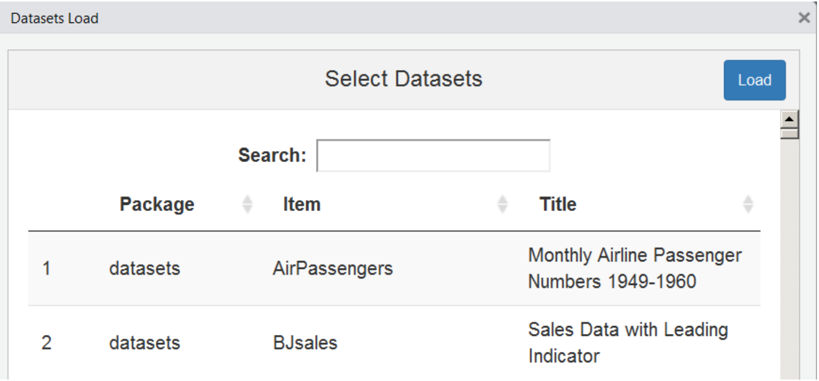
`Kyphosis`

a factor with levels `absent` `present` indicating if a kyphosis (a type of deformation) was present after the operation.

Excursus RStudio Addins

- In the upper right corner there is a button Addins





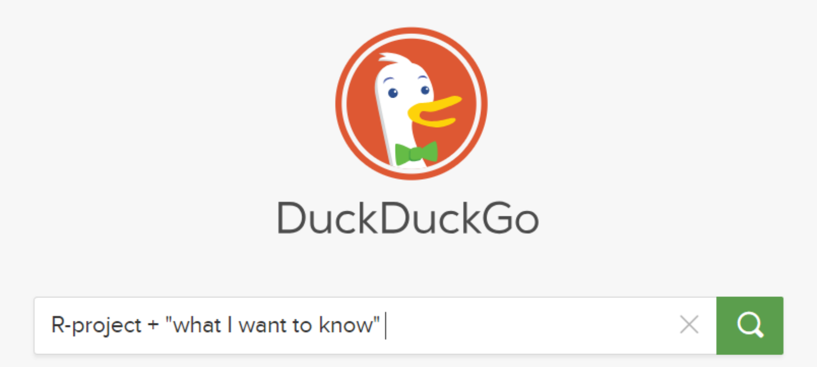
	Package	Item	Title
1	datasets	AirPassengers	Monthly Airline Passenger Numbers 1949-1960
2	datasets	BJsales	Sales Data with Leading Indicator

How to get help

- I use **duckduckgo:**

```
R-project + "what I want to know"
```

- this works of course for all search engines!



R-project + "what I want to know"

Exercise: load built-in data

Load the the built-in dataset `swiss`

1) How many observations and variables are available?
2) What is the scale level of the variables?

Interactive data table

3) Create an interactive data table

The R-package data.table

Get an overview

```
data(airquality)
head(airquality)
##   Ozone Solar.R Wind Temp Month Day
## 1    41     190  7.4   67     5   1
## 2    36     118  8.0   72     5   2
## 3    12     149 12.6   74     5   3
## 4    18     313 11.5   62     5   4
## 5    NA      NA 14.3   56     5   5
## 6    28      NA 14.9   66     5   6
```

Overview with data.table

```
library(data.table)
(airq <- data.table(airquality))
```

```
##      Ozone Solar.R Wind Temp Month Day
##   1:    41     190  7.4   67     5   1
##   2:    36     118  8.0   72     5   2
##   3:    12     149 12.6   74     5   3
##   4:    18     313 11.5   62     5   4
##   5:    NA      NA 14.3   56     5   5
##  ---
## 149:    30     193  6.9   70     9  26
## 150:    NA     145 13.2   77     9  27
## 151:    14     191 14.3   75     9  28
## 152:    18     131  8.0   76     9  29
## 153:    20     223 11.5   68     9  30
```

