Data Science Workflows

https://github.com/chendaniely/biovis_jp_workflow

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こんにちは!

I'm Daniel

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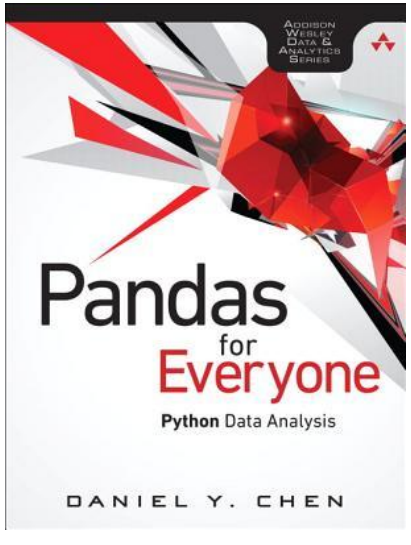

ありがとう


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Joined June 2009
D@niel Chen
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Pretty random, but is there an #rstats usergroup near Shinjuku, Tokyo, Japan that would be able to host a small talk while I'm in town for vacation? Leaving 27th morning.
4:08 PM - 22 Dec 2018 from Chiyoda-ku, Tokyo
3 Retweets 7 Likes
2
3
7
Jared Lander @jaredlander · Dec 22

Structuring Your Data Science Projects

We are happy when our code just runs

R has given us the tools to make your projects more structured and organized

Many people converge on very similar project templates

It doesn't matter where you are in your learning path

tl;dr

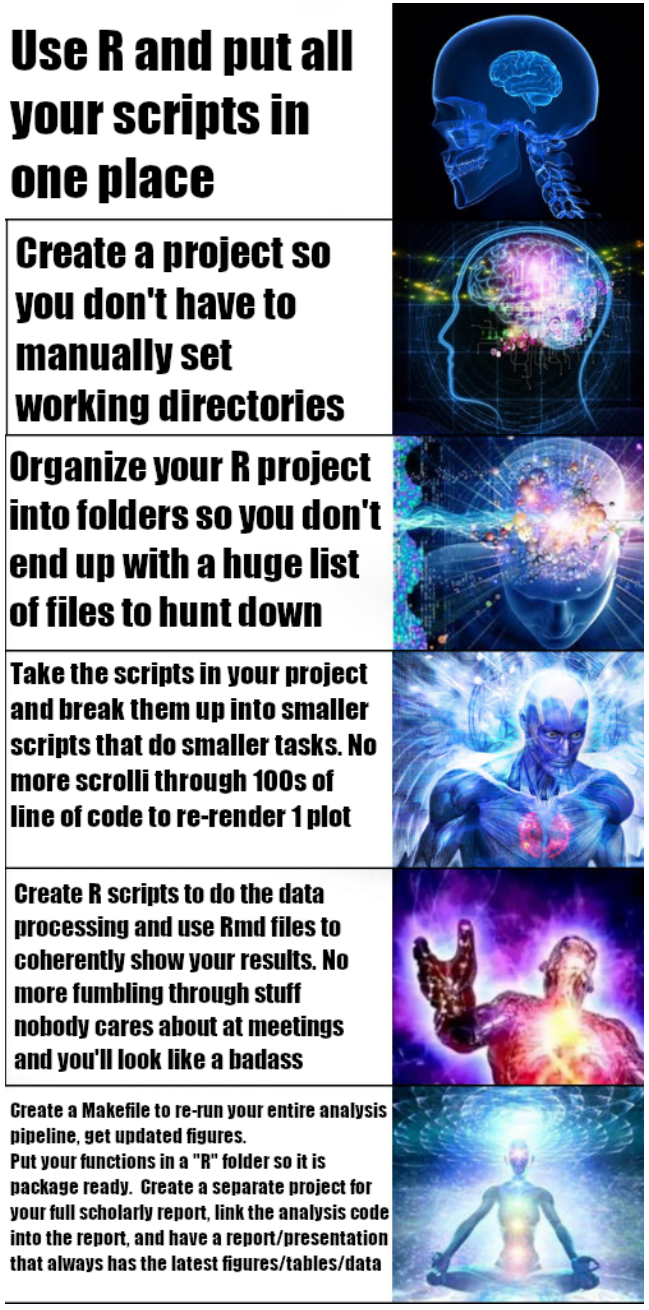
> I just want stuff to run the first time around

Tidy Data Paper -- Billboard Dataset

- Tidy data paper
- Billboard dataset
- Github repository has "original" and "cleaned" data

tl;dr

1. Use R
2. Make a project
3. Organize the project into folders and use `here::here()` to get project relative paths
4. Break up scripts into smaller pieces
5. RMarkdown for things you want to show
6. Put functions in `R` so your analysis is package ready and write `Makefiles`, shell scripts, or other build scripts and link your projects to scholarship so your figures and tables are always up to date



Package management

- Packrat (https://rstudio.github.io/packrat/)
- Checkpoint (https://cran.r-project.org/web/packages/checkpoint/index.html)
- conda (https://conda.io/docs/commands.html#conda-environment-commands)

(More) Resources

- slide template: xaringan (remark.js)
- Jenny Bryan - Stop working directory insanity
- Jenny Bryan - Naming things
- John Myles White - ProjectTemplate
- John Blischak - workflowr: organized + reproducible + shareable data science in R
- rr-init
- Compuational Project Cookie Cutter

