

# Computing for Big Data (BST-262)

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# 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

**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 (h2o, 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.

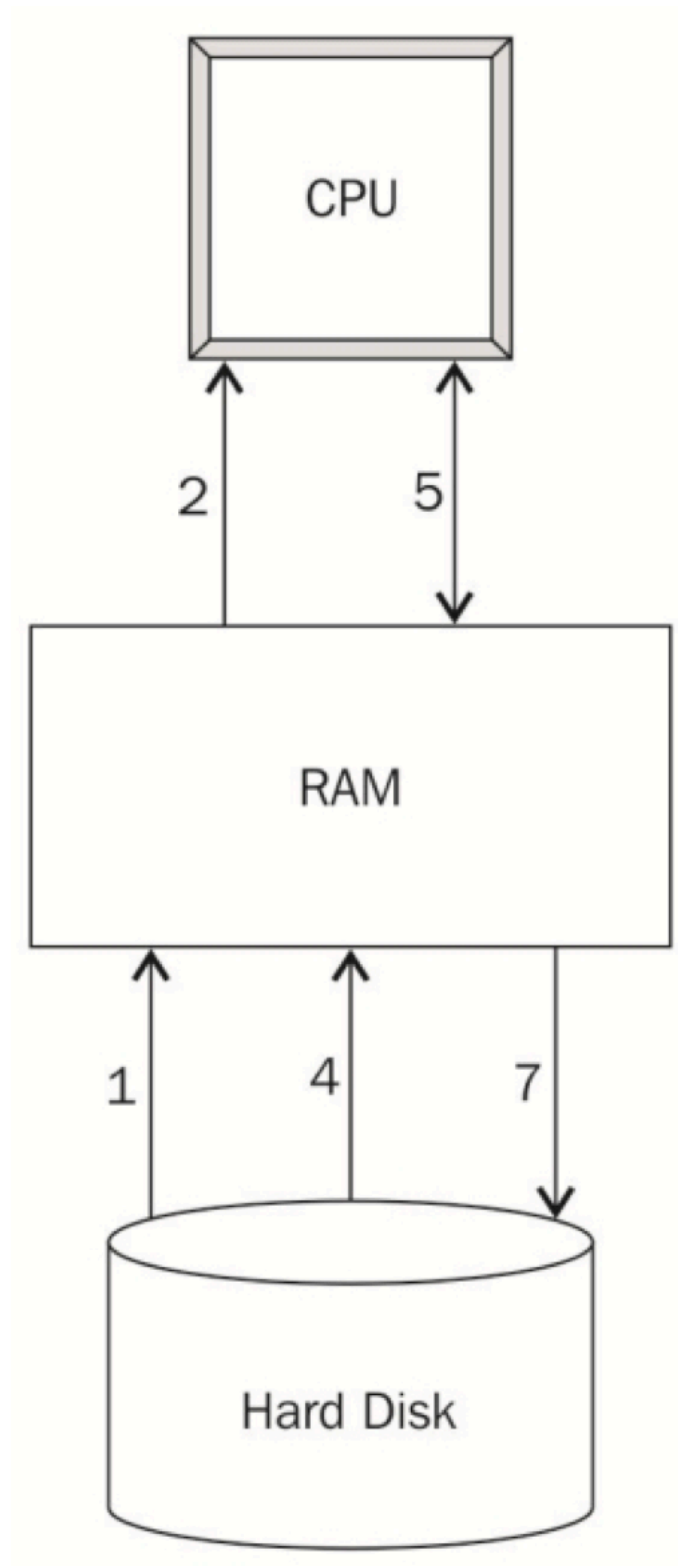


Figure 1.1: Steps to execute an R program, from @Lim2015, Chapter 1.

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<sub>2.5</sub> exposure

We will use PM<sub>2.5</sub> 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
```

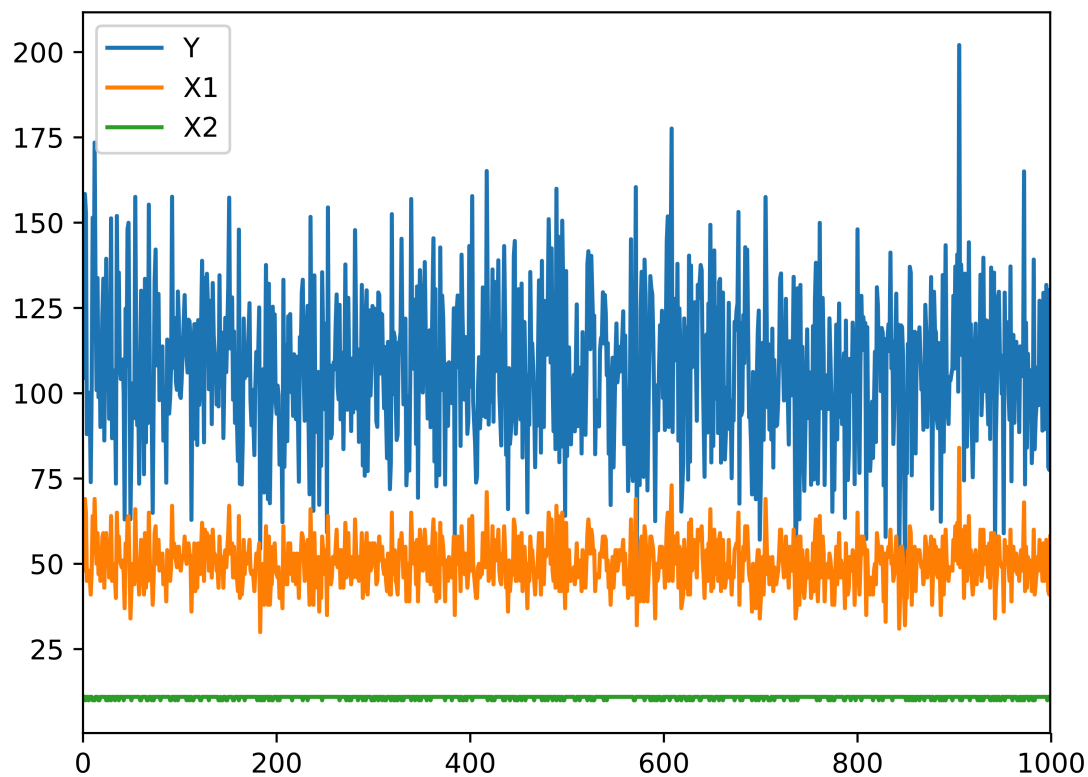
### 2.2.2 Create a plot in Python

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")
```



### 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 recommend 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)
```



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")
```

