Thirteen things I wish I'd known when starting my PhD

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24 October 2019

Overview

A collection of tools and tips to make:

- Developing your statistical software
- Publishing your code
- Writing your thesis and papers

easier, more efficient — and even fun.

Towards better Science

Using these tools and approaches will allow one to:

- Become more efficient on a computer
- Write better code
- Create more reproducible research

Disclaimer

- Just my opinion
- I am not an expert
- These are just **suggestions**
- There are lots of other options
- Many of these may seem obvious

I hope you will find **one** suggestion today that is of interest to you

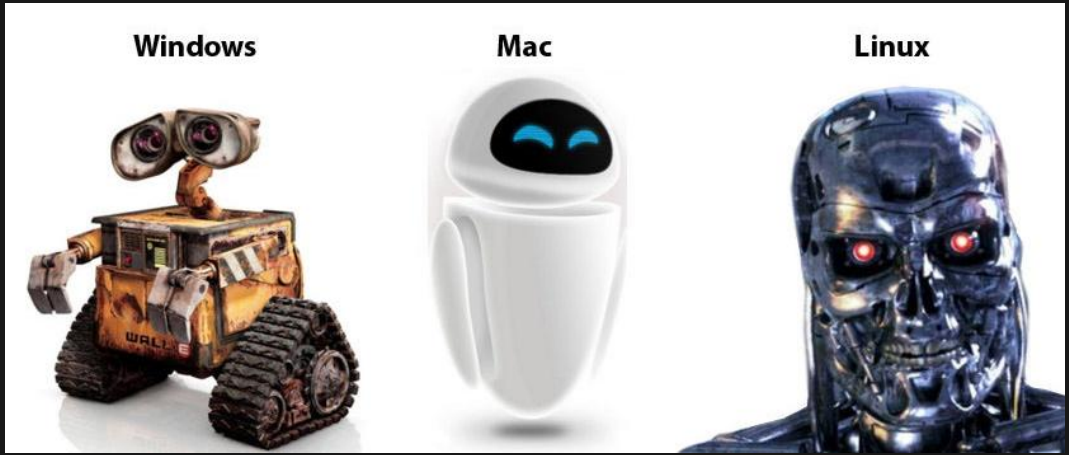
1. Use a Unix-based OS

Two popular distributions:

- Linux (many versions)
- OSX

Everything you see today is free and works with both.

Why use Unix?



source: imgur.com

Why use Unix?

- The power of the command line tools:
  - `ssh`
  - `grep`
  - `find`
  - `wget`
  - `aspell` (LaTeX spellcheck)
  - `top`
- These tools can be 'piped' together
  - e.g. find all files containing word X, made after date Y
- **Shell script**: a single file that runs multiple commands/scripts
- Don't know how to use a tool?
  - `man grep`
- Windows users: Cygwin

Useful example

```
grep --include=*.{Rmd,R} -rnw '.' -e "Linux"
```

```
grep --include=*.{Rmd,R} -rnw '.' -e "Linux"
./thirteenthings.Rmd:309:* Linux (many versions)
./thirteenthings.Rmd:353:grep --include=*.{Rmd,R} -rnw '.' -e "Linux"
./thirteenthings.Rmd:357:grep --include=*.{Rmd,R} -rnw '.' -e "Linux"
./thirteenthings.Rmd:361:## Different flavours of Linux
./thirteenthings.Rmd:484:Linux (Ubuntu):
./thirteenthings.Rmd:534: - Developed by Linus Torvalds (Linux)
./thirteenthings.Rmd:591:Linux:
```

Different flavours of Linux

Last 12 months			Last 6 months		
1	MX Linux	4303▲	1	MX Linux	4926▲
2	Manjaro	3116▼	2	Manjaro	2554▼
3	Mint	2142▬	3	Mint	2045▼
4	elementary	1527▼	4	Debian	1558▲
5	Ubuntu	1434▲	5	Ubuntu	1406▼
6	Debian	1416▲	6	elementary	1285▼
7	Solus	1041▲	7	Solus	1093▲
8	Fedora	999▲	8	Fedora	989▬
9	openSUSE	815▬	9	deepin	856▲
10	Zorin	785▬	10	Zorin	832▬

source: distrowatch.com, October 2019, top 10 of approx. 200

Cinnamon, source: linuxmint.com

Try it out

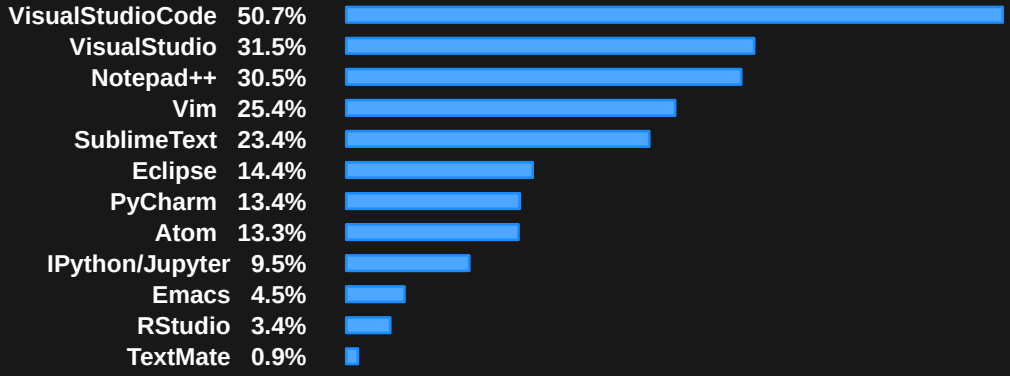
- Live USB - let's you test it out before installing
  - check wifi
  - check sound
  - check video
  - check filesystem
- Virtual machine: VirtualBox

Starting out?