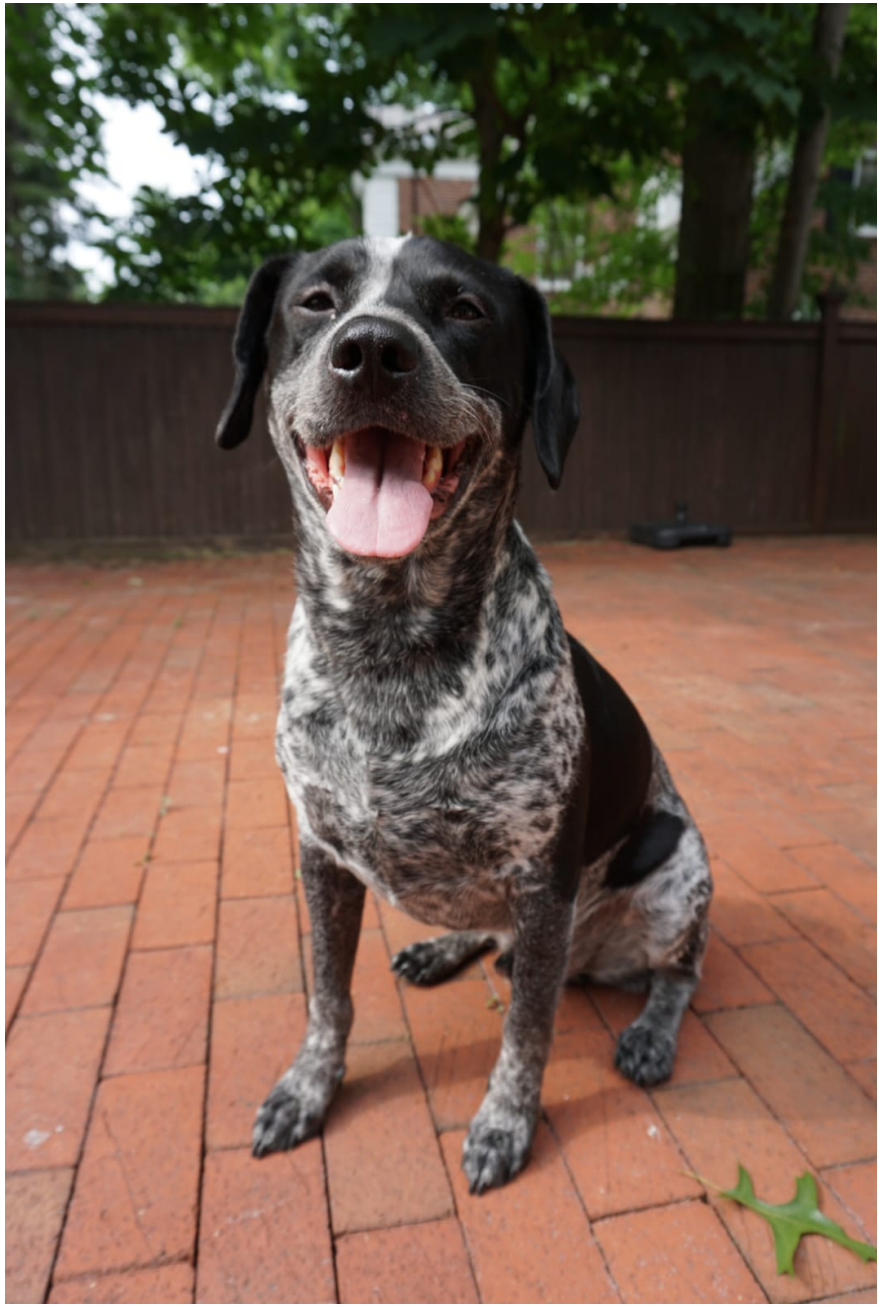
Thanks!

github/twitter/instagram/gmail: `@chendaniely`

https://github.com/chendaniely/biovis_jp_workflow

#rdogladies

#hobbesthebluehelermix



Backup Slides for reference.

A Tale of Two Dialects

Clean Data (Original)

```
library(stringr)
library(plyr)

rm(list = ls())
setwd('~/git/hub/rstatsdc_2018-structure/01-just_starting_out/')

raw <- read.csv("billboard.csv")

raw <- raw[, c("year", "artist.inverted", "track", "time", "date.entered", "x1st.week",
               "x2nd.week", "x3rd.week", "x4th.week", "x5th.week", "x6th.week", "x7th.week", "x
               "x76th.week")]
names(raw)[2] <- "artist"

raw$artist <- iconv(raw$artist, "MAC", "ASCII//translit")
raw$track <- stringr::str_replace(raw$track, " \\(.*?\\)", "")
names(raw)[-(1:5)] <- str_c("wk", 1:76)
raw <- plyr::arrange(raw, year, artist, track)

long_name <- nchar(raw$track) > 20
raw$track[long_name] <- paste0(substr(raw$track[long_name], 0, 20), "...")
```

