Computing for Big Data (BST-262)

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2017-10-25

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: Thursday 3-4pm
- 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

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

```r
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.

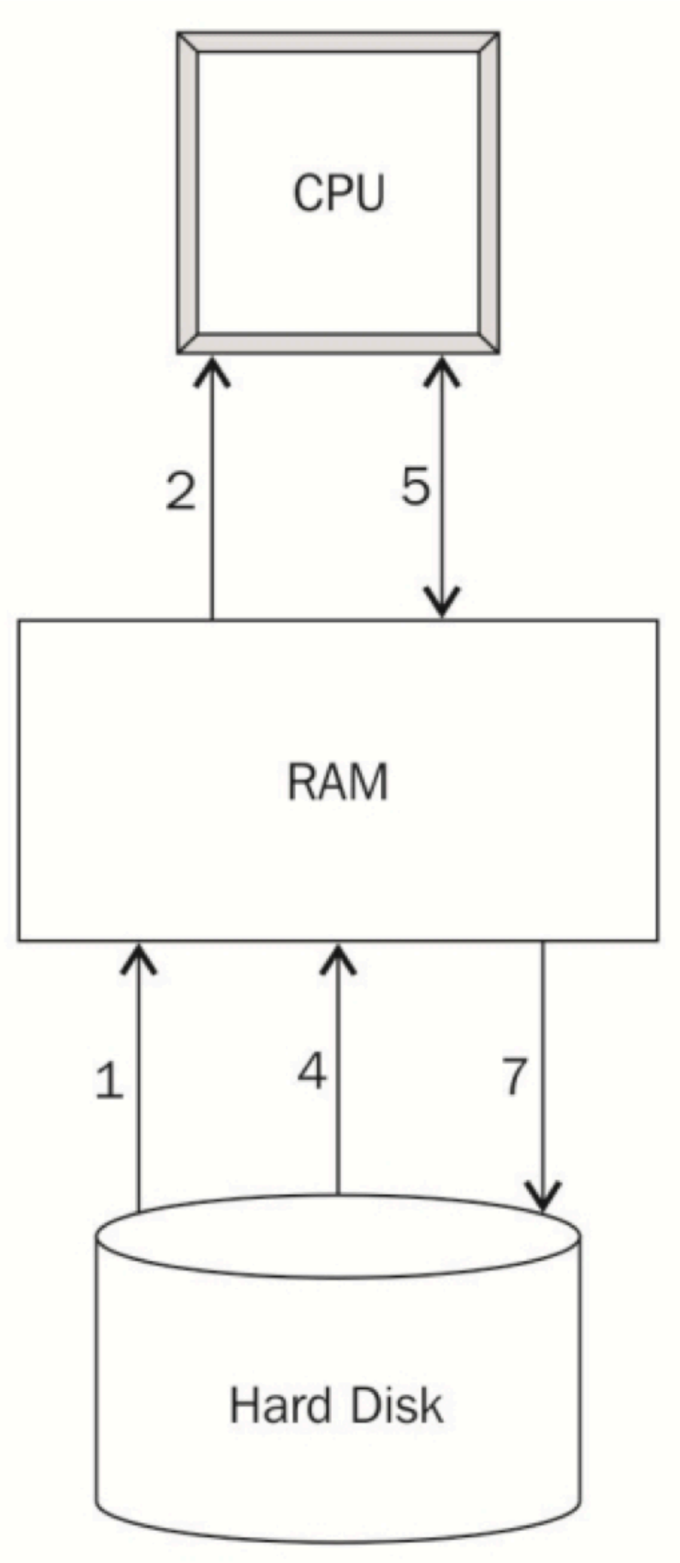


Figure 1.1: Steps to execute an R program, from @Lim2015, Chapter 1.

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:

```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:

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

or

```r
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.

```r
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

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

File `simulate_data.R`

```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)
```

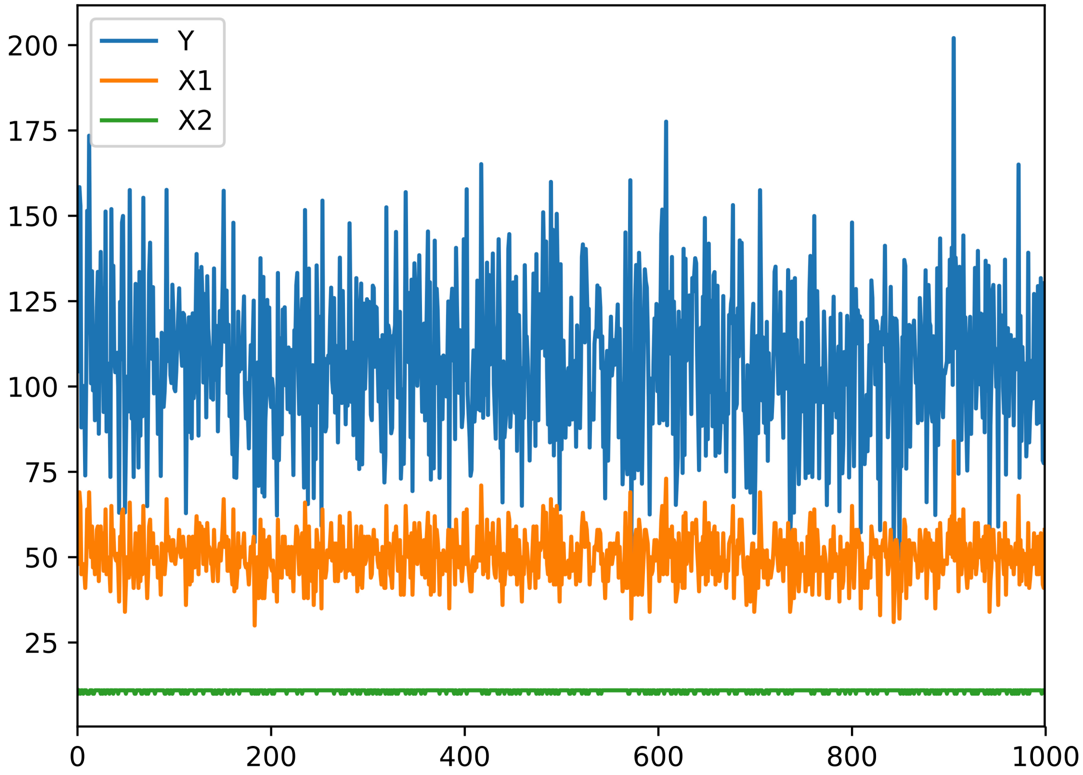
```r
head(data.frame(Y = Y, X1 = X1, X2 = X2))
```

```
##           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`

```python
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")
```



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`

```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:

```r
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)
```

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

```
e <- rnorm(1000)
package.skeleton(list = c("f","g","d","e"), name = "pkgname")
```