Column (and row) names of airq

```r
colnames(airq)
```

```
## [1] "Ozone"   "Solar.R" "Wind"    "Temp"    "Month"   "Day"
```

```r
rownames(airq)
```

```
##   [1] "1"   "2"   "3"   "4"   "5"   "6"   "7"   "8"   "9"   "
##  [13] "13"  "14"  "15"  "16"  "17"  "18"  "19"  "20"  "21"  "
##  [25] "25"  "26"  "27"  "28"  "29"  "30"  "31"  "32"  "33"  "
##  [37] "37"  "38"  "39"  "40"  "41"  "42"  "43"  "44"  "45"  "
##  [49] "49"  "50"  "51"  "52"  "53"  "54"  "55"  "56"  "57"  "
##  [61] "61"  "62"  "63"  "64"  "65"  "66"  "67"  "68"  "69"  "
##  [73] "73"  "74"  "75"  "76"  "77"  "78"  "79"  "80"  "81"  "
##  [85] "85"  "86"  "87"  "88"  "89"  "90"  "91"  "92"  "93"  "
##  [97] "97"  "98"  "99"  "100" "101" "102" "103" "104" "105" "
## [109] "109" "110" "111" "112" "113" "114" "115" "116" "117" "
## [121] "121" "122" "123" "124" "125" "126" "127" "128" "129" "
## [133] "133" "134" "135" "136" "137" "138" "139" "140" "141" "
## [145] "145" "146" "147" "148" "149" "150" "151" "152" "153"
```

Command `mutate` - create or transform variables

```
?dplyr::mutate
```

```
airq %>%
  mutate(Temp / max(Temp, na.rm = TRUE))
```

```
##     Ozone Solar.R Wind Temp Month Day Temp/max(Temp, na.rm =
## 1      41     190  7.4   67     5   1                    0.69
## 2      36     118  8.0   72     5   2                    0.74
## 3      12     149 12.6   74     5   3                    0.76
## 4      18     313 11.5   62     5   4                    0.63
## 5      NA      NA 14.3   56     5   5                    0.57
## 6      28      NA 14.9   66     5   6                    0.68
## 7      23     299  8.6   65     5   7                    0.67
## 8      19      99 13.8   59     5   8                    0.60
## 9       8      19 20.1   61     5   9                    0.62
## 10     NA     194  8.6   69     5  10                    0.71
## 11      7      NA  6.9   74     5  11                    0.76
## 12     16     256  9.7   69     5  12                    0.71
```

Exercise: random numbers

1) Draw 8 random numbers from the uniform distribution and save them in a vector `x`
2) Compute the logarithm of `x`, return suitably lagged and iterated differences,
3) compute the exponential function and round the result

```
## [1]  6.8  1.2  0.0 20.7  1.1  0.8  0.3
```

The pipe operator

```
library(magrittr)

# Perform the same computations on `x` as above
x %>% log() %>%
    diff() %>%
    exp() %>%
    round(1)
```

```
## [1]  6.8  1.2  0.0 20.7  1.1  0.8  0.3
```

How to deal with missing values

```
?na.omit
```

```
airq
```

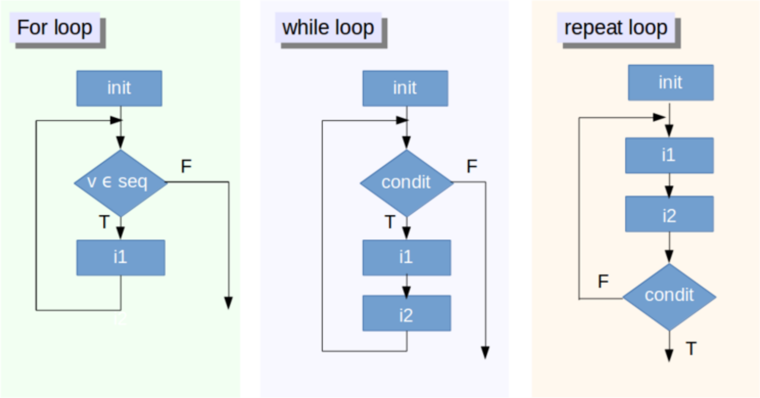
```
##      Ozone Solar.R Wind Temp Month Day
##   1:    41     190  7.4   67     5   1
##   2:    36     118  8.0   72     5   2
##   3:    12     149 12.6   74     5   3
##   4:    18     313 11.5   62     5   4
##   5:    NA      NA 14.3   56     5   5
##  ---
## 149:    30     193  6.9   70     9  26
## 150:    NA     145 13.2   77     9  27
## 151:    14     191 14.3   75     9  28
## 152:    18     131  8.0   76     9  29
## 153:    20     223 11.5   68     9  30
```