- Consider starting with:
  - Mint (Ubuntu), Cinnamon
  - Manjaro KDE
- Loads of software, users, support

2. Pick a good editor

Most Popular Development Environments



87,317 responses; select all that apply

source: Stackoverflow Developer Survey 2019

Desirable editor features

- Cross platform
- Multi-language support
  - Python, R, C++, etc
  - LaTeX
- If not command line-based editor, become familiar with one
  - e.g. nano, Vim, Emacs

3. Use a terminal multiplexer

Terminal multiplexers

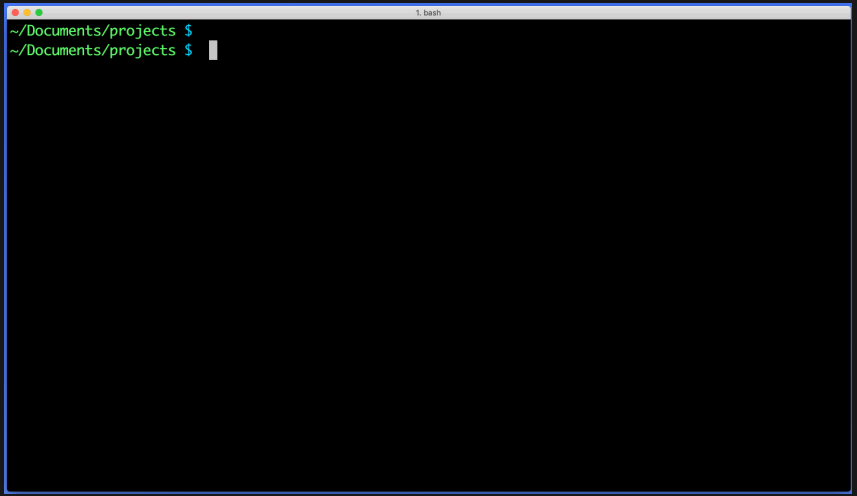
- `screen` (classic, but no longer maintained)
- `tmux` (new and growing in popularity)

`tmux` benefits

- Organise multiple terminals in one screen*
- Easily split windows into panes*
- Continue server sessions*
- Pane shading
- Save sessions after reboots: tmux-resurrect

*also `screen`

tmux demo



4. Use the server

Easily run large-scale simulations

- Your local machine is for **development**
- Queue a job on the server, and let it run overnight
- This is where knowing:
  - terminal commands
  - Vim/Emacs
  - `screen`/`tmux`

  will pay off **A LOT**.
- If no queueing system, try `nohup`
  - Example: `nuhup CMD bg &`, where `CMD` is the command to be run

5. Use Git

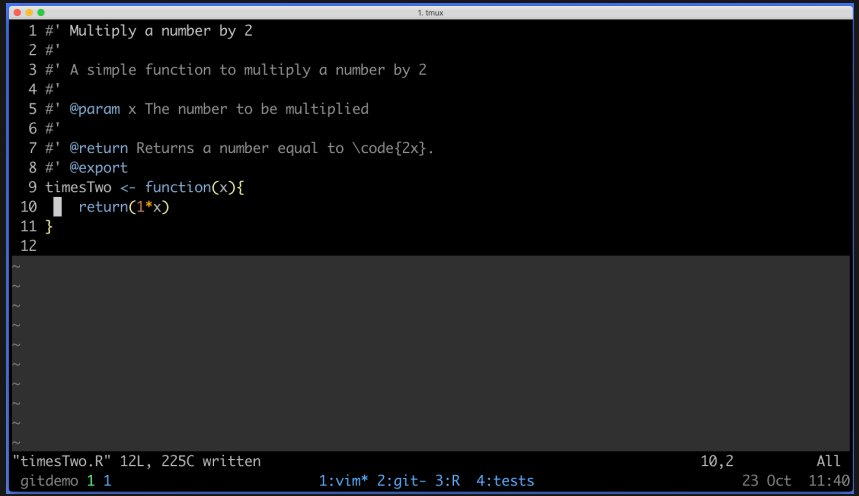
Git: version control

- Ever had code (R, C++, LaTeX...) 'stop working'?
- Git allows you to easily create checkpoints and versions
- Developed by Linus Torvalds (Linux)
- Git is FAST
- Allows you to work offline
- There are other version control systems, but Git is most popular

Git: basic commands

- Quick and easy to get started:
  - `git init`
  - `git add .`
  - `git commit`
- Recovering versions is also easy
  - Three different methods, depending on situation