3.4.2 devtools::create

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

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

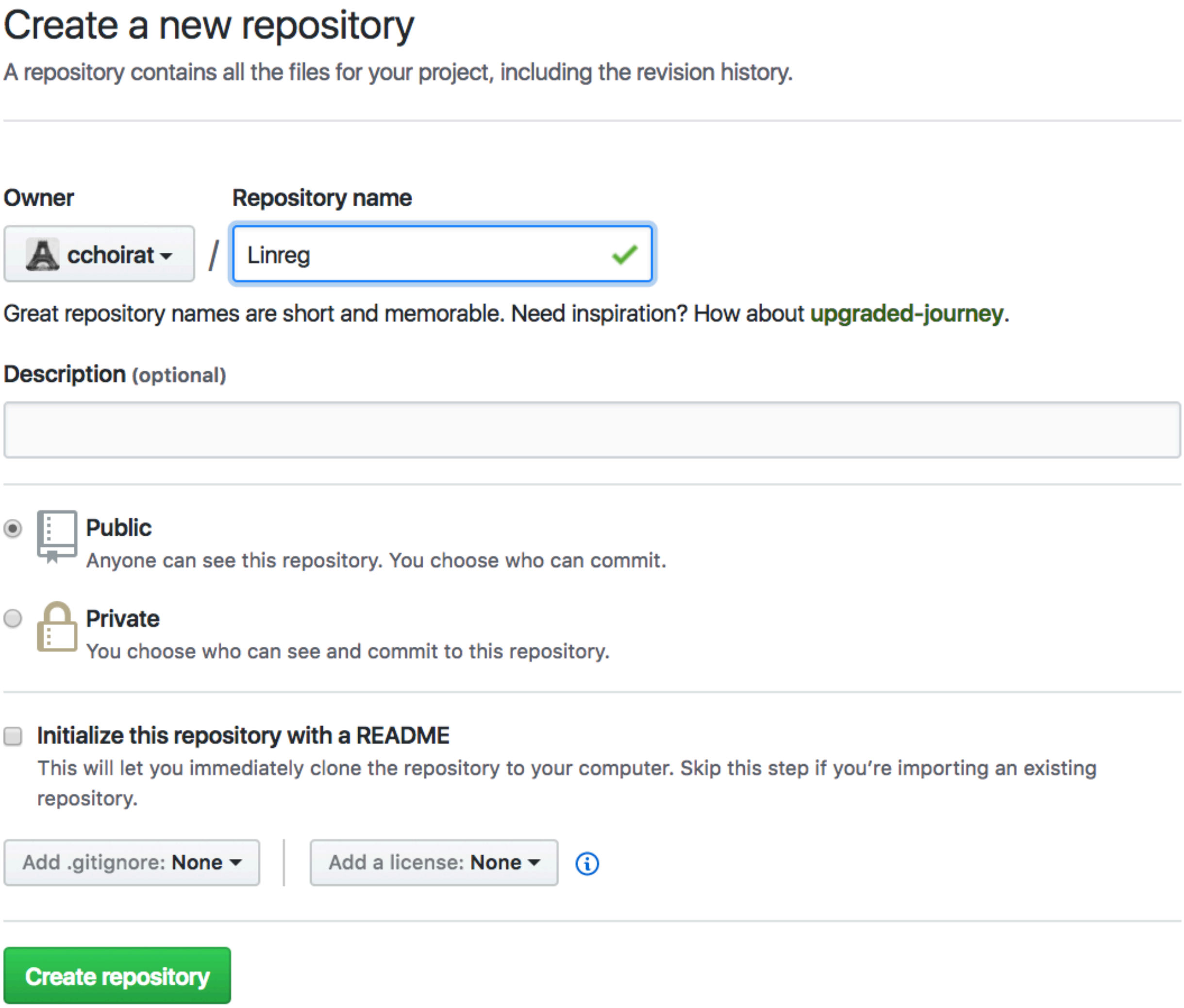
3.5.0.1 RStudio and GitHub integration

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



Create a new repository

A repository contains all the files for your project, including the revision history.

Owner: cchoirat / Repository name: Linreg ✓

Great repository names are short and memorable. Need inspiration? How about upgraded-journey.

Description (optional)

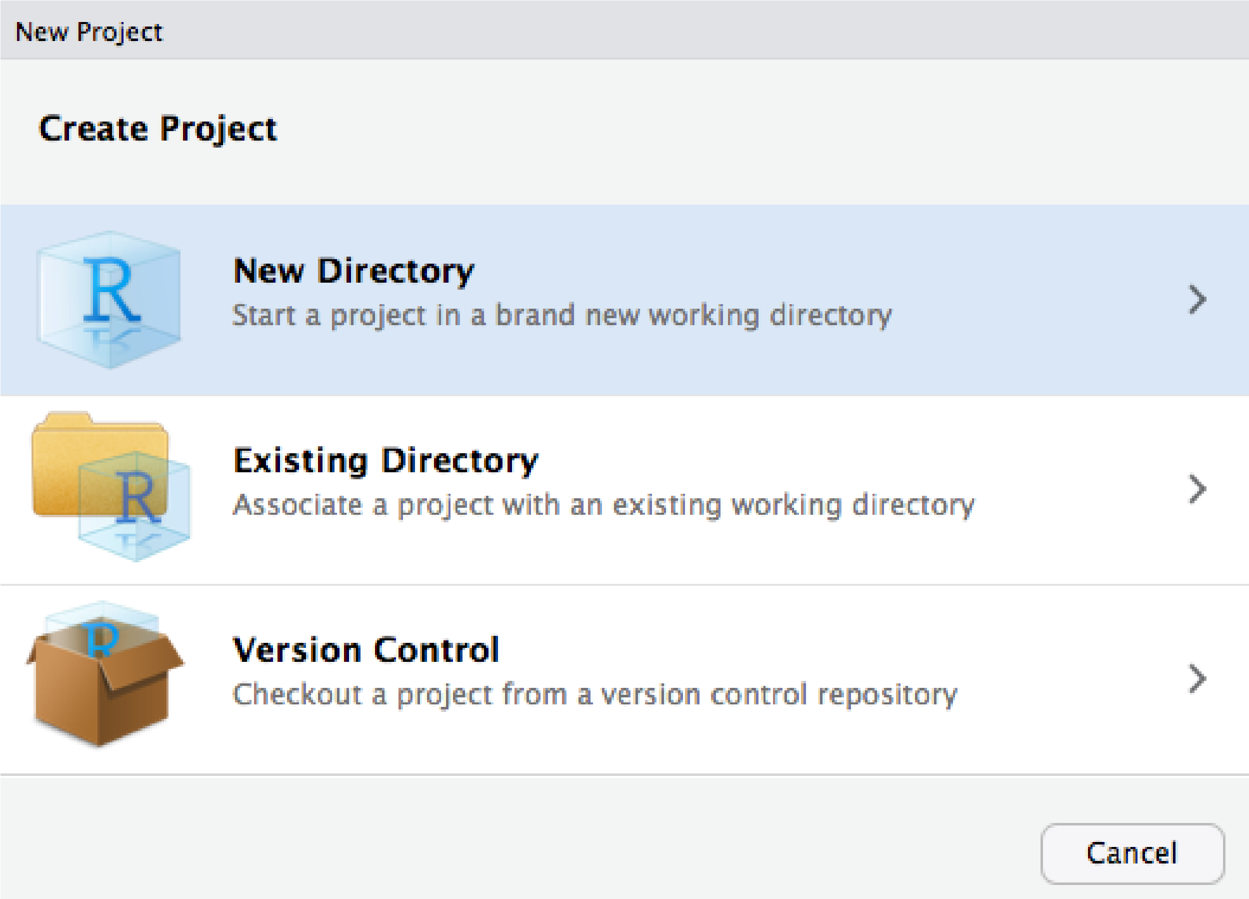
● Public
Anyone can see this repository. You choose who can commit.

○ Private
You choose who can see and commit to this repository.

□ Initialize this repository with a README
This will let you immediately clone the repository to your computer. Skip this step if you're importing an existing repository.