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
```


## Create a new repository

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

---

Owner

Repository name

 cchoirat ▾


 / 

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** ▾ 

---

**Create repository**

Figure 3.2: Create a new Linreg repository on GitHub

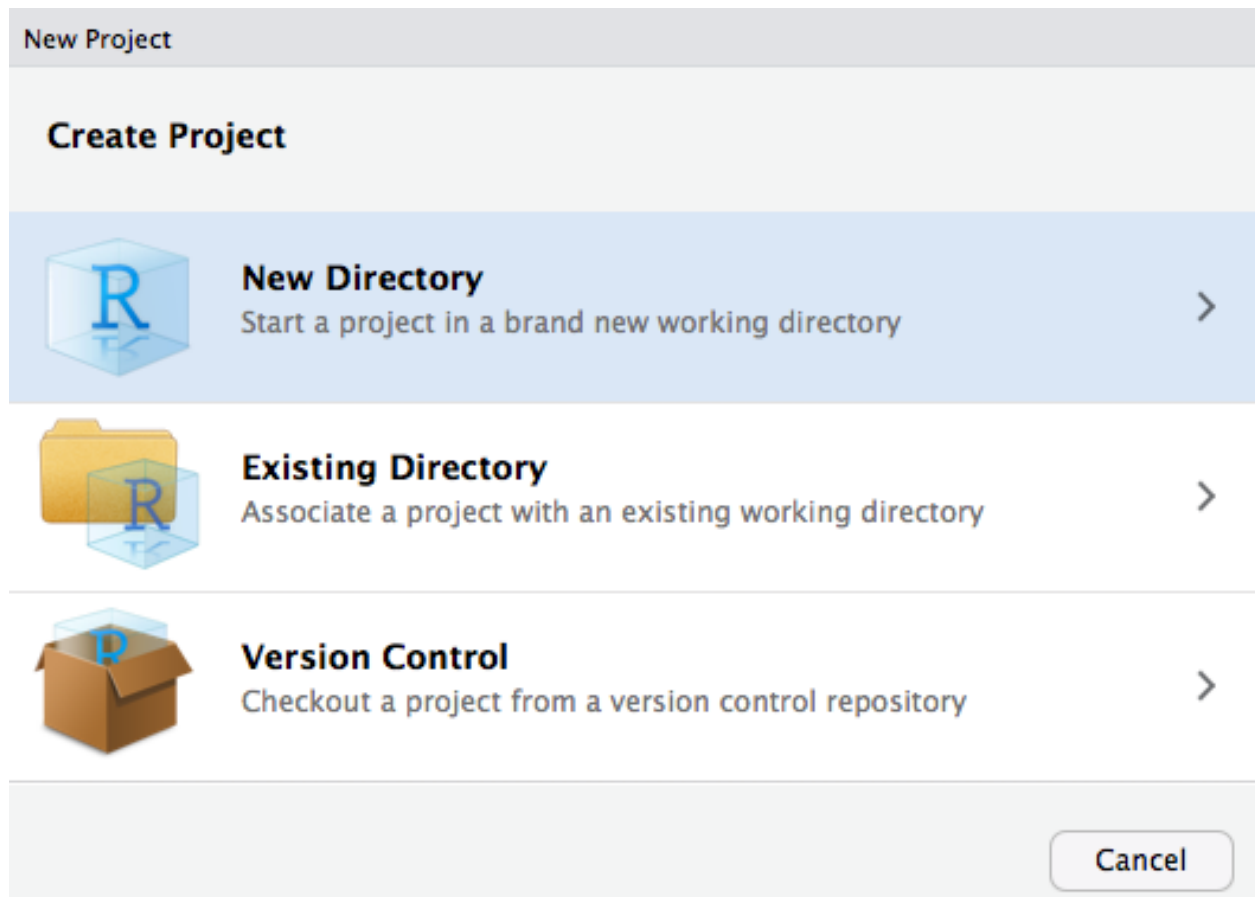


Figure 3.3: Create a new project in RStudio

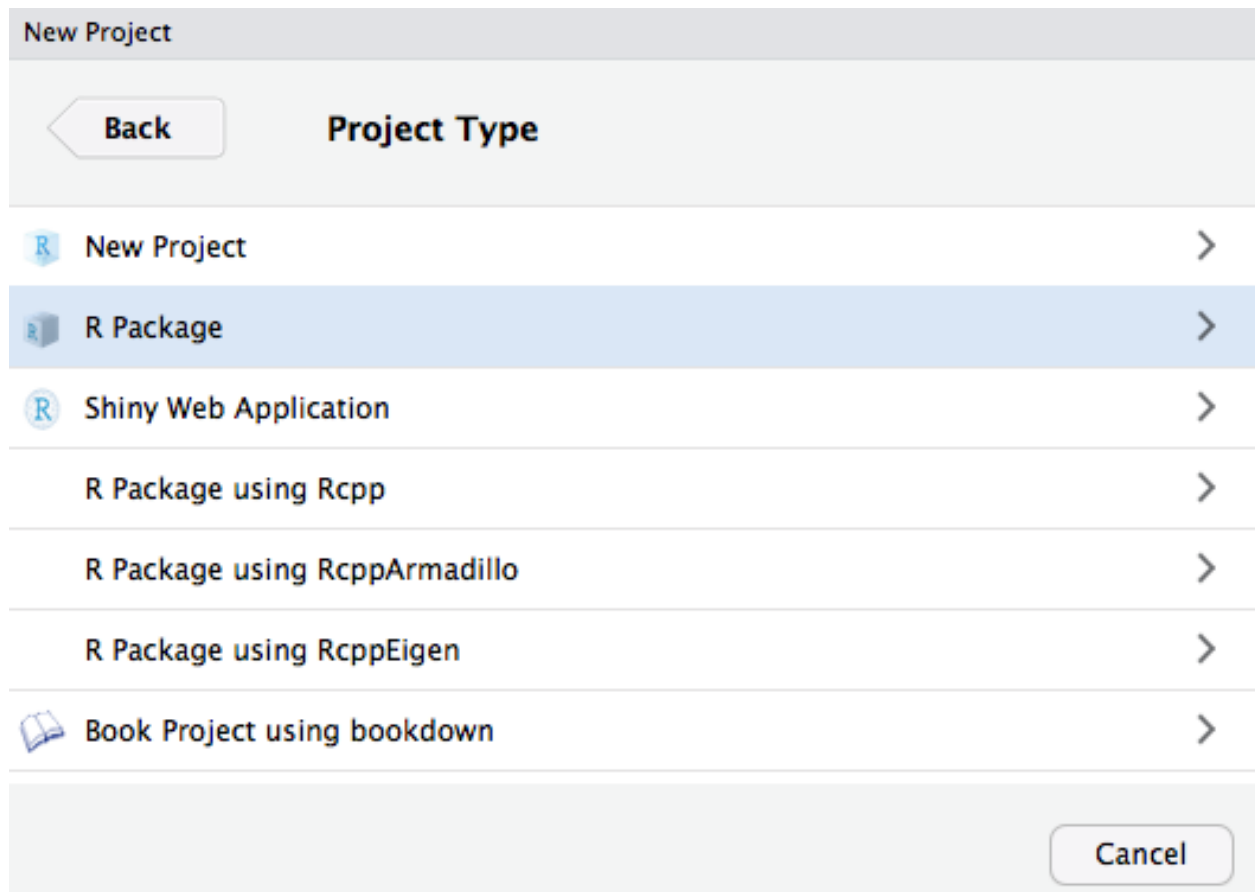



