#### POIR 613: Computational Social Science

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#### **Outline**

#### What we will discuss here:

- Good (enough) practices in scientific computing
- Efficient data analysis with R
- Guided coding session:
  - Loops and functions in R
  - Algorithm complexity
  - Examples of good coding practices in R

# Good (enough) practices in scientific computing

Based on Nagler (1995) "Coding Style and Good Computing Practices" (PS) and Wilson *et al* (2017) "Good Enough Practices in Scientific Computing" (PLOS Comput Biol)

# Good practices in scientific computing

#### Why should I waste my time?

- Replication is a key part of science:
  - Keep good records of what you did so that others can understand it
- "Yourself from 3 months ago doesn't answer emails"
  - ► More efficient research: avoid retracing own steps
  - Your future self will be grateful

#### General principles:

- 1. Good documentation: README and comments
- 2. Modularity with structure
- Parsimony (without being too smart)
- 4. Track changes

# Summary of good practices

- 1. Safe and efficient data management
- 2. Well-documented code
- 3. Organized collaboration
- 4. One project = one folder
- 5. Track changes
- 6. Manuscripts as part of the analysis

#### 1. Data management

- Save raw data as originally generated
- Create the data you wish to see in the world:
  - Open, non-proprietary formats: e.g. .csv
  - ► Informative variable names that indicate direction: is\_political instead of topic or V322; voted vs turnout
  - Recode missing values to NA
  - ► File names that contain metadata: e.g. 05-alaska.csv instead of state5.csv
- Record all steps used to process data and store intermediate data files if computationally intensive (easier to rerun parts of a data analysis pipeline)
- Separate data manipulation from data analysis
- Prepare README with codebook of all variables
- Periodic backups (or Dropbox, Google Drive, etc.)
- Sanity checks: summary statistics after data manipulation

#### 2. Well-documented code

- Number scripts based on execution order:
  - → e.g. 01-clean-data.r, 02-recode-variables.r, 03-run-regression.r, 04-produce-figures.R...
- Write an explanatory note at the start of each script:
  - → Author, date of last update, purpose, inputs and outputs, other relevant notes
- Rules of thumb for modular code:
  - Any task you run more than once should be a function (with a meaningful name!)
  - 2. Functions should not be more than 20 lines long
  - Separate functions from execution (e.g. in functions.r file and then use source (functions.r) to load functions to current environment
  - 4. Errors should be corrected when/where they occur
- Keep it simple and don't get too clever
- Add informative comments before blocks of code

#### 3. Organized collaboration

- Create a README file with an overview of the project: title, brief description, contact information, structure of folder
- Shared to-do list with tasks and deadlines
- Choose one person as corresponding author / point of contact / note taker
- Split code into multiple scripts to avoid simultaneous edits
- ShareLatex, Overleaf, Google Docs to collaborate in writing of manuscript

# 4. One project = one folder

#### Logical and consistent folder structure:

- ► code or src for all scripts
- data for raw data
- temp for temporary data files
- output or results for final data files and tables
- figures or plots for figures produced by scripts
- manuscript for text of paper
- docs for any additional documentation

# 5 & 6. Track changes; producing manuscript

- Ideally: use version control (e.g. GitHub)
- Manual approach: keep dates versions of code & manuscript, and a CHANGELOG file with list of changes
- Dropbox also has some basic version control built-in
- Avoid typos and copy&paste errors: tables and figures are produced in scripts and compiled directly into manuscript with LATEX

#### Examples

Replication materials for some of my published articles:

- ▶ 2019 APSR
- ► 2017 ISQ

John Myles White's ProjectTemplate R package.

Replication materials for Leeper 2017:

Code and data

Efficient data analysis with R



# Myths about R as programming language

- 1. R is an interpreted language, so it must be slow
  - Interpreted = executes code directly without compiling
  - Compiled code = code executed natively on CPU (fast!)
  - BUT: many functions are written in C and C++ and thus run in fast machine code
  - Slow code can be written more efficiently
- 2. All objects in R are stored in memory
  - You cannot open datasets larger than RAM
  - BUT: most laptops now have 8+ GB of RAM (+virtual mem)
  - bigmemory package: work with files on disk
  - Easy to work with large databases in the cloud
- R only uses one core of your CPU
  - Unlike STATA, no multi-core computing out of the box
  - BUT: many functions and packages now take advantage of multi-core computers
  - Easy to write your own code to do parallel computing

# My data is too big! My code is too slow!

#### What to do?

- Buy a better computer or expand RAM memory
- 2. Write more efficient code
- 3. Use parallel computing more on that later this semester
- 4. Move your code/data to the cloud
- Use out-of-memory storage: SQL databases, bigmemory package, Hadoop...

# Detour: algorithm complexity

- You can define the efficiency (aka complexity) of code (algorithm) in two different ways:
  - 1. Time: how long it takes to run
  - 2. Space: how much memory it uses
- ► These can be defined in terms proportional to the size of your data "Big O" notation; e.g. O(n),  $O(\log n)$ ,  $O(n^2)$
- Time and space complexity can be quite different! (more on this later)

# Writing efficient R code (Part I)

- Conventional wisdom: avoid for loops at all costs!
- But simply rewriting loops will not make code faster
- Key: use vectorized functions instead of loops
- Why are vectorized function fast? They use vector filtering, which means loop is done in machine native code
  - Takes vector as input and return vector as output
  - Some vectorized functions: ifelse(), which(), rowSums(), colSums(), sum(), any(), rnorm()...

# Writing efficient R code (Part II)

A common bottleneck is memory re-allocation, e.g.:

```
result <- c()
for (i in 1:n) {
    result[i] <- x[i] + y[i]
}</pre>
```

- ▶ In iteration, R re-sizes the vector and re-allocates memory
- For large operations (e.g. data frames), this can make your code really slow
- Solution: pre-allocate vector size:

```
result <- rep(NA, n)
for (i in 1:n) {
    result[i] <- x[i] + y[i]
}</pre>
```