Git demo


1. tmux
#' Multiply a number by 2
#'
#' A simple function to multiply a number by 2
#'
#' @param x The number to be multiplied
#'
#' @return Returns a number equal to \code{2x}.
#' @export
timesTwo <- function(x){
return(1*x)
}
"timesTwo.R" 12L, 225C written
10,2 All
gitdemo 1 1
1:vim* 2:git- 3:R 4:tests
23 Oct 11:40

Git for backups

- Ever worried about backing up scripts?
- Get a free GitHub or Bitbucket account
  - upload Git repo's with: `git push -u origin master`
- Lost your code or want to sync on a different computer?
  - `git clone`
  - `git pull`

Using Git

- Use Git for version control with:
  - code scripts
  - LaTeX scripts
- Do not use Git with:
  - data files
- Can use it to save images, but be careful. Try `git-lfs`
- Create a `.gitignore` file to ignore certain file(type)s
- Can be used for team-based projects

6. Create R packages, not scripts

R packages

- Binds your scripts together
- Forces you to comment/document your code
- Easily integrate **tests** (more later)
- Getting started: `devtools` and `roxygen2` packages
- Check out Hadley Wickham's online book
- **Note:** similar in Python

7. Comment your code

Two types of comments

- Code description (documentation)
  - show users how to use functions
  - input, output, what the function does
  - part of `roxygen2` commands
- Algorithmic description
  - for others (and yourself!) to understand the code
  - inside the functions
  - explain why you did something in a certain way, e.g.
    - `# using a matrix here because...`

Seems annoying and time-consuming - but the payoff is **worth it**

(ever come back to code after a couple of months...?)

Example of roxygen2 comments

```
#' Multiply a number by 2
#'
#' A simple function to multiply a number by 2
#'
#' @param x The number to be multiplied
#'
#' @return Returns a number equal to \code{2*x}.
#' @export
timesTwo <- function(x){
    return(2*x)
}
```

8. Write unit tests for your code

Test your code

- **Unit tests** are pieces of code that test your functions
- Make sure your code **works** as it should
- Avoid breaking your (previously working) code
- Forces you to break your code down into logical chunks
- Can be useful for debugging
- Longer in the short term, but **shorter in the long term**
- Check out the `testthat` R package
  - Makes testing quick and easy

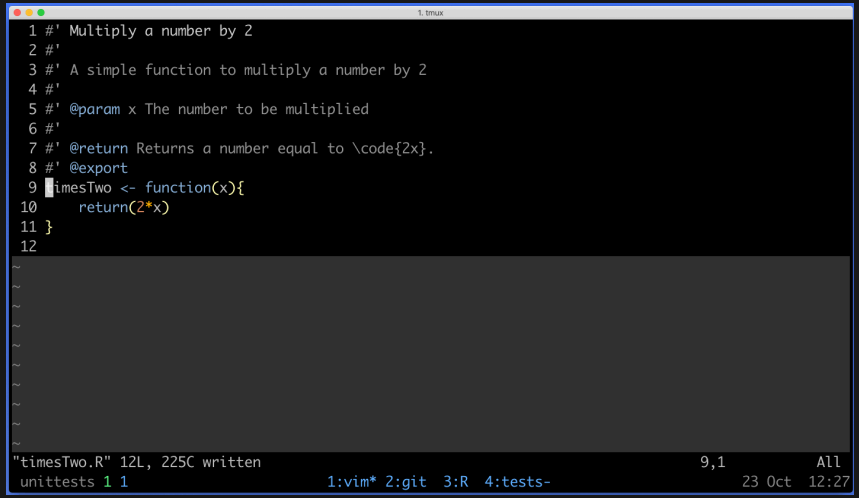
Unit testing in R

```
timesTwo <- function(x){
    return(2*x)
}
```

Unit testing in R

```
test_that("timesTwo tests", {
    expect_equal(timesTwo(1), 2)
    expect_equal(timesTwo(2), 4)
})
```

Unit testing in R



Start testing

- Hadley Wickham's tutorial
- R journal article

Note: Similar framework in Python

9. Speed up your code with Rcpp and Cython

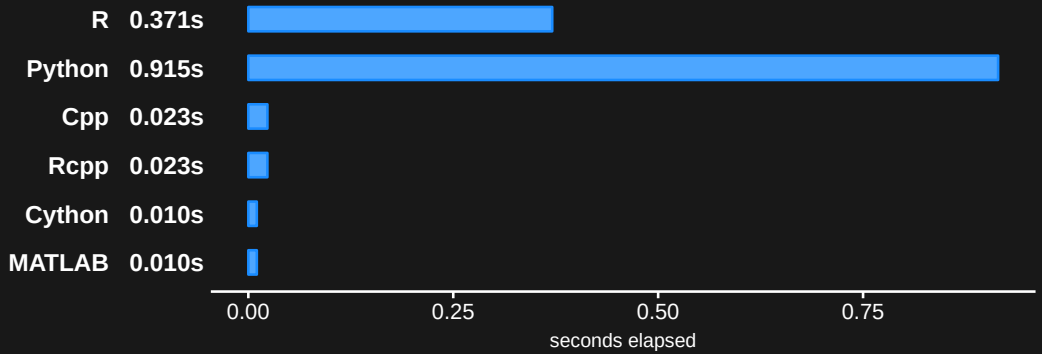
Bring the the speed of C++ to R and Python