Figure 3.4: Select R package



New Project

[Back](#) **Create R Package**



Type: Package

Package name:

Create package based on source files:

[Add...](#)
[Remove](#)

Create project as subdirectory of:


[Browse...](#)

☒ Create a git repository

☐ Open in new session

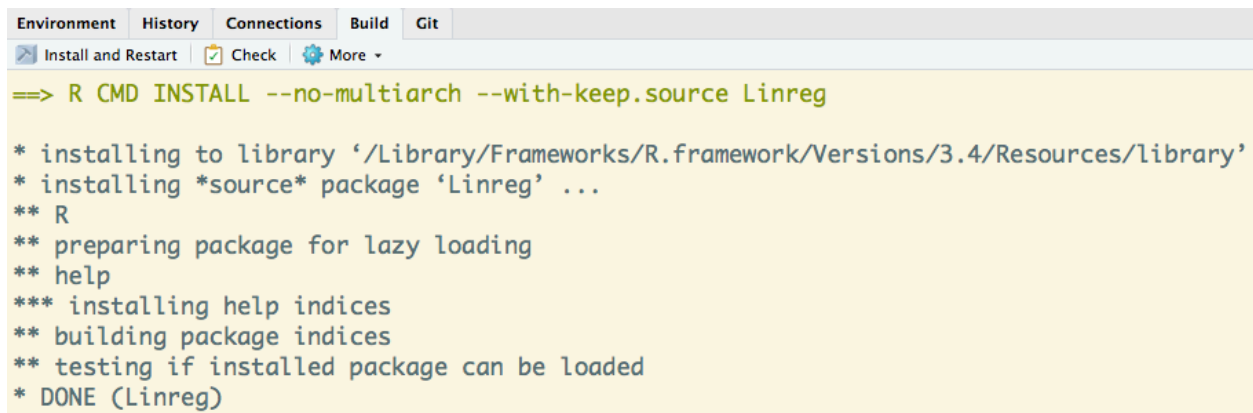
[Create Project](#) [Cancel](#)

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



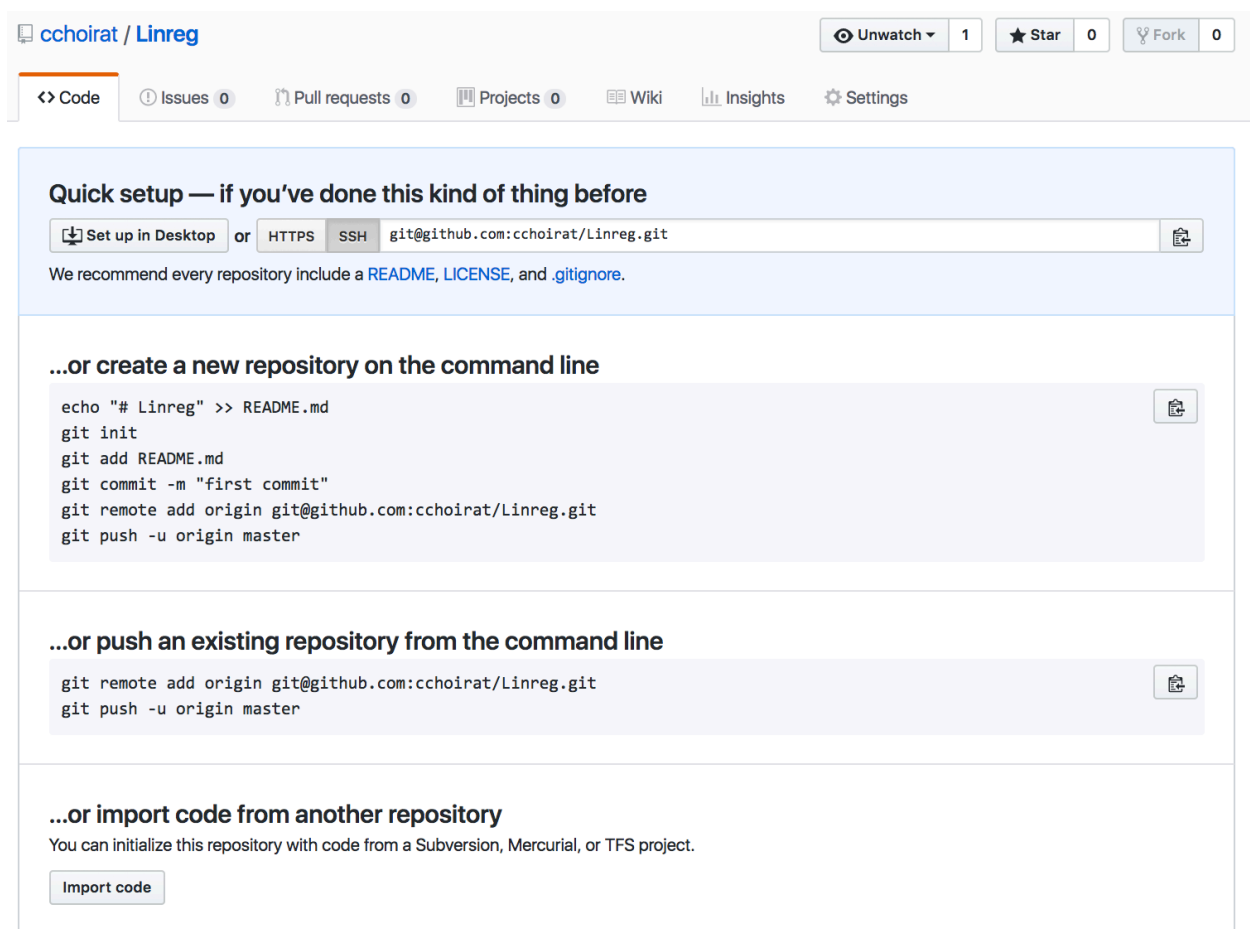
```