Add .gitignore: None | Add a license: None

Figure 3.2: Create a new Linreg repository on GitHub



New Project

Create Project

New Directory
Start a project in a brand new working directory

Existing Directory
Associate a project with an existing working directory

Version Control
Checkout a project from a version control repository

Figure 3.3: Create a new project in RStudio

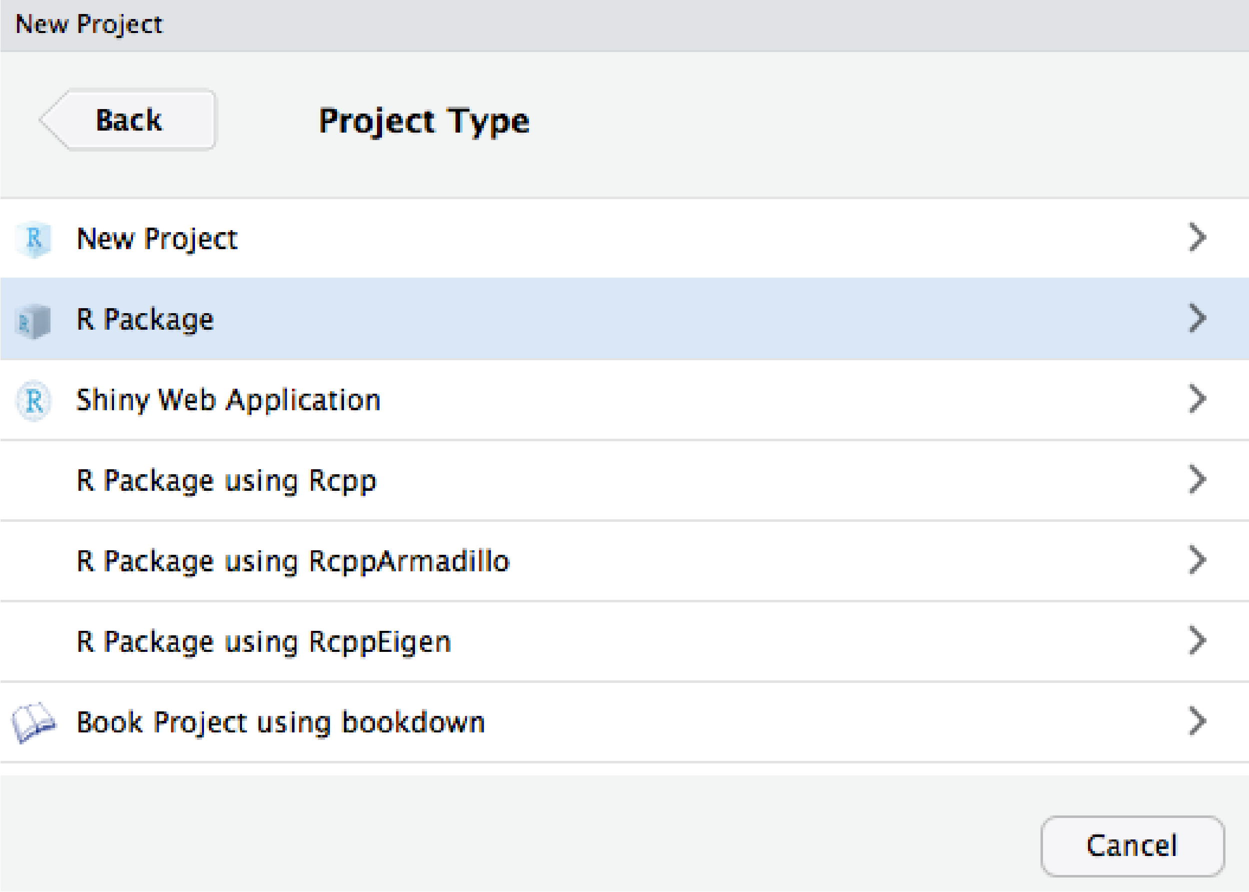
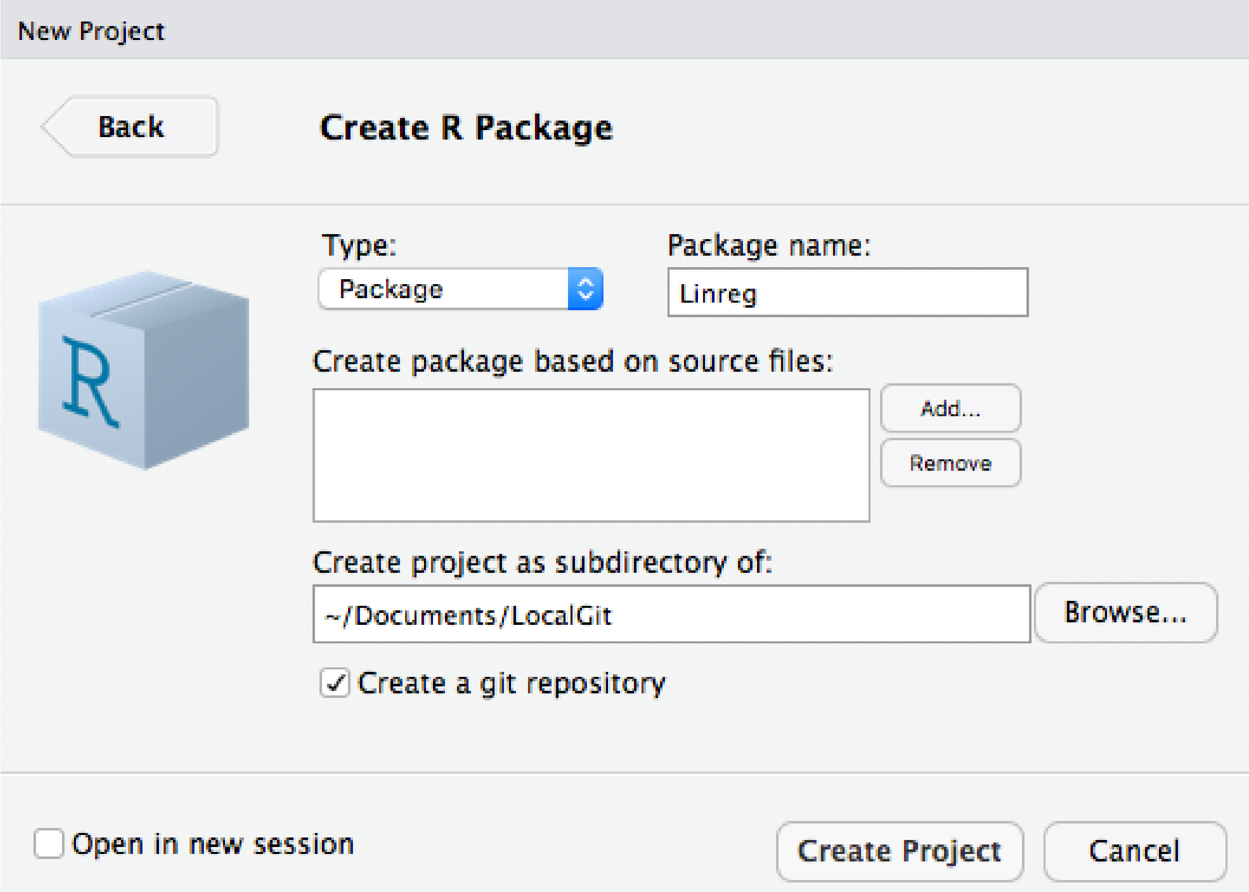


Figure 3.4: Select R package



Type: Package

Package name: Linreg

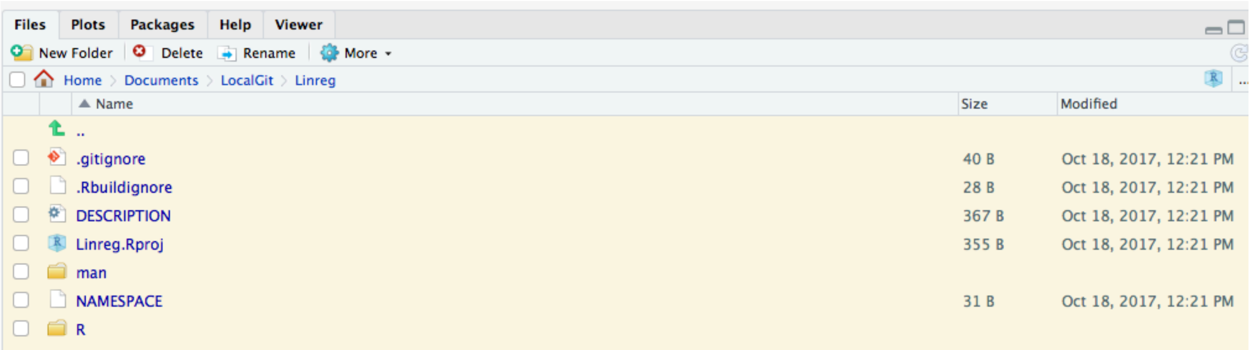
Create package based on source files:

Create project as subdirectory of: ~/Documents/LocalGit

☑ Create a git repository

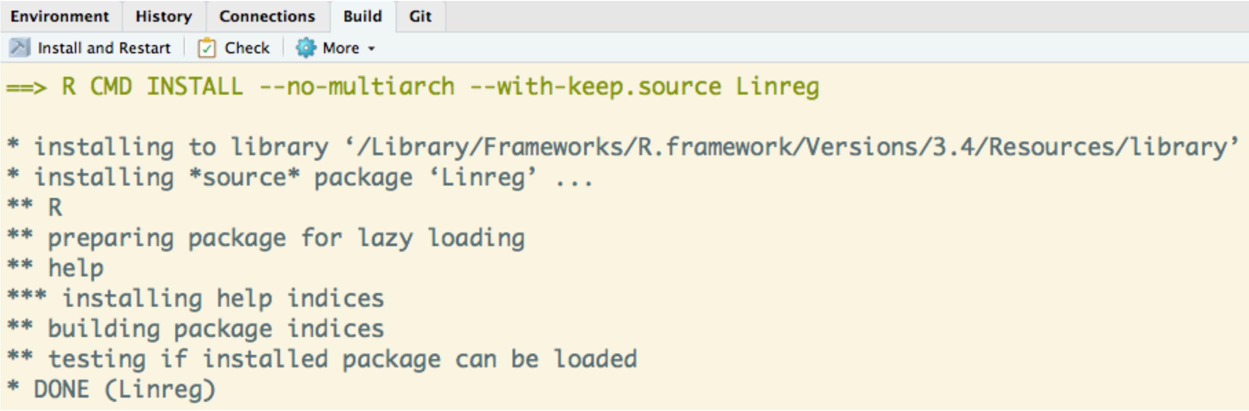
□ Open in new session

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



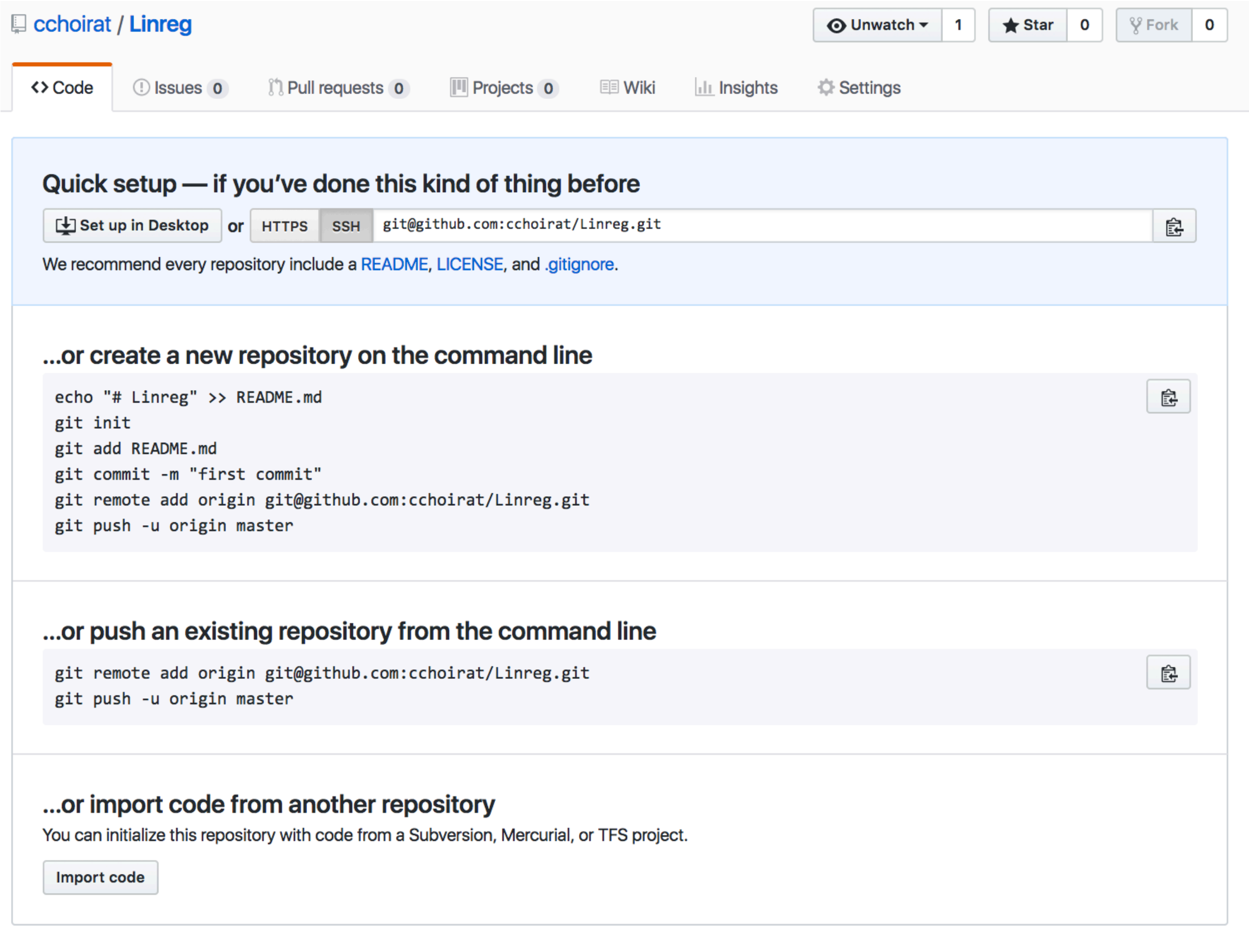
Name	Size	Modified
..		
.gitignore	40 B	Oct 18, 2017, 12:21 PM
.Rbuildignore	28 B	Oct 18, 2017, 12:21 PM
DESCRIPTION	367 B	Oct 18, 2017, 12:21 PM
Linreg.Rproj	355 B	Oct 18, 2017, 12:21 PM
man		
NAMESPACE	31 B	Oct 18, 2017, 12:21 PM
R		