- R is often criticised for being slow
  - bad at `for` loops
- C++ is **fast**, but lacks many of R's functions
- `Rcpp` is an R package that links R and C++
- Cython is a framework for running C++ code from Python

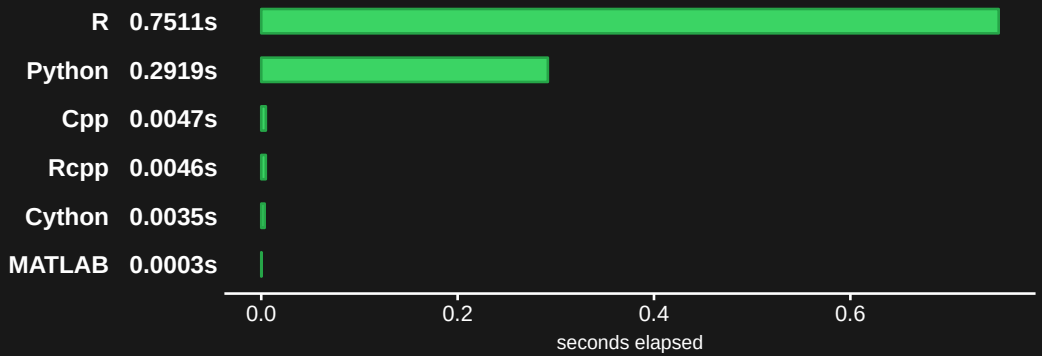
Bring the the speed of C++ to R and Python

- Code for benchmarks from julialang.org
- To reproduce these results, see https://github.com/deanbodenham/benchmarks_rpycpp
- Using `microbenchmark` package
- For linear algebra in C++, using Armadillo package
- MATLAB 2019a is used
- Check out the Rcpp gallery