Environment History Connections Build Git
Install and Restart Check More
==> 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



cchoirat / Linreg

Unwatch 1 Star 0 Fork 0

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

Set up in Desktop or HTTPS SSH 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.

Import code

Figure 3.8: Github webpage

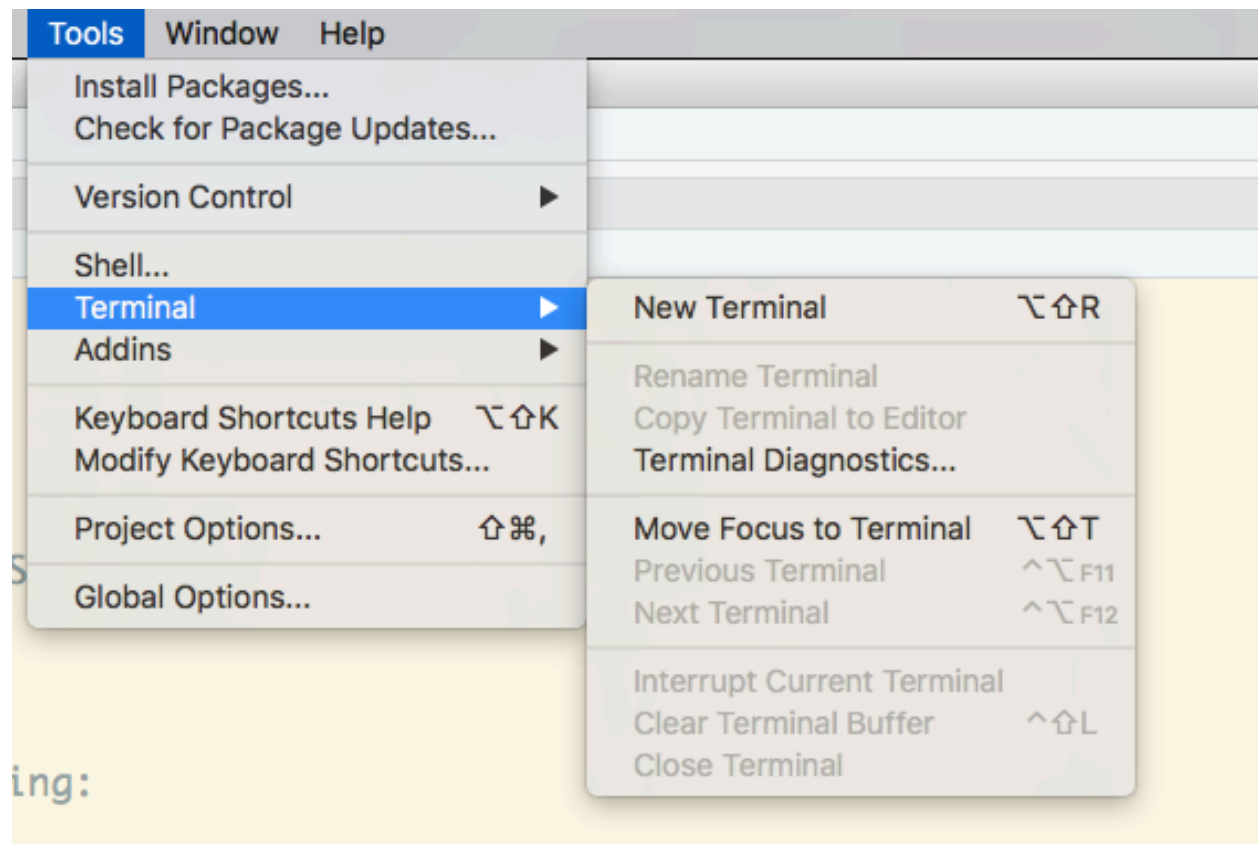


Figure 3.9: Open a terminal

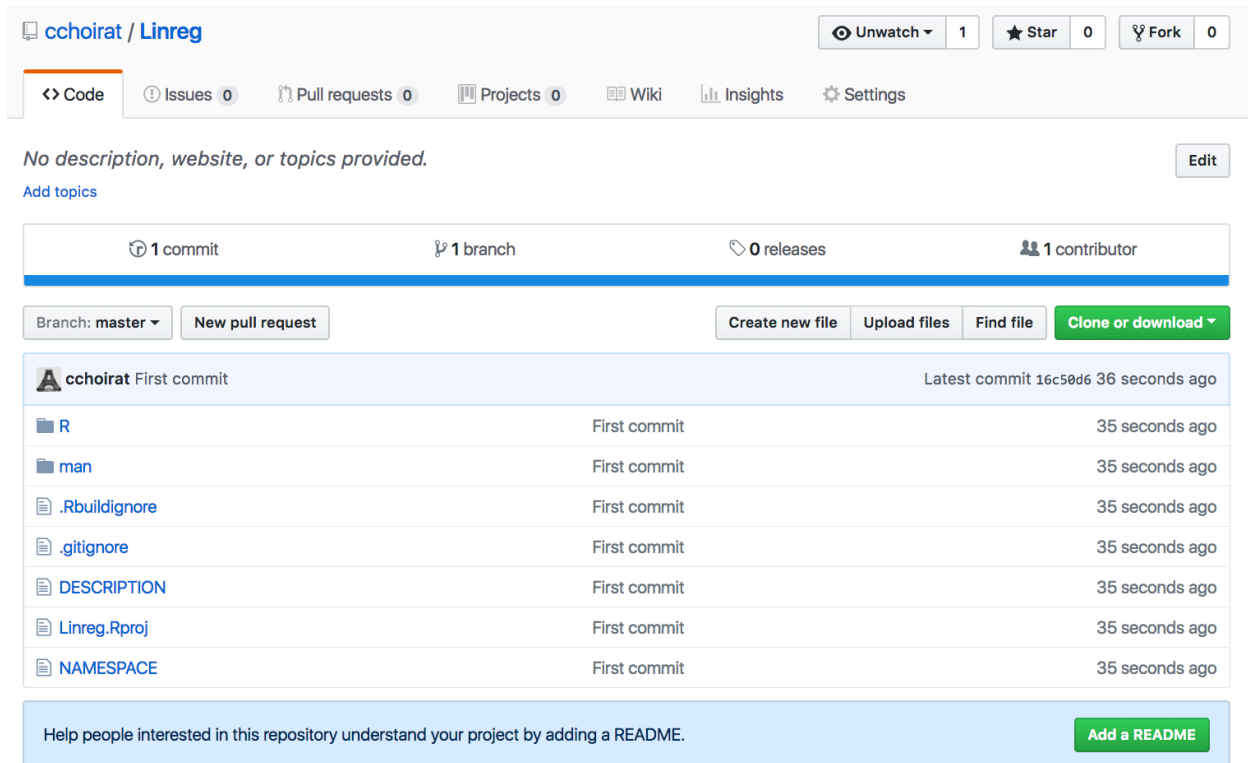


Figure 3.10: Github webpage is updated

### 3.5.1 .gitignore

RStudio default

```
.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 `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`.