Clean Data

```
##   year       artist                   track time date.entered wk1 wk2 wk3
## 1 2000        2 Pac          Baby Don't Cry 4:22   2000-02-26  87  82  72
## 2 2000      2Ge+her The Hardest Part Of ... 3:15   2000-09-02  91  87  92
## 3 2000 3 Doors Down              Kryptonite 3:53   2000-04-08  81  70  68
## 4 2000 3 Doors Down                   Loser 4:24   2000-10-21  76  76  72
## 5 2000     504 Boyz           Wobble Wobble 3:35   2000-04-15  57  34  25
## 6 2000      A*Teens           Dancing Queen 3:44   2000-07-08  97  97  96
##   wk4 wk5 wk6 wk7 wk8 wk9 wk10 wk11 wk12 wk13 wk14 wk15 wk16 wk17 wk18
## 1  77  87  94  99  NA  NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 2  NA  NA  NA  NA  NA  NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 3  67  66  57  54  53  51   51   51   51   47   44   38   28   22   18
## 4  69  67  65  55  59  62   61   61   59   61   66   72   76   75   67
## 5  17  17  31  36  49  53   57   64   70   75   76   78   85   92   96
## 6  95 100  NA  NA  NA  NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
##   wk19 wk20 wk21 wk22 wk23 wk24 wk25 wk26 wk27 wk28 wk29 wk30 wk31 wk32
## 1   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 2   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 3   18   14   12    7    6    6    6    5    5    4    4    4    4    3
## 4   73   70   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 5   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 6   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
##   wk33 wk34 wk35 wk36 wk37 wk38 wk39 wk40 wk41 wk42 wk43 wk44 wk45 wk46
## 1   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 2   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA   NA
## 3    3    3    4    5    5    9    9   15   14   13   14   16   17   21
```

Clean Data (Tidyverse)

```
library(readr)
library(dplyr)
library(stringr)

rm(list = ls())
setwd('~/git/hub/rstatsdc_2018-structure/01-just_starting_out/')

(raw <- readr::read_csv('billboard.csv') %>%
    dplyr::select(year, artist.inverted, track, time, date.entered,
                  x1st.week:x76th.week) %>%
    dplyr::rename(artist = artist.inverted) %>%
    dplyr::mutate(artist = iconv(artist, "MAC", "ASCII//translit")) %>%
    dplyr::mutate(track = stringr::str_replace(track,  " \\(.*?\\)", "")) %>%
    dplyr::arrange(year, artist, track) %>%
    dplyr::mutate(track = dplyr::case_when(
        nchar(track) > 20 ~ stringr::str_c(stringr::str_sub(track, 0, 20), "..."),
        TRUE ~ track
    ))
)
(names(raw)[-(1:5)] <- str_c("wk", 1:76)) # changed the order here
```

Clean Data

```
## # A tibble: 317 x 81
##     year artist track time  date.entered   wk1   wk2   wk3   wk4   wk5
##    <int> <chr>  <chr> <tim> <date>       <int> <int> <int> <int> <int>
##  1  2000 2 Pac  Baby… 04:22 2000-02-26      87    82    72    77    87
##  2  2000 2Ge+h… The … 03:15 2000-09-02      91    87    92    NA    NA
##  3  2000 3 Doo… Kryp… 03:53 2000-04-08      81    70    68    67    66
##  4  2000 3 Doo… Loser 04:24 2000-10-21      76    76    72    69    67
##  5  2000 504 B… Wobb… 03:35 2000-04-15      57    34    25    17    17
##  6  2000 A*Tee… Danc… 03:44 2000-07-08      97    97    96    95   100
##  7  2000 Aaliy… I Do… 04:15 2000-01-29      84    62    51    41    38
##  8  2000 Aaliy… Try … 04:03 2000-03-18      59    53    38    28    21
##  9  2000 Adams… Open… 05:30 2000-08-26      76    76    74    69    68
## 10  2000 Adkin… More  03:05 2000-04-29      84    84    75    73    73
## # ... with 307 more rows, and 71 more variables: wk6 <int>, wk7 <int>,
## #   wk8 <int>, wk9 <int>, wk10 <int>, wk11 <int>, wk12 <int>, wk13 <int>,
## #   wk14 <int>, wk15 <int>, wk16 <int>, wk17 <int>, wk18 <int>,
## #   wk19 <int>, wk20 <int>, wk21 <int>, wk22 <int>, wk23 <int>,
## #   wk24 <int>, wk25 <int>, wk26 <int>, wk27 <int>, wk28 <int>,
## #   wk29 <int>, wk30 <int>, wk31 <int>, wk32 <int>, wk33 <int>,
## #   wk34 <int>, wk35 <int>, wk36 <int>, wk37 <int>, wk38 <int>,
## #   wk39 <int>, wk40 <int>, wk41 <int>, wk42 <int>, wk43 <int>,
## #   wk44 <int>, wk45 <int>, wk46 <int>, wk47 <int>, wk48 <int>,
## #   wk49 <int>, wk50 <int>, wk51 <int>, wk52 <int>, wk53 <int>,
## #   wk54 <int>, wk55 <int>, wk56 <int>, wk57 <int>, wk58 <int>,
## #   wk59 <int>, wk60 <int>, wk61 <int>, wk62 <int>, wk63 <int>,
```

Tidy

```
clean_out <- raw %>%
    tidyr::gather(key = 'week', value = "value", # can rename rank = value here
              tidyselect::matches('^wk')) %>%
    dplyr::mutate(week = as.integer(stringr::str_replace_all(week, "[^0-9]+", "")),
                  date.entered = lubridate::ymd(date.entered),
                  date = date.entered + lubridate::weeks(week - 1)
                  ) %>%
    dplyr::select(-date.entered) %>%
    dplyr::rename('rank' = 'value') %>%
    dplyr::arrange(year, artist, track, time, week) %>%
    dplyr::select(year, artist, time, track, date, week, rank)
```

