Computing for Big Data (BST-262)

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2017-11-16

Contents

Chapter 1

Introduction

1.1 Logistics

- Fall 2 course
- Tuesday and Thursday, 11:30am-1pm
- Contact info: Christine Choirat (cchoirat@iq.harvard.edu). Please use BST232 in the email title.
- TA's: Qian Di (qiandi@mail.harvard.edu) and Ben Sabath (mbsabath@hsph.harvard.edu)
- Office hours:
  - Ben: Tuesday 1:30-2:30pm
  - Qian: Thursday 10:30-11:30am
  - Christine: Tuesday 10:30-11:30am (office 437A)
- Course GitHub repository https://github.com/cchoirat/bigdata17
- Open file in folder `_book/index.html`
- These course notes are **work in progress**.

1.2 Prerequisites

For BST262 (Computing for Big Data), we assume familiarity with the material covered in BST260 (Introduction to Data Science).

We will use R to present concepts that are mostly language-agnostic. We could have used Python, as in BST261 (Data Science II).

1.3 Rationale

1. Available data grows at a much faster rate than available computing capacity.
2. Statistical software programs such as R were not designed to handle datasets of massive size.

1.4 Big data bottlenecks

As described by Lim and Tjhi (2015), there are three bottlenecks:

- CPU
- RAM
- I/O

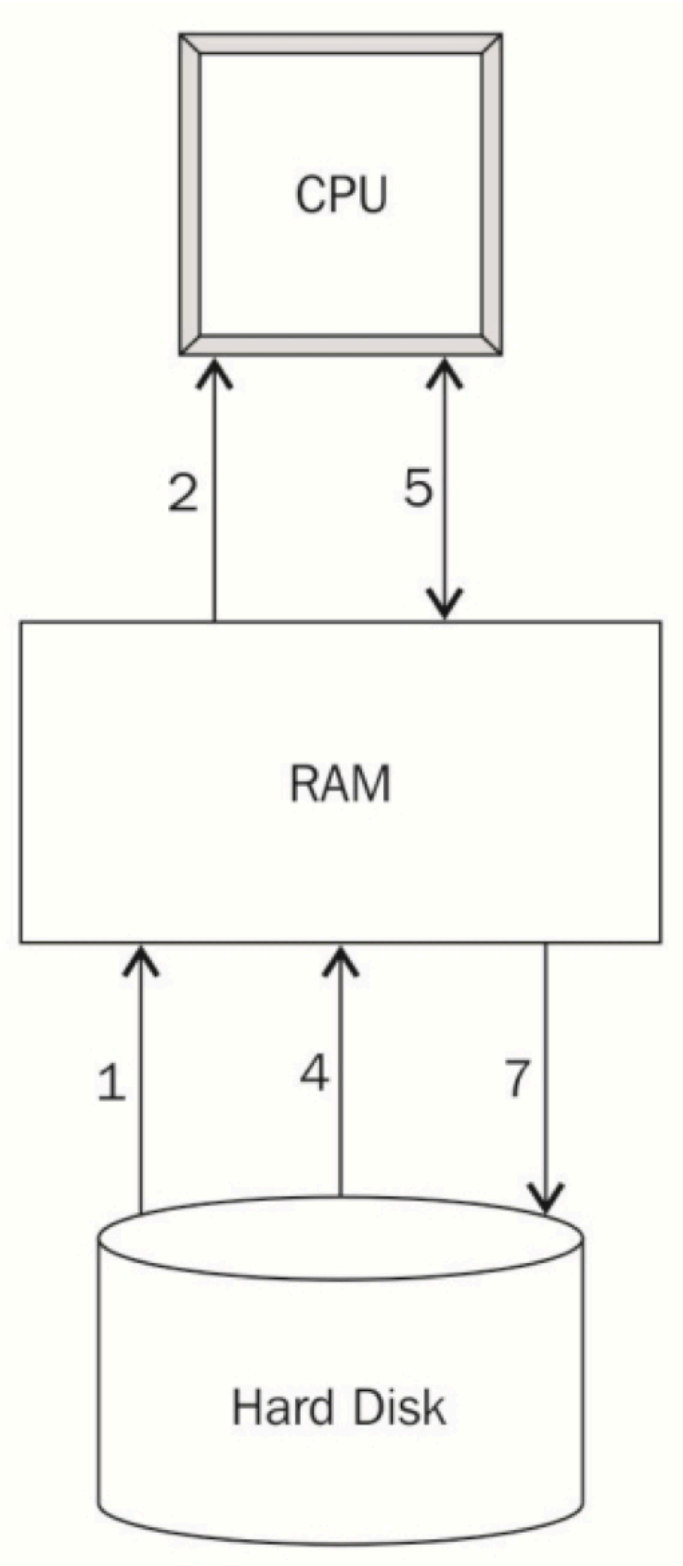


Figure 1.1: Steps to execute an R program, from @Lim2015, Chapter 1.

Exercise 1.1. Can you identify points 1–7 in the following code snippet?

```
data <- read.csv("mydata.csv")
totals <- colSums(data)
write.csv(totals, "totals.csv")
```

1.5 Syllabus

Part I – Good code still matters *(even with lots of computing resources)*

Week 1 - Basic tools

- Lecture 1. Unix scripting, make
- Lecture 2. Version control: Git and GitHub (guest lecture: Ista Zhan)

Week 2 - Creating and maintaining R packages

- Lecture 3. Rationale, package structure, available tools
- Lecture 4. Basics of software engineering: unit testing, code coverage, continuous integration

Week 3 - Software optimization

- Lecture 5. Measuring performance: profiling and benchmarking tools
- Lecture 6. Improving performance: an introduction to C/C++, Rcpp

Part II – Scaling up *(don't use big data tools for small data)*

Week 4 – Databases

- Lecture 7. Overview of SQL (SQLite, PostgreSQL) and noSQL databases (HBase, MongoDB, Cassandra, BigTable, …)
- Lecture 8. R database interfaces (in particular through dplyr and mongolite)

Week 5 - Analyzing data that does not fit in memory

- Lecture 9. Pure R solutions (sampling, `ff` and `bigmemory`, other interpreters). JVM solutions (h20, Spark)
- Lecture 10. An introduction to parallel computing; clusters and cloud computing. "Divide and Conquer" (MapReduce approaches)

Week 6 – Visualization

- Lecture 11. Principles of visualization (guest lecture: James Honaker)
- Lecture 12. Maps and GIS: principles of GIS, using R as a GIS, PostGIS

Weeks 7 & 8 - Guest lectures (order and precise schedule TBD)

- Software project management (Danny Brooke)
- R and Spark (Ellen Kraffmiller and Robert Treacy)
- Advanced GIS and remote sensing (TBD)
- Cluster architecture (William J. Horka)

1.6 Evaluation

Grades will be based on **two mandatory problem sets**. Each problem set will correspond to 50% (= 50 points) of the final grade. The first problem set will be available by the end of week 3 and the second problem set by the end of week 6.

You will be required to submit problem set solutions within two weeks. Grades, and feedback when appropriate, will be returned two weeks after submission.

You will submit a markdown document that combines commented code for data analysis and detailed and structured explanations of the algorithms and software tools that you used.

1.7 Software tools and packages

We will mostly use R in this course. Some examples will be run in Python.

In general, we will use free and open-source software programs such as PostgreSQL / PostGIS or Spark.

1.8 Datasets

We have collected datasets to illustrate concepts. They are hosted on a Dropbox folder.

1.8.1 MovieLens

MovieLens by Harper and Konstan (2015, https://grouplens.org/datasets/movielens/) collects datasets from the website https://movielens.org/.

There are datasets of different sizes. We will use:

1. Small (1MB): https://grouplens.org/datasets/movielens/latest/
2. Benchmark (~190MB zipped): https://grouplens.org/datasets/movielens/20m/

1.8.2 Airlines data

The airlines dataset comes from the U.S. Department of Transportation and were used in the 2009 Data Expo of the American Statistical Association (ASA).

We will use a version curated by h2o: https://github.com/h2oai/h2o-2/wiki/Hacking-Airline-DataSet-with-H2O.

1.8.3 Insurance claims

Claims data contain Protected Health Information (PHI). There are strong privacy restrictions to store, use and share this type of data.

We will use synthetic data (Sample 1) from the Centers for Medicare and Medicaid Services (CMS).

1.8.4 Census

Census data is commonly merged with administrative claims data such as Medicare. We will use data from the Census Bureau.

1.8.5 $PM_{2.5}$ exposure

We will use $PM_{2.5}$ exposure data from the EPA Air Quality System (AQS) to illustrate GIS linkage concepts.

1.8.6 Methylation

If there is enough interest, we might present methylation examples.

1.9 Contributing with GitHub

If you have suggestions, you can open a GitHub issue at https://github.com/cchoirat/bigdata17/issues.

If you want to contribute, we welcome pull requests.

1.10 Before we start...

How much R do you know?

Introduction to R: http://tutorials.iq.harvard.edu/R/Rintro/Rintro.html

Regression models in R: http://tutorials.iq.harvard.edu/R/Rstatistics/Rstatistics.html

R graphics: http://tutorials.iq.harvard.edu/R/Rgraphics/Rgraphics.html

R programming: http://tutorials.iq.harvard.edu/R/RProgramming/Rprogramming.html

1.11 Style

Reading: http://adv-r.had.co.nz/Style.html

Chapter 2

Basic tools

In this Chapter, we present basic tools that will be important when interacting with big data systems: the command-line interface (CLI) in a Unix shell and several utilities (`less`, `awk`, `vi` and `make`).

2.1 Command line tools

We assume some familiarity with the Unix shell, for example as in http://swcarpentry.github.io/shell-novice/.

We also assume that you have access to a shell, either because you use Linux or OS X or because you have the right tools on Windows (for example Cygwin or the Bash shell in Windows 10).

2.1.1 Why use the command line?

- Batch processing
- Cluster and cloud computing

2.1.2 Basic Unix tools

2.1.3 Useful tools

2.1.3.1 `less`

`less` is a pager that lets you view one page at a time files that can be very large.

File `DE1_0_2008_to_2010_Carrier_Claims_Sample_1A.csv` in `Data17/SyntheticMedicare` is 1.2GB. Even if we have enough RAM to process the data, `less` helps get a very quick sense of the data (variable names, separators, etc.)

2.1.3.2 `awk`

`awk` is a text-processing programming language available on most Unix systems. It can be used for data extraction.

2.1.3.3 `vi`

`vi` is a screen-based text editor available on almost all Unix systems. Most versions are actually `Vim` (that stands for "Vi IMproved").

There are many cheat sheets and tutorials available on-line (for example, the interactive http://www.openvim.com/). I invite you to learn basics `vi` commands.

2.1.4 Example

Let's apply some of the techniques described in Blackwell and Sen (2012) on Fisher's Iris data set saved in tab-delimited format. Of course, it is a small dataset easily processed with R:

```
iris <- read.table("~/Dropbox/Data17/iris/iris.tab")
head(iris, n = 5)
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5         0.2  setosa
## 5          5.0         3.6          1.4         0.2  setosa
```

In a shell, we can use:

```
head -n 6 ~/Dropbox/Data17/iris/iris.tab
```

```
## "Sepal.Length"   "Sepal.Width"   "Petal.Length"  "Petal.Width"   "Species"
## "1"  5.1 3.5 1.4 0.2 "setosa"
## "2"  4.9 3   1.4 0.2 "setosa"
## "3"  4.7 3.2 1.3 0.2 "setosa"
## "4"  4.6 3.1 1.5 0.2 "setosa"
## "5"  5   3.6 1.4 0.2 "setosa"
```

Suppose we only need to select two variables in our model, `Sepal.Length` and `Species`. In R, we can use:

```
iris_subset <- iris[, c("Sepal.Length", "Species")]
```

or

```
iris_subset <- iris[, c(1, 5)]
head(iris_subset)
```

```
##   Sepal.Length Species
## 1          5.1  setosa
## 2          4.9  setosa
## 3          4.7  setosa
## 4          4.6  setosa
## 5          5.0  setosa
## 6          5.4  setosa
```

With the tidyverse, we can use *pipes*. The `%>%` operator allows for performing chained operations.

```
suppressMessages(library(dplyr))

iris %>%
  select(1, 5) %>%
  head()
```

```
##   Sepal.Length Species
## 1          5.1  setosa
## 2          4.9  setosa
## 3          4.7  setosa
## 4          4.6  setosa
## 5          5.0  setosa
## 6          5.4  setosa
```

In a shell, the pipe operator to combine shell commands is `|` and we can use:

```
cut -f 1,5 ~/Dropbox/Data17/iris/iris.tab | head -n 7
```

```
## "Sepal.Length"   "Species"
## "1"  0.2
## "2"  0.2
## "3"  0.2
## "4"  0.2
## "5"  0.2
## "6"  0.4
```

To keep observations with "Sepal.Length" greater than 5:

```
iris %>%
  filter(Sepal.Length > 5) %>%
  head()
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          5.4         3.9          1.7         0.4  setosa
## 3          5.4         3.7          1.5         0.2  setosa
## 4          5.8         4.0          1.2         0.2  setosa
## 5          5.7         4.4          1.5         0.4  setosa
## 6          5.4         3.9          1.3         0.4  setosa
```

In the shell, we can use the `AWK` programming language. We start from row `NR` 2 (we could start from row 1, it contains variable names) and select rows such that the second variable (`Sepal.Length`) is greater than 5.

```
awk 'NR == 2 || $2 > 5' ~/Dropbox/Data17/iris/iris.tab | head
```

```
## "1"  5.1 3.5 1.4 0.2 "setosa"
## "6"  5.4 3.9 1.7 0.4 "setosa"
## "11" 5.4 3.7 1.5 0.2 "setosa"
## "15" 5.8 4   1.2 0.2 "setosa"
## "16" 5.7 4.4 1.5 0.4 "setosa"
## "17" 5.4 3.9 1.3 0.4 "setosa"
## "18" 5.1 3.5 1.4 0.3 "setosa"
## "19" 5.7 3.8 1.7 0.3 "setosa"
## "20" 5.1 3.8 1.5 0.3 "setosa"
## "21" 5.4 3.4 1.7 0.2 "setosa"
```

Exercise 2.1. The iris dataset is also saved in .csv format at `~/Dropbox/Data17/iris/iris.csv`. Use `AWK` and `tail` to select the last 5 observations where `Sepal.Width` is larger than 3.5 and `Petal.Length` is smaller than 1.5.