```
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

Reading: [http://kbroman.org/pkg\\_primer/pages/docs.html](http://kbroman.org/pkg_primer/pages/docs.html)

```
## 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) {
  ## 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
  )
}
```

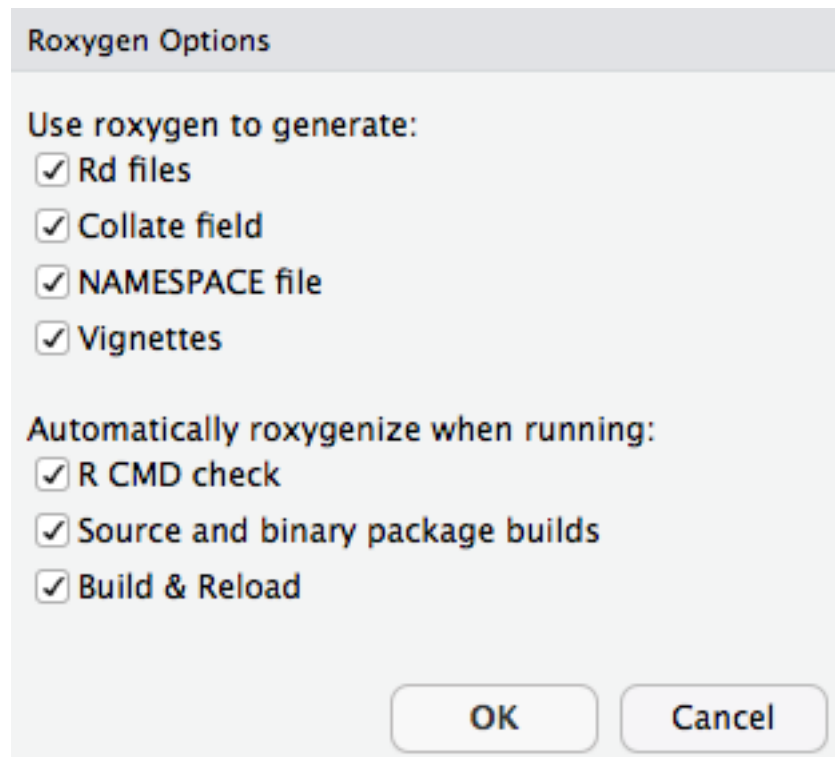


Figure 3.11: Roxygen options

```
)
}
```

### 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"]
linreg(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

#### 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()
```

```
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)
```







```
## [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, ...

### 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.

Calling

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

creates the `.travis.yml` file:

We're only showing your public repositories. You can find your private projects on [travis-ci.com](https://travis-ci.com).