EDA

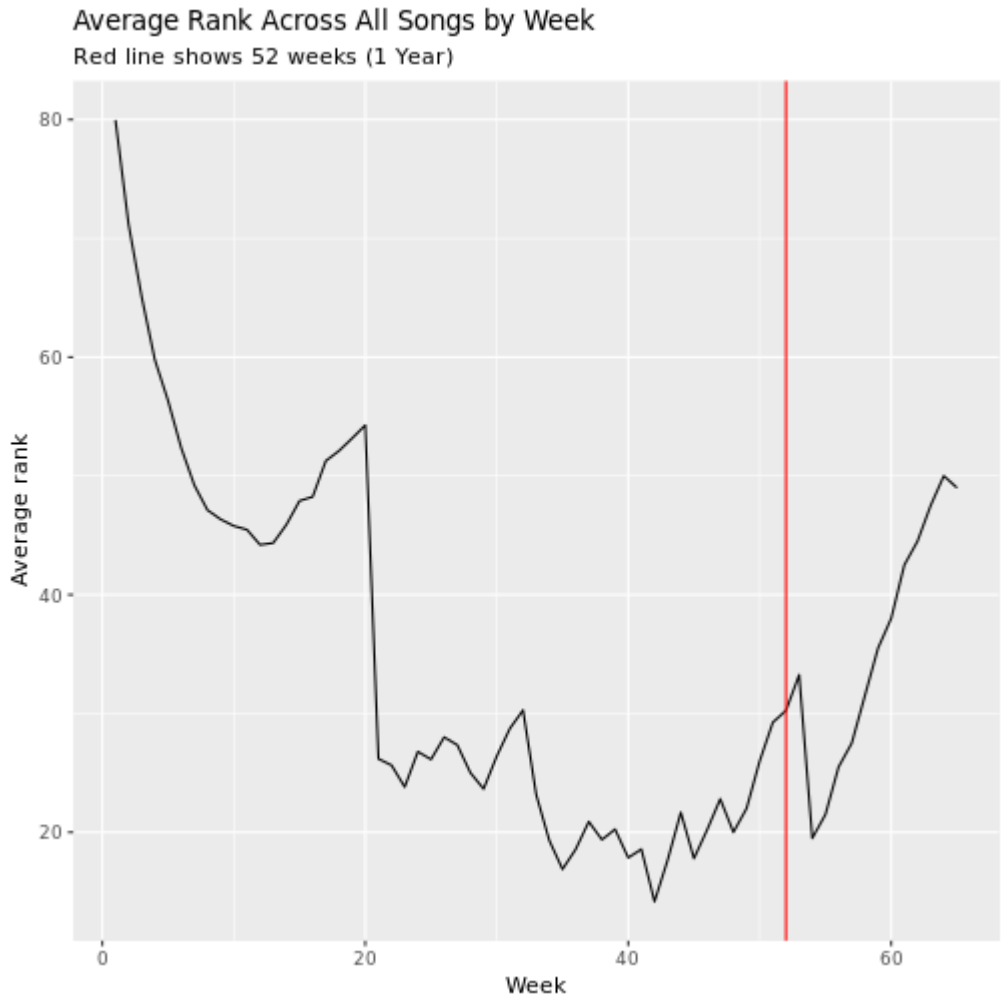
```
clean_out$month <- lubridate::month(clean_out$date)

# average rank by week
wk_rnk_avg <- clean_out %>%
    dplyr::group_by(week) %>%
    dplyr::summarise(avg_rnk = mean(rank))
```

EDA Vis

```
library(ggplot2)
ggplot2::ggplot(wk_rnk_avg, ggplot2::aes(x = week, y = avg_rnk)) +
    ggplot2::geom_line() +
    ggplot2::geom_vline(aes(xintercept = 52), color = 'red') +
    ggplot2::ggtitle(label = 'Average Rank Across All Songs by Week',
                     subtitle = 'Red line shows 52 weeks (1 Year)') +
    ggplot2::xlab('Week') +
    ggplot2::ylab('Average rank')
```

EDA Vis


Average Rank Across All Songs by Week
Red line shows 52 weeks (1 Year)
Average rank
80
60
40
20
0
20
40
60
Week

Model

```
fit <- lm(rank ~ week + artist, data = clean_out)
coefs <- broom::tidy(fit)
coefs
```