Figure 3.6: Automatically created files



```
==> R CMD INSTALL --no-multiarch --with-keep.source Linreg

* installing to library ‘/Library/Frameworks/R.framework/Versions/3.4/Resources/library’
* installing *source* package ‘Linreg’ ...
** R
** preparing package for lazy loading
** help
*** installing help indices
** building package indices
** testing if installed package can be loaded
* DONE (Linreg)
```

Figure 3.7: Build tab in RStudio



Quick setup — if you've done this kind of thing before

git@github.com:cchoirat/Linreg.git

We recommend every repository include a README, LICENSE, and .gitignore.

...or create a new repository on the command line

```
echo "# Linreg" >> README.md
git init
git add README.md
git commit -m "first commit"
git remote add origin git@github.com:cchoirat/Linreg.git
git push -u origin master
```

...or push an existing repository from the command line

```
git remote add origin git@github.com:cchoirat/Linreg.git
git push -u origin master
```

...or import code from another repository

You can initialize this repository with code from a Subversion, Mercurial, or TFS project.

Figure 3.8: Github webpage

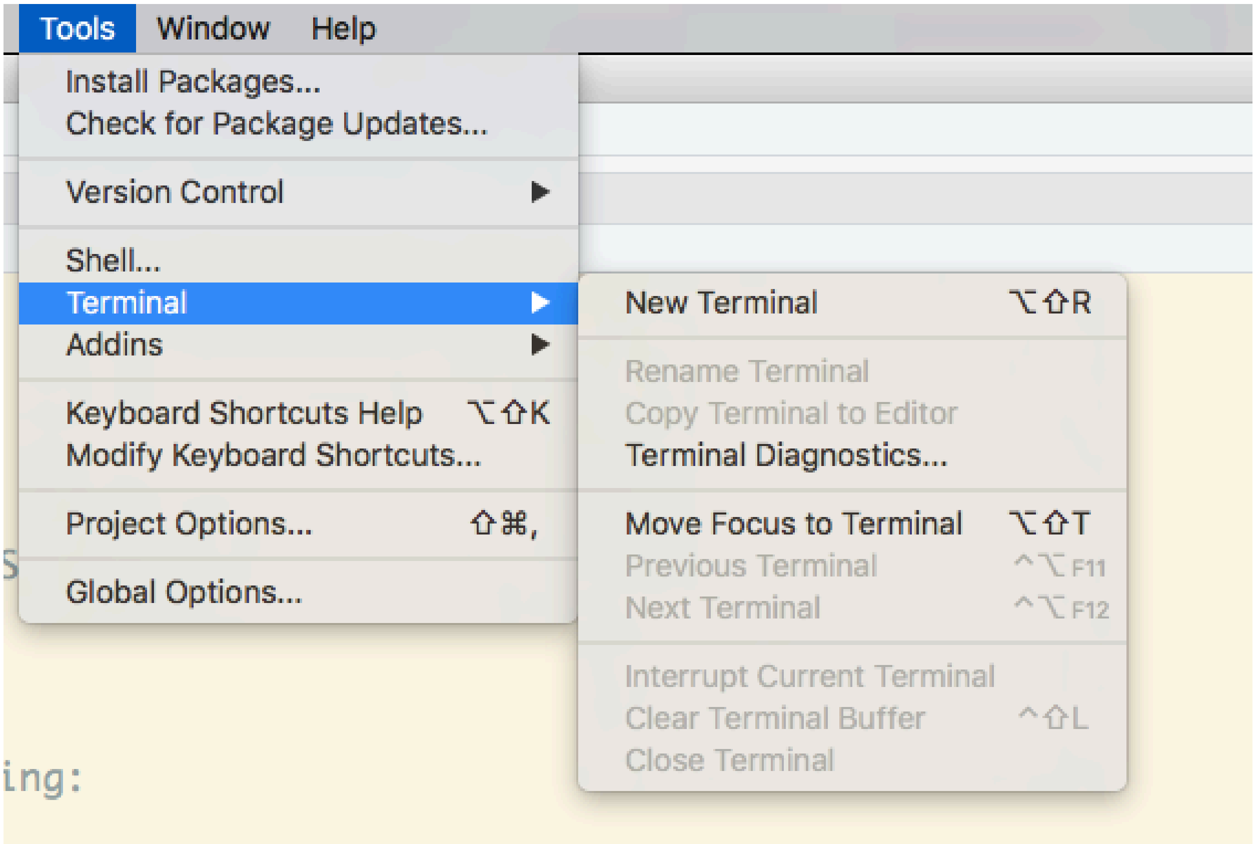
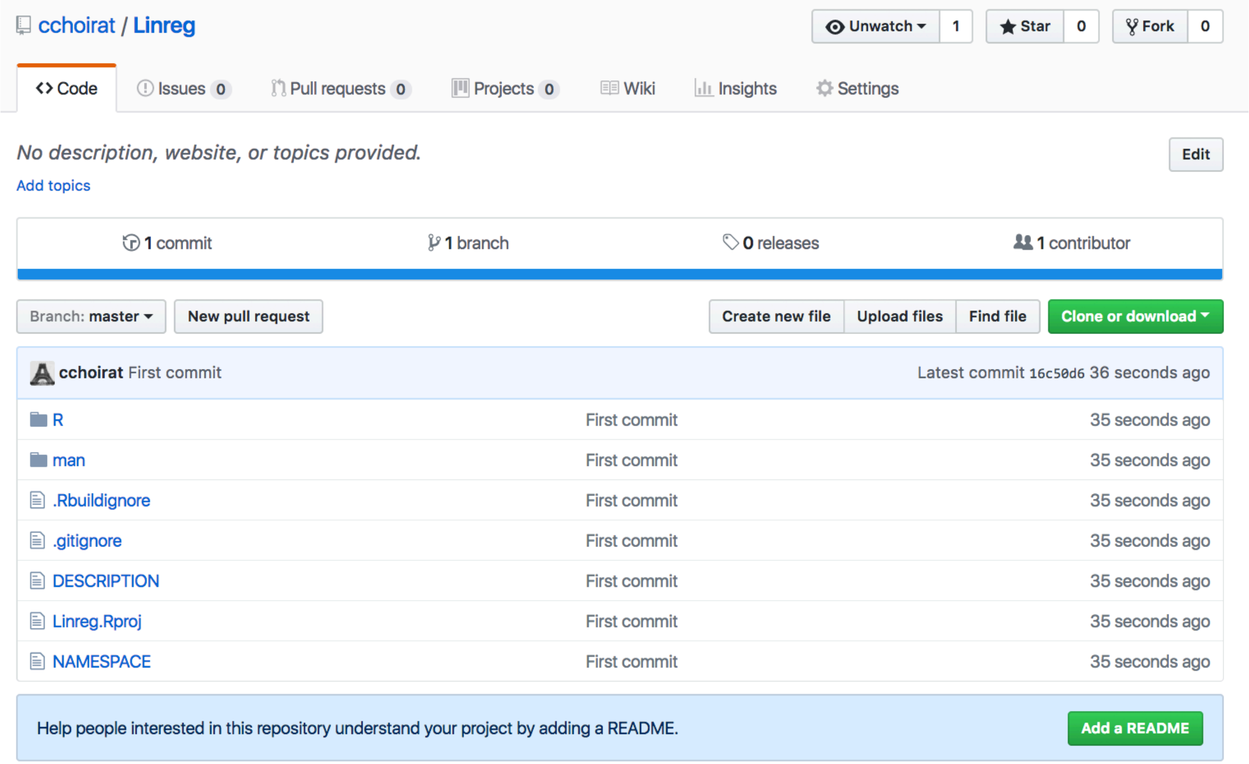


Figure 3.9: Open a terminal



No description, website, or topics provided.

cchoirat First commit — Latest commit 16c50d6 36 seconds ago

R	First commit	35 seconds ago
man	First commit	35 seconds ago
.Rbuildignore	First commit	35 seconds ago
.gitignore	First commit	35 seconds ago
DESCRIPTION	First commit	35 seconds ago
Linreg.Rproj	First commit	35 seconds ago
NAMESPACE	First commit	35 seconds ago

Help people interested in this repository understand your project by adding a README.