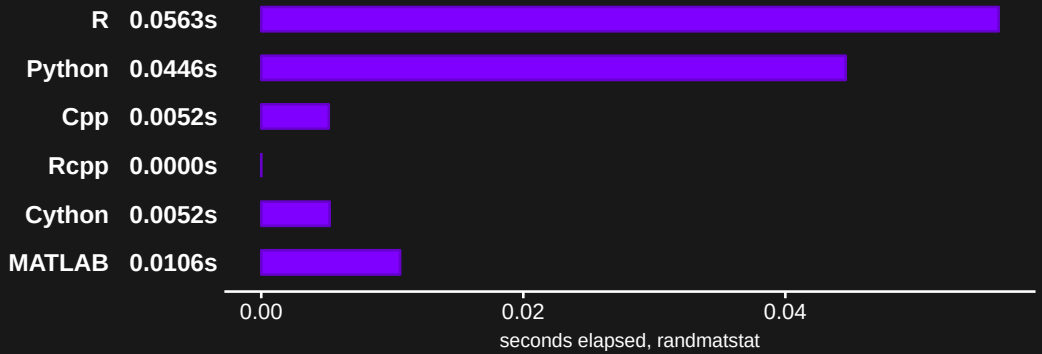
Pisum, nested for loop



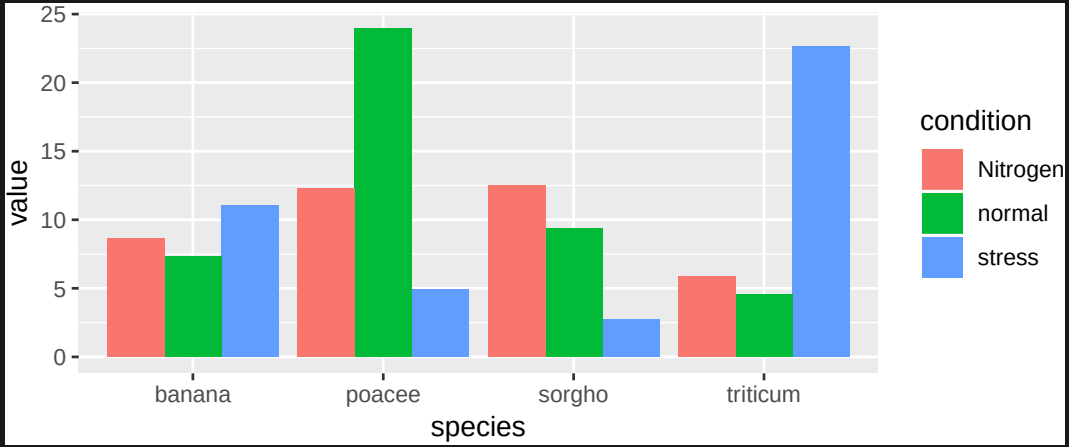
Recursive Fibonnaci



Random matrix statistics



10. For nice plots, use `ggplot2`


25
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15
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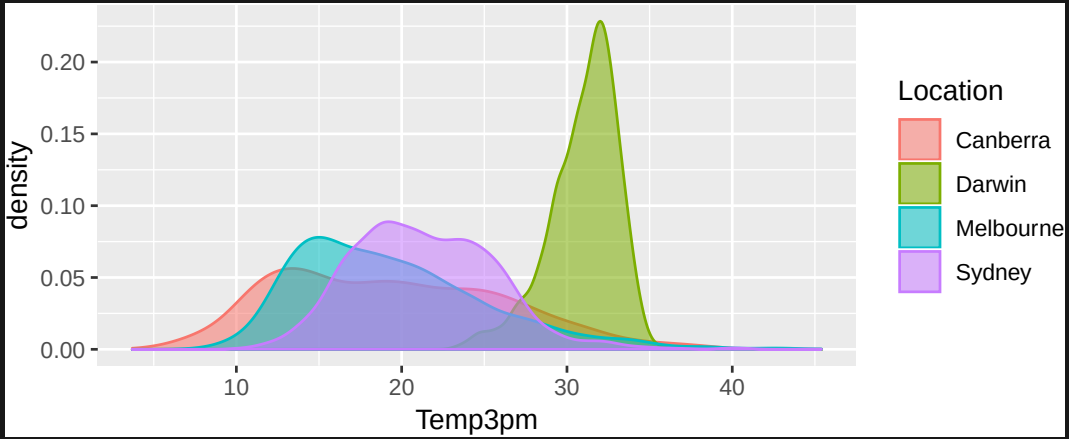
value
banana
poacee
sorgho
triticum
species
condition
Nitrogen
normal
stress


density
0.20
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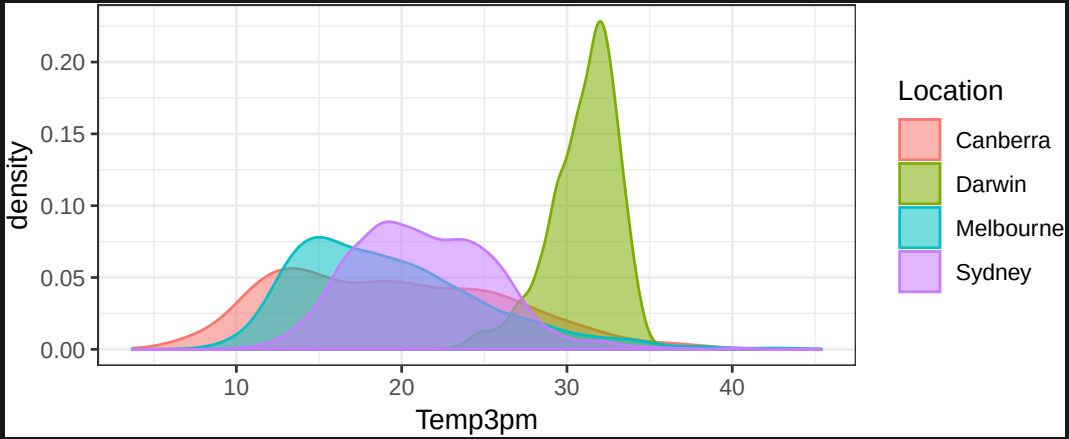
Temp3pm
Location
Canberra
Darwin
Melbourne
Sydney