2.2 Makefiles

`make` is a tool that helps put all the (interdependent) pieces of an analytic workflow together:

- data retrieving
- data cleaning
- analysis
- graphs
- reports
- …

2.2.1 Simulate data in R

```
set.seed(123)
```

File `simulate_data.R`

```
# set.seed(123)
N <- 1000 # sample size

X1 <- rpois(n = N, lambda = 50)
X2 <- 10 + rbinom(n = N, prob = 0.8, size = 1)
Y <- 10 + 3 * X1 + -5 * X2 + 3 * rnorm(n = N)

write.csv(data.frame(Y = Y, X1 = X1, X2 = X2),
          "sample_data.csv", row.names = FALSE)
```

```
head(data.frame(Y = Y, X1 = X1, X2 = X2))
```

```
##           Y X1 X2
## 1  88.74430 46 11
## 2 125.77081 58 11
## 3  70.76396 38 10
## 4 110.32157 50 10
## 5 145.79546 62 11
## 6 109.45403 53 11
```

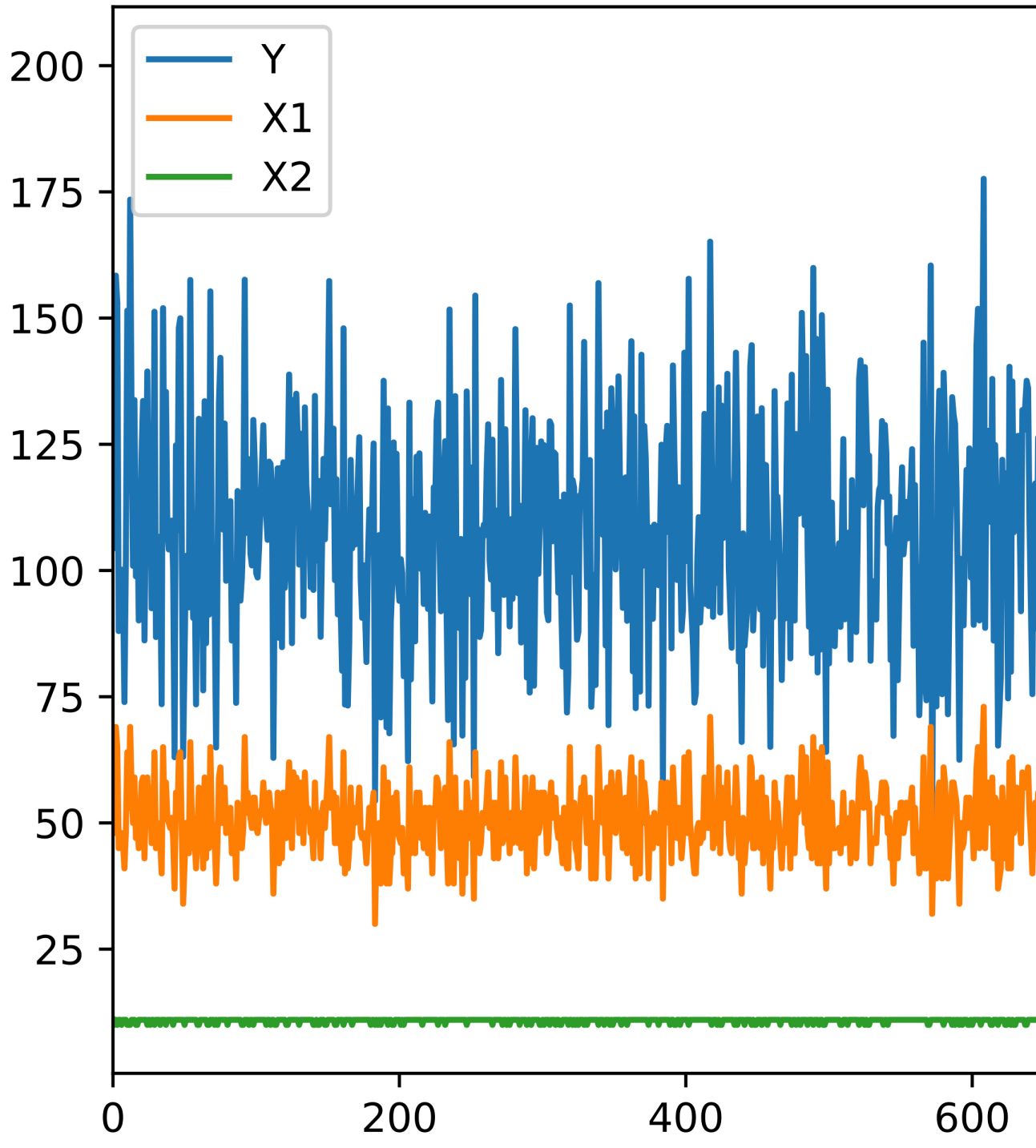
2.2.2 Create a plot in Python

File `create_graph.py`

```
import pandas as pd
import matplotlib.pyplot as plt

sim_data = pd.read_csv("sample_data.csv")

plt.figure()
sim_data.plot()
plt.savefig("plot.pdf", format = "pdf")
```


Y
X1
X2
200
175
150
125
100
75
50
25
0
200
400
600

2.2.3 Run statistical model in R

We can estimate the model with R:

```
sim_data <- read.csv("sample_data.csv")
summary(lm(Y ~ X1 + X2, data = sim_data))
```

```
##
## Call:
## lm(formula = Y ~ X1 + X2, data = sim_data)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -8.3988 -1.9452 -0.0261  2.0216  9.1066
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  9.09087    2.54667    3.57 0.000374 ***
## X1           3.00531    0.01326  226.68  < 2e-16 ***
## X2          -4.94658    0.22876  -21.62  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.936 on 997 degrees of freedom
## Multiple R-squared:  0.9811, Adjusted R-squared:  0.981
## F-statistic: 2.585e+04 on 2 and 997 DF,  p-value: < 2.2e-16
```

2.2.4 Run statistical model in R

To save the output, we use the `sink` function.

File `estimate_model.R`

```
sink("estimation_summary.txt")
summary(lm(Y ~ X1 + X2, data = sim_data))
sink()
```

2.2.5 Makefile syntax

- `make` is a *command* that runs on a text file often named `Makefile`.
- A `Makefile` contains one or several blocks with the following structure:

```
targetfile: sourcefile(s)
[tab] command
```

2.2.6 Naive version

File: `Makefile`

```
sample_data.csv: simulate_data.R
    R CMD BATCH simulate_data.R

plot.pdf: create_graph.py
    python create_graph.py
```

```
estimation_summary.txt: estimate_model.R
    R CMD BATCH estimate_model.R
```

A simple call to `make` only builds the first target (`sample_data.csv`). To build the other targets, we have to use: `make plot.pdf` and `make estimation_summary.txt`.

2.2.7 Making all targets

File: `Makefile`

```
all: analysis

analysis: sample_data.csv plot.pdf estimation_summary.txt

sample_data.csv: simulate_data.R
    R CMD BATCH simulate_data.R

plot.pdf: create_graph.py
    python create_graph.py

estimation_summary.txt: estimate_model.R
    R CMD BATCH estimate_model.R
```

New data is simulated and saved in `sample_data.csv`. But `plot.pdf` and `estimation_summary.txt` are not updated.

2.2.8 Dealing with dependencies

- Problem `plot.pdf` and `estimation_summary.txt` depend on `sample_data.csv`.
- Solution: explicit dependencies.

File: `Makefile`

```
all: analysis

analysis: sample_data.csv plot.pdf estimation_summary.txt

sample_data.csv: simulate_data.R
    R CMD BATCH simulate_data.R

plot.pdf: sample_data.csv create_graph.py
    python create_graph.py

estimation_summary.txt: sample_data.csv estimate_model.R
    R CMD BATCH estimate_model.R
```

2.3 Git and GitHub

Guest lecture by Ista Zahn.

Chapter 3

Packages

We strongly recommand Wickham (2015).

We assume the following packages are installed:

```
install.packages(c("devtools", "roxygen2", "testthat", "knitr"))
```

3.1 Why?

- Organize your code
- Distribute your code
- Keep versions of your code

3.2 Package structure

- Folder hierarchy
  - `NAMESPACE`: package import / export
  - `DESCRIPTION`: metadata
  - `R/`: R code
  - `man/`: object documentation (with short examples)
  - `tests/`
  - `data/`
  - `src/`: compiled code
  - `vignettes/`: manual-like documentation
  - `inst/`: installed files
  - `demo/`: longer examples
  - `exec`, `po`, `tools`

3.3 Building steps

- `R CMD build`
- `R CMD INSTALL`
- `R CMD check`

3.3.1 R CMD build

```
R CMD build --help
```

Build R packages from package sources in the directories specified by 'pkgdirs'

3.3.2 R CMD INSTALL

```
R CMD INSTALL --help
```

Install the add-on packages specified by pkgs. The elements of pkgs can be relative or absolute paths to directories with the package sources, or to gzipped package 'tar' archives. The library tree to install to can be specified via '–library'. By default, packages are installed in the library tree rooted at the first directory in .libPaths() for an R session run in the current environment.

3.3.3 R CMD check

```
R CMD check --help
```

http://r-pkgs.had.co.nz/check.html

Check R packages from package sources, which can be directories or package 'tar' archives with extension '.tar.gz', '.tar.bz2', '.tar.xz' or '.tgz'.

A variety of diagnostic checks on directory structure, index and control files are performed. The package is installed into the log directory and production of the package PDF manual is tested. All examples and tests provided by the package are tested to see if they run successfully. By default code in the vignettes is tested, as is re-building the vignette PDFs.

3.3.4 Building steps with `devtools`

- `devtools::build`
- `devtools::install`
- `devtools::check`
- and many others: `load_all`, `document`, `test`, `run_examples`, …

3.4 Create an R package

3.4.1 `utils::package.skeleton`

```
package.skeleton() # "in "clean" session ("anRpackage")
package.skeleton("pkgname") # in "clean" session

set.seed(02138)
f <- function(x, y) x+y
g <- function(x, y) x-y
d <- data.frame(a = 1, b = 2)
e <- rnorm(1000)
package.skeleton(list = c("f","g","d","e"), name = "pkgname")
```

Figure 3.1: Submitting to CRAN. It's not that bad...

3.4.2 `devtools::create`

```
devtools::create("path/to/package/pkgname")
```

Also from RStudio ('File -> New Project').

3.4.3 Submit to CRAN

Reading: http://r-pkgs.had.co.nz/release.html

3.5 R packages on GitHub

Reading: http://r-pkgs.had.co.nz/git.html

- Version control
- Website, wiki, project management
- Easy install: `install_github` from `devtools`
- Collaboration
- Issue tracking

3.5.0.1 RStudio and GitHub integration

Command line

```
# git init # already run when creating package with RStudio
git add *
git commit -m "First commit"
git remote add origin https://github.com/cchoirat/Linreg
git push -u origin master
```