1 Click the repository switch on

2 Add .travis.yml file to your repository

3 Trigger your first build with a git push



cchoirat/Linreg

# 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...



**cchoirat / Linreg (master)**



**Build #1 failed.**



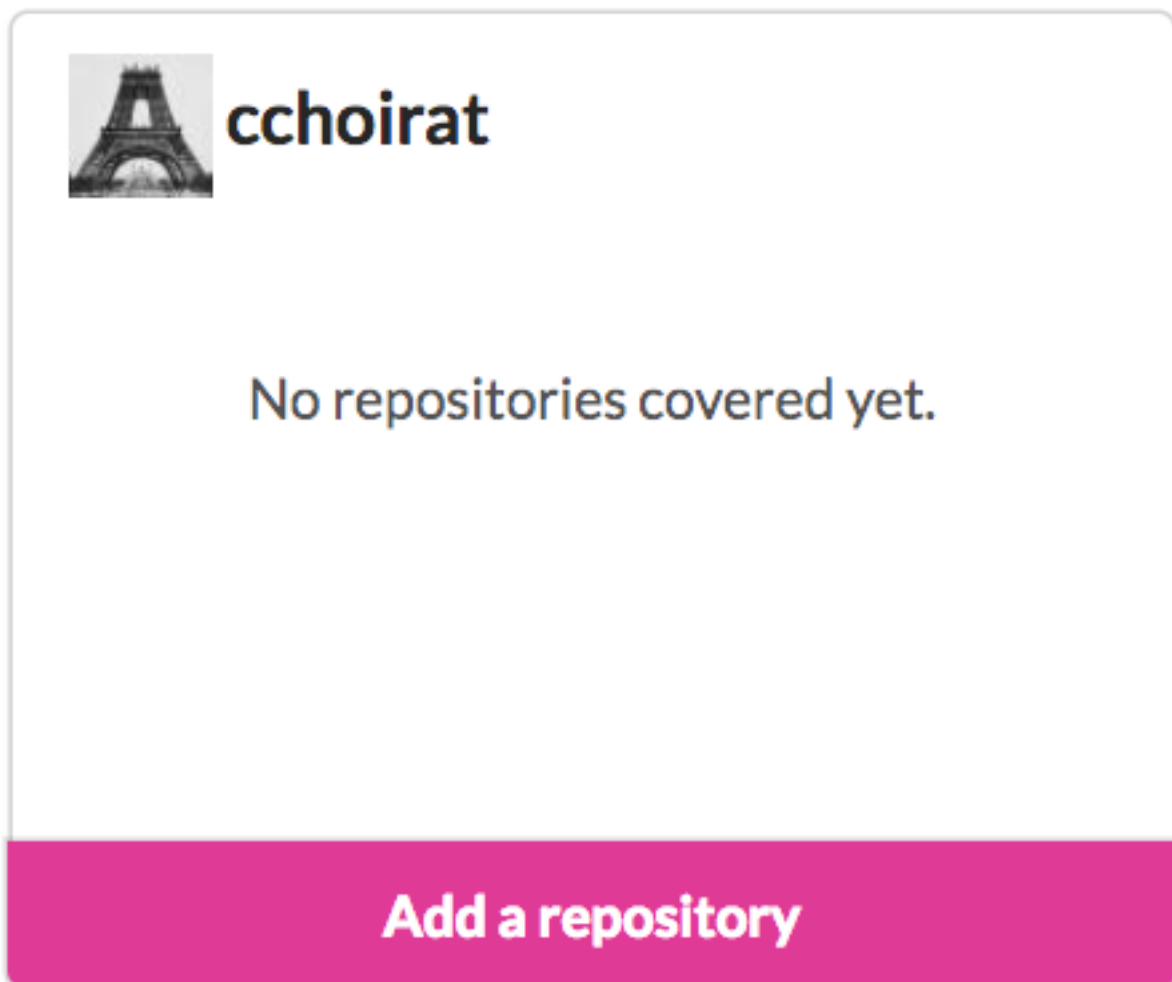
4 minutes and 19 seconds



**cchoirat**

Trying to trigger a build

**c14dcc2 Changeset** →



### 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:

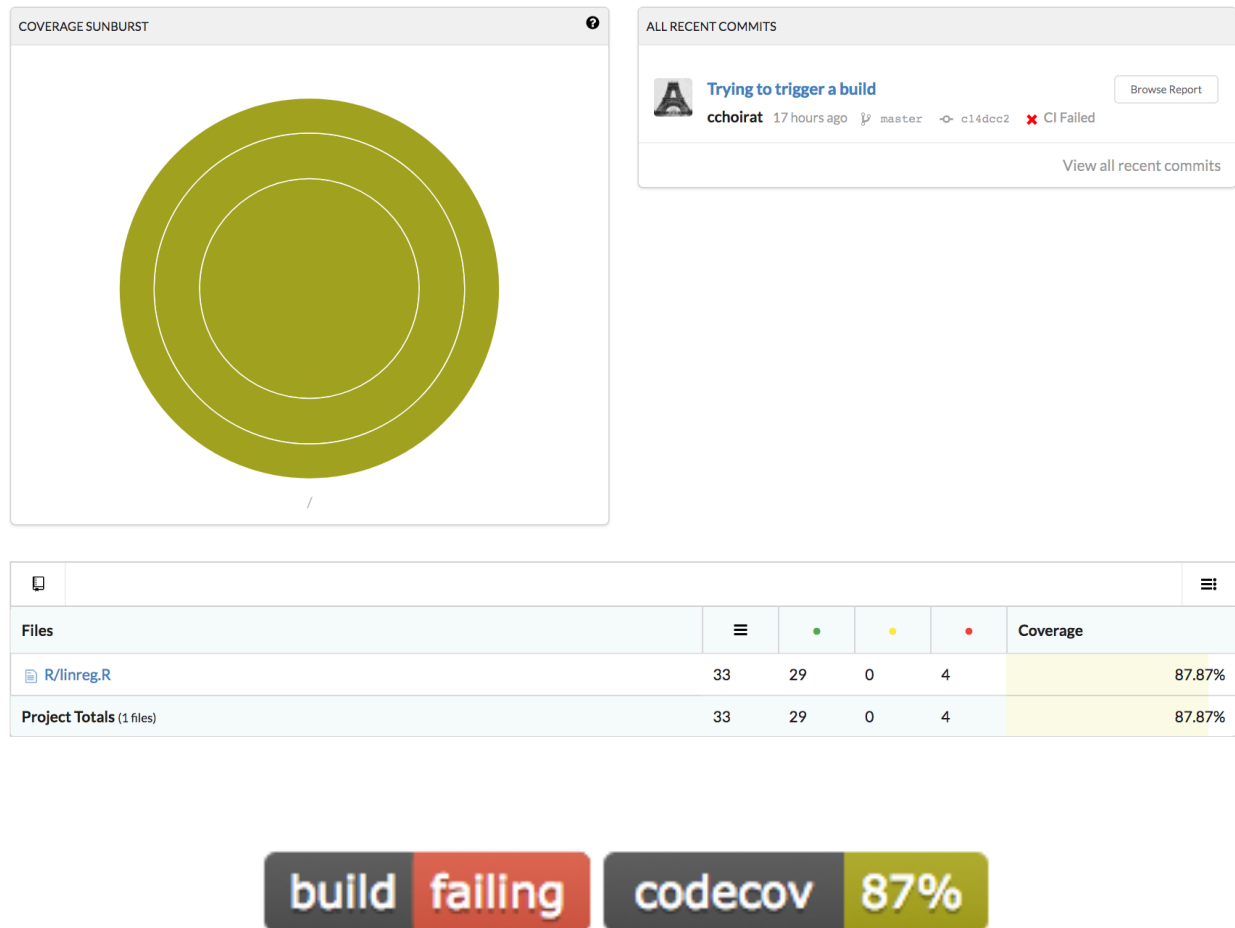
```
comment: false
```

A call to

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

will give you code coverage information:





## 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-ci.org/cchoirat/Linreg)
[! [codecov] (https://codecov.io/gh/cchoirat/Linreg/branch/master/graph/badge.svg)] (https://codecov.io/gh/cchoirat/Linreg)

## `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](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 illustration on how to use your package. A *vignette* is the right place to explain a workflow 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>