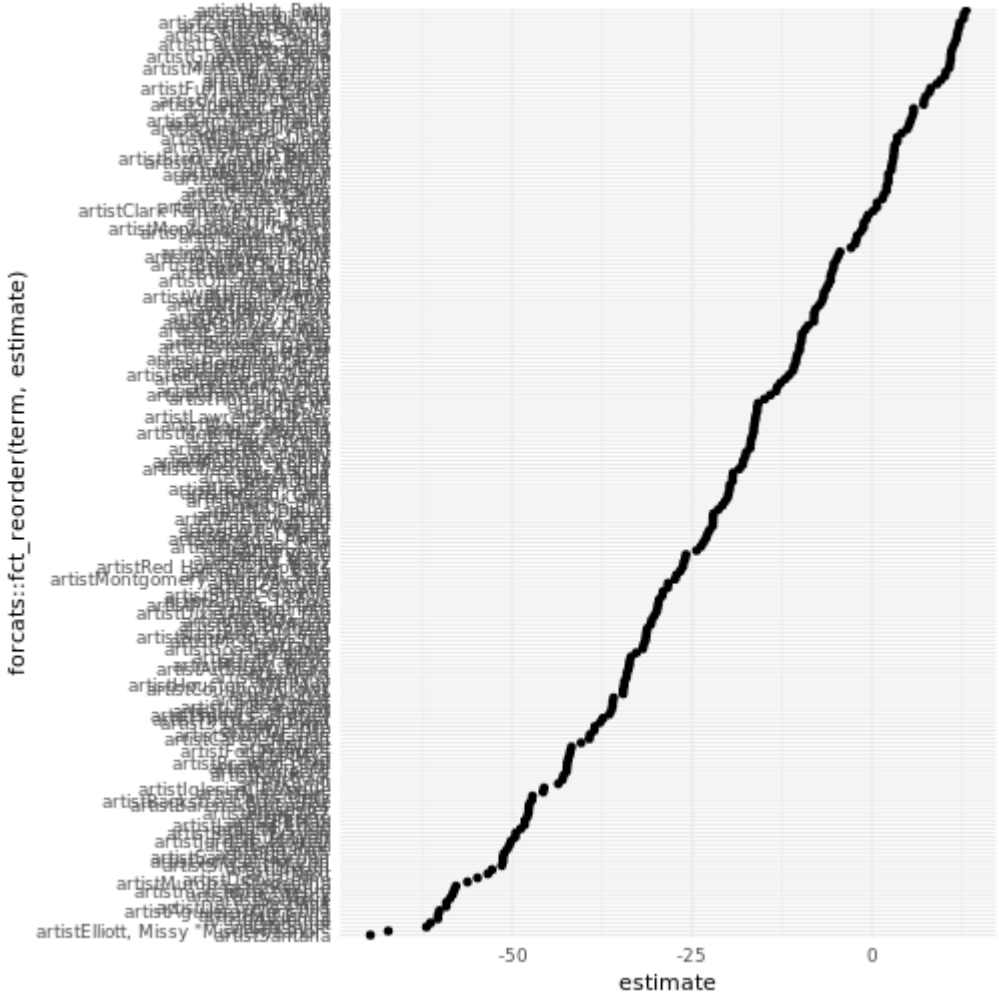
```
## # A tibble: 228 x 5
##    term                      estimate std.error statistic  p.value
##    <chr>                        <dbl>     <dbl>     <dbl>    <dbl>
##  1 (Intercept)                 87.6      7.69      11.4   1.02e-29
##  2 week                        -0.542    0.0368   -14.7   4.66e-48
##  3 artist2Ge+her                3.49    14.0        0.249 8.04e- 1
##  4 artist3 Doors Down         -37.8      8.07      -4.68  2.90e- 6
##  5 artist504 Boyz             -26.2      9.06      -2.89  3.81e- 3
##  6 artistA*Teens               11.0     11.9        0.926 3.54e- 1
##  7 artistAaliyah              -49.6      8.20      -6.06  1.49e- 9
##  8 artistAdams, Yolanda       -14.2      8.93      -1.58  1.13e- 1
##  9 artistAdkins, Trace         -8.07     9.83      -0.821 4.12e- 1
## 10 artistAguilera, Christina  -60.2      8.08      -7.44  1.14e-13
## # ... with 218 more rows
```

Vis Model

```r
library(forcats)

ggplot(coefs[!coefs$term %in% c('(Intercept)'), ],
       aes(x = estimate,
           y = forcats::fct_reorder(term, estimate))) +
    geom_point() +
    theme_minimal()
```

Vis Model


forcats::fct_reorder(term, estimate)
artistClark
artistRed
artistMontgomery
artistElliott, Missy
-50
-25
0
estimate

Demo 01

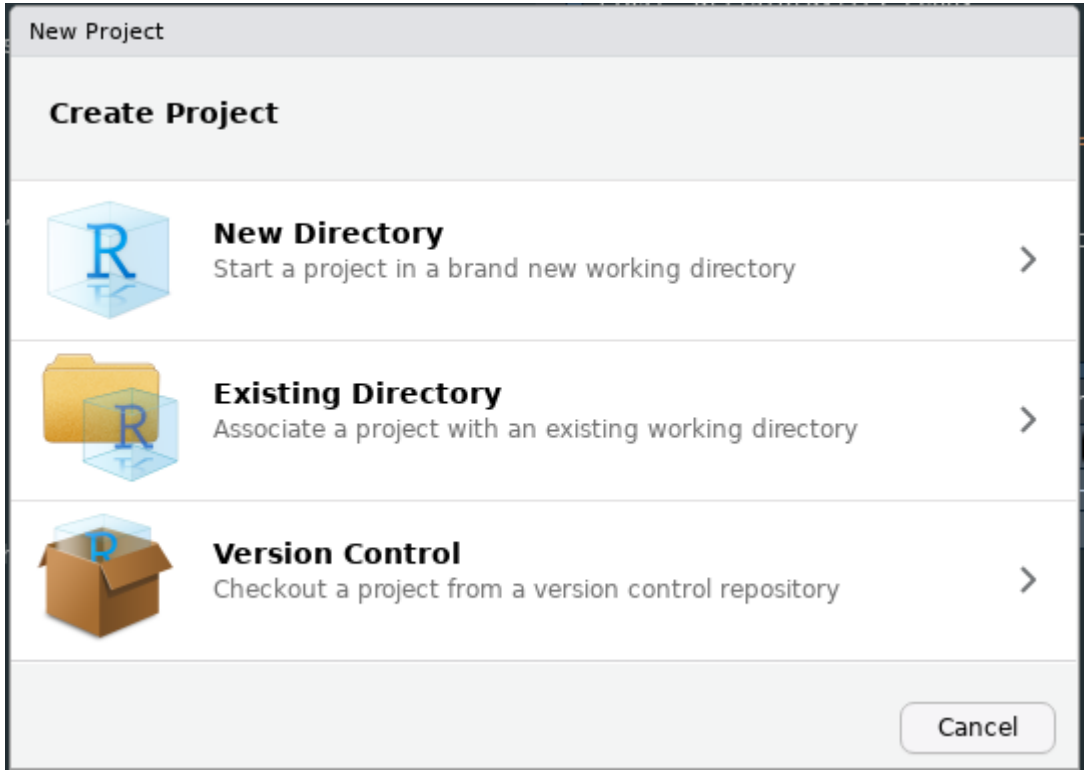
Do you want your computer set on fire...?