Figure 3.10: Github webpage is updated

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

GitHub default

```
# 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 `pkgtemplate.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` (or `Sweave`)

3.7 Package workflow example

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

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

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

```
linmodEst <- function(x, y) {
  ## compute QR-decomposition of x
  qx <- qr(x)
  ## compute (x’x)^(-1) x’y
  coef <- solve.qr(qx, 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 * chol2inv(qx$qr)
  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)
```

```
## $coefficients
## [1] -0.3566624  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`.

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

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

```
coef(lm1)
```

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

```
vcov(lm1)
```

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

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

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

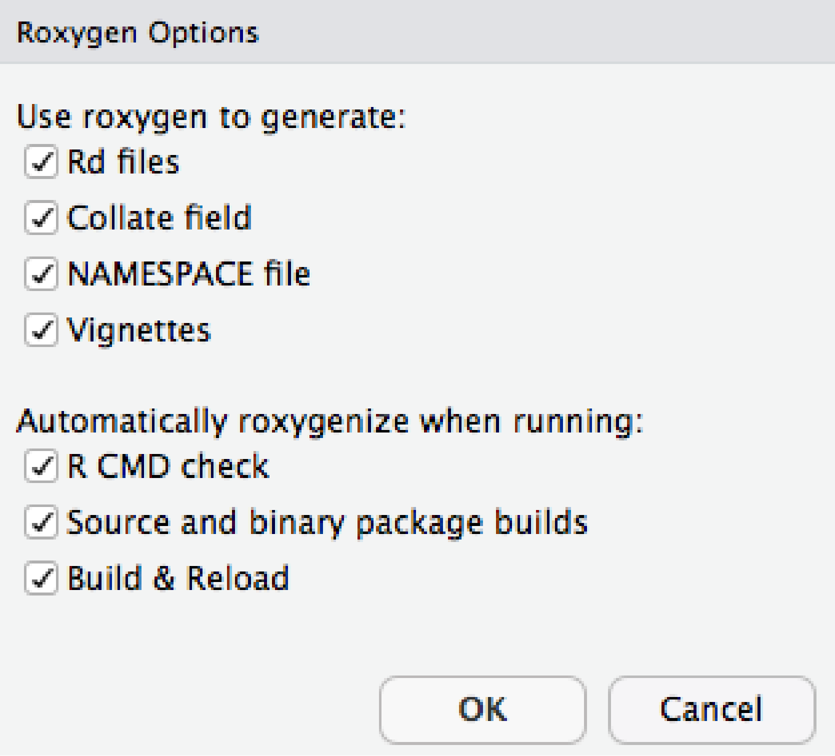
3.7.3 Add ROxygen2 documentation

```
#' 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"]
#' linreg(y, X)
#'
#' @export
#'
linmodEst <- function(x, y) {
  ## compute QR-decomposition of x
  qx <- qr(x)
  ## compute (x’x)^(-1) x’y
  coef <- solve.qr(qx, 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 * chol2inv(qx$qr)
  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:



Roxygen Options

Use roxygen to generate:

☑ Rd files

☑ Collate field

☑ NAMESPACE file

☑ Vignettes

Automatically roxygenize when running:

☑ R CMD check

☑ Source and binary package builds

☑ Build & Reload

Figure 3.11: Roxygen options

```
% 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"]
linreg(y, X)

}
```

3.7.6 Formatted output

3.7.7 DESCRIPTION

```
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

export's automatically generated when parsing ROxygen2 snippets

```
export(linmodEst)
```

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"
```

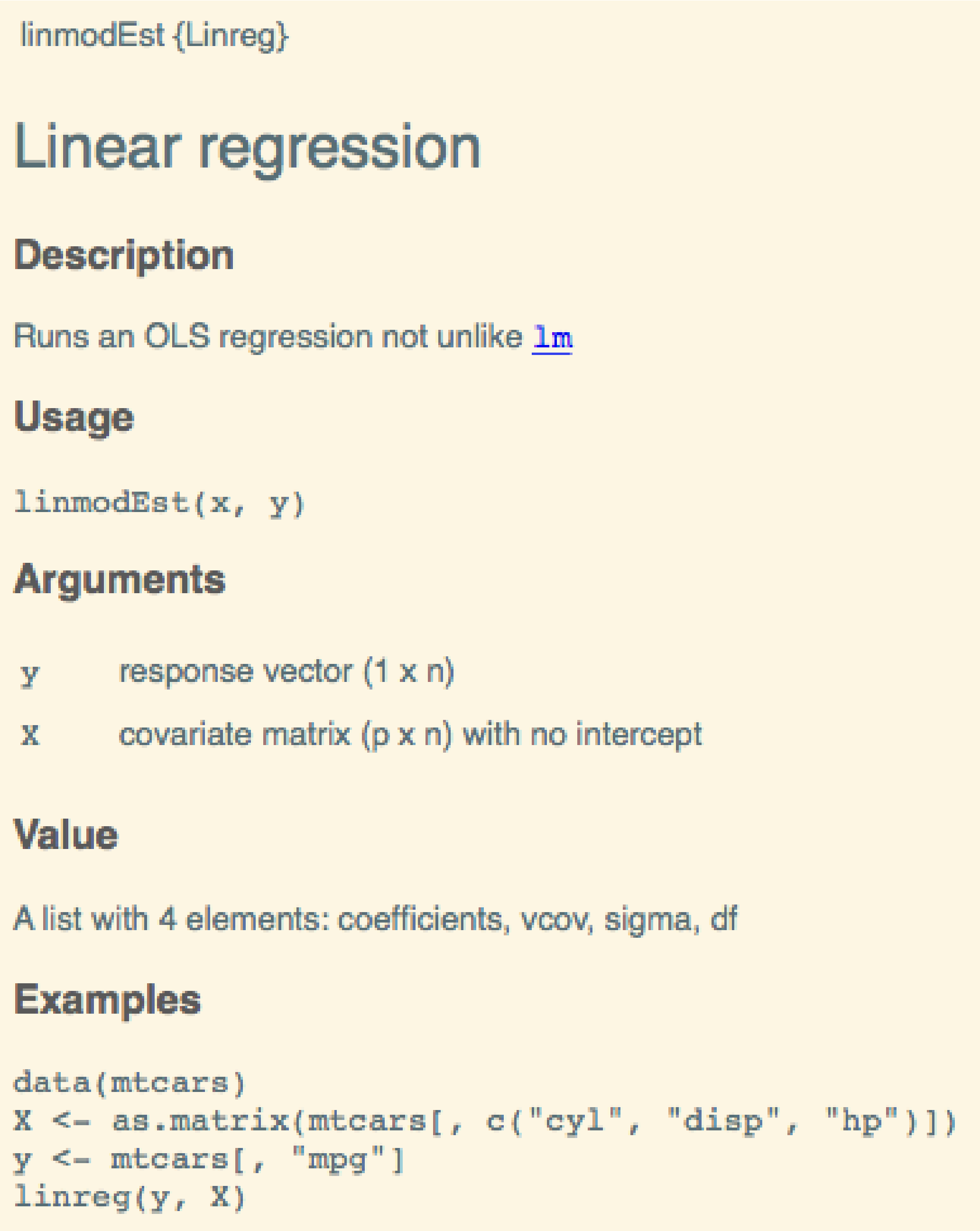
```
print.hi <- function(...) {
  print("Surprise!")
}

hello()
```

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

3.7.10 S3 and S4 generics

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

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



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"]
linreg(y, X)
```

```
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)
mod1
```

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

3.7.12 Other methods

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

3.7.13 Formulas and model frames

```
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 ========================================================================================
```

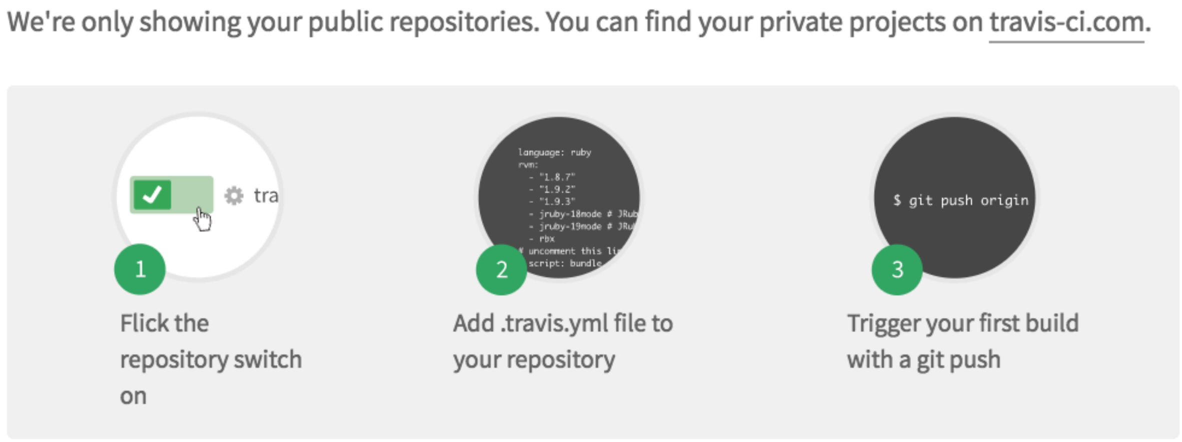
3.9 Continuous integration

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



We're only showing your public repositories. You can find your private projects on travis-ci.com.