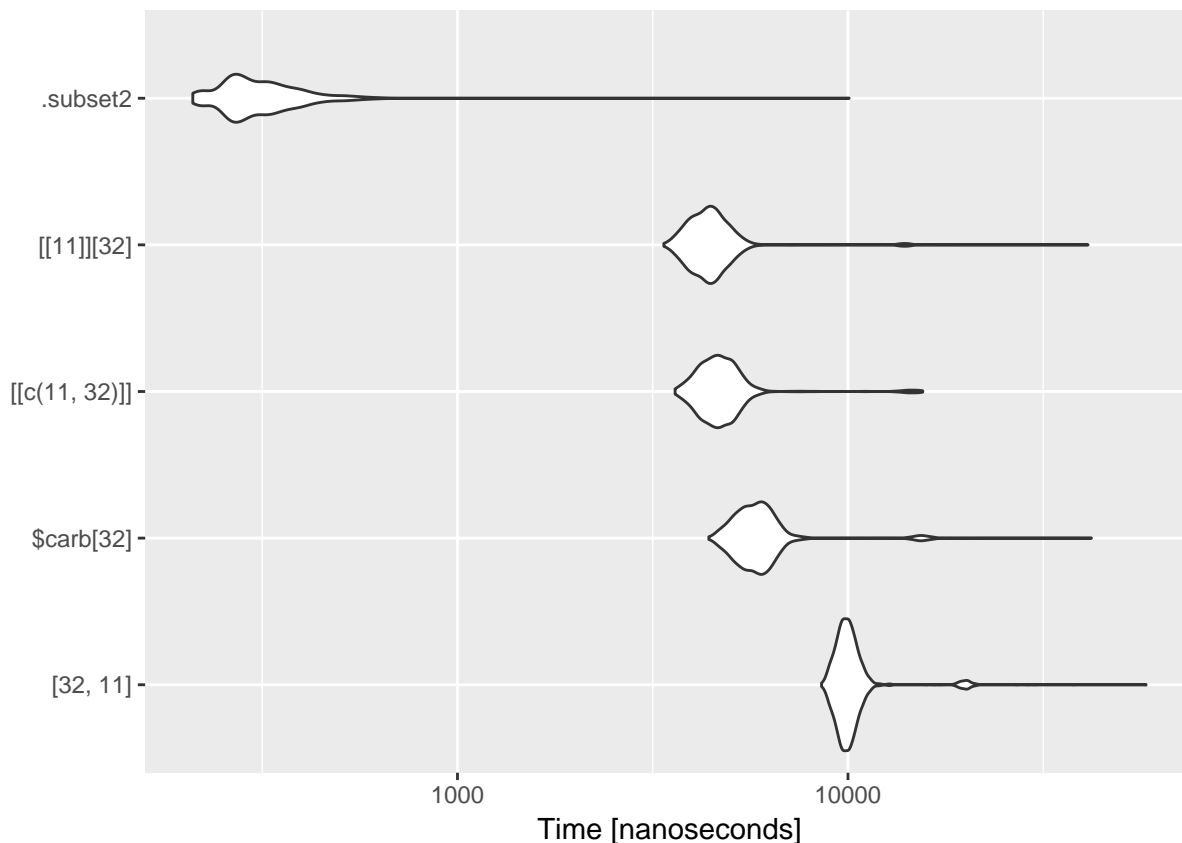
There are several ways to benchmark code (see [http://www.alexejgossmann.com/benchmarking\\_r/](http://www.alexejgossmann.com/benchmarking_r/)) from `system.time` to dedicated packages such as `rbenchmark` (Kusnierczyk (2012)) or `microbenchmark` (Mersmann (2015)).

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]  8556  9535.0 10452.708  9940.0 10386.5 57994   1000
##   $carb[32]  4402  5332.0  6125.413  5807.5  6250.5 42018   1000
##  [[c(11, 32)]] 3608  4288.0  4852.306  4651.5  5031.0 15538   1000
##  [[11]][32]  3376  4050.5  4576.783  4393.5  4716.5 41183   1000
##    .subset2    210   265.0   338.083   297.0   354.0 10068   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)

##               [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
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]
## (Intercept) -0.3566624
## Bwt         4.0340627
##           [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##           [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##           [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##           [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##           [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##           [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##           [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##           [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##           [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##           [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##           [,1]
## (Intercept) -0.3566624
```

```

## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624

```



```

## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          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]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624

```

```

## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          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]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624

```

```

## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624

```



```
## Bwt      4.0340627  
##           [,1]  
## [1,] -0.3566624  
## [2,]  4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## [1,] -0.3566624  
## [2,]  4.0340627  
##           [,1]  
## [1,] -0.3566624  
## [2,]  4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      4.0340627  
##           [,1]  
## [1,] -0.3566624  
## [2,]  4.0340627  
##           [,1]  
## (Intercept) -0.3566624  
## Bwt      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]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         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]
## (Intercept) -0.3566624
## Bwt         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]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## [1,] -0.3566624

```

```

## [2,] 4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## [1,] -0.3566624
## [2,] 4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624
## Bwt         4.0340627
##      [,1]
## (Intercept) -0.3566624

```

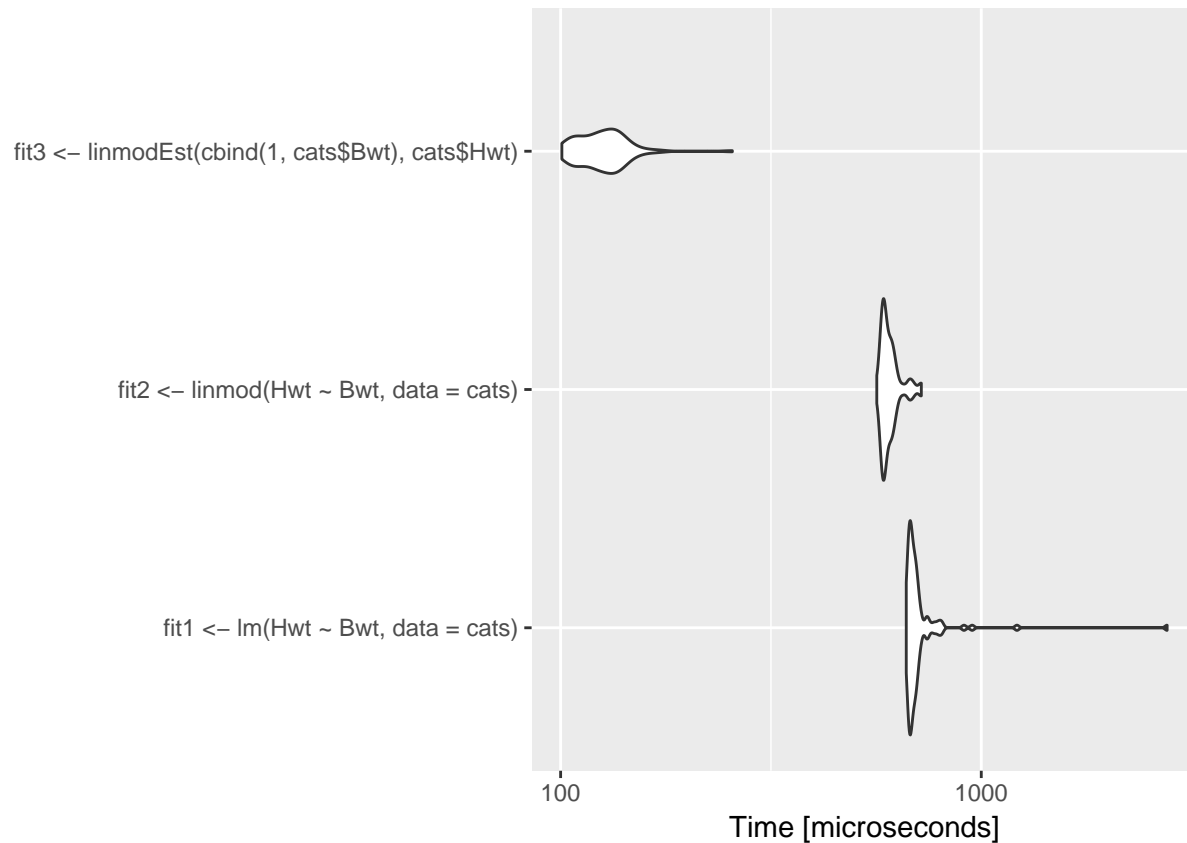