The command na.omit

```
na.omit(airq)
```

```
##        Ozone Solar.R Wind Temp Month Day
##   1:      41     190  7.4   67     5   1
##   2:      36     118  8.0   72     5   2
##   3:      12     149 12.6   74     5   3
##   4:      18     313 11.5   62     5   4
##   5:      23     299  8.6   65     5   7
##  ---                                    
## 107:      14      20 16.6   63     9  25
## 108:      30     193  6.9   70     9  26
## 109:      14     191 14.3   75     9  28
## 110:      18     131  8.0   76     9  29
## 111:      20     223 11.5   68     9  30
```

Available loops in R



Loops in R

- This loop calculates the square of the first 10 elements of vector u1

```
u1 <- rnorm(30)
# Initialize `usq`
usq <- 0
for(i in 1:10) {
  # i-th element of `u1` squared into `i`-th position of `usq`
  usq[i] <- u1[i]*u1[i]
  print(usq[i])
}
```

```
## [1] 0.8037931
## [1] 0.1441734
## [1] 1.177838
## [1] 0.215837
## [1] 1.488146
## [1] 1.910998
## [1] 10.69898
## [1] 0.4196871
```

Library purrr

purrr - Functional Programming Tools

- The pattern of looping over a vector, doing something to each element and saving the results is so common that the purrr package provides a family of functions to do it for you.

```
library(purrr)
```

- `map()` makes a list.
- `map_lgl()` makes a logical vector.
- `map_int()` makes an integer vector.
- `map_dbl()` makes a double vector.
- `map_chr()` makes a character vector.

Example map_dbl

```
map_dbl(airq, mean)
```

```
##     Ozone   Solar.R      Wind      Temp     Month       Day
##        NA        NA  9.957516 77.882353  6.993464 15.803922
```

```
map_dbl(airq, mean,na.rm=T)
```

```
##      Ozone    Solar.R       Wind       Temp      Month
##  42.129310 185.931507   9.957516  77.882353   6.993464  15.80
```

Clean the titanic data set

```
clean_titanic <- titanic %>%
  mutate(pclass=factor(pclass,levels = c(1, 2, 3),
                      labels=c('Upper','Middle','Lower')),
    survived = factor(survived,levels = c(0, 1),
                     labels=c('No', 'Yes'))) %>%
na.omit()
```

mutate(pclass = factor(...:

- Add label to the variable pclass.
- 1 becomes Upper, 2 becomes MIddle and 3 becomes lower

factor(survived,...:

- Add label to the variable survived.
- 1 Becomes No and 2 becomes Yes
- `na.omit()`: Remove the NA observations