... because that's how you get your computer set on fire.

What's wrong with `setwd()`?

- **You are assuming a folder structure**
  - Your collaborator might not have the same structure
  - Your other computer might not have the same structure
  - You want to move files and folders around and now... you guessed it, don't have the same structure!
- You end up having a different line in your code for every possible location and commenting it in and out
  - Annoying for yourself, others, and
  - Version control systems

Make a Project




```
diff -r 01-just_starting_out 02-projects | grep "Only in 02-projects"
```

```
## Only in 02-projects: 02-projects.Rproj
```

RStudio projects assume everyone is using RStudio

```
TRUE
```

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

but...

- Emacs ESS allows you to pick the working directory
- `cd` in linux changes the working directory
  - Run code from working directory

What's wrong with `rm(list = ls())`?

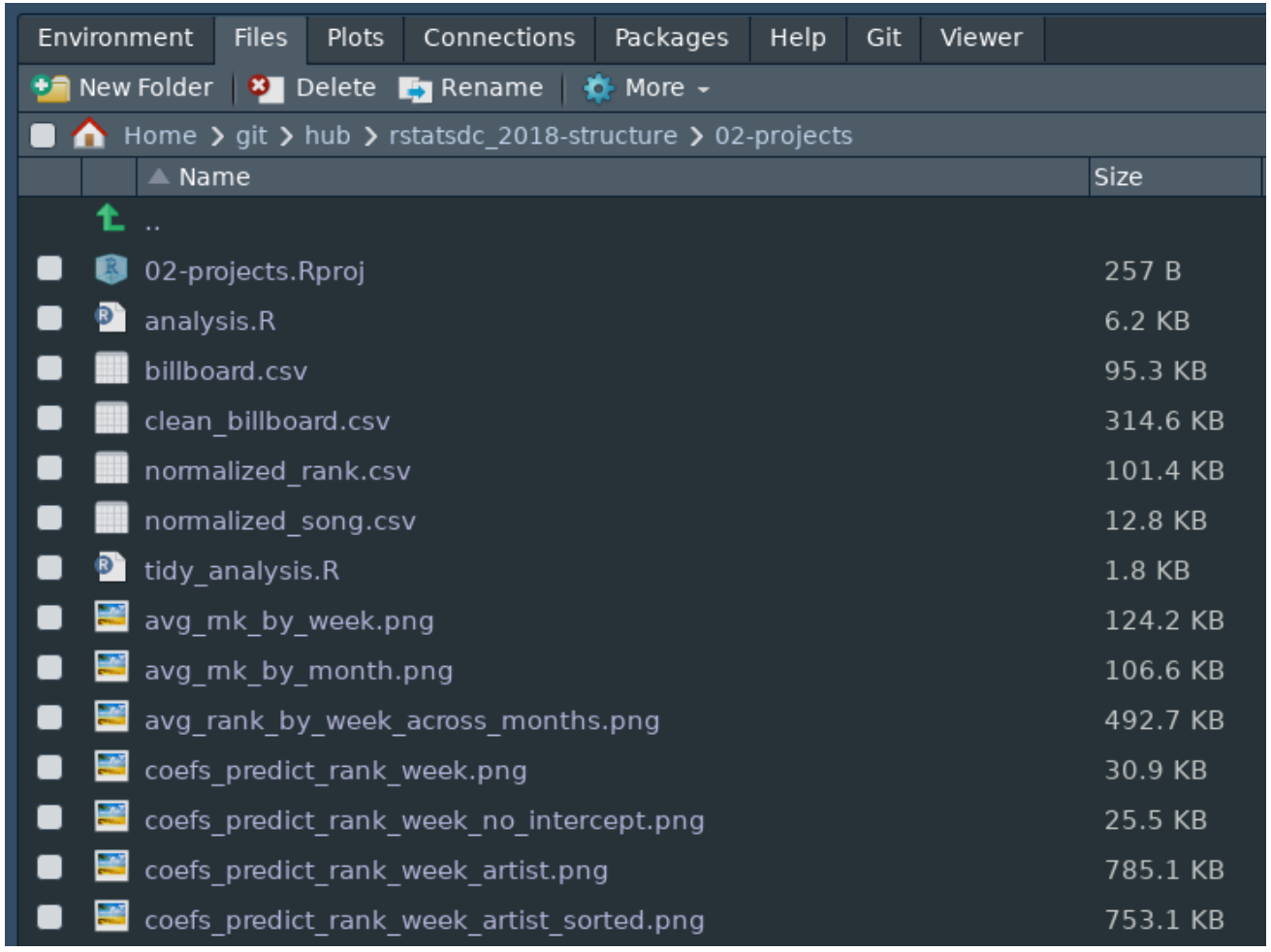
- **It doesn't detatch libraries**
  - You might end up using a function without an explicit `library` call in your script

What do I do instead?