3.5.1 `.gitignore`

RStudio default

```
.Rproj.user
.Rhistory
.RData
```

GitHub default

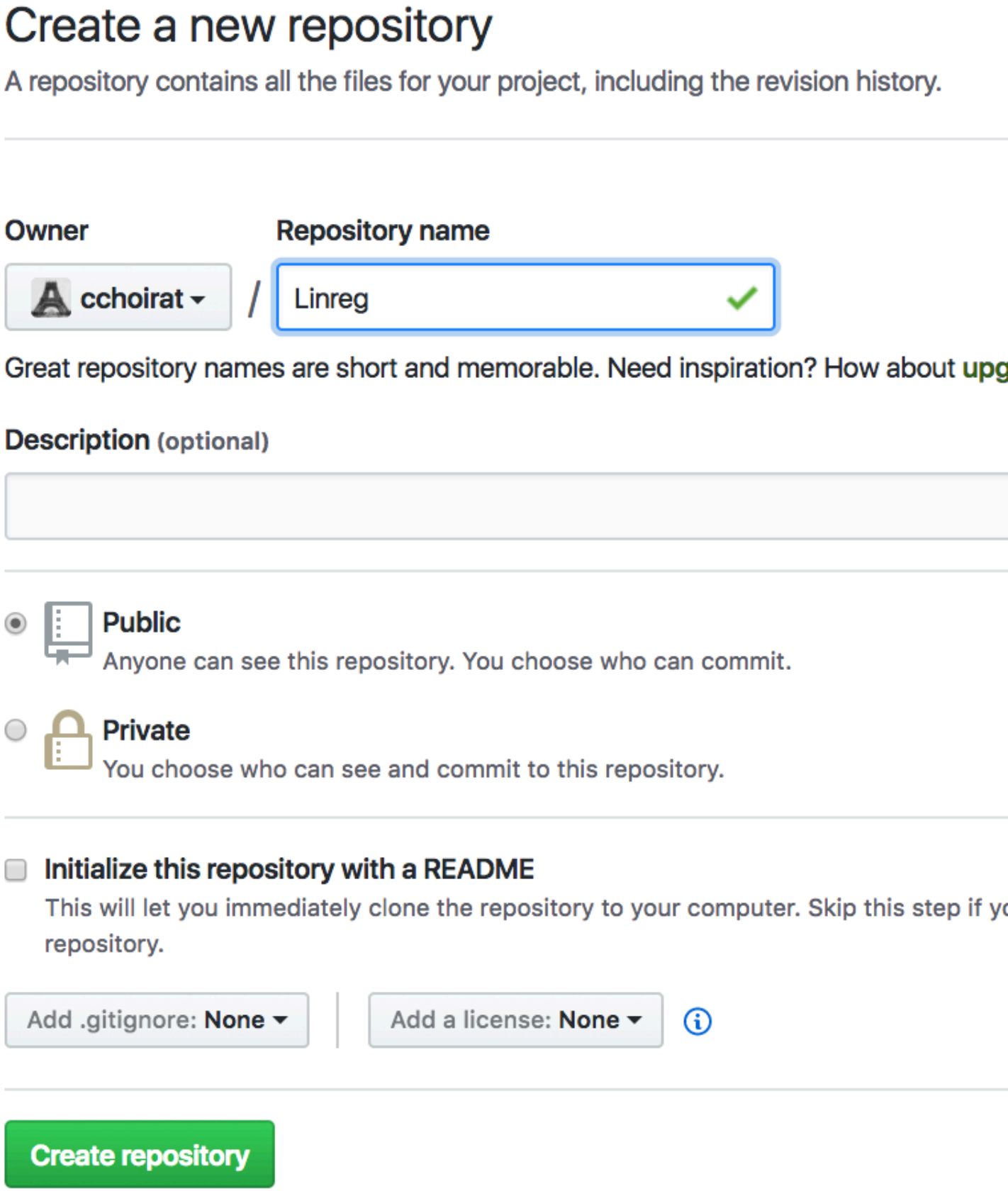


Figure 3.2: Create a new Linreg repository on GitHub

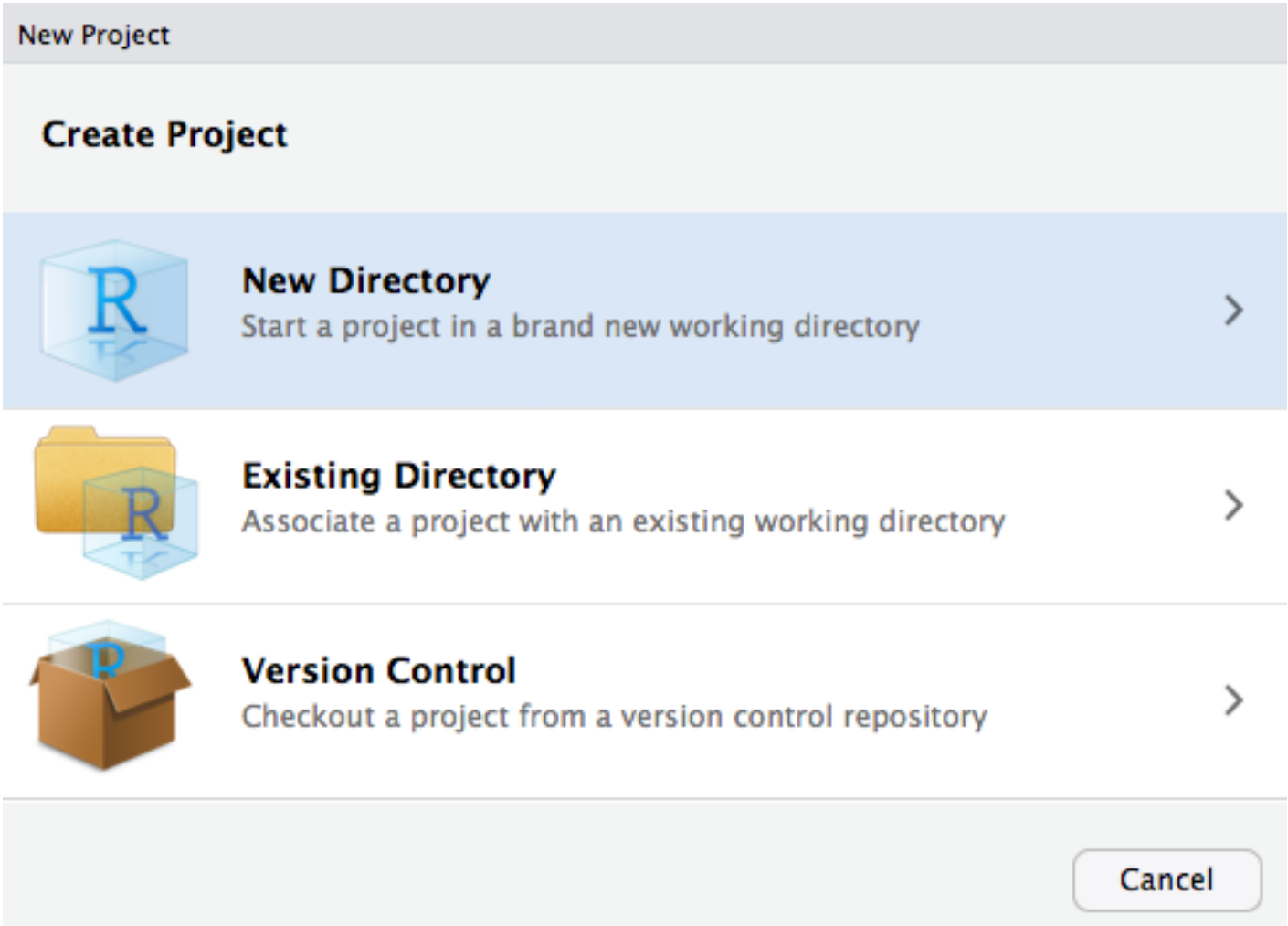


Figure 3.3: Create a new project in RStudio

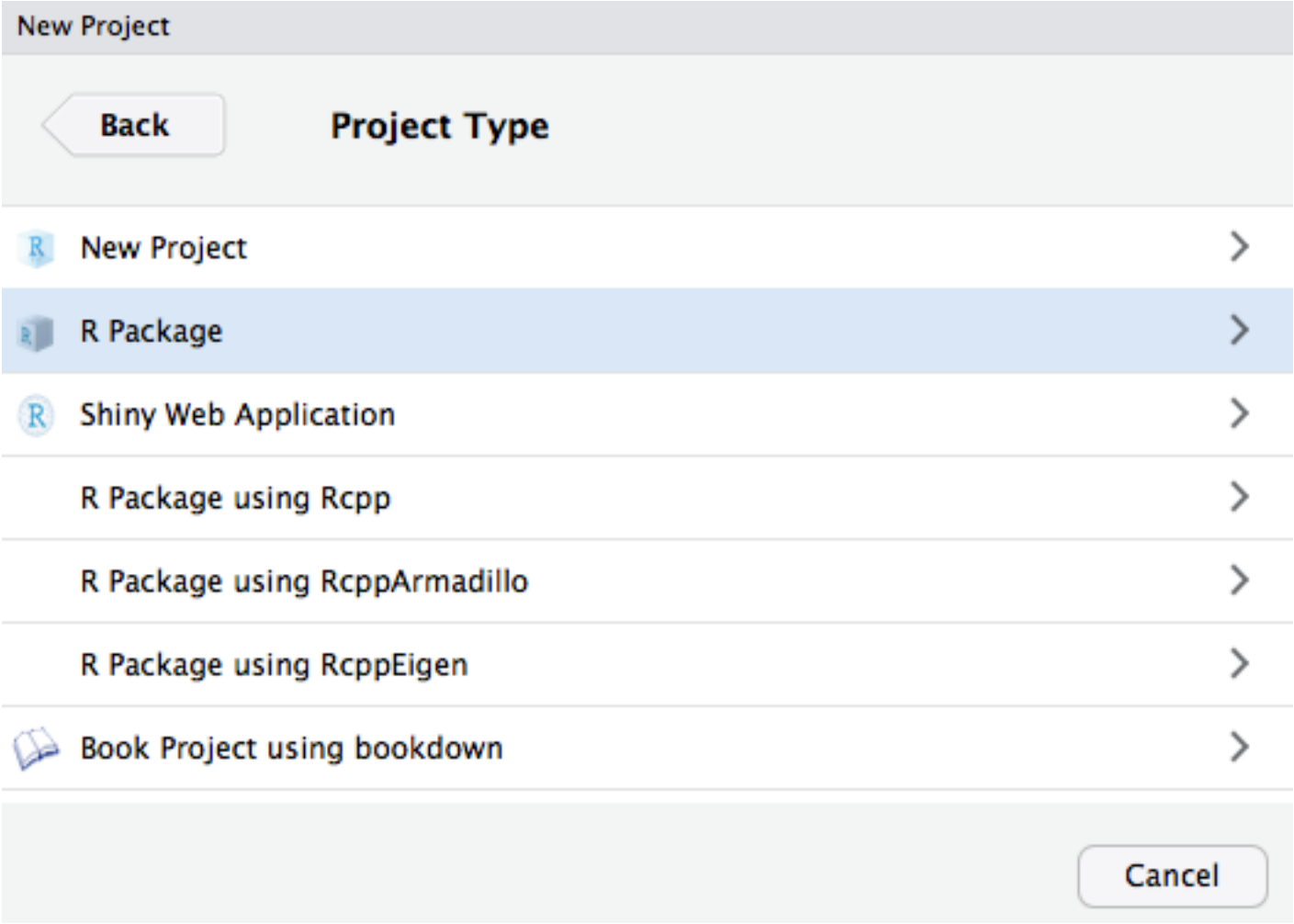


Figure 3.4: Select R package

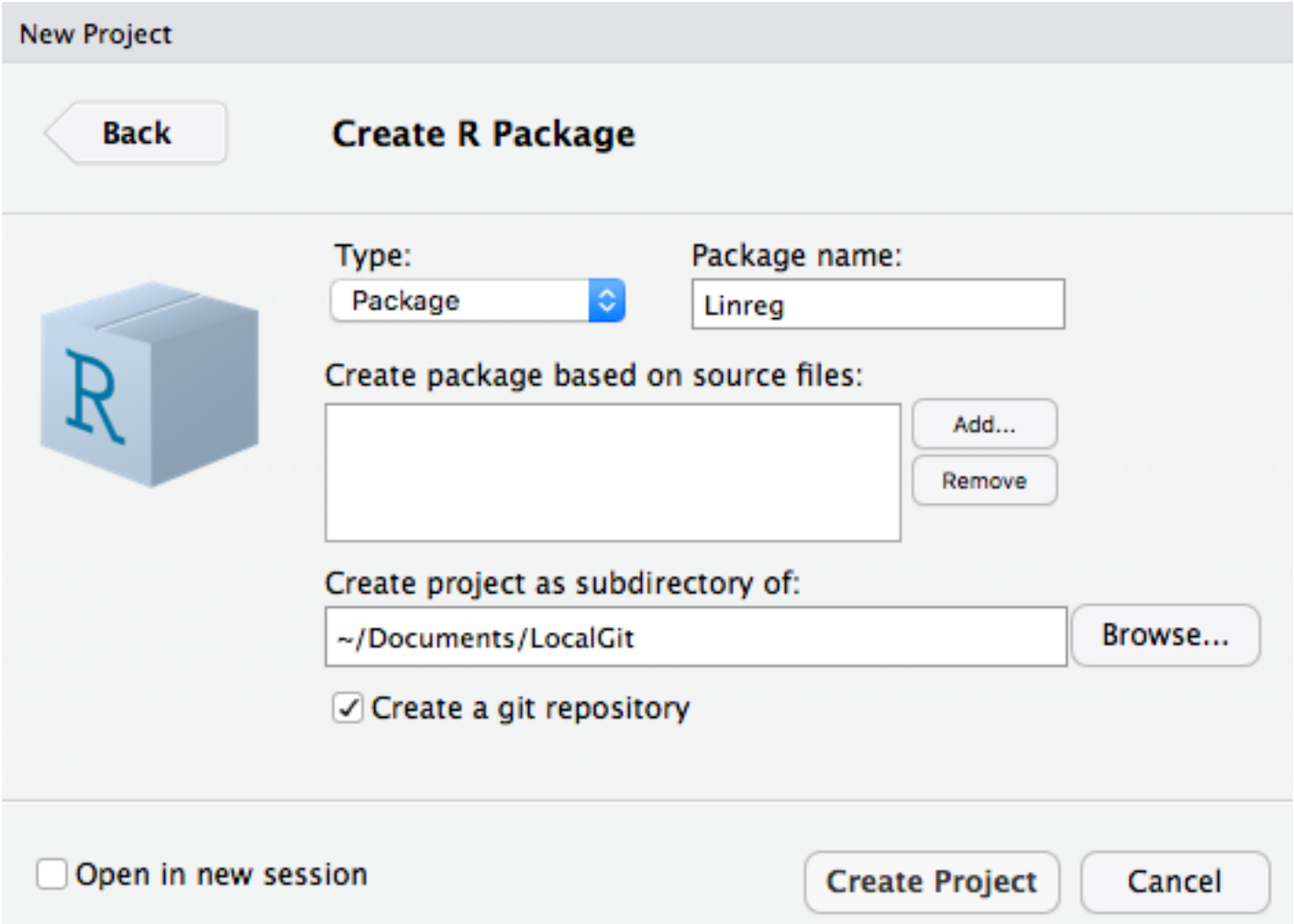


Figure 3.5: Create the Linreg R package as a Git repository

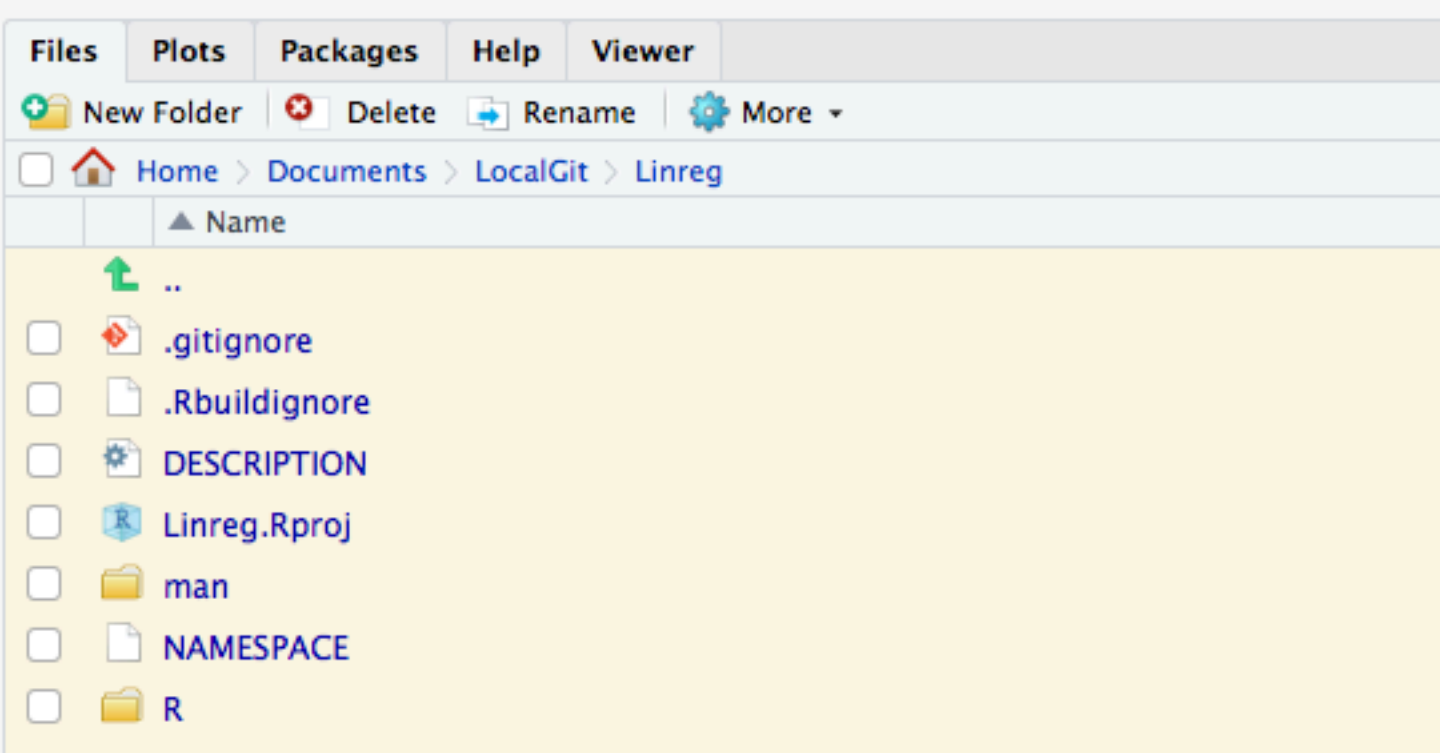


Figure 3.6: Automatically created files

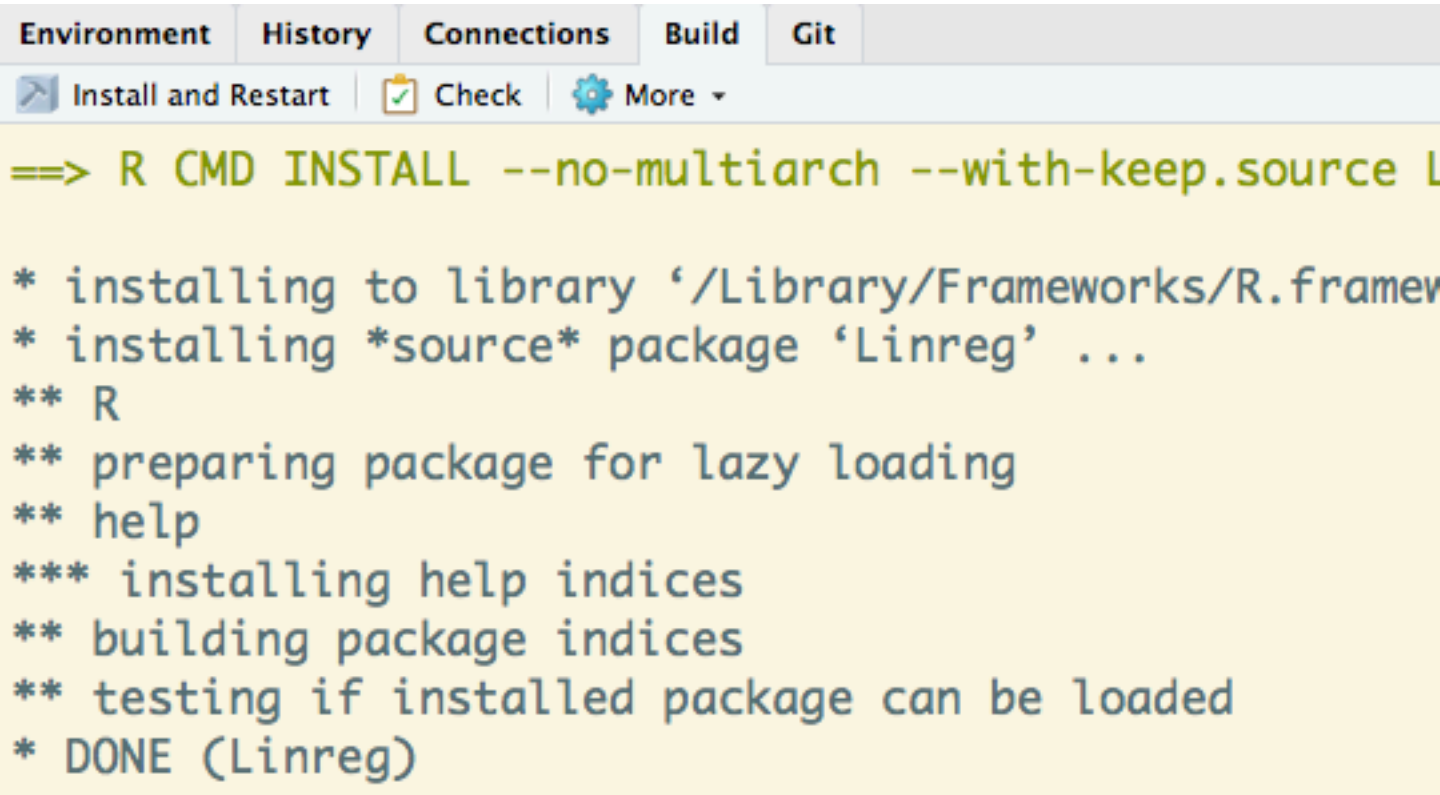


Figure 3.7: Build tab in RStudio

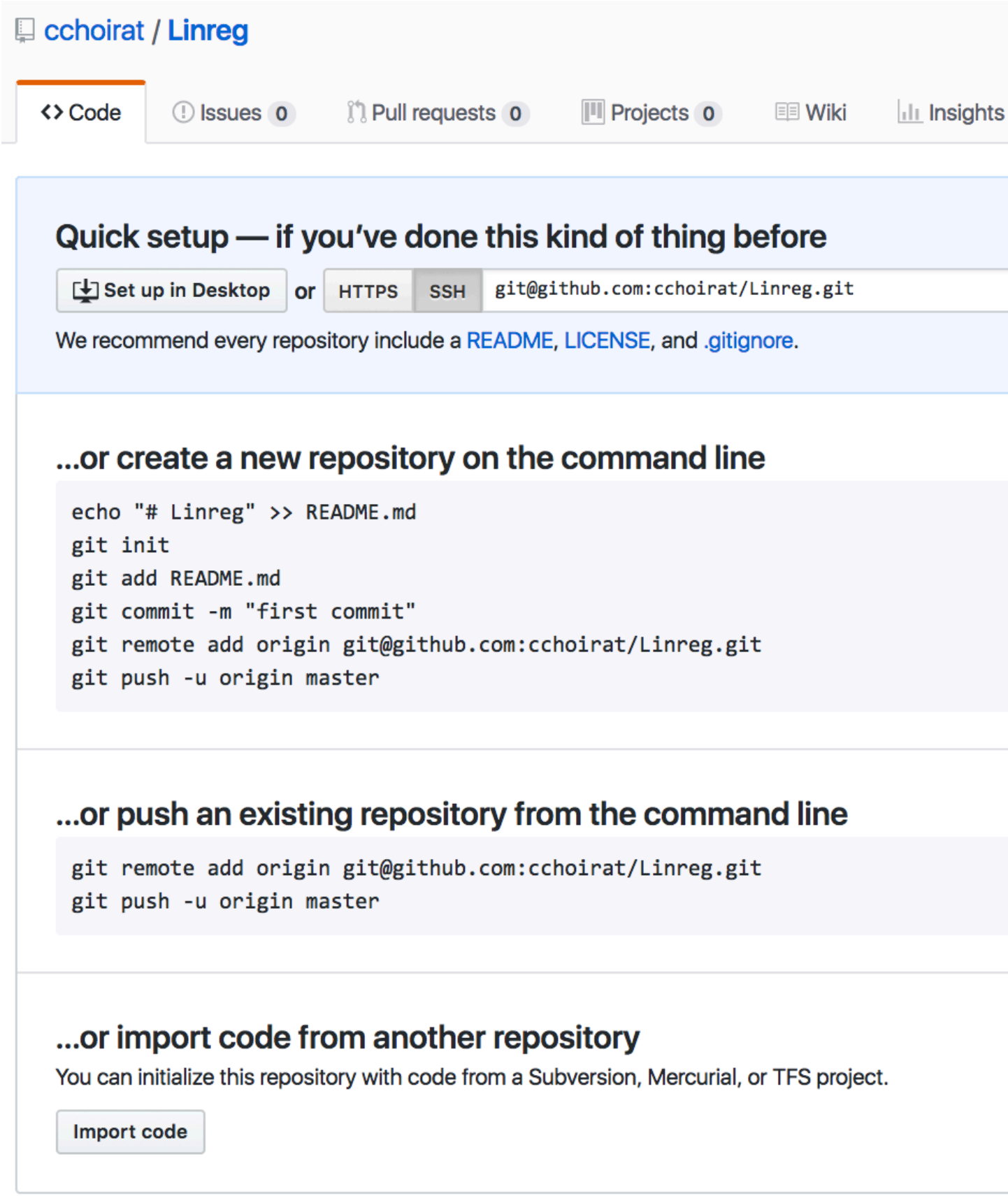


Figure 3.8: Github webpage

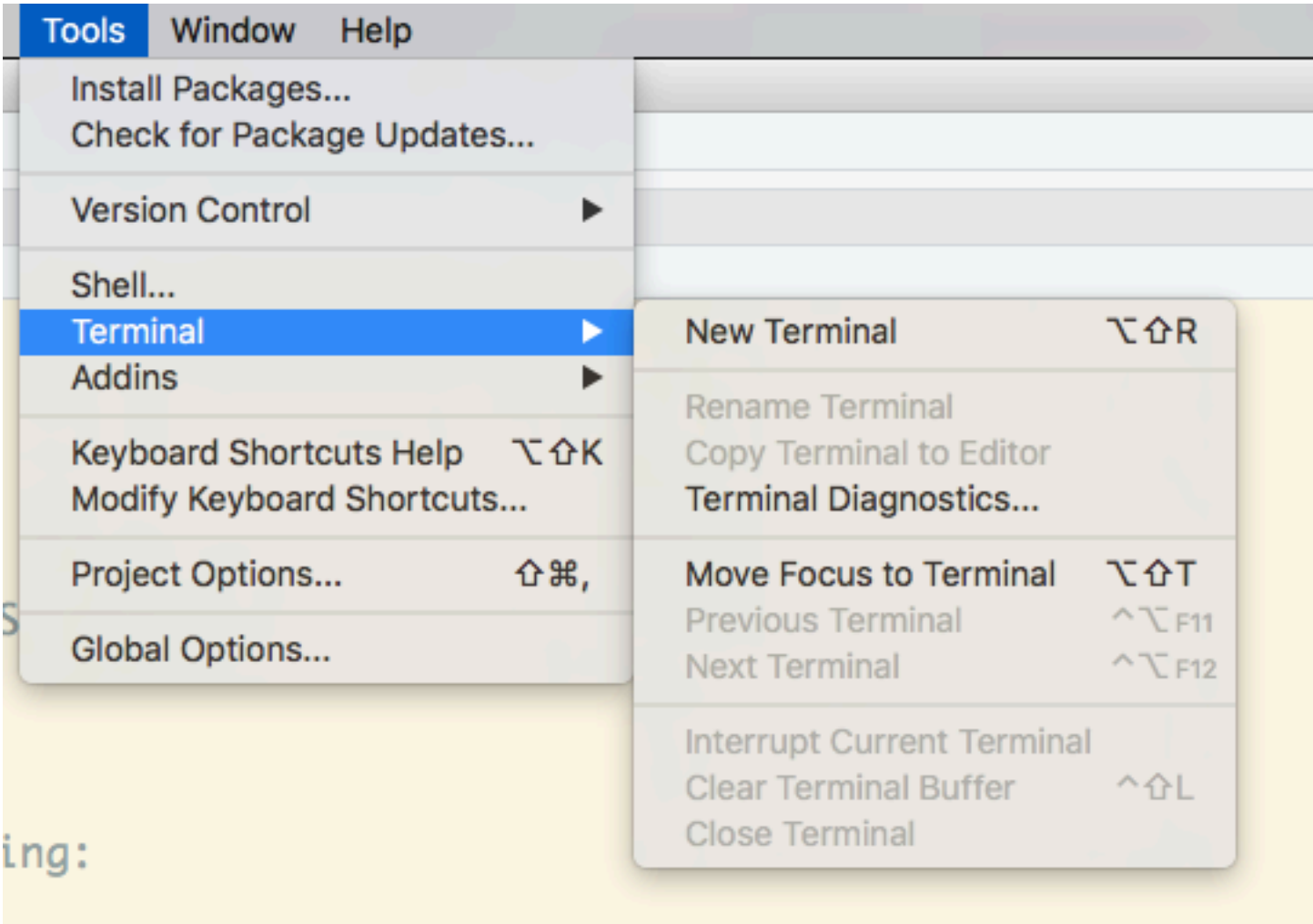


Figure 3.9: Open a terminal

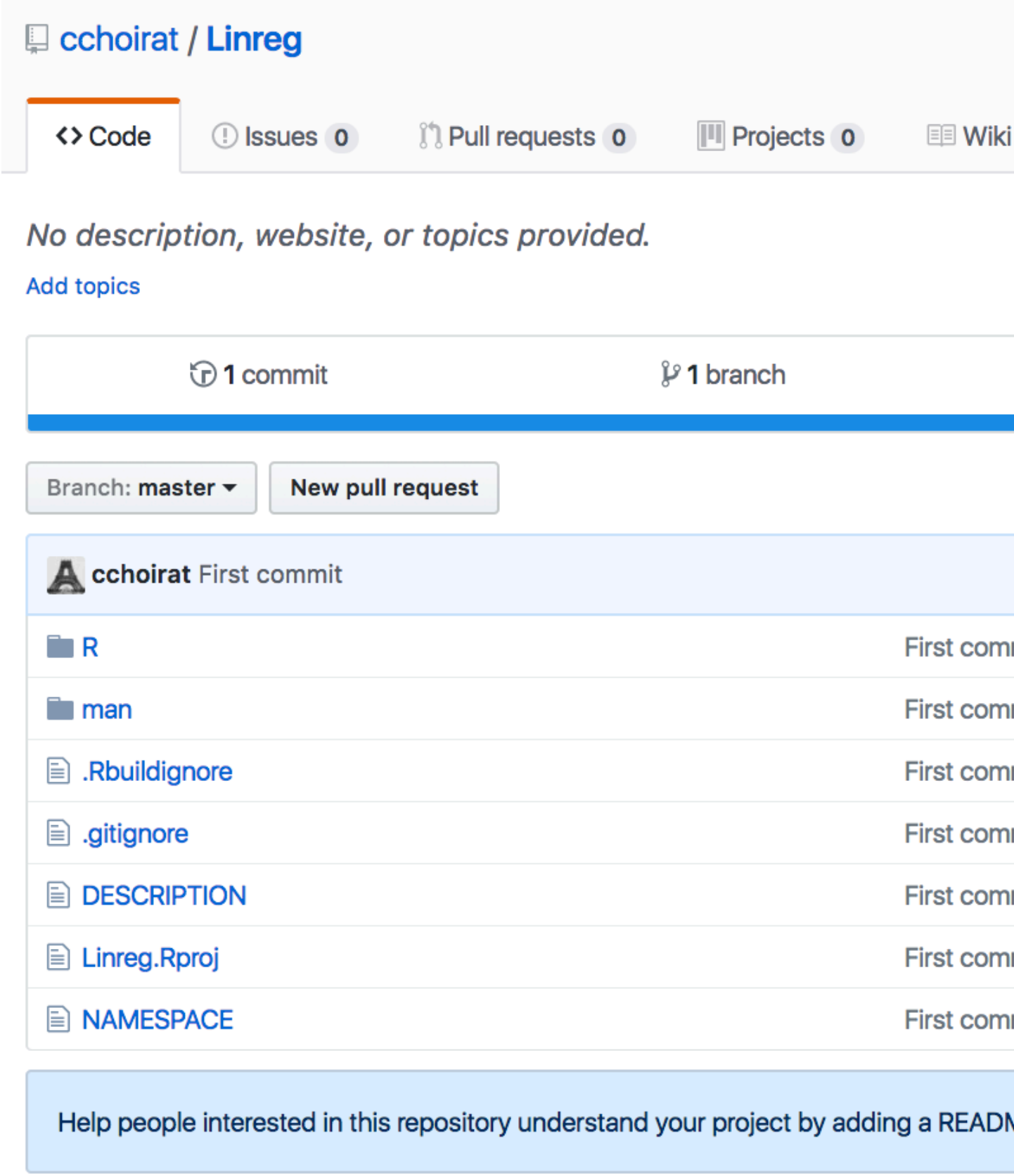


Figure 3.10: Github webpage is updated

```
# History files
.Rhistory
.Rapp.history

# Example code in package build process
*-Ex.R

# RStudio files
.Rproj.user/

# produced vignettes
vignettes/*.html
vignettes/*.pdf
```

3.6 RStudio projects

- `.Rproj` file extension, in our example `Linreg.Rproj`
- A project has its own:
  - R session
  - .Rprofile (*e.g.*, to customize startup environment)
  - .Rhistory
- Default working directory is project directory
- Keeps track of project-specific recent files

3.6.1 Project options

```
Version: 1.0

RestoreWorkspace: Default
SaveWorkspace: Default
AlwaysSaveHistory: Default

EnableCodeIndexing: Yes
UseSpacesForTab: Yes
NumSpacesForTab: 2
Encoding: UTF-8

RnwWeave: knitr
LaTeX: pdfLaTeX

AutoAppendNewline: Yes
StripTrailingWhitespace: Yes

BuildType: Package
PackageUseDevtools: Yes
PackageInstallArgs: --no-multiarch --with-keep.source
```

3.6.2 Package documentation

- Functions and methods
- Vignettes
  - PDF
  - `knitr`

3.7 Package workflow example

Creating R Packages: A Tutorial (Friedrich Leisch, 2009)

Our example is adapted from https://cran.r-project.org/doc/contrib/Leisch-CreatingPackages.pdf.

3.7.1 Add `linreg.R` to `R/` directory

```
linmodEst <- function(x, y) {
  ## CC: crossprod or a QR decomposition (as in the original version) are more efficient
  coef <- solve(t(x) %*% x) %*% t(x) %*% y
  print(coef)
  ## degrees of freedom and standard deviation of residuals
  df <- nrow(x) - ncol(x)
  sigma2 <- sum((y - x %*% coef) ^ 2) / df
  ## compute sigma^2 * (x'x)^-1
  vcov <- sigma2 * solve(t(x) %*% x)
  colnames(vcov) <- rownames(vcov) <- colnames(x)
  list(
    coefficients = coef,
    vcov = vcov,
    sigma = sqrt(sigma2),
    df = df
  )
}
```

3.7.2 Run our function

```
data(cats, package = "MASS")
linmodEst(cbind(1, cats$Bwt), cats$Hwt)
```

```
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
```

```
## $coefficients
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##
## $vcov
##            [,1]        [,2]
## [1,]  0.4792475 -0.17058197
## [2,] -0.1705820  0.06263081
```

```
##
## $sigma
## [1] 1.452373
##
## $df
## [1] 142
```

We can compare the output with `lm`.

```r
lm1 <- lm(Hwt ~ Bwt, data = cats)
lm1
```

```
##
## Call:
## lm(formula = Hwt ~ Bwt, data = cats)
##
## Coefficients:
## (Intercept)          Bwt
##     -0.3567       4.0341
```

```r
coef(lm1)
```

```
## (Intercept)         Bwt
##  -0.3566624   4.0340627
```

```r
vcov(lm1)
```

```
##             (Intercept)         Bwt
## (Intercept)   0.4792475 -0.17058197
## Bwt          -0.1705820  0.06263081
```

```r
summary(lm1)$sigma
```

```
## [1] 1.452373
```

3.7.3 Add ROxygen2 documentation

Reading: http://kbroman.org/pkg_primer/pages/docs.html

```r
#' Linear regression
#'
#' Runs an OLS regression not unlike \code{\link{lm}}
#'
#' @param y response vector (1 x n)
#' @param X covariate matrix (p x n) with no intercept
#'
#' @return A list with 4 elements: coefficients, vcov, sigma, df
#'
#' @examples
#' data(mtcars)
#' X <- as.matrix(mtcars[, c("cyl", "disp", "hp")])