```

## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624
## [2,]  4.0340627
##              [,1]
## (Intercept) -0.3566624
## Bwt          4.0340627
##              [,1]
## [1,] -0.3566624

```





## 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] 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

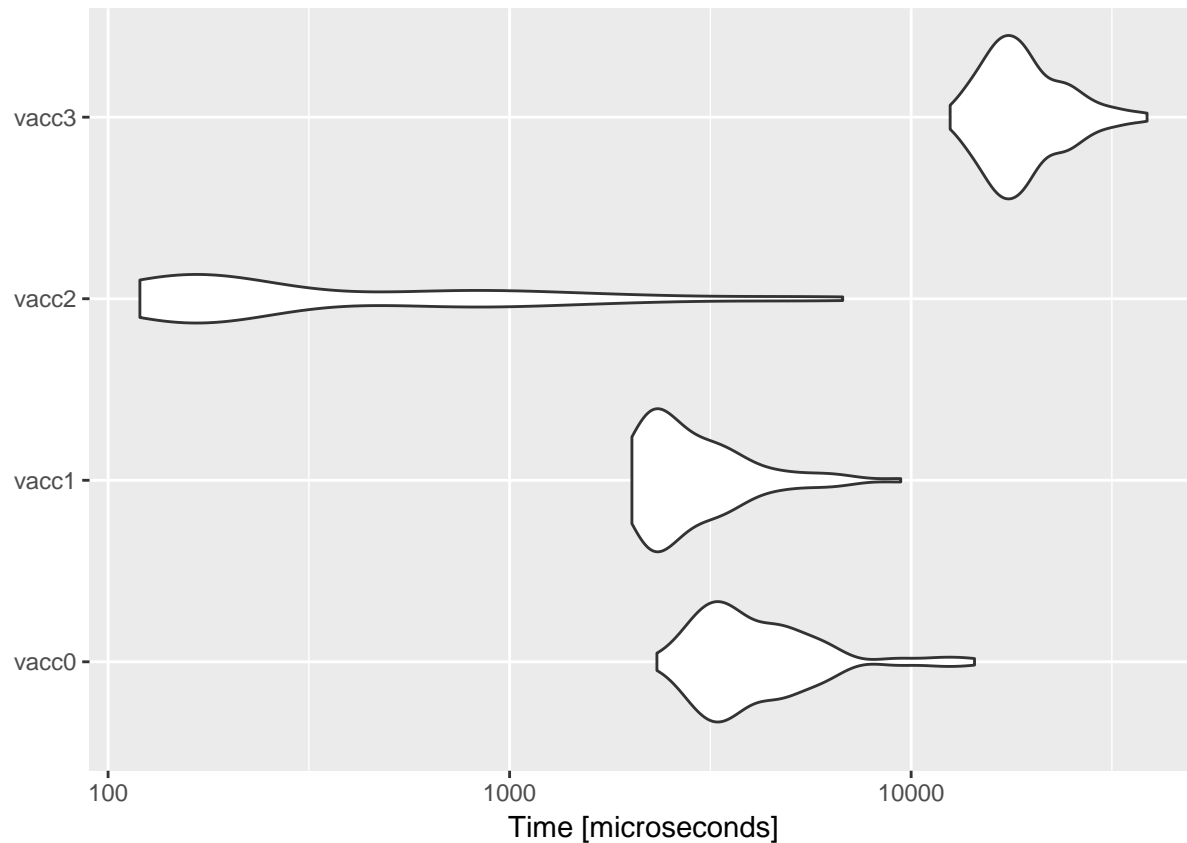
```

```

## Unit: microseconds
##      expr      min       lq      mean     median      uq      max
##  vacc0 2327.358 3199.2290 4420.0718 3752.461 4835.2780 14382.605
##  vacc1 2016.536 2271.4975 3047.2921 2630.461 3408.3345  9421.878
##  vacc2  120.001  152.2795  731.9802  201.683  721.5475  6754.642
##  vacc3 12508.071 16257.4655 19605.5051 18513.723 21728.3050 38685.539
##   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: 0x104fbccc0>))
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`, `<`, `<=`, `>`, `>=`, `==`, `!=`, `!`

-x'

**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
  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
  )
}

```

## 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>



## Chapter 5

# Databases

### 5.1 Overview

### 5.2 SQL

### 5.3 noSQL

### 5.4 R interfaces



# Chapter 6

## Big data

### 6.1 List of tools

Reading: Varian (2014) (PDF available)

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

- CPU
- RAM
- I/O

### 6.2 Data that fits in memory

#### 6.2.1 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"))
```

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, by specifying column types). But in general `fread` is much faster.

## Tools for Manipulating Big Data

<i>Google name</i>	<i>Analog</i>	<i>Description</i>
Google File System	Hadoop File System	This system supports files so large that they must be distributed across hundreds or even thousands of computers.
Bigtable	Cassandra	This is a table of data that lives in the Google File System. It too can stretch over many computers.
MapReduce	Hadoop	This is a system for accessing and manipulating data in large data structures such as Bigtables. MapReduce allows you to access the data in parallel, using hundreds or thousands of machines to extract the data you are interested in. The query is “mapped” to the machines and is then applied in parallel to different shards of the data. The partial calculations are then combined (“reduced”) to create the summary table you are interested in.
Sawzall	Pig	This is a language for creating MapReduce jobs.
Go	None	Go is flexible open-source, general-purpose computer language that makes it easier to do parallel data processing.
Dremel, BigQuery	Hive, Drill, Impala	This is a tool that allows data queries to be written in a simplified form of of Structured Query Language (SQL). With Dremel it is possible to run an SQL query on a petabyte of data (1,000 terabytes) in a 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

```
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`.

### 6.2.2 Reference vs copy

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

## 6.4 Pure R solutions

### 6.4.1 Sampling

### 6.4.2 bigmemory

### 6.4.3 Database connections and lazy evaluation

## 6.5 Scaling up

### 6.5.1 Parallel computing and clusters

### 6.5.2 Cloud computing

### 6.5.3 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 loooooong 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

#### 6.5.4 h2o and Sparkling Water

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

#### 6.5.5 More?

GPU



## Chapter 7

# Visualization

### 7.1 Principles of visualization

### 7.2 Maps and GIS



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