1. RStudio: Session > Restart R (Ctrl + Shift + F10)
2. Terminal: `Rscript myscript.R`

Demo 02

Am I done yet? Yes, but...

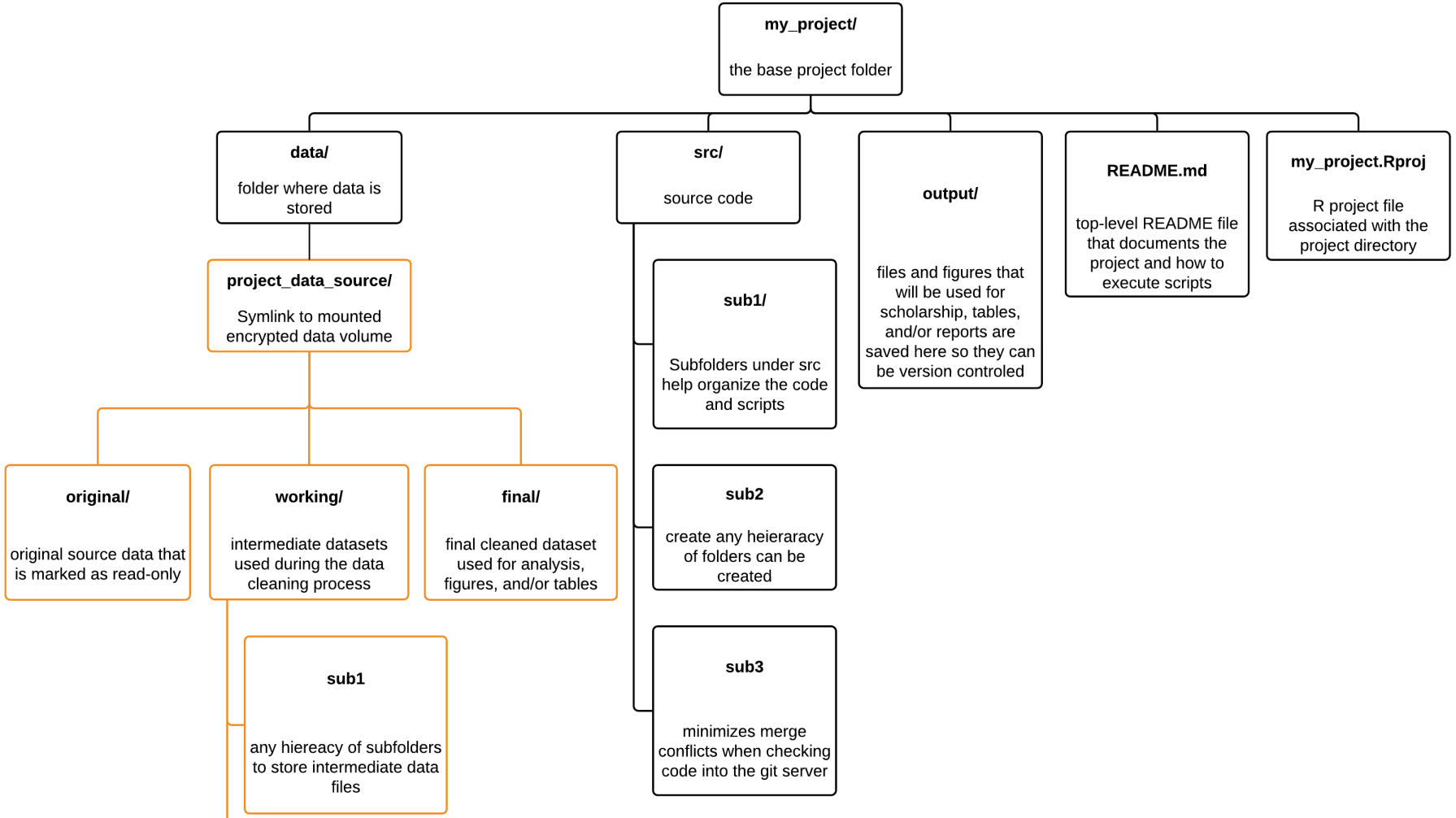


`project += structure`

Yes this is the whole point of this talk...

Noble's recommendations

What I/we do


my_project/
the base project folder
data/
folder where data is stored
project_data_source/
Symlink to mounted encrypted data volume
original/
original source data that is marked as read-only
working/
intermediate datasets used during the data cleaning process
sub1
any hiereacy of subfolders to store intermediate data files
final/
final cleaned dataset used for analysis, figures, and/or tables
src/
source code
sub1/
Subfolders under src help organize the code and scripts
sub2
create any heieraracy of folders can be created
sub3
minimizes merge conflicts when checking code into the git server
output/
files and figures that will be used for scholarship, tables, and/or reports are saved here so they can be version controled
README.md
top-level README file that documents the project and how to execute scripts
my_project.Rproj
R project file associated with the project directory

But basically...