#' y <- mtcars[, "mpg"]
#' linmodEst(y, X)
#'
#' @export
#'
linmodEst <- function(x, y) {
  ## CC: crossprod or a QR decomposition (as in the original version) are more efficient
```

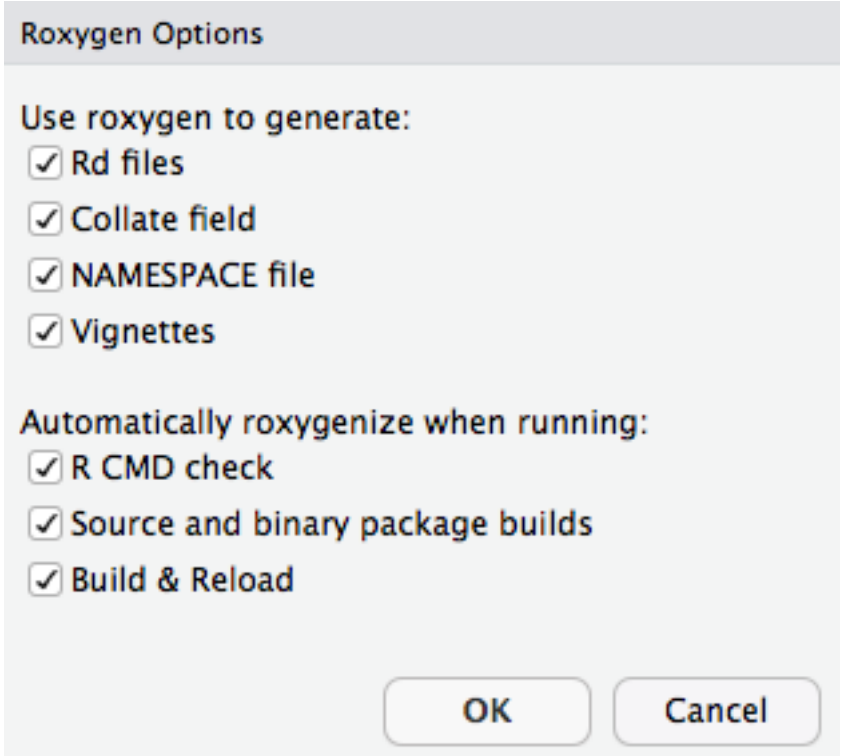


Figure 3.11: Roxygen options

```
  coef <- solve(t(x) %*% x) %*% t(x) %*% y
  print(coef)
  ## degrees of freedom and standard deviation of residuals
  df <- nrow(x) - ncol(x)
  sigma2 <- sum((y - x %*% coef) ^ 2) / df
  ## compute sigma^2 * (x'x)^-1
  vcov <- sigma2 * solve(t(x) %*% x)
  colnames(vcov) <- rownames(vcov) <- colnames(x)
  list(
    coefficients = coef,
    vcov = vcov,
    sigma = sqrt(sigma2),
    df = df
  )
}
```

3.7.4 Configure Build Tools

3.7.5 man page

File ‘man/linmodEst.Rd contains:

```
% Generated by roxygen2: do not edit by hand
% Please edit documentation in R/linreg.R
\name{linmodEst}
\alias{linmodEst}
```

```
\title{Linear regression}
\usage{
linmodEst(x, y)
}
\arguments{
\item{y}{response vector (1 x n)}

\item{X}{covariate matrix (p x n) with no intercept}
}
\value{
A list with 4 elements: coefficients, vcov, sigma, df
}
\description{
Runs an OLS regression not unlike \code{\link{lm}}
}
\examples{
data(mtcars)
X <- as.matrix(mtcars[, c("cyl", "disp", "hp")])
y <- mtcars[, "mpg"]
linmodEst(y, X)

}
```

3.7.6 Formatted output

3.7.7 DESCRIPTION

Reading: http://r-pkgs.had.co.nz/description.html

```
Package: Linreg
Type: Package
Title: What the Package Does (Title Case)
Version: 0.1.0
Author: Who wrote it
Maintainer: The package maintainer <yourself@somewhere.net>
Description: More about what it does (maybe more than one line)
    Use four spaces when indenting paragraphs within the Description.
License: What license is it under?
Encoding: UTF-8
LazyData: true
RoxygenNote: 6.0.1
```

3.7.8 NAMESPACE

Reading: http://r-pkgs.had.co.nz/namespace.html, in particular `Imports` vs `Suggests`

`export`'s automatically generated when parsing ROxygen2 snippets

```
export(linmodEst)
```

- A scary hack
- A scary tree

Reading: https://git-scm.com/book/en/v2/Git-Branching-Basic-Branching-and-Merging

linmodEst {Linreg}

Linear regression

Description

Runs an OLS regression not unlike `lm`

Usage

```
linmodEst(x, y)
```

Arguments

`y`	response vector (1 x n)
`X`	covariate matrix (p x n) with no intercept

Value

A list with 4 elements: coefficients, vcov, sigma, df

Examples

```
data(mtcars)
X <- as.matrix(mtcars[, c("cyl", "disp", "hp")])
y <- mtcars[, "mpg"]
linmodEst(y, X)
```

3.7.9 S3 basics

Reading: http://adv-r.had.co.nz/S3.html

```
hello <- function() {
 s <- "Hello World!"
 class(s) <- "hi"
 return(s)
}

hello()
```

```
## [1] "Hello World!"
## attr(,"class")
## [1] "hi"
```

```
print.hi <- function(...) {
  print("Surprise!")
}

hello()
```

```
## [1] "Surprise!"
```

3.7.10 S3 and S4 generics

Reading: http://adv-r.had.co.nz/S4.html

```
linmod <- function(x, ...)
  UseMethod("linmod")
```

```
linmod.default <- function(x, y, ...) {
  x <- as.matrix(x)
  y <- as.numeric(y)
  est <- linmodEst(x, y)
  est$fitted.values <- as.vector(x %*% est$coefficients)
  est$residuals <- y - est$fitted.values
  est$call <- match.call()
  class(est) <- "linmod"
  return(est)
}
```

3.7.11 print

```
print.linmod <- function(x, ...) {
  cat("Call:\n")
  print(x$call)
  cat("\nCoefficients:\n")
  print(x$coefficients)
}
```

```
x <- cbind(Const = 1, Bwt = cats$Bwt)
y <- cats$Hw
mod1 <- linmod(x, y)
```

```
##             [,1]
## Const -0.3566624
## Bwt    4.0340627
```

```
mod1
```

```
## Call:
## linmod.default(x = x, y = y)
##
## Coefficients:
##             [,1]
## Const -0.3566624
## Bwt    4.0340627
```

3.7.12 Other methods

- `summary.linmod`
- `print.summary.linmod`
- `predict.linmod`
- `plot.linmod`
- `coef.linmod`, `vcov.linmod`, …

Exercise 3.1. Write two functions that implement the `coef.linmod` and `vcov.linmod` methods.