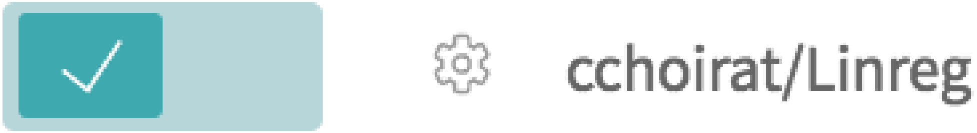
```
language: ruby
rvm:
  - "1.8.7"
  - "1.9.2"
  - "1.9.3"
  - jruby-18mode # JRub
  - jruby-19mode # JRu
  - rbx
# uncomment this li
  script: bundle
```

```
$ git push origin
```

1 Flick the repository switch on

2 Add .travis.yml file to your repository

3 Trigger your first build with a git push



cchoirat/Linreg

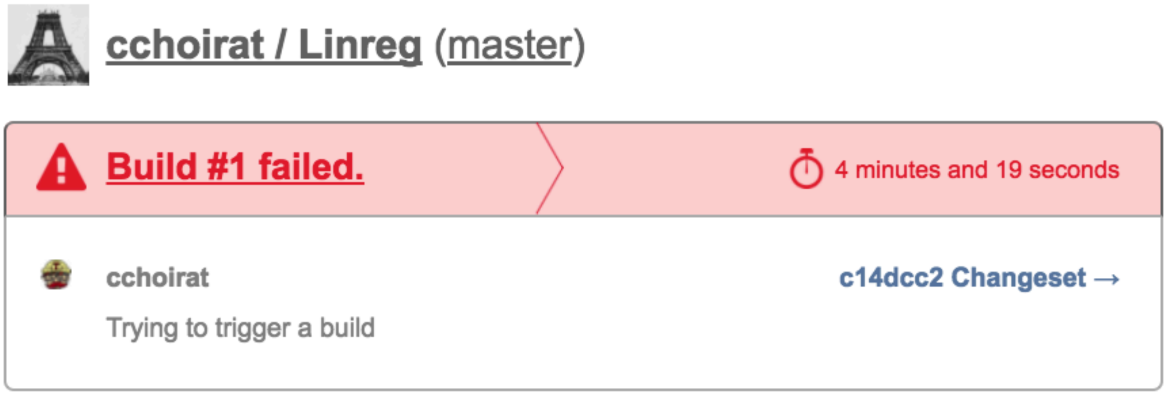
Calling

```r
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!



cchoirat / Linreg (master)

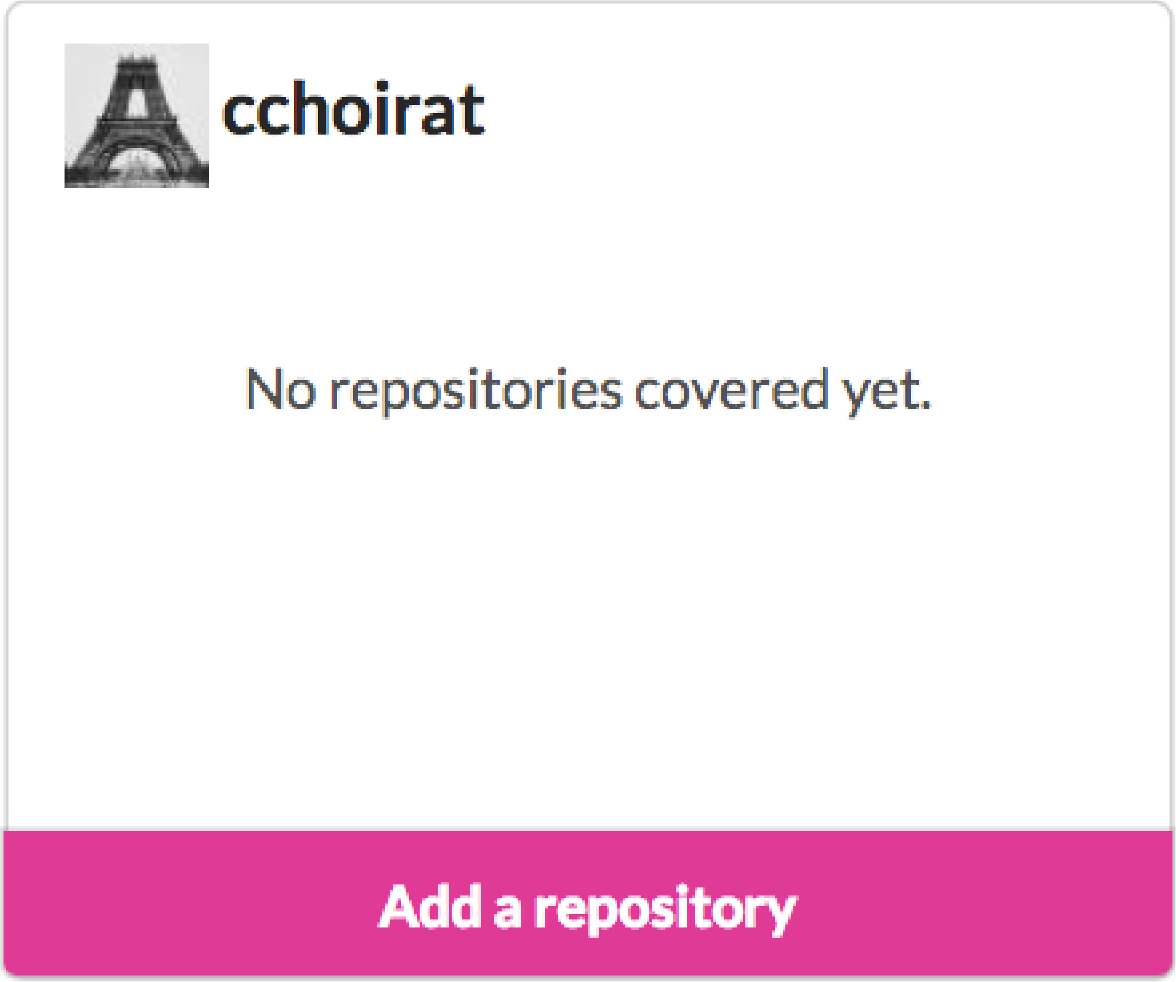
Build #1 failed.

4 minutes and 19 seconds

cchoirat

Trying to trigger a build

c14dcc2 Changeset →



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"))
```

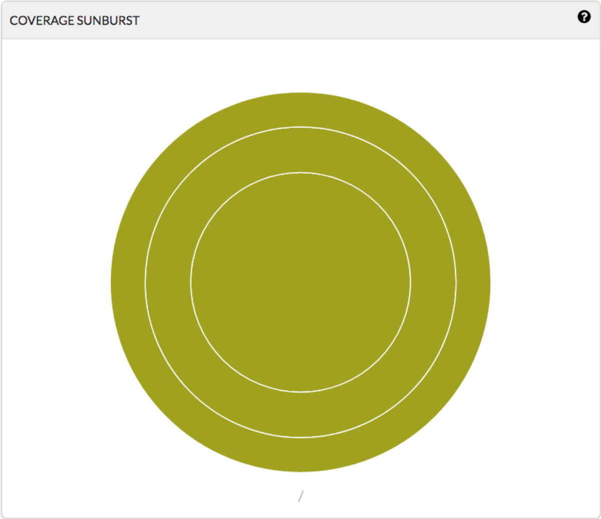
creates the `codecov.yml` file:

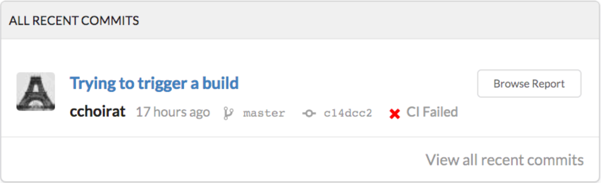
```
comment: false
```

A call to

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

will give you code coverage information:


COVERAGE SUNBURST

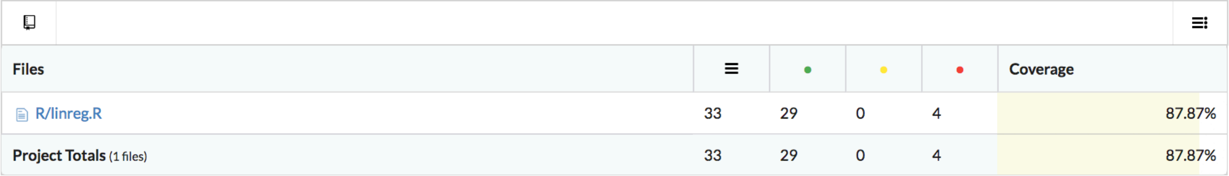

ALL RECENT COMMITS

Trying to trigger a build

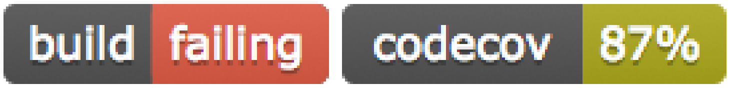
cchoirat 17 hours ago master c14dcc2 ✖ CI Failed

Browse Report

View all recent commits



Files	≡	●	●	●	Coverage
R/linreg.R	33	29	0	4	87.87%
Project Totals (1 files)	33	29	0	4	87.87%



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://travi
[![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 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
```

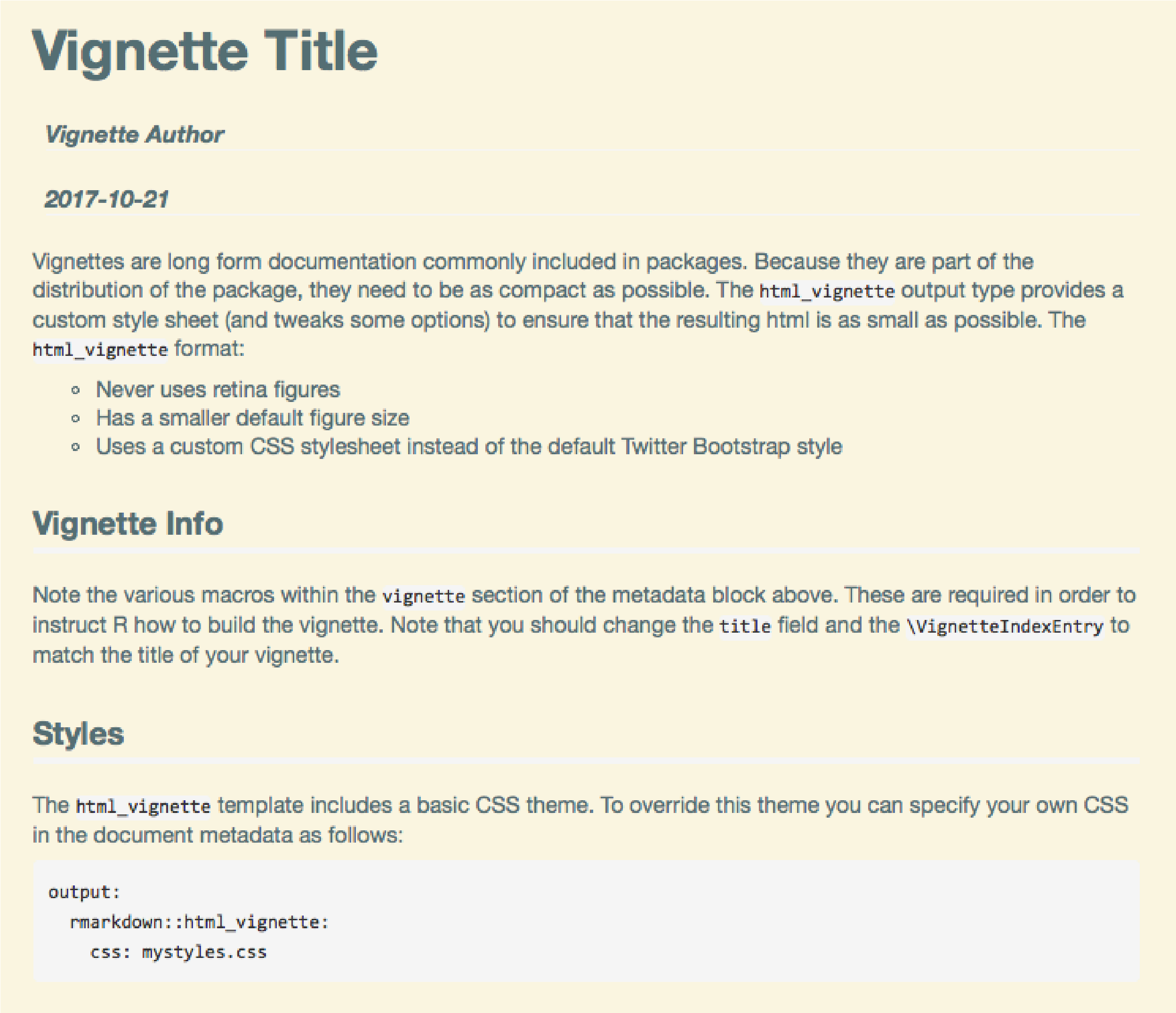
The vignette is built into a HTML document with

```
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 they are part of the distribution of the package, they need to be as compact as possible. The `html_vignette` output type provides a custom style sheet (and tweaks some options) to ensure that the resulting html is as small as possible. The `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. These are required in order to instruct R how to build the vignette. Note that you should change the `title` field and the `\VignetteIndexEntry` to match the title of your vignette.

Styles

The `html_vignette` template includes a basic CSS theme. To override this theme you can specify your own CSS 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

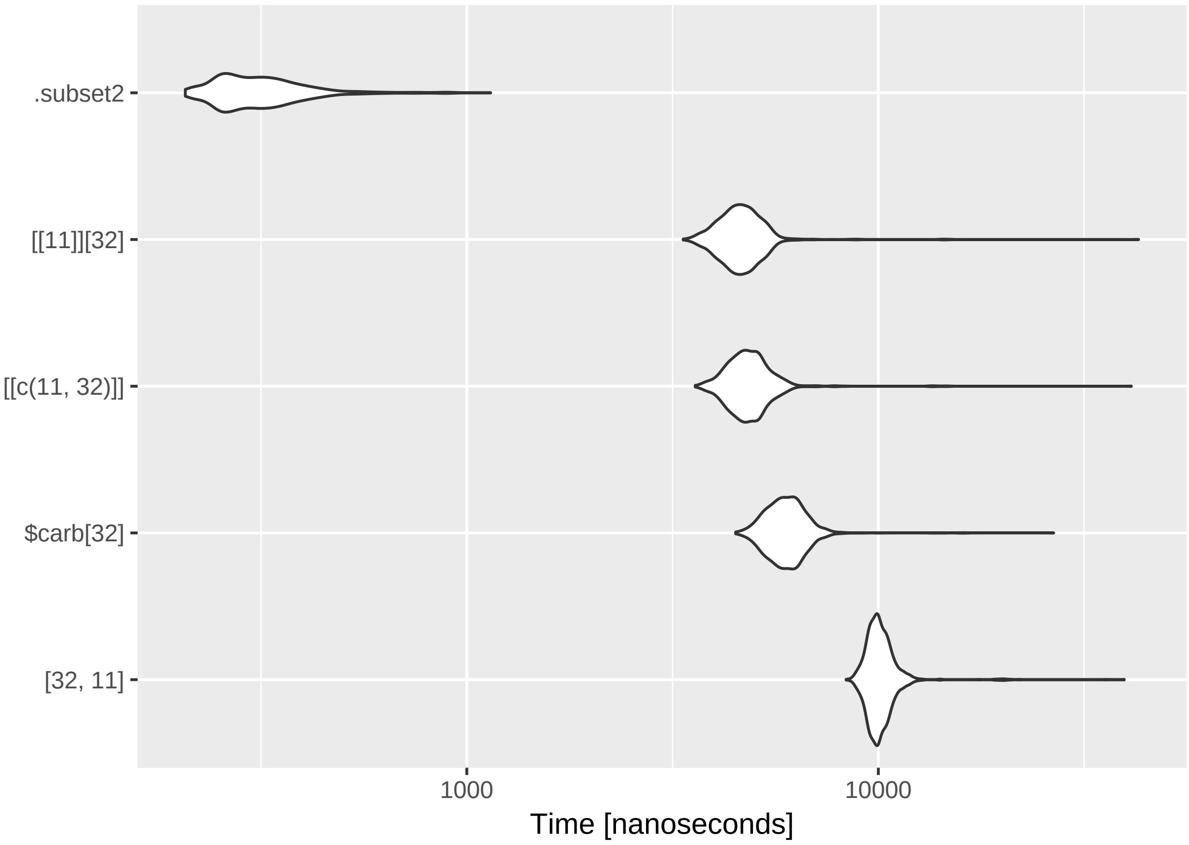
There are several ways to benchmark code (see http://www.alexejgossmann.com/benchmarking_r/) from `system.time` to dedicated packages such as `rbenchmark` (Kusnierczyk (2012)) or `microbenchmark` (Mersmann (2015)).