1. **Data** (e.g., `data`)
    1. `orginal` folder from your original (read-only) data
    2. `processed` folder that your scripts create
        - If you want you can break down `processed` to `intermediate` and/or `final`
        - Do whatever feels right
    - Create symbolic links (i.e., shortcuts) as needed if you are using a version control system.
2. **Code** (e.g., `src`, `analysis`)
    - Same thing as the data folder: create subfolders as necessary
3. **Output** (e.g., `output`, `plots`, `results`)[1]
    1. Things your script outputs that is not a dataset
    2. `git` does not track empty folders, so put in a `README.md` or `.gitkeep` file
4. **Functions** (e.g., `R`)
5. **README** files

Make sub-folders as needed, everything is in a project and/or has a fixed working directory.

[1] Can get weird in `git` with image conflicts. But works great on shared drives/dropbox!

Demo 03

Can we do better? Of course.

How long is my script?

```
wc 01-just_starting_out/analysis.R
```

```
##  171  682 6348 01-just_starting_out/analysis.R
```

What does my script do?

1. Loads
2. Cleans
3. Tidy
4. Normalize
5. EDA
6. Model

Split it up into separate scripts ... in a subfolder

1. Loads
2. Cleans
3. Tidy
4. Normalize
5. EDA
6. Model

1. `01-load.R`
2. `02-01-clean.R`
3. `02-02-tidy.R`
4. `02-03-normalize.R`
5. `03-eda.R`
6. `04-model.R`

Be sensible, a 2 line script is probably not worth it, but a 2000 line script is unwieldy.

Demo 04

What else?

Rachael Tatman (from Kaggle) @rctatman

- R-Ladies organizer (Seattle chapter)
- Data scientist at Kaggle
- RLadies DC Meetup: Put together a data science portfolio
  - http://www.rctatman.com/files/Tatman_2018_DataSciencePortfolios_DC.pdf

Domain knowledge

If you're showing code (not just a dashboard or something) make sure it looks professional!

- Clean, readable code (remove all your "checking stuff out" bits, like printing out any parts of a dataframe)
- Use version control
- Pick a style guide and use it consistently! (A linter can help here)
- Break your project into multiple files. Example:
    1. Utility functions/package
    2. Data cleaning
    3. Modelling
    4. Model evaluation & visualizations

@rctatman

Portfolios are also about what you *don't* include

- **Quality over quantity**! Don't throw in every student project
- Avoid sharing data cleaning (just link to the file with the code)
- Avoid EDA, portfolio pieces should have a clear story
- Check for grammar errors/clarity

@rctatman

Knitr

1. Loads
2. Cleans
3. Tidy
4. Normalize
5. EDA
6. Model

1. `01-load.R`
2. `02-01-clean.R`
3. `02-02-tidy.R`
4. `02-03-normalize.R`
5. `03-eda.Rmd`
6. `04-model.Rmd`

But...

- Sometimes working with knitr in RStudio projects get weird because of working directories [1]
- I don't work in RStudio

Fix this with the `here` package

- It's based off rprojroot

In `here::here()`:

- Is a file named .here present?
- Is this an RStudio Project? Literally, can I find a file named something like foo.Rproj?
- Is this an R package? Does it have a DESCRIPTION file?
- Is this a remake project? Does it have a file named remake.yml?
- Is this a projectile project? Does it have a file named .projectile?
- Is this a checkout from a version control system? Does it have a directory named .git or .svn? - Currently, only Git and Subversion are supported.

[1] Also loses file tab completion within `Rmd` document. Worth?

Demo 05

Functions

Not shown in this example

But...

1. Put them in an `R` folder for easy reference and `source`ing.
2. Get's the analysis project ready to turn into an R package

What about scholarship/formal reports (LaTeX)?

1. Sibbling project

```
\begin{figure}[H]
    \centering
    \includegraphics[width=.7\linewidth]{../06-make/output/billboard_rank_plots/avg_rank_by_wee
\end{figure}
```

1. Child project (git submodules?)
    - Symbolic links (i.e., shortcuts) could work too

```
ln -s ~/git/hub/rstatsdc_2018-structure/06-make .
```

```
\begin{figure}[H]
    \centering
    \includegraphics[width=.7\linewidth]{./06-make/output/billboard_rank_plots/avg_rank_by_week
\end{figure}
```

`knitr` button puts output in the source file location

The output document is put in the `analysis` folder. I want it in the `output` folder!

Solution

use `rmarkdown::render()`

```
# not executed during build
rmarkdown::render(here::here('./analysis/billboard_eda/03-eda.Rmd'),
                  output_dir = './output/billboard_reports')
```

Too many commands to run!

1. Shell Script
2. Make
3. RStudio > Build (?)

Makefile

```
BILLBOARD=./analysis/billboard_eda/

all : commands

## commands      : show all commands.
commands :
    @grep -E '^##' Makefile | sed -e 's/## //g'

## billboard_eda  : re-generate billboard eda analsyis
billboard_eda :
    Rscript ${BILLBOARD}/01*
    Rscript ${BILLBOARD}/02-01*
    Rscript ${BILLBOARD}/02-02*
    Rscript ${BILLBOARD}/02-03*
    Rscript -e "rmarkdown::render(here::here('./analysis/billboard_eda/03-eda.Rmd'), output_dir
    Rscript -e "rmarkdown::render(here::here('./analysis/billboard_eda/04-model.Rmd'), output_d

## clean         : clean up junk files.
clean :
    find data/processed/ -type f -name '*.csv' | xargs rm
    find analysis/ type f -name '*.html' | xargs rm
```

Demo 06