3.7.13 Formulas and model frames

Reading: http://genomicsclass.github.io/book/pages/expressing_design_formula.html

`model.frame` (a generic function) and its methods return a data.frame with the variables needed to use formula and any … arguments.

`model.matrix` creates a design (or model) matrix, e.g., by expanding factors to a set of dummy variables (depending on the contrasts) and expanding interactions similarly.

`model.response` returns the response of a model frame passed as optional arguments to model.frame.

Exercise 3.2. What is `model.extract`?

```
linmod.formula <- function(formula, data = list(), ...) {
  mf <- model.frame(formula = formula, data = data)
  x <- model.matrix(attr(mf, "terms"), data = mf)
  y <- model.response(mf)
  est <- linmod.default(x, y, ...)
  est$call <- match.call()
  est$formula <- formula
  return(est)
}
```

```
linmod(Hwt ~ - 1 + Bwt * Sex, data = cats)
```

```
Call:
linmod.formula(formula = Hwt ~ -1 + Bwt * Sex, data = cats)

Coefficients:
      Bwt      SexF      SexM  Bwt:SexM
 2.636414  2.981312 -1.184088  1.676265
```

3.8 Unit testing

3.8.1 Unit tests and `testthat`

Reading: http://r-pkgs.had.co.nz/tests.html

In package directory:

```
devtools::use_testthat()
```

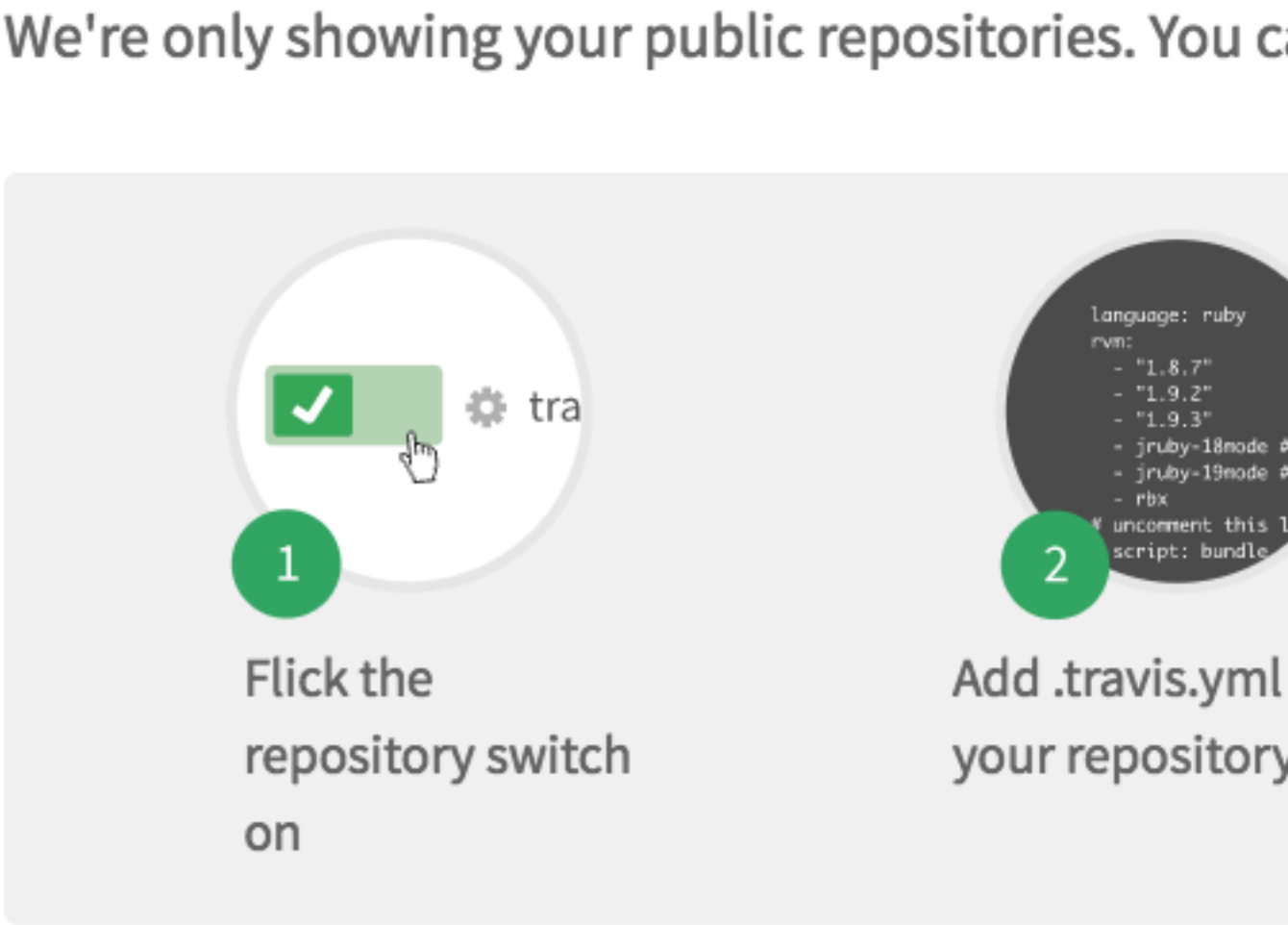
pre-populates `test/testthat/`

Test files should start with `test` to be processed.

3.8.2 `test_coef.R`

```
data(cats, package = "MASS")
l1 <- linmod(Hwt ~ Bwt * Sex, data = cats)
l2 <- lm(Hwt ~ Bwt * Sex, data = cats)

test_that("same estimated coefficients as lm function", {
  expect_equal(round(l1$coefficients, 3), round(l2$coefficients, 3))
})
```




```
> devtools::test()
Loading Linreg
Loading required package: testthat
Testing Linreg
.
DONE ==========================================================================================
```

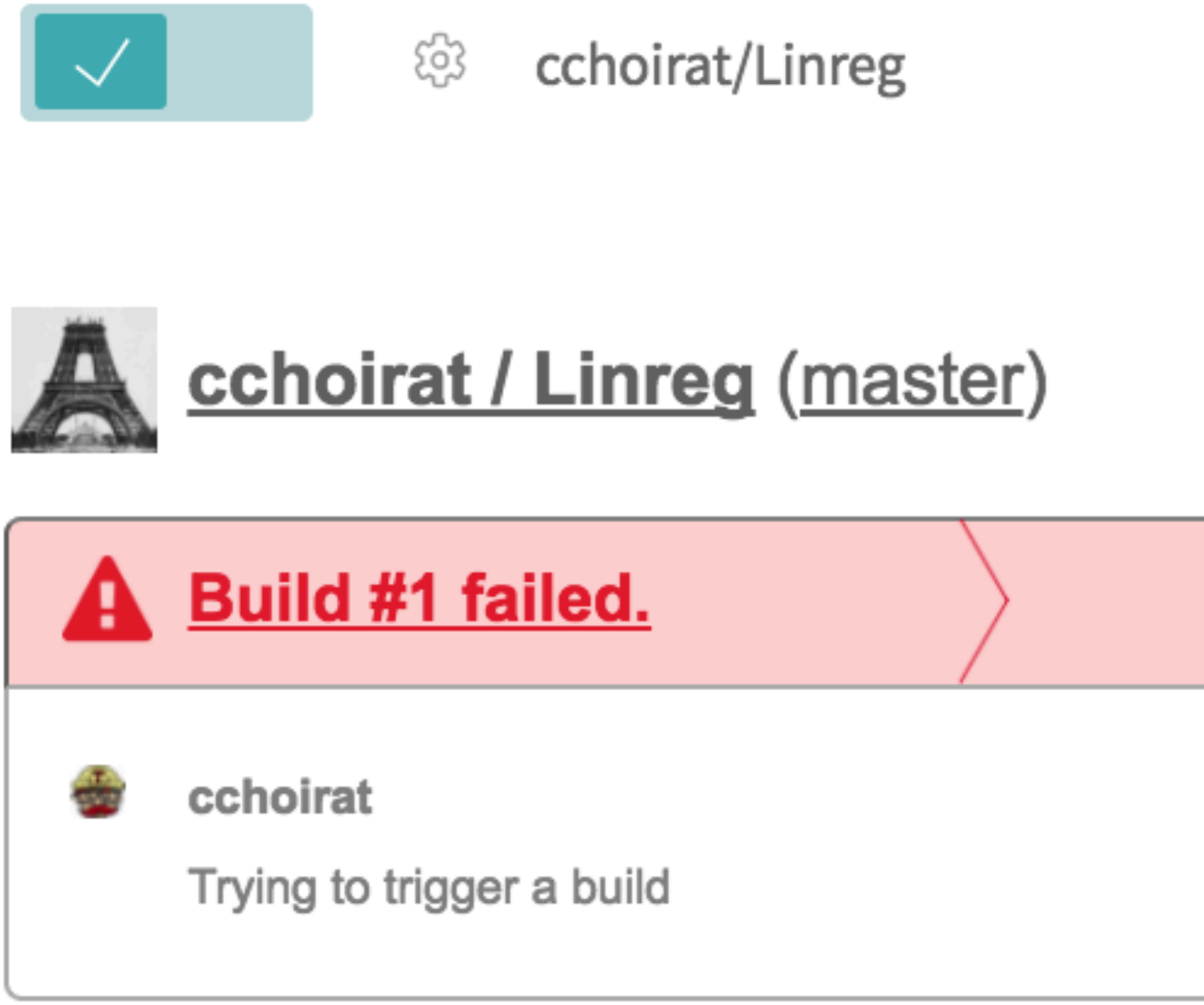
3.9 Continuous integration

Readings: - http://r-pkgs.had.co.nz/check.html#travis - https://juliasilge.com/blog/beginners-guide-to-travis/

Website: https://travis-ci.org/

First step is to create a Travis account and link it to you GitHub account.

Travis will list all your public GitHub repositories for you to select the ones you want to test.



Calling

```
devtools::use_coverage(pkg = ".", type = c("codecov"))
```

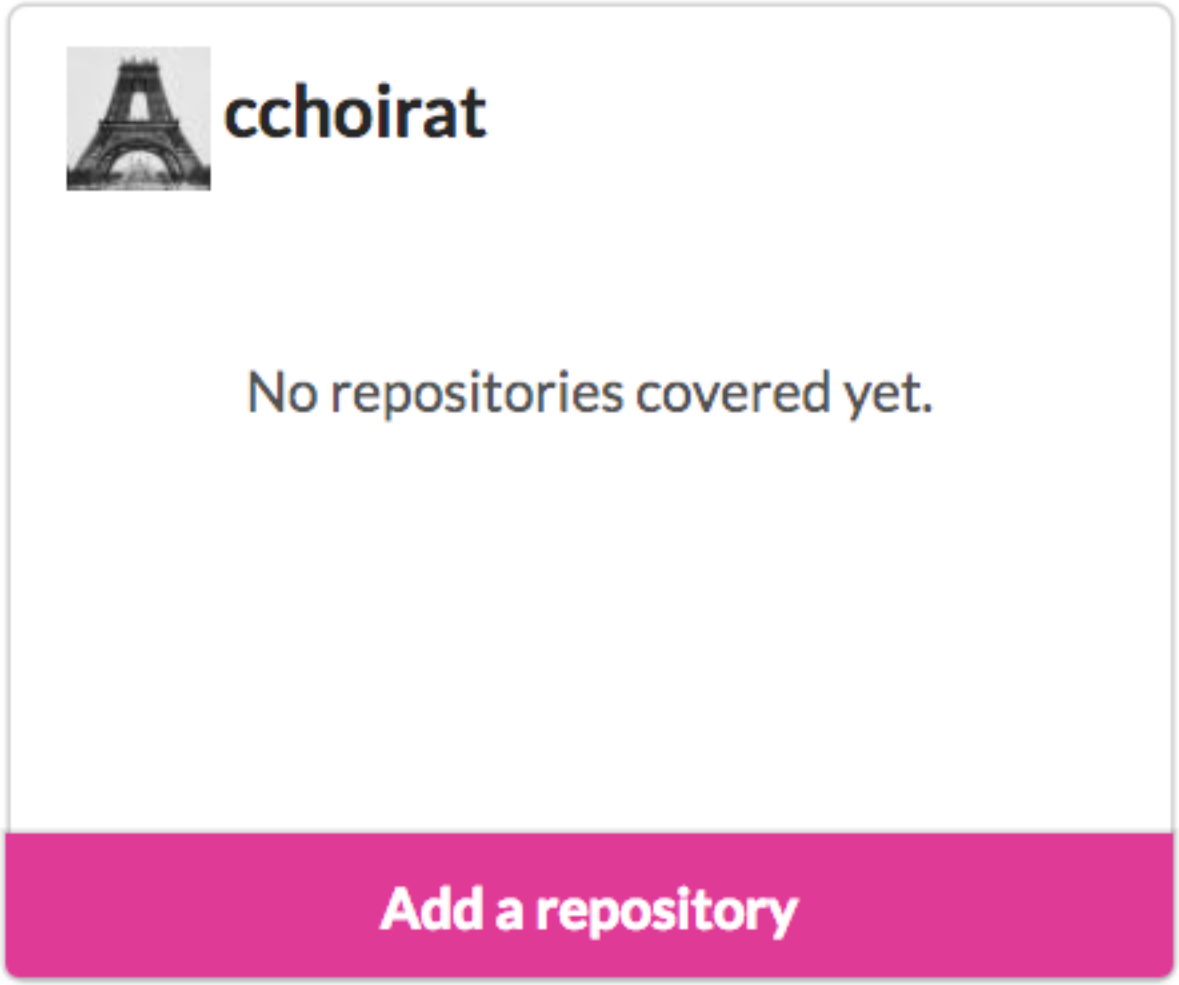
creates the `.travis.yml` file:

```
# R for travis: see documentation at https://docs.travis-ci.com/user/languages/r

language: R
sudo: false
cache: packages
```

and pushing `Linreg` code to GitHub will automatically triggers a Travis build… which fails!