density
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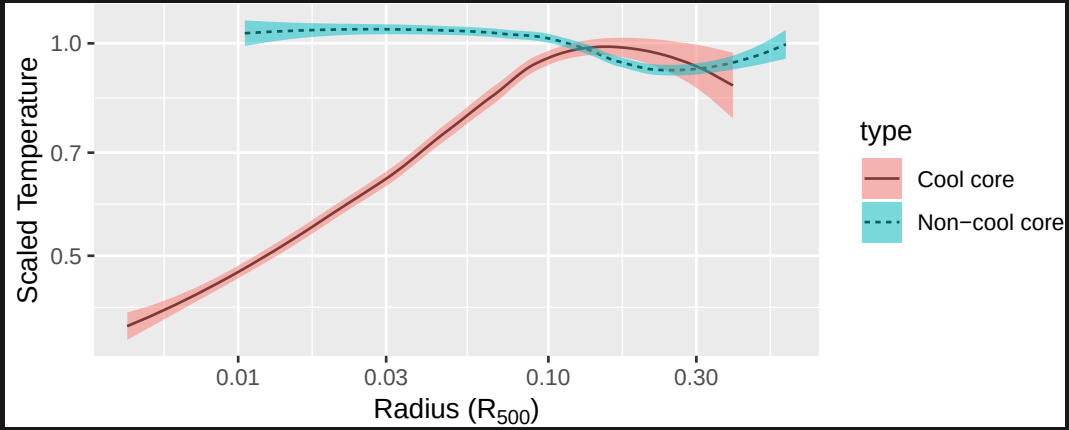
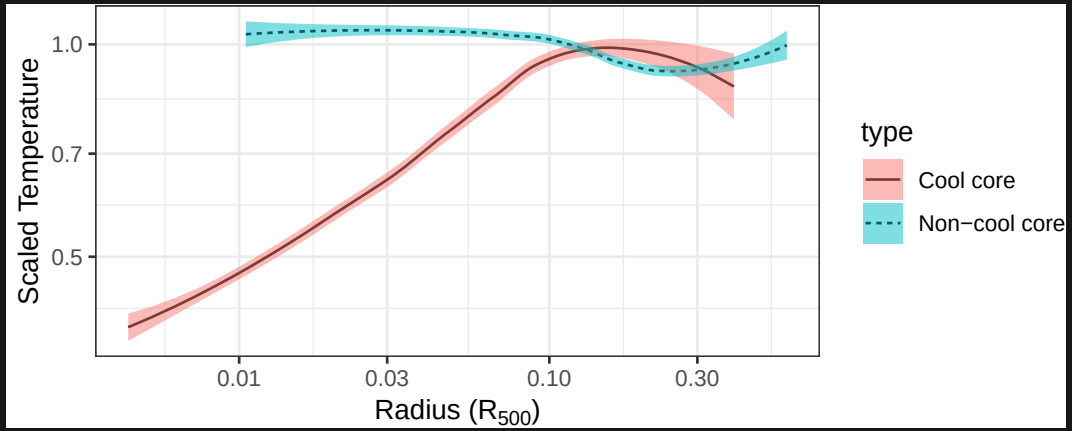
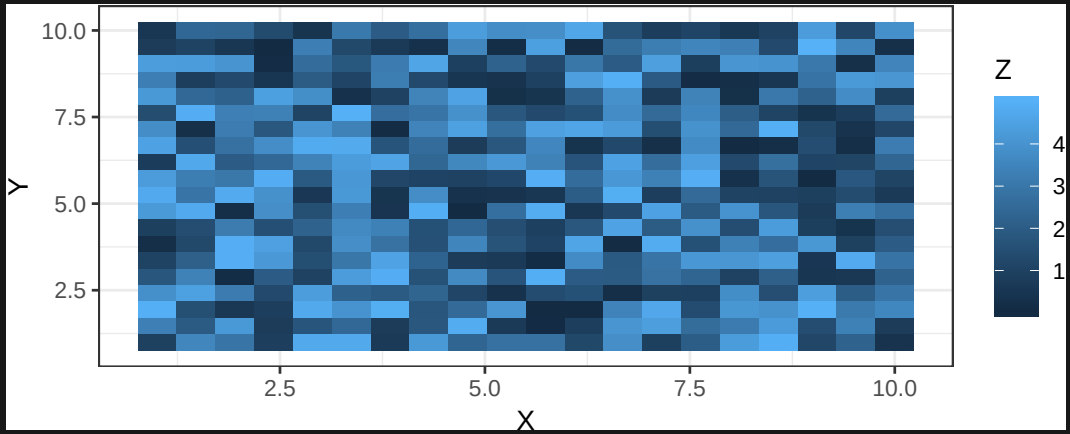
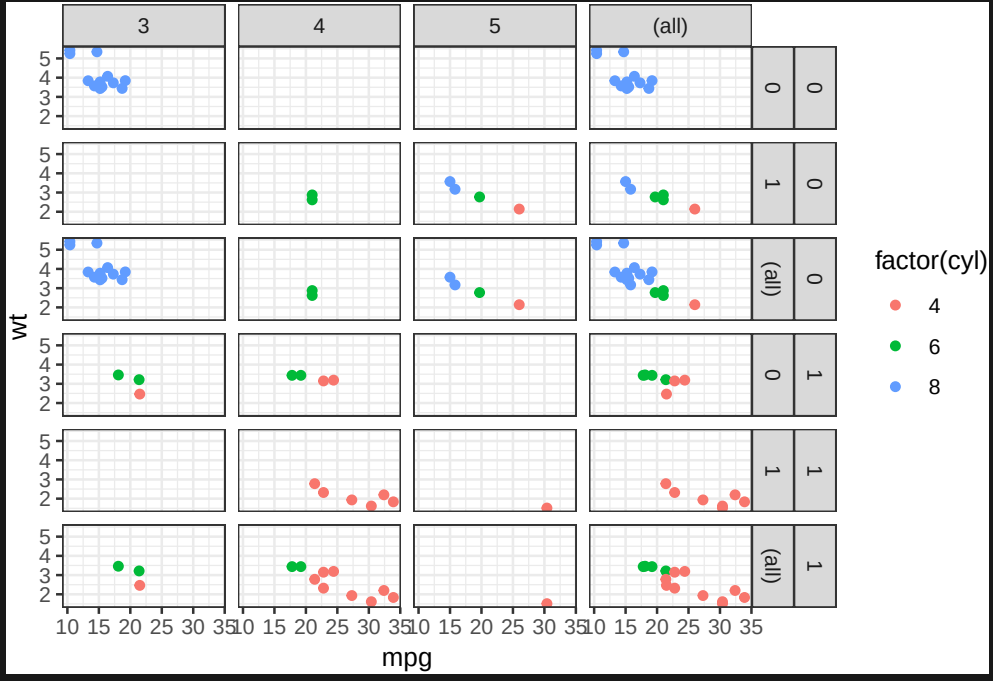
Location
Canberra
Darwin
Melbourne
Sydney