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
##       [32, 11] 8350 9595.0 10216.091 9992.0 10472.5 39588  1000
##      $carb[32] 4501 5520.0  6037.642 5954.5  6385.0 26665  1000
##  [[c(11, 32)]] 3590 4460.5  4930.627 4806.0  5153.0 41202  1000
##     [[11]][32] 3355 4269.5  4705.329 4609.0  4958.5 42893  1000
##       .subset2  207  258.5   323.393  303.0   355.0  1143  1000
```

```
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.

```
data(cats, package = "MASS")
fit1 <- lm(Hwt ~ Bwt, data = cats)
fit2 <- linmod(Hwt ~ Bwt, data = cats)
fit3 <- linmodEst(cbind(1, cats$Bwt), cats$Hwt)
all.equal(round(coef(fit1), 5), round(coef(fit2), 5))
```

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

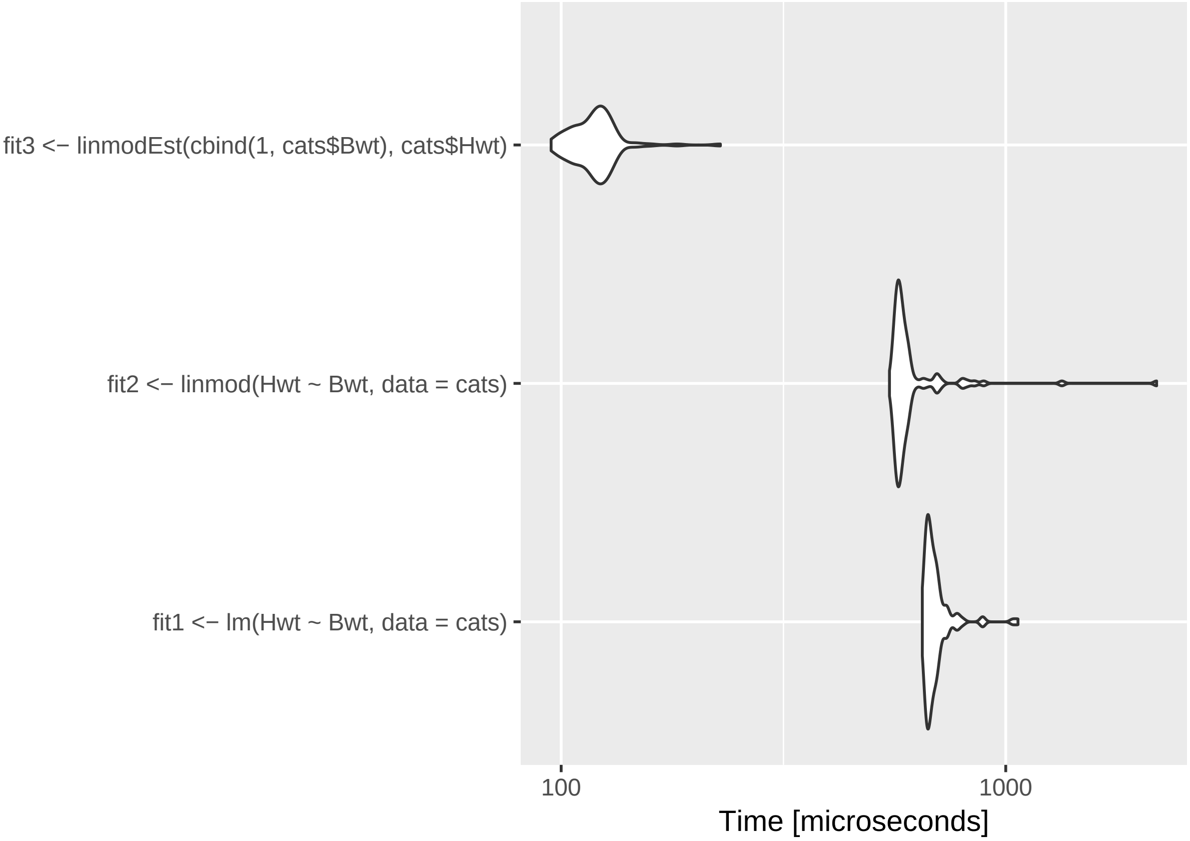
```
all.equal(round(coef(fit1), 5), round(fit3$coefficients, 5), check.names = FALSE)
```

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

```
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
)
m
```

```
## Unit: microseconds
##                                              expr     min       lq     mean
##               fit1 <- lm(Hwt ~ Bwt, data = cats) 649.134 665.2440 698.7733
##           fit2 <- linmod(Hwt ~ Bwt, data = cats) 547.634 570.2980 624.7540
##  fit3 <- linmodEst(cbind(1, cats$Bwt), cats$Hwt)  94.924 109.7005 119.8547
##    median       uq      max neval
##  679.1715 701.6545 1065.559   100
##  580.9210 602.6640 2184.982   100
##  119.4020 125.7615  228.101   100
```

```
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).

```r
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
```

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

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

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

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

`vacc1a` is not designed for vector inputs

```r
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

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

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

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

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

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

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

We can use a loop:

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

or one of the `apply` functions:

```r
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
```

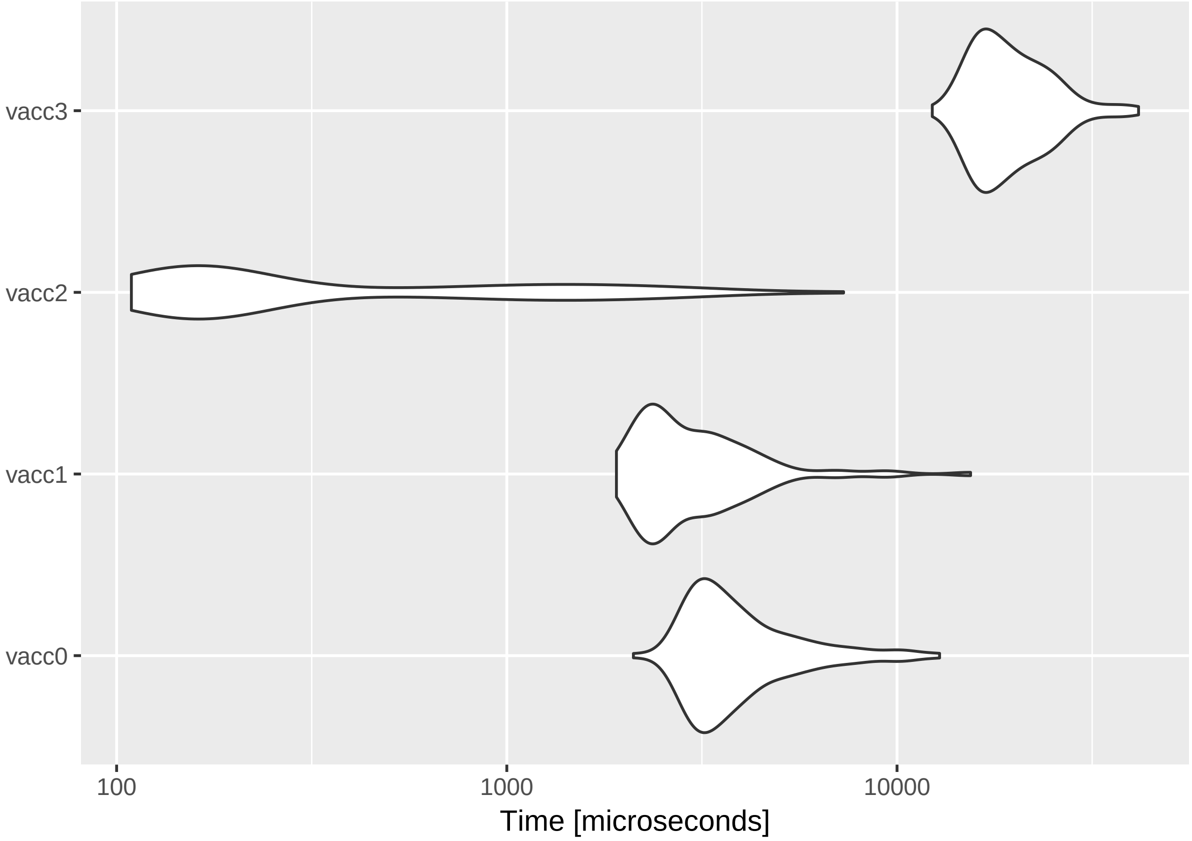
```
## [1] 4
```

```
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 2110.544 3085.9260 4223.4172 3547.9315 4486.068 12855.482
##   vacc1 1909.436 2325.8515 3282.6658 2646.2705 3506.734 15436.084
##  vacc2   109.103   149.2355   689.2302   191.2885   948.037  7294.517
##  vacc3 12313.887 16455.7605 20109.1667 18752.7630 22837.876 41589.137
##  neval
##    100
##    100
##    100
##    100
```

```
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: 0x114462cc0>))
```

```
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.

4.5.6 Example

```
#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]]
```

```cpp
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;
}
```

Chapter 5

Databases

5.1 Overview

5.2 SQL

5.3 noSQL

5.4 R interfaces

Chapter 6

Big data

In this Chapter, we are going to review different approaches to handle and perform analyses on *data that does not fit in memory.*

6.1 Reading big data (that fits in memory)

6.1.1 R package comparison

6.1.2 Python

6.2 Sampling (can be read, not analyzed easily)

6.3 Pure R solutions

6.4 JVM solutions

6.4.1 h20

6.4.2 Spark

Chapter 7

Visualization

7.1 Principles of visualization

7.2 Maps and GIS

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