To be continued…



3.10 Code coverage

Reading: https://walczak.org/2017/06/how-to-add-code-coverage-codecov-to-your-r-package/

Website: https://codecov.io/

Like Travis, codecov has to be linked to a GitHub account:

```
devtools::use_coverage(pkg = ".", type = c("codecov"))
```

creates the `codecov.yml` file:

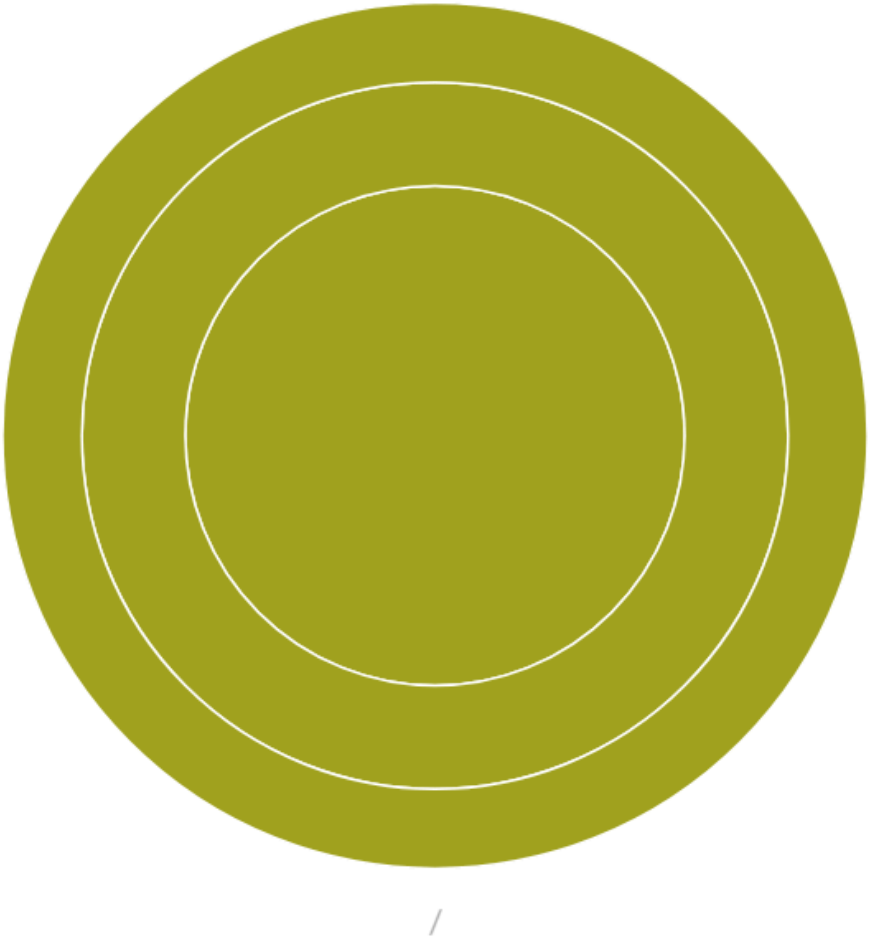
```
comment: false
```

A call to

```
covr::codecov(token = "YOUR_TOKEN")
```

will give you code coverage information:

COVERAGE SUNBURST



Files

R/linreg.R

Project Totals (1 files)

3.11 Back to GitHub

Badges can be added to `README.md`:

```
<!--- Badges ----->
[![Travis (LINUX) Build Status](https://travis-ci.org/cchoirat/Linreg.svg?branch=master)](https://travis
[![codecov](https://codecov.io/gh/cchoirat/Linreg/branch/master/graph/badge.svg)](https://codecov.io/gh/

## `Linreg` package template

Based on "Creating R Packages: A Tutorial" (Friedrich Leisch, 2009)

- https://cran.r-project.org/doc/contrib/Leisch-CreatingPackages.pdf
```

are automatically displayed on GitHub:

3.12 Vignettes

Reading: http://r-pkgs.had.co.nz/vignettes.html

Reading: http://kbroman.org/pkg_primer/pages/vignettes.html

Even if all the functions and datasets of your package are documented, it is still useful to have a more detailed illustation on how to use your package. A *vignette* is the right place to explain a worflow and a statistical method.

Running:

```
devtools::use_vignette("my-linear-regression")
```

creates a `vignettes` folder and provide a template in RMarkdown format `my-linear-regression.Rmd`:

https://github.com/cchoirat/Linreg/blob/master/vignettes/my-linear-regression.Rmd

It also indicates in `DESCRIPTION` that vignettes should be built with `knitr`.

```
VignetteBuilder: knitr
```

The vignette is built into a HTML document with

```
devtools::build_vignettes()
```

```
Building Linreg vignettes
Moving my-linear-regression.html, my-linear-regression.R to inst/doc/
Copying my-linear-regression.Rmd to inst/doc/
```

The vignette is accessible with

```
vignette("my-linear-regression")
vignette("my-linear-regression", package = "Linreg")
```

Vignette Title

Vignette Author

2017-10-21

Vignettes are long form documentation commonly included in packages. Because t
distribution of the package, they need to be as compact as possible. The `html_vign`
custom style sheet (and tweaks some options) to ensure that the resulting html is as
`html_vignette` format:

- Never uses retina figures
- Has a smaller default figure size
- Uses a custom CSS stylesheet instead of the default Twitter Bootstrap style

Vignette Info

Note the various macros within the `vignette` section of the metadata block above. T
instruct R how to build the vignette. Note that you should change the `title` field and
match the title of your vignette.

Styles

The `html_vignette` template includes a basic CSS theme. To override this theme you
in the document metadata as follows:

```
output:
  rmarkdown::html_vignette:
    css: mystyles.css
```

Chapter 4

Optimization

In this Chapter, we will see how to measure and improve code performance.

4.1 Measuring performance

4.1.1 Benchmarking

Reading: http://adv-r.had.co.nz/Performance.html#microbenchmarking

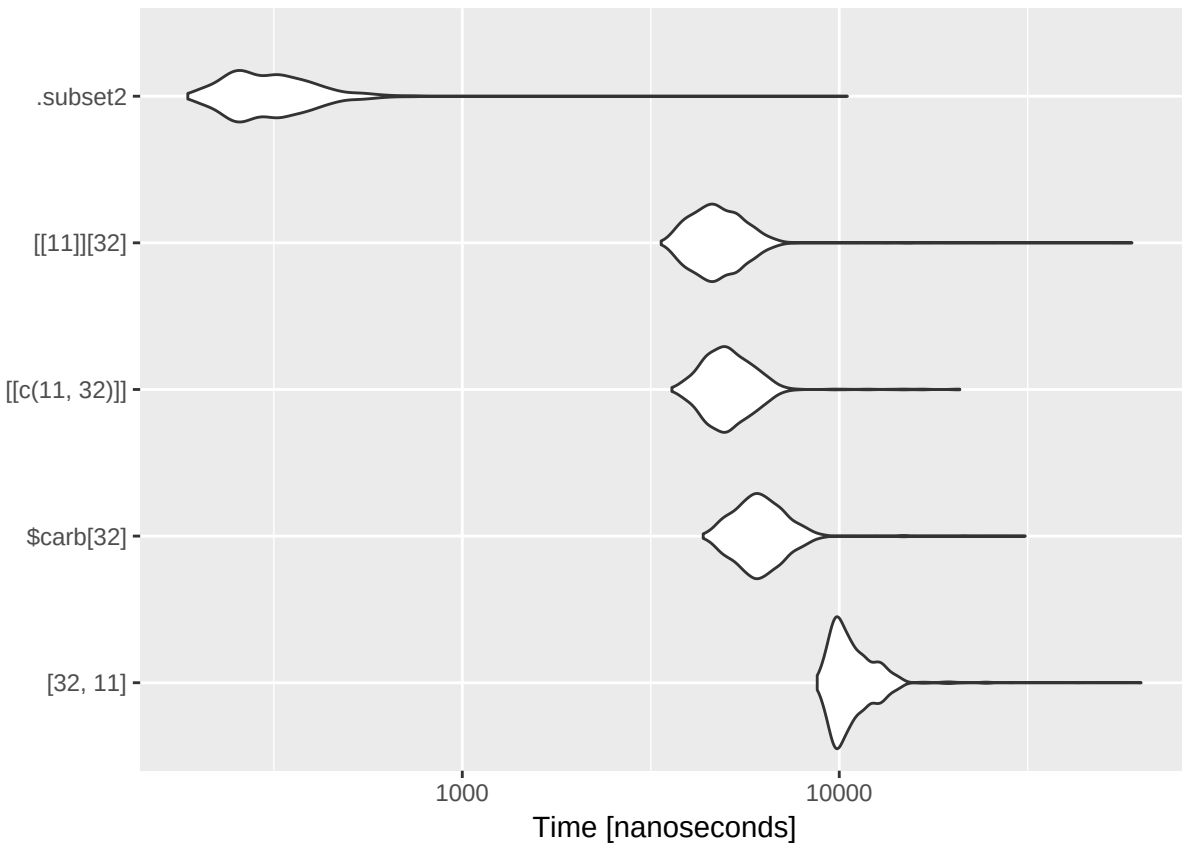
There are several ways to benchmark code (see http://www.alexejgossmann.com/benchmarking_r/) from `system.time` to dedicated packages such as `rbenchmark` (Kusnierczyk (2012)) or `microbenchmark` (Mersmann (2015)).

Let's start with an example from Wickham (2014).

```
library(microbenchmark)
m <- microbenchmark(
  times = 1000, # default is 100
  "[32, 11]"      = mtcars[32, 11],
  "$carb[32]"     = mtcars$carb[32],
  "[[c(11, 32)]]" = mtcars[[c(11, 32)]],
  "[[11]][32]"    = mtcars[[11]][32],
  ".subset2"      = .subset2(mtcars, 11)[32]
)
m
```

```
## Unit: nanoseconds
##           expr  min     lq      mean  median      uq   max neval   cld
##       [32, 11] 8742 9760.5 10981.424 10406.0 11617.5 63196  1000     e
##      $carb[32] 4355 5537.0  6317.541  6115.5  6818.0 31148  1000    d
##  [[c(11, 32)]] 3598 4544.5  5209.066  5036.0  5620.5 20888  1000   c
##     [[11]][32] 3370 4224.5  4942.880  4697.0  5308.5 59784  1000  b
##       .subset2  187  252.0   328.241   300.0   362.0 10511  1000 a
```

```
ggplot2::autoplot(m)
```



4.1.2 Profiling and optimization

Reading: http://adv-r.had.co.nz/Profiling.html#measure-perf

Let's compare three ways of estimating a linear regression: with built-in `lm` and with two functions we defined in package `Linreg` in Chapter 3.

```
library(Linreg)
data(cats, package = "MASS")
fit1 <- lm(Hwt ~ Bwt, data = cats)
fit2 <- linmod(Hwt ~ Bwt, data = cats)
fit3 <- linmodEst(cbind(1, cats$Bwt), cats$Hwt)
```

```
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
```

```
all.equal(round(coef(fit1), 5), round(coef(fit2), 5))
```

```
## [1] "names for target but not for current"
## [2] "Attributes: < names for current but not for target >"
## [3] "Attributes: < Length mismatch: comparison on first 0 components >"
## [4] "target is numeric, current is matrix"
```

```
all.equal(round(coef(fit1), 5), round(fit3$coefficients, 5), check.names = FALSE)
```

```
## [1] "Attributes: < names for current but not for target >"
## [2] "Attributes: < Length mismatch: comparison on first 0 components >"
## [3] "target is numeric, current is matrix"
```

```
m <- microbenchmark(
  fit1 <- lm(Hwt ~ Bwt, data = cats),
  fit2 <- linmod(Hwt ~ Bwt, data = cats),
  fit3 <- linmodEst(cbind(1, cats$Bwt), cats$Hwt)
  # custom checks can be performed with the 'check' argument
)
```

```
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
```

```
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
```

```
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
```

```
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
```

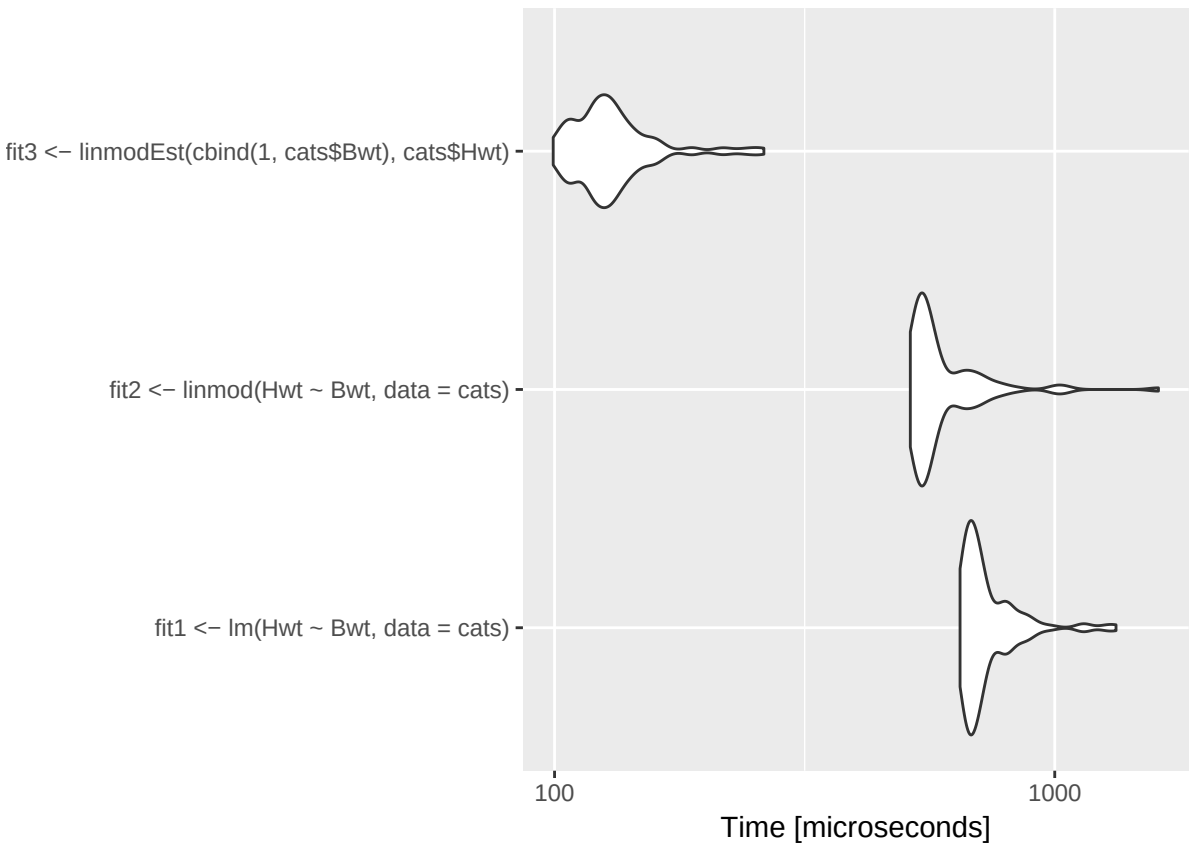
```
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
```

```
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##            [,1]
## [1,] -0.3566624
## [2,]  4.0340627
```

```
m
```

```
## Unit: microseconds
##                                            expr     min       lq     mean
##               fit1 <- lm(Hwt ~ Bwt, data = cats) 646.628 672.8640 739.4639
##           fit2 <- linmod(Hwt ~ Bwt, data = cats) 514.311 536.1520 604.3039
##  fit3 <- linmodEst(cbind(1, cats$Bwt), cats$Hwt)  99.370 118.0265 132.6574
##    median       uq      max neval cld
##  697.3575 770.9850 1325.828   100   c
##  550.2295 633.6295 1611.840   100  b
##  127.0395 137.2735  262.125   100 a
```

```
ggplot2::autoplot(m)
```



4.2 Improving performance

- Vectorize
- Parallelize
- Use a faster language (C/C++, Fortran, …)
- Use different tools (as in Chapter 6)

4.3 Vectorization

Let's take an example from a blog post (that seems to be gone). It's used in Wickham (2014, Section Case studies).

```
vacc1a <- function(age, female, ily) {
  p <- 0.25 + 0.3 * 1 / (1 - exp(0.04 * age)) + 0.1 * ily
  p <- p * if (female) 1.25 else 0.75
  p <- max(0, p)
  p <- min(1, p)
  p
}

set.seed(1959)
n <- 1000
age <- rnorm(n, mean = 50, sd = 10)
```

```
female <- sample(c(T, F), n, rep = TRUE)
ily <- sample(c(T, F), n, prob = c(0.8, 0.2), rep = TRUE)

vacc1a(age[1], female[1], ily[1])
```

```
## [1] 0.1667005
```

```
vacc1a(age[2], female[2], ily[2])
```

```
## [1] 0.4045439
```

```
vacc1a(age[3], female[3], ily[3])
```

```
## [1] 0.2699324
```

`vacc1a` is not designed for vector inputs

```
vacc1a(age, female, ily)
```

```
## Warning in if (female) 1.25 else 0.75: the condition has length > 1 and
## only the first element will be used
```

```
## [1] 0.2526293
```

It should be called

```
vacc1a(age[1], female[1], ily[1])
```

```
## [1] 0.1667005
```

```
vacc1a(age[2], female[2], ily[2])
```

```
## [1] 0.4045439
```

```
vacc1a(age[3], female[3], ily[3])
```

```
## [1] 0.2699324
```

We can use a loop:

```
out <- numeric(n)
for (i in 1:n)
  out[i] <- vacc1a(age[i], female[i], ily[i])
```

or one of the `apply` functions:

```
vacc0<- function(age, female, ily) {
  sapply(1:n, function(i) vacc1a(age[i], female[i], ily[i]))
}

out0 <- vacc0(age, female, ily)
```

```
all.equal(out, out0)
```

```
## [1] TRUE
```