Scaled Temperature
1.0
0.7
0.5
0.01
0.03
0.10
0.30
Radius (R_{500})
type
Cool core
Non−cool core


Scaled Temperature
1.0
0.7
0.5
0.01
0.03
0.10
0.30
Radius (R_{500})
type
Cool core
Non−cool core


10.0
7.5
5.0
2.5
Y
2.5
5.0
7.5
10.0
X
Z
4
3
2
1


3
4
5
(all)
0
1
(all)
wt
mpg
factor(cyl)
4
6
8

11. Reproducible results and plots

Reproducible results

- Save every experiment with key results
  - May need to run again/tweak at a later stage
  - Combine with Git
- All results should appear by running **one command**
- Write a README for each experiment

Reproducible figures

- Less obvious, but just as important
- Use a two-step approach:
  - One script to generate the data
  - Another script to generate the figure from the data

Putting it all together

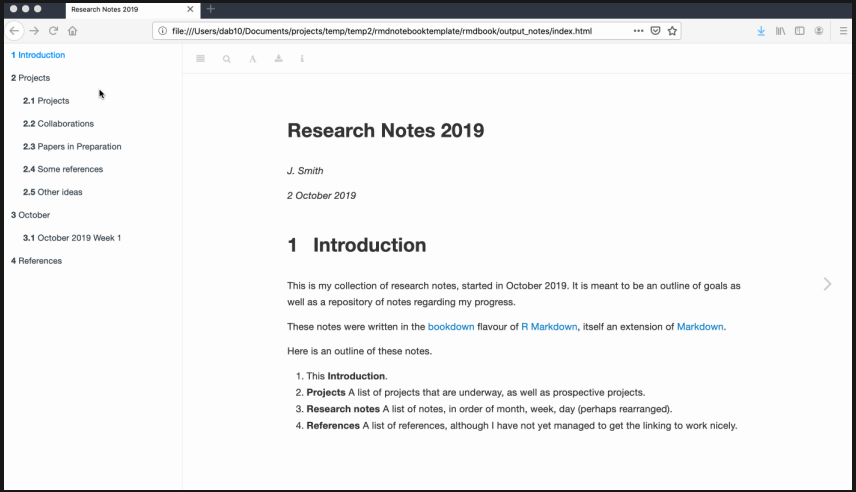
- Step 1: Run code to generate results (long time, server)
  - results saved in csv/RData file.
- Step 2: Script to create plot from data file (short time, laptop)
  - e.g. pdf, probably many revisions
- Step 3: Shell script to both generate results and create plot
  - Test on laptop with short simulation
  - Used in the future when needing to reproduce results
  - Make a note of the Git commit/package version number for generating data
- Example of the general advice: “write as you go”

12. R Markdown Journal

Keep track of research goals and results

- As a scientist, keep track of:
  - research efforts
  - results
  - things that worked
  - things that didn't work
  - goals
- Pen/paper notebooks are great
- R Markdown provides a framework for a digital version
- Allows output to html, pdf and other formats

Rmd notebook output



Template

A template I use can be found at:

https://github.com/deanbodenham/rmd_notebook_template

13. Use a reference manager

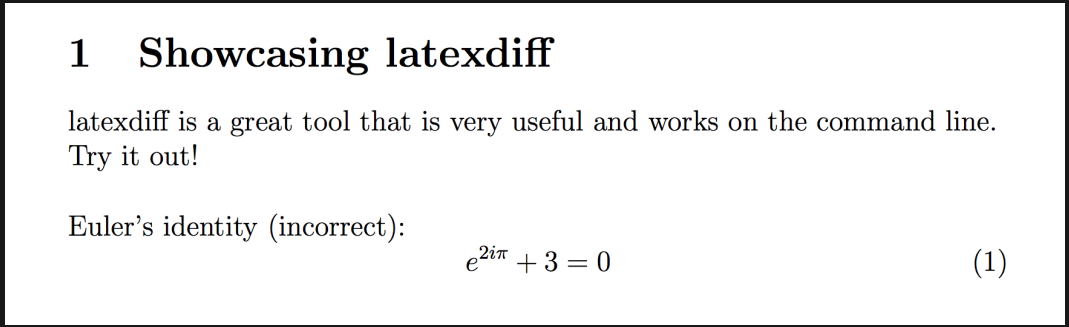
Keep track of papers and citations

- Examples:
  - Mendeley
  - Zotero
- Organise your papers
  - What you've already read
  - What you've still got to read
  - Notes on papers (later searchable)
- When citing paper/reference in your work, include comment with page/line number

14. git-latexdiff

Check differences between tex files

- Originally, `latexdiff` works with two files as input
- `git-latexdiff` works with **versions of the same file** with Git