Get an overview of the data

```
glimpse(clean_titanic)
```

```
## Observations: 1,045
## Variables: 13
## $ X         <int> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13,
## $ pclass    <fct> Upper, Upper, Upper, Upper, Upper, Upper, U
## $ survived  <fct> Yes, Yes, No, No, No, Yes, Yes, No, Yes, No
## $ name      <fct> "Allen, Miss. Elisabeth Walton", "Allison,
## $ sex       <fct> female, male, female, male, female, male, f
## $ age       <dbl> 29.0000, 0.9167, 2.0000, 30.0000, 25.0000,
## $ sibsp     <int> 0, 1, 1, 1, 1, 0, 1, 0, 2, 0, 1, 1, 0, 0, 0
## $ parch     <int> 0, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
## $ ticket    <fct> 24160, 113781, 113781, 113781, 113781, 1995
## $ fare      <dbl> 211.3375, 151.5500, 151.5500, 151.5500, 151
## $ cabin     <fct> B5, C22 C26, C22 C26, C22 C26, C22 C26, E12
## $ embarked  <fct> S, S, S, S, S, S, S, S, S, C, C, C, C, S, S
## $ home.dest <fct> "St Louis, MO", "Montreal, PQ / Chestervill
```

With gather from wide to long format

```
library(dplyr)
library(tidyr)
stocks <- tibble(
  time = as.Date('2009-01-01') + 0:9,
  X = rnorm(10, 0, 1),
  Y = rnorm(10, 0, 2),
  Z = rnorm(10, 0, 4)
)

gather(stocks, "stock", "price", -time)
```

```
## # A tibble: 30 x 3
##    time       stock   price
##    <date>     <chr>   <dbl>
##  1 2009-01-01 X      1.93
##  2 2009-01-02 X      0.751
##  3 2009-01-03 X      0.658
##  4 2009-01-04 X      1.64
```

Sequences

- Later we will create hyperparameter grids.
- To do so, we will need sequences

```
# the easiest sequence
1:4
```

```
## [1] 1 2 3 4
```

```
# the other way
4:1
```

```
## [1] 4 3 2 1
```

```
# the command sequence
seq(start=1,to = 10,by = 2)
```

```
## [1] 1 3 5 7 9
```

```
# we will need the following for loops
seq_along(14:21)
```

```
## [1] 1 2 3 4 5 6 7 8
```

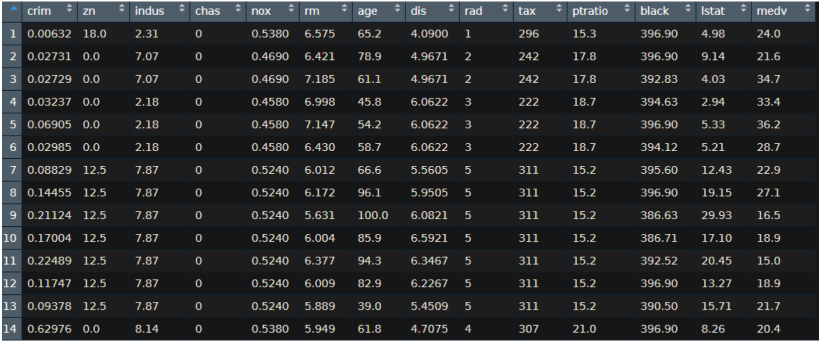
The command expand.grid

```r
expand.grid(letters[1:4],5:3,LETTERS[1:2])
```

```
##    Var1 Var2 Var3
## 1     a    5    A
## 2     b    5    A
## 3     c    5    A
## 4     d    5    A
## 5     a    4    A
## 6     b    4    A
## 7     c    4    A
## 8     d    4    A
## 9     a    3    A
## 10    b    3    A
## 11    c    3    A
## 12    d    3    A
## 13    a    5    B
## 14    b    5    B
## 15    c    5    B
```

Example Data - Housing Values in Suburbs of Boston

```r
library(MASS)
bdat <- Boston
```