But, it's convenient for the function to support vector inputs, instead of relying on users writing their own wrappers. We can loop inside the function body.

```
vacc1 <- function(age, female, ily) {
  n <- length(age)
  out <- numeric(n)
  for (i in seq_len(n)) {
    out[i] <- vacc1a(age[i], female[i], ily[i])
```

```
  }
  out
}
```

or we can rely on base R functions that accept vector inputs

```
vacc2 <- function(age, female, ily) {
  p <- 0.25 + 0.3 * 1 / (1 - exp(0.04 * age)) + 0.1 * ily
  p <- p * ifelse(female, 1.25, 0.75)
  p <- pmax(0, p)
  p <- pmin(1, p)
  p
}
```

4.4 Parallelization

```
library(parallel)
cores <- detectCores()
cores
```

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

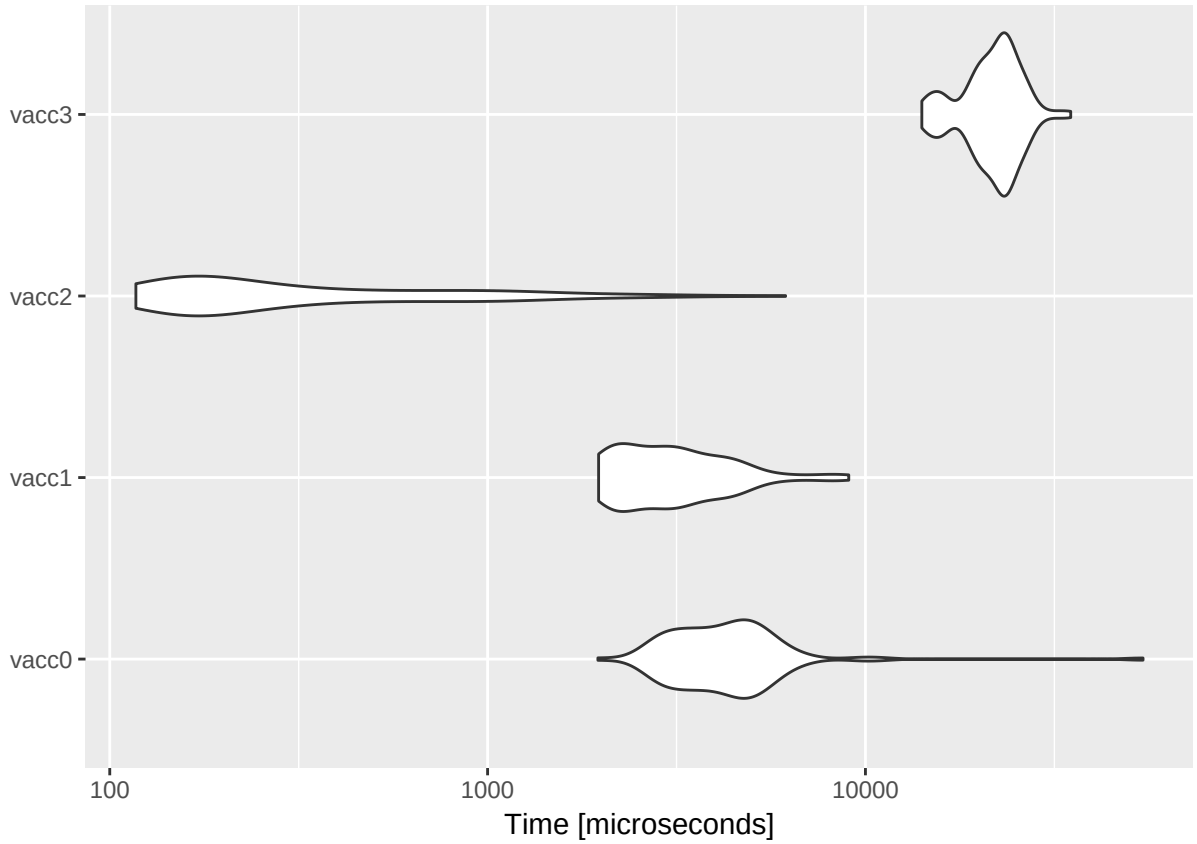
```
vacc3 <- function(age, female, ily) {
  mcmapply(function(i) vacc1a(age[i], female[i], ily[i]), 1:n, mc.cores = cores - 1)
}

out3 <- vacc3(age, female, ily)
```

```
library(microbenchmark)
m <- microbenchmark(
  vacc0 = vacc0(age, female, ily),
  vacc1 = vacc1(age, female, ily),
  vacc2 = vacc2(age, female, ily),
  vacc3 = vacc3(age, female, ily)
)
m
```

```
## Unit: microseconds
##   expr       min         lq       mean    median         uq       max
##  vacc0  1958.306  3318.8395  4820.8838  4207.614  5047.4830 54284.494
##  vacc1  1966.963  2283.9290  3302.5990  3040.963  3917.6425  9034.687
##  vacc2   117.251   157.9805   512.7771   200.859   521.6105  6147.073
##  vacc3 14100.910 19808.5095 21916.5820 22403.471 24170.6880 34937.594
##  neval  cld
##    100   c
##    100  b
##    100 a
##    100    d
```

```
ggplot2::autoplot(m)
```



So, what's going on?

We will talk more about parallelization tools and techniques in Chapter '**?**(bigdata).

4.5 Introduction to C++

- C++ is a very powerful object-oriented language.
- Many tutorials are available on-line, for example http://www.cplusplus.com/doc/tutorial/.
- R is *intepreted*, C++ is *compiled* and typically much faster (in loops for examples).
- Our introduction to C++ is from an R perspective. Python (and most interpreted languages) can be extended with C++ too.

4.5.1 Rcpp

Reading: http://adv-r.had.co.nz/Rcpp.html

- `Rcpp` Eddelbuettel (2013) makes it very easy to use C++ code in R (for example to speed up a function or to wrap methods already implemented in C++).
- `Rcpp` provides "syntactic sugar" that makes is easy to leverage C++ even without a deep knowledge of it.
- To use `Rcpp`, you need a C++ compiler:

  - Windows: Rtools
  - OS X: Xcode
  - Linux: `r-base-dev` from package manager

4.5.2 Hello World!

```
library(Rcpp)
cppFunction('void hello(){
  Rprintf("Hello, world!");
}')
hello
```

```
## function ()
## invisible(.Primitive(".Call")(<pointer: 0x10d6a6100>))
```

```
hello()
```

```
## Hello, world!
```

`Rprintf` is the counterpart of C++ `printf` function.

Let's take the first example of Wickham (2014), Section Getting started with C++.

```
cppFunction('int add(int x, int y, int z) {
  int sum = x + y + z;
  return sum;
}')
```

We have to specify the input type and the output type. As expected

```
add(1, 2, 3)
```

returns 6. How about?

```
add(1.1, 2.2, 3.3)
```

```
cppFunction('double addd(double x, double y, double z) {
  double sum = x + y + z;
  return sum;
}')
```

With `addd` we do get 6.6:

```
addd(1.1, 2.2, 3.3)
```

4.5.3 `sourceCpp`

When C++ code takes more than a couple of lines, it's more convenient to create a stand-alone C++ source file.

From the RStudio default template:

```
#include <Rcpp.h>
using namespace Rcpp;

NumericVector timesTwo(NumericVector x) {
  return x * 2;
}
```

```
/*** R
timesTwo(42)
*/
```

From R, we can use `sourceCpp` to access `timesTwo` in R:

```
sourceCpp("src/times-two.cpp")
timesTwo(100)
```

4.5.4 Data types

`int double bool string`

`NumericVector LogicalVector IntegerVector CharacterVector`

`NumericMatrix IntegerMatrix LogicalMatrix CharacterMatrix`

`NA_REAL NA_INTEGER NA_STRING NA_LOGICAL`

`List DataFrame Function`

…

4.5.5 Sugar

Reading: http://adv-r.had.co.nz/Rcpp.html#rcpp-sugar.

- Vectorization of `+`, `*`, `-`, `/`, `pow`, `<`, `<=`, `>`, `>=`, `==`, `!=`, …
- Vectorization of R-like functions: `abs()`, `exp()`, `factorial()`, …

Exercise 4.1. Can you write an `Rcpp` function similar to `addd` but accepting vector arguments?

```
cppFunction('NumericVector addv(NumericVector x, NumericVector y, NumericVector z) {
  NumericVector sum = x + y + z;
  return sum;
}')
```

4.5.6 Example (continued)

```
#include <Rcpp.h>
using namespace Rcpp;

double vacc3a(double age, bool female, bool ily){
  double p = 0.25 + 0.3 * 1 / (1 - exp(0.04 * age)) + 0.1 * ily;
  p = p * (female ? 1.25 : 0.75);
  p = std::max(p, 0.0);
  p = std::min(p, 1.0);
  return p;
}

// [[Rcpp::export]]
NumericVector vacc3(NumericVector age, LogicalVector female,
                    LogicalVector ily) {
  int n = age.size();
  NumericVector out(n);
```

```
  for(int i = 0; i < n; ++i) {
    out[i] = vacc3a(age[i], female[i], ily[i]);
  }

  return out;
}
```

4.5.7 Back to Linreg

- `armadillo` is a very powerful C++ linear algebra library: http://arma.sourceforge.net/
- It can be used in `Rcpp` via the `RcppArmadillo` package.

Exercise 4.2. Can you write an `Rcpp` function similar to `linmodEst`?

```
linmodEst <- function(x, y) {
  ## CC: crossprod or a QR decomposition (as in the original version) are more efficient
  coef <- solve(t(x) %*% x) %*% t(x) %*% y
  ## degrees of freedom and standard deviation of residuals
  df <- nrow(x) - ncol(x)
  sigma2 <- sum((y - x %*% coef) ^ 2) / df
  ## compute sigma^2 * (x'x)^-1
  vcov <- sigma2 * solve(t(x) %*% x)
  colnames(vcov) <- rownames(vcov) <- colnames(x)
  list(
    coefficients = coef,
    vcov = vcov,
    sigma = sqrt(sigma2),
    df = df
  )
}
```

4.6 Rcpp packages

Readings: - https://cran.r-project.org/web/packages/Rcpp/vignettes/Rcpp-package.pdf - http://adv-r.had.co.nz/Rcpp.html#rcpp-package

4.7 Getting serious about C++

4.7.1 STL

STL: Standard Template Library

Reading: http://adv-r.had.co.nz/Rcpp.html#stl

4.8 Profiling

Reading: https://rstudio.github.io/profvis/

```r
library(profvis)

profvis({
  data(diamonds, package = "ggplot2")

  plot(price ~ carat, data = diamonds)
  m <- lm(price ~ carat, data = diamonds)
  abline(m, col = "red")
})
```

Chapter 5

SQL

5.1 What is SQL?

SQL (Structured Query Language) is a standard way of specifying the information you want to receive from a database. There are a number of variations on the language, and a number of online resources available for learning their various complexities. However, the general structure of all SQL queries is consistent across implementations.

SQL is an imperative computer language. This means that it describes the output desired without actually describing the calculations required to get the output described. This allows for the verbs and structures of the language to be used across database systems, as well as in other areas of data handling.

5.1.1 What is a database?

A database is simply an organized structure for storing and accessing data on disk. There are a number of structures used to store data on disk, each with their own languages. However, despite the variations in structure, the goals (and song) remain the same. The process of data storage on disk is controlled by the database management system (DBMS).

5.1.2 Relational Databases (SQL)

The most common type of DBMS is a relational database (RDBMS). A Relational Database stores information in a the form of entities and the relationships between them. Entities are typically nouns and relationships are typically verbs. For example, if we wanted to store information about class enrollment at a university, the entities would consist of objects like a student, class, and professor. The relationships would consist of takes and teaches. Relationships can be one to one, many to many, or one to many.

5.1.3 Types of Relational Databases

- Commercial
  - Oracle Database
  - Microsoft
  - SQL Server
  - …
- Open-source
  - MySQL
  - PostgreSQL

  - SQLite
  - …
- SQLite is the easiest way to start: unlike the others, it's not a client-server DB. The whole DB can live in a (portable) folder. All the required tools are included in `dplyr`.

5.1.4 SQL

In relational databases, entities and relationships are represented by tables, where each row or record in a table represents a particular instance of of that general object. Continuing the class example, students would be stored in `Student`, classes in `Class`, and professors in `Professor`. The table containing the relationships between students and classes would be likely named `StudentClass` and the

The three key parts of a SQL query are the `SELECT` clause, the `FROM` clause, and the `WHERE` clause. The `SELECT` clause specifies the pieces of information you want about an individual record, the `FROM` clause specifies the tables that will be used

To get all information about all students we would type the following:

```
SELECT * FROM STUDENT
```

To Select the name and birthday of all students in classes taught by Dr. Choirat would be a more complex query, which would likely look something like this:

```
   SELECT Name,
          DOB
   FROM Student s
        inner join StudentClass sc on
            s.ID = sc.studentid
        inner join ProfessorClass pc on
            sc.classid = pc.classid
        inner join Professor p on
            pc.profid = p.id
    WHERE p.lastname = "Choirat"
```

5.2 SQLite: An Exercise

Create an in memory DB

`sqlite3`

5.2.1 Make a Table

```
CREATE TABLE table1(x,y,z);
```

5.2.2 Insert Values

```
INSERT INTO table1 VALUES (1,2,3),(4,5,6),(7,8,9);
```

5.2.3 Select Values

Select All Values

```
SELECT * FROM table1;
```

Select specific values

```
SELECT z from table1 WHERE x = 4;
```

5.3 SQL and R

There are a number of R packages for interfacing directly with RDBs. RODBC is one sucn example that allows for queries to be submitted to previsously set up database connections with the results being returned as a data frame for further analysis in R. There's a large amount of documentation available online for these methods. Each system has its own idiosyncracies.

5.3.1 Data: `oscars` and `movies` again: 2016 Oscars Nominations

```
library(readr)
library(dplyr)

db <- src_sqlite("db.sqlite3", create = TRUE)

oscars <-"
name,movie,category
Adam McKay,The Big Short,Best Director
Alejandro González Iñárritu,The Revenant,Best Director
Lenny Abrahamson,Room,Best Director
Tom McCarthy,Spotlight,Best Director
George Miller,Mad Max: Fury Road,Best Director
Bryan Cranston,Trumbo,Best Actor
Matt Damon,The Martian,Best Actor
Michael Fassbender,Steve Jobs,Best Actor
Leonardo DiCaprio,The Revenant,Best Actor
Eddie Redmayne,The Danish Girl,Best Actor
Cate Blanchett,Carol,Best Actress
Brie Larson,Room,Best Actress
Jennifer Lawrence,Joy,Best Actress
Charlotte Rampling,45 Years,Best Actress
Saoirse Ronan,Brooklyn,Best Actress
"
oscars <- read_csv(oscars, trim_ws = TRUE, skip = 1)

movies <-"
movie,length_mins
The Big Short,130
Star Wars: The Force Awakens,135
Brooklyn,111
Mad Max: Fury Road,120
Room,118
The Martian,144
The Revenant,156
Spotlight,128
"
movies <- read_csv(movies, trim_ws = TRUE, skip = 1)
```

```
oscars_table <- copy_to(db, oscars)
movies_table <- copy_to(db, movies)

db
```

5.4 Non-Relational Databases (noSQL)

5.4.1 Drawbacks of Relational Databases

- Looking up all information about one entity can be expensive
- Require a large amount of overhead
- Difficult to distribute across multiple disks
- Considered to by some to be inflexible

5.4.2 Common Types of NoSQL Databases

- Graph Databases
  - Neo4j
  - OrientDB
- Document Databases
  - MongoDB
  - JSON Databases
  - XML Databases

5.5 References

The Oscar movie example comes from this lecture by Rafa Irizarry: https://github.com/datasciencelabs/2016/blob/master/lectures/wrangling/data-wrangling-with-dplyr.Rmd

Chapter 6

Big data

6.1 How to deal with (very / too) large datasets?

1. Use more RAM / processors / drive space…
2. Use less data: (re)sample, …
3. Use a database
4. Use specific R packages (`ff`, `bigmemory`)
5. Use other tools

6.2 How big is big?

1. Fits in RAM and on drive (but slow)
2. Doesn't fit in RAM but fits on drive
3. Doesn't fit in RAM and doesn't fit on drive

6.3 List of tools

Reading: Varian (2014) (PDF available)

Spark? h2o? More? Let's go back to the bottlenecks

- CPU
- RAM
- I/O

6.4 Data that fits in memory

6.4.1 Faster I/O

Reading: https://cran.r-project.org/web/packages/data.table/vignettes/datatable-intro.html

`data.table` provides an enhanced of a `data.frame` and faster I/O with `fread` and `fwrite`.