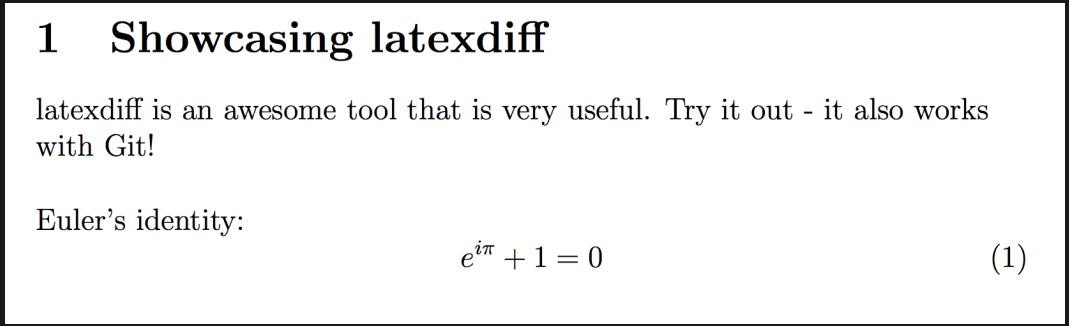
1 Showcasing latexdiff

latexdiff is a great tool that is very useful and works on the command line. Try it out!

Euler's identity (incorrect):

$$e^{2i\pi} + 3 = 0 \tag{1}$$

Figure 1: Version 1



1 Showcasing latexdiff

latexdiff is an awesome tool that is very useful. Try it out - it also works with Git!

Euler's identity:

$$e^{i\pi} + 1 = 0 \tag{1}$$

Figure 2: Version 2

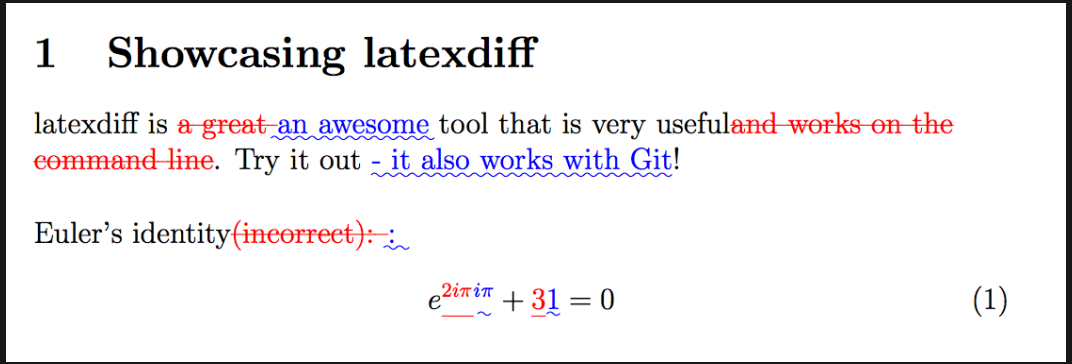


Figure 3: Differences with `latexdiff`

Easy Command:

- Compare current version and two versions back:

```
git latexdiff HEAD~2 --main main.tex
```

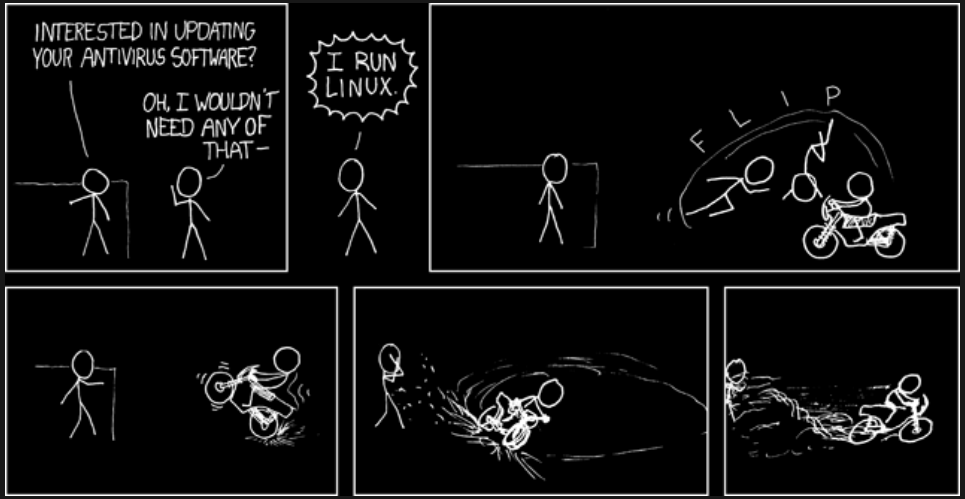
- Full credit to:
  - Frederik Tilmann, creator of `latexdiff`
  - Matthieu Moy, creator of `git-latexdiff`

Summary

1. Use a Unix-based OS
2. Choose a good editor
3. Use tmux for terminal management
4. Use the server for running experiments
5. Use Git for version control (mention `git-lfs`)
6. Create R packages, rather than scripts
7. Comment your code
8. Write unit tests for your code
9. Speed up your code with Rcpp and Cython
10. For nice plots `ggplot2`
11. Reproducible results and plots
12. Rmarkdown research journal
13. Use a reference manager
14. `git-latexdiff`

15. Things I Learnt

Questions?



source: http://xkcd.com/272/

Slides at https://github.com/deanbodenham/tenthings

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