	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	black	lstat	medv
1	0.00632	18.0	2.31	0	0.5380	6.575	65.2	4.0900	1	296	15.3	396.90	4.98	24.0
2	0.02731	0.0	7.07	0	0.4690	6.421	78.9	4.9671	2	242	17.8	396.90	9.14	21.6
3	0.02729	0.0	7.07	0	0.4690	7.185	61.1	4.9671	2	242	17.8	392.83	4.03	34.7
4	0.03237	0.0	2.18	0	0.4580	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
5	0.06905	0.0	2.18	0	0.4580	7.147	54.2	6.0622	3	222	18.7	396.90	5.33	36.2
6	0.02985	0.0	2.18	0	0.4580	6.430	58.7	6.0622	3	222	18.7	394.12	5.21	28.7
7	0.08829	12.5	7.87	0	0.5240	6.012	66.6	5.5605	5	311	15.2	395.60	12.43	22.9
8	0.14455	12.5	7.87	0	0.5240	6.172	96.1	5.9505	5	311	15.2	396.90	19.15	27.1
9	0.21124	12.5	7.87	0	0.5240	5.631	100.0	6.0821	5	311	15.2	386.63	29.93	16.5
10	0.17004	12.5	7.87	0	0.5240	6.004	85.9	6.5921	5	311	15.2	386.71	17.10	18.9
11	0.22489	12.5	7.87	0	0.5240	6.377	94.3	6.3467	5	311	15.2	392.52	20.45	15.0
12	0.11747	12.5	7.87	0	0.5240	6.009	82.9	6.2267	5	311	15.2	396.90	13.27	18.9
13	0.09378	12.5	7.87	0	0.5240	5.889	39.0	5.4509	5	311	15.2	390.50	15.71	21.7
14	0.62976	0.0	8.14	0	0.5380	5.949	61.8	4.7075	4	307	21.0	396.90	8.26	20.4

Normalize your data

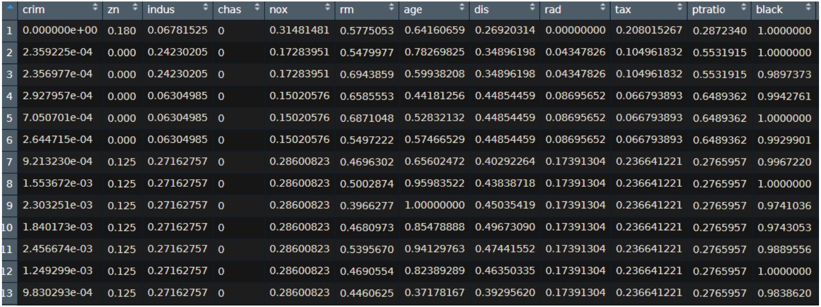
Compute maximum and minimum per column

```
maxs <- apply(bdat, 2, max)
mins <- apply(bdat, 2, min)
```

scale - Scaling and Centering of Matrix-like Objects

```
scaled <- as.data.frame(scale(bdat, center = mins,
                              scale = maxs - mins))
```

The scaled data



	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	black
1	0.000000e+00	0.180	0.06781525	0	0.31481481	0.5775053	0.64160659	0.26920314	0.00000000	0.208015267	0.2872340	1.0000000
2	2.359225e-04	0.000	0.24230205	0	0.17283951	0.5479977	0.78269825	0.34896198	0.04347826	0.104961832	0.5531915	1.0000000
3	2.356977e-04	0.000	0.24230205	0	0.17283951	0.6943859	0.59938208	0.34896198	0.04347826	0.104961832	0.5531915	0.9897373
4	2.927957e-04	0.000	0.06304985	0	0.15020576	0.6585553	0.44181256	0.44854459	0.08695652	0.066793893	0.6489362	0.9942761
5	7.050701e-04	0.000	0.06304985	0	0.15020576	0.6871048	0.52832132	0.44854459	0.08695652	0.066793893	0.6489362	1.0000000
6	2.644715e-04	0.000	0.06304985	0	0.15020576	0.5497222	0.57466529	0.44854459	0.08695652	0.066793893	0.6489362	0.9929901
7	9.213230e-04	0.125	0.27162757	0	0.28600823	0.4696302	0.65602472	0.40292264	0.17391304	0.236641221	0.2765957	0.9967220
8	1.553672e-03	0.125	0.27162757	0	0.28600823	0.5002874	0.95983522	0.43838718	0.17391304	0.236641221	0.2765957	1.0000000
9	2.303251e-03	0.125	0.27162757	0	0.28600823	0.3966277	1.00000000	0.45035419	0.17391304	0.236641221	0.2765957	0.9741036
10	1.840173e-03	0.125	0.27162757	0	0.28600823	0.4680973	0.85478888	0.49673090	0.17391304	0.236641221	0.2765957	0.9743053
11	2.456674e-03	0.125	0.27162757	0	0.28600823	0.5395670	0.94129763	0.47441552	0.17391304	0.236641221	0.2765957	0.9889556
12	1.249299e-03	0.125	0.27162757	0	0.28600823	0.4690554	0.82389289	0.46350335	0.17391304	0.236641221	0.2765957	1.0000000
13	9.830293e-04	0.125	0.27162757	0	0.28600823	0.4460625	0.37178167	0.39295620	0.17391304	0.236641221	0.2765957	0.9838620