To read the 0.5GB ratings file from MovieLens

```
library(data.table)
system.time(ratings <- fread("~/Dropbox/Data17/ml-20m/ratings.csv"))
```

Tools for Manipulating Big Data

Google name	*Analog*	*Description*
Google File System	Hadoop File System	This system supports files s distributed across hundre computers.
Bigtable	Cassandra	This is a table of data that System. It too can stretch c
MapReduce	Hadoop	This is a system for accessi data in large data structur MapReduce allows you to a using hundreds or thousan the data you are interested to the machines and is the different shards of the data are then combined ("redu summary table you are int
Sawzall	Pig	This is a language for creat
Go	None	Go is flexible open-source, computer language that m parallel data processing.
Dremel, BigQuery	Hive, Drill, Impala	This is a tool that allows da a simplified form of of St (SQL). With Dremel it is query on a petabtye of da few seconds.

Table 6.1: I/O comparison

package	function.	speed	output
base	read.csv	slow	data.frame
data.table	fread	very fast	data.table
readr	read_csv	fast	tibble

takes

```
Read 20000263 rows and 4 (of 4) columns from 0.497 GB file in 00:00:05
   user  system elapsed
  4.007   0.229   4.244
```

while

```
system.time(ratings <- read.csv("~/Dropbox/Data17/ml-20m/ratings.csv"))
```

takes

```
   user  system elapsed
 85.199   2.711  90.997
```

There are ways to improve the speed of `read.csv` (for example, but specifying column types). But in general `fread` is much faster.

```
library(readr) # in tidyverse
system.time(ratings <- read_csv("~/Dropbox/Data17/ml-20m/ratings.csv"))
```

```
   user  system elapsed
 10.290   3.037  18.450
```

also tends to perform better than `read.csv`.

6.4.2 Reference vs copy

Reading: http://adv-r.had.co.nz/memory.html Reading: https://jangorecki.gitlab.io/data.table/library/data.table/html/assign.html

```
library(pryr)
library(data.table)

d <- read.csv("~/Dropbox/Data17/ml-latest-small/ratings.csv")
D <- fread("~/Dropbox/Data17/ml-latest-small/ratings.csv")

object_size(d)
object_size(D)

mem_change(d$Idx <- 1:nrow(d))
mem_change(D[, Idx:= 1:.N])

object_size(d$Idx)
object_size(D$Idx)
```

```
d <- read.csv("~/Dropbox/Data17/ml-latest-small/ratings.csv")
D <- fread("~/Dropbox/Data17/ml-latest-small/ratings.csv")
```

```
.Internal(inspect(d))
d$Idx <- 1:nrow(d)
.Internal(inspect(d))

.Internal(inspect(D))
D[, Idx:= 1:.N]
.Internal(inspect(D))
```

6.4.3 data.table: another data manipulation grammar

Reading: https://cran.r-project.org/web/packages/data.table/vignettes/datatable-intro.html

Exercise 6.1. Benchmark adding a column to a large data frame vs a large data table.

6.5 Data that doesn't fit in memory (but fits on drive)

Let's try to work with a 12GB file and 4/8 GB of memory…

6.6 Pure R solutions

6.6.1 A regressions example

```
library(data.table)
airlines <- fread("/Users/cchoirat/Dropbox/Data17/AirFlights/allyears2k.csv")
rfit <- lm(ArrDelay ~ Distance, data = airlines)
summary(rfit)
```

6.6.2 Sampling

- Read the data (even line by line)
- Select a sample of rows
- Run your model on the random sample

6.6.3 `bigmemory`

https://cran.r-project.org/web/packages/bigmemory/index.html

Reading: https://cran.r-project.org/web/packages/bigmemory/vignettes/Overview.pdf

bigmemory: Manage Massive Matrices with Shared Memory and Memory-Mapped Files

Create, store, access, and manipulate massive matrices. Matrices are allocated to shared memory and may use memory-mapped files. Packages 'biganalytics', 'bigtabulate', 'synchronicity', and 'bigalgebra' provide advanced functionality.

(+) pure R solution from a user perspective

(-) mostly for numeric data matrices, mostly to speed up computations on data of +/- RAM size

```
library(bigmemory)
library(biganalytics)
# library(bigtabulate)
# library(biglm)

flights <- read.big.matrix(
  "/Users/cchoirat/Dropbox/Data17/AirFlights/allyears2k.csv",
  header = TRUE,
  backingfile = "allyears2k.bin",
  backingpath = "/Users/cchoirat/Dropbox/Data17/AirFlights/",
  descriptorfile = "allyears2k.desc",
  shared = TRUE)

air_flights <- attach.big.matrix("/Users/cchoirat/Dropbox/Data17/AirFlights/allyears2k.desc")
dim(air_flights)
colnames(air_flights)
mean(air_flights[, "ArrDelay"], na.rm = TRUE)

fit <- biglm.big.matrix(ArrDelay ~ Distance, data = air_flights)
fit
summary(fit)
```

6.6.4 Database connections and lazy evaluation

```
D <- fread("~/Dropbox/Data17/AirFlights/")
```

6.7 Scaling up

6.8 Parallel computing and clusters

6.9 Cloud computing

More soon with the Odyssey guest lecture (https://www.rc.fas.harvard.edu/odyssey/).

6.10 `h2o`: "Fast Scalable Machine Learning"

http://www.h2o.ai/

http://www.r-bloggers.com/scalable-machine-learning-for-big-data-using-r-and-h2o/

http://venturebeat.com/2014/11/07/h2o-funding/ https://www.h2o.ai/driverless-ai/ https://www.infoworld.com/article/3236048/machine-learning/review-h2oai-automates-machine-learning.html

6.10.1 Ecosystem

Readings:

- http://docs.h2o.ai/h2o/latest-stable/h2o-docs/welcome.html

- http://www.h2o.ai/download/h2o/r
- https://cran.r-project.org/web/packages/h2o/index.html

  To build H2O or run H2O tests, the 64-bit JDK is required.

  To run the H2O binary using either the command line, R, or Python packages, only 64-bit JRE is required.

```
if ("package:h2o" %in% search()) { detach("package:h2o", unload=TRUE) }
if ("h2o" %in% rownames(installed.packages())) { remove.packages("h2o") }
install.packages("h2o")
```

6.11 Running h20 locally within R

```
library(h2o)
localH2O <- h2o.init(min_mem_size = "20g")
```

```
# h2o.init(ip = "localhost", port = 54321, startH2O = TRUE,
#          forceDL = FALSE, enable_assertions = TRUE, license = NULL,
#          nthreads = -2, max_mem_size = NULL, min_mem_size = NULL,
#          ice_root = tempdir(), strict_version_check = TRUE,
#          proxy = NA_character_, https = FALSE, insecure = FALSE,
#          username = NA_character_, password = NA_character_)
```

(No persistence beyond the R session when h2O is started from R.)

```
 Connection successful!

R is connected to the H2O cluster:
    H2O cluster uptime:         19 days 12 hours
    H2O cluster version:        3.14.0.3
    H2O cluster version age:    1 month and 24 days
    H2O cluster name:           H2O_started_from_R_cchoirat_bgt310
    H2O cluster total nodes:    1
    H2O cluster total memory:   15.18 GB
    H2O cluster total cores:    8
    H2O cluster allowed cores:  8
    H2O cluster healthy:        TRUE
    H2O Connection ip:          localhost
    H2O Connection port:        54321
    H2O Connection proxy:       NA
    H2O Internal Security:      FALSE
    H2O API Extensions:         XGBoost, Algos, AutoML, Core V3, Core V4
    R Version:                  R version 3.4.2 (2017-09-28)
```

6.12 JVM (from Wikipedia)

A Java virtual machine (JVM) is an abstract computing machine that enables a computer to run a Java program. There are three notions of the JVM: specification, implementation, and instance. The specification is a document that formally describes what is required of a JVM implementation.

(https://en.wikipedia.org/wiki/Java_virtual_machine)

6.13 Which languages? (from Wikipedia)

This list of JVM Languages comprises notable computer programming languages that are used to produce software that runs on the Java Virtual Machine (JVM). Some of these languages are interpreted by a Java program, and some are compiled to Java bytecode and JIT-compiled during execution as regular Java programs to improve performance.

6.14 Which languages?

https://en.wikipedia.org/wiki/List_of_JVM_languages

- Java
- Scala, an object-oriented and functional programming language
- Jython
- R (an implementation of R: https://en.wikipedia.org/wiki/Renjin)
- …

6.15 State of the h2o JVM

```
h2o.clusterInfo()
```

```
R is connected to the H2O cluster:
    H2O cluster uptime:         19 days 13 hours
    H2O cluster version:        3.14.0.3
    H2O cluster version age:    1 month and 24 days
    H2O cluster name:           H2O_started_from_R_cchoirat_bgt310
    H2O cluster total nodes:    1
    H2O cluster total memory:   15.18 GB
    H2O cluster total cores:    8
    H2O cluster allowed cores:  8
    H2O cluster healthy:        TRUE
    H2O Connection ip:          localhost
    H2O Connection port:        54321
    H2O Connection proxy:       NA
    H2O Internal Security:      FALSE
    H2O API Extensions:         XGBoost, Algos, AutoML, Core V3, Core V4
    R Version:                  R version 3.4.2 (2017-09-28)
```

Let's check http://localhost:54321/flow/index.html.

H2O FLOW Flow Cell Data Model Scor

Untitled Flow

CS

```
assist
```

Assistance

	Routine	Description
	importFiles	Import file(s) into H_2O
	getFrames	Get a list of frames in H_2O
	splitFrame	Split a frame into two or more frames
	mergeFrames	Merge two frames into one
	getModels	Get a list of models in H_2O
	getGrids	Get a list of grid search results in H_2O
	getPredictions	Get a list of predictions in H_2O
	getJobs	Get a list of jobs running in H_2O
	buildModel	Build a model
	runAutoML	Automatically train and tune many models
	importModel	Import a saved model
	predict	Make a prediction

Ready

6.15.1 Importing data into h2o from the R session

```
data(cars)
cars_to_h2o <- as.h2o(cars, destination_frame = "cars_from_r")
is.data.frame(cars_to_h2o) # FALSE
class(cars_to_h2o) # H2OFrame
```

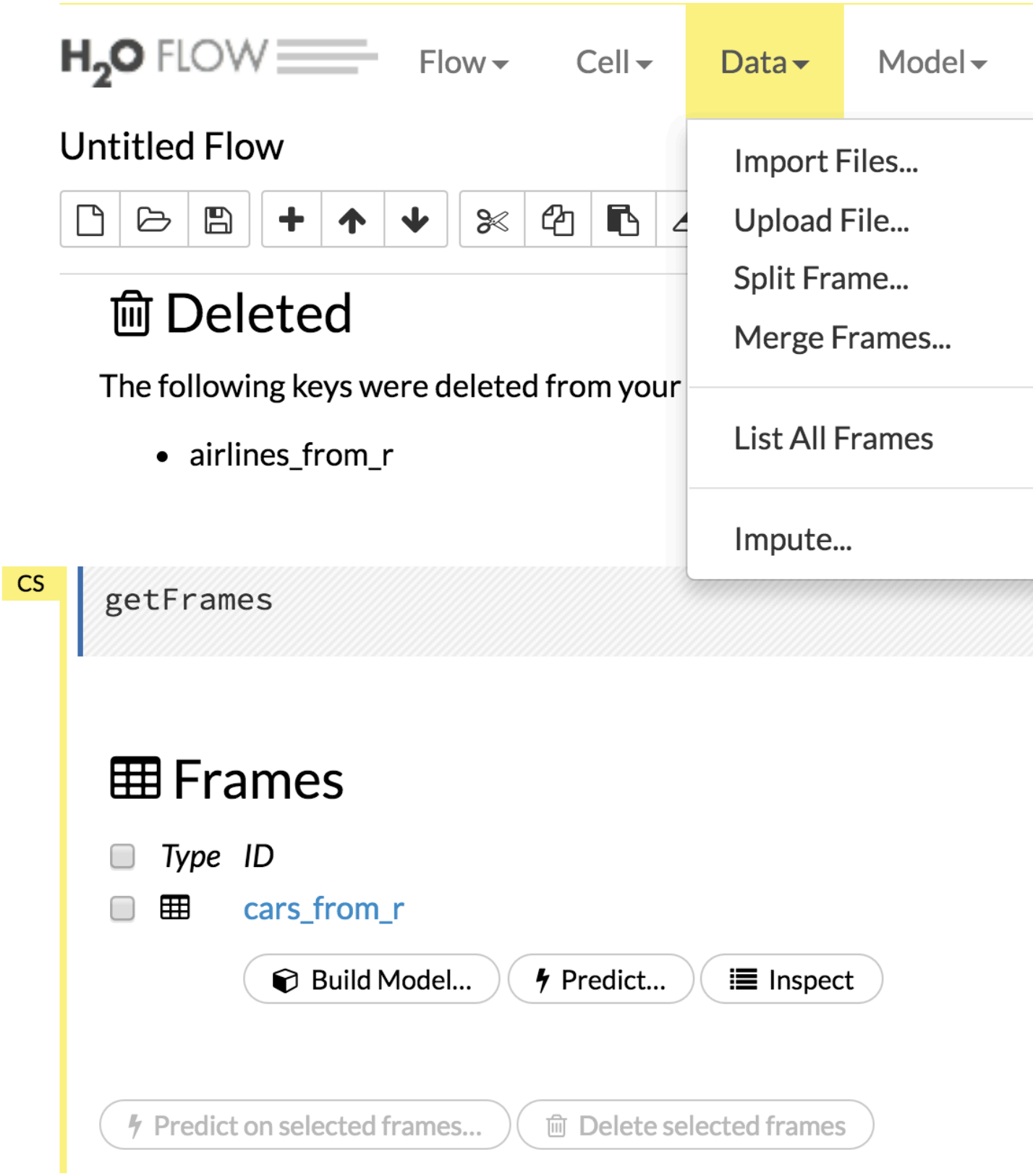
6.15.2 h2o functions

```
summary(cars_to_h2o) # actually calls h2o:::summary.H2OFrame(cars_to_h2o)
```

```
Approximated quantiles computed! If you are interested in exact quantiles, please pass the `exact_quant
 Min.   : 4.0   Min.   :  2.00
 1st Qu.:12.0   1st Qu.: 26.00
 Median :15.0   Median : 36.00
 Mean   :15.4   Mean   : 42.98
 3rd Qu.:19.0   3rd Qu.: 56.00
 Max.   :25.0   Max.   :120.00
```

6.15.3 Let's check from the h2o JVM

From the browser: 'Data' -> 'List All Frames'


H2O FLOW
Flow
Cell
Data
Model
Untitled Flow
Import Files...
Upload File...
Split Frame...
Merge Frames...
List All Frames
Impute...
Deleted
The following keys were deleted from your
airlines_from_r
CS
getFrames
Frames
Type
ID
cars_from_r
Build Model...
Predict...
Inspect
Predict on selected frames...
Delete selected frames

6.16 Spark

Reading: https://spark.rstudio.com/

```
library(sparklyr)
spark_install(version = "2.1.0")
```

```
conf <- spark_config()
conf$`sparklyr.shell.driver-memory` <- "32G"
conf$spark.memory.fraction <- 0.5
sc <- spark_connect(master = "local")
```

```
library(dplyr)
iris_tbl <- copy_to(sc, iris)
flights_tbl <- copy_to(sc, nycflights13::flights, "flights")
batting_tbl <- copy_to(sc, Lahman::Batting, "batting")
src_tbls(sc)
```

```
top_rows <- read.csv("~/Dropbox/Data17/AirFlights/allyears.csv", nrows = 5)
file_columns <- top_rows %>%
  purrr::map(function(x)"character")
rm(top_rows)
```

```
sp_flights <- spark_read_csv(sc,
                             name = "flights2",
                             path = "~/Dropbox/Data17/AirFlights/allyears.csv",
                             memory = FALSE,
                             columns = file_columns,
                             infer_schema = FALSE)
```

```
flights_table <- sp_flights %>%
  mutate(DepDelay = as.numeric(DepDelay),
         ArrDelay = as.numeric(ArrDelay),
         SchedDeparture = as.numeric(CRSDepTime)) %>%
  select(Origin, Dest, SchedDeparture, ArrDelay, DepDelay, Month, DayofMonth)

flights_table %>% head
```

Cache data:

```
sp_flights %>%
  tally # takes a looooong time
```

123534969…

```
subset_table <- flights_table %>%
  compute("flights_subset")
```

```
subset_table %>%
  tally # a bit faster.
```

123534969 as well!

```
lm(arr_delay ~ distance, data = flights_tbl)
ml_linear_regression(subset_table, response = "ArrDelay", features = "SchedDeparture")
```

TODOL change the `config` arguments of the connection

6.17 Sparkling Water

Reading: https://spark.rstudio.com/h2o.html

6.17.1 More?

GPU

Chapter 7

Visualization

7.1 Principles of visualization

7.2 Maps and GIS

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