The command sample

- We can use this command to draw a sample.
- We need the command later to split our dataset into a test and a training dataset.

```
sample(1:10,3,replace=T)
```

```
## [1]  6 10  2
```

```
sample(1:10,3,replace=T)
```

```
## [1] 9 8 9
```

Create test and training datasets

```
ntest <- round(nrow(bdat)*.2)
ind <- sample(1:nrow(bdat),ntest)
bdat_test <- bdat[ind,]
bdat_train <- bdat[-ind,]
```

Alternative to split a dataset

- Y - Vector of data labels. If there are only a few labels (as is expected) than relative ratio of data in both subsets will be the same.
- SplitRatio - Splitting ratio

```
split <- caTools::sample.split(Y = bdat$lstat,SplitRatio = .8)
Train <- bdat[split,]
Test <- bdat[!split,]
nrow(Train);nrow(Test)
```

```
## [1] 404
```

```
## [1] 102
```

Dealing with missingness

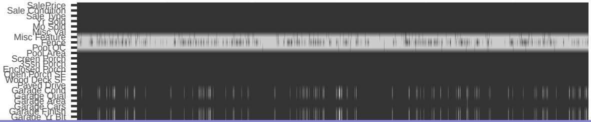
- It is important to understand the distribution of missing values

```
sum(is.na(AmesHousing::ames_raw))
```

```
## [1] 13997
```

```
library(magrittr)
library(tidyverse)

AmesHousing::ames_raw %>%
  is.na() %>%
  reshape2::melt() %>%
  ggplot(aes(Var2, Var1, fill=value)) +
    geom_raster() +
    coord_flip() +
    scale_y_continuous(NULL, expand = c(0, 0)) +
    scale_fill_grey(name = "",
                    labels = c("Present",
                               "Missing")) +
    xlab("Observation") +
    theme(axis.text.y  = element_text(size = 4))
```



Set a seed

- `set.seed` is the recommended way to specify seeds.
- If we set a seed, we get the same result for random events.
- This function is mainly required for simulations.

```
set.seed(234)
sample(1:10,3,replace=T)
```

```
## [1] 1 2 2
```

```
set.seed(234)
sample(1:10,3,replace=T)
```

```
## [1] 1 2 2
```

Time measurement

```
start_time <- Sys.time()
ab <- runif(10000000)
end_time <- Sys.time()

end_time - start_time
```

```
## Time difference of 0.4707301 secs
```

How many cores are available

```
library(doParallel)
detectCores()
```

```
## [1] 4
```

Make cluster

```
cl <- makeCluster(detectCores())
registerDoParallel(cl)
```

```
start_time <- Sys.time()
ab <- runif(10000000)
end_time <- Sys.time()

end_time - start_time
```

```
## Time difference of 0.4287639 secs
```

```
stopCluster(cl)
```

```
?parallel::makeCluster
```

Resources

- **Course materials for the Data Science Specialization**
- Data wrangling - `dplyr` **vignette** -
- The usage of pipes - `magrittr` **vignette**
- Gareth James et al (2013) **An Introduction to Statistical Learning**