Data Management With R

Hunter Wade York

01/27/2022

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- How to assign variables; how to manipulate them using basic operations
- How to run a linear regression
- Basic familiarity with tidyverse syntax and operations

But first, who am I?

- Second-year PhD student in Sociology at Princeton

Figure 1: Me!

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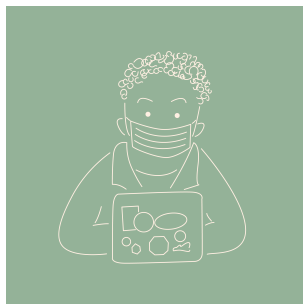- Formerly: AB at Harvard in Human Evolutionary Biology and Music

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- If you have questions during the presentation, STOP ME! No question is too simple.

Useful Links

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Questions?

Project Design and Data Management

Some Code-Writing Theory

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- Version often, save versions remotely (git + github or even dropbox)

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- A project is simply, start to finish, everything to get you from idea to finished paper
- It includes code, data, output files like clean datasets, figures, and possibly a manuscript
- Most importantly, by having all your files in one directory and using relational paths, you make the entire project replicable!

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My Workflow (starting a new project)

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  - NB: Git has a lot of features built out for collaboration that are not necessary for basic data management. If you learn a simple "add," "commit," "push" workflow, it will serve most of your needs.
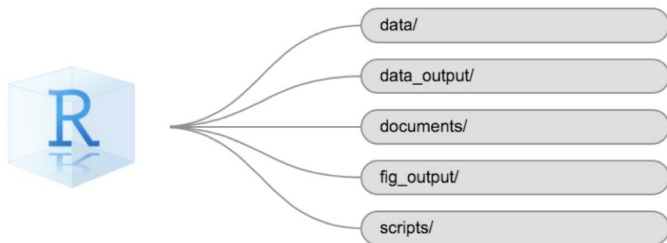
Workflows

Figure 3: Another Example Directory Setup
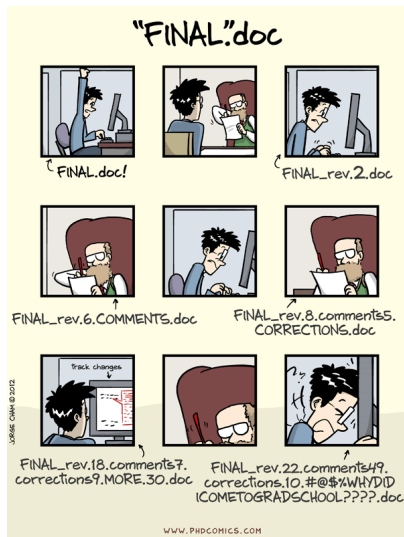
A Note on Git

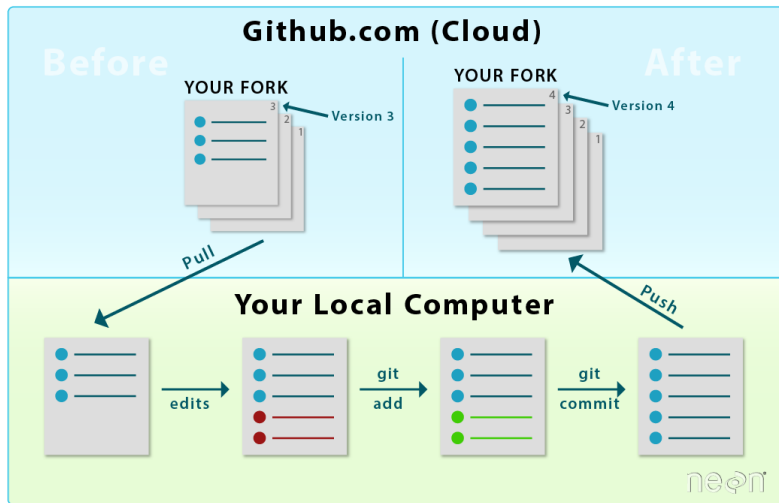Figure 4: www.phdcomics.com

A Note on Git

Figure 5: https://www.neonscience.org/resources/learning-hub/tutorials/github-git-add

Code Tips

1. Break down large projects into smaller chunks.

- For me, this usually looks something like having a "processing.R", "anlaysis.R", and a "figures.R" script.
  - Tailor these to your specific project. If you have many lines of data acquisition and many lines of data processing, break that up!
- Real programmers, data scientists working to make reproducible pipelines, etc. will all have drastically different standards of coding. Don't listen to them. Unless you're making a package to put on CRAN, you don't need a script for helper functions, etc.
- That said, if one of your files exceeds 1,000 lines, or you have a very time-consuming step in the middle of a script, consider breaking it up.
- I love to save intermediate files in my scripts. Later, these form a natural place for me to break a script up if it gets too long.

Code Tips

Figure 6: "../code"

https://speakerdeck.com/jennybc/zen-and-the-art-of-workflow-maintenance?slide=59
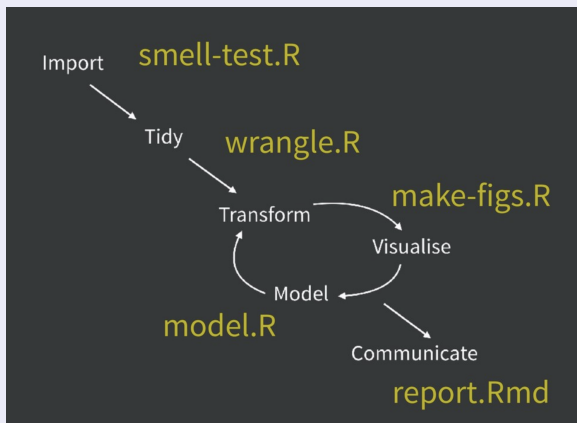
Code Tips

2. Comment (when it helps you)!

- I actually rarely comment well until the final stages of a pipeline. BUT, that is because I'm so used to using a certain set of tools, that I can almost always tell what I'm doing. My comments are thus more limited to reminding myself why I made a certain choice or flags for me to revisit a small bug.

3. Test clunky operations on smaller bits of data

- Sometimes we get too ambitious. If your code is slow and you can't or don't want to optimize it, subset your data early on in the script, write your code using the subset, and in the last stage, run it on the full sample.

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Example of using your own line breaks to make code neater

```
c("Hunter", "Mary", "Sol",
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Figure 7: Tweet

Some actual examples of less-than-ideal code I found on the internet

Original Code - Repeated tasks

```r
# ORIGINAL
#remove idnumb, other ids
data[which(colnames(data) == "idnumb")] <- NULL
data[which(colnames(data) == "challengeIDs")] <- NULL
data[which(colnames(data) == "mothids1")] <- NULL
data[which(colnames(data) == "mothids2")] <- NULL
data[which(colnames(data) == "mothids3")] <- NULL
data[which(colnames(data) == "mothids4")] <- NULL
data[which(colnames(data) == "hv3mothids3")] <- NULL
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data[which(colnames(data) == "fathids1")] <- NULL
```

Alternative Code - Using Built-In Functions

```
# ALTERNATIVE DPLYR
data <- data %>% select (-c(idnumb, challengeIDs, mothids1,
                           mothids2, mothids4, "........"))
# ALTERNATIVE DATA.TABLE
data[, c("idnum", "challengeID", "mothids1",
        "mothids2", "mothid4s", "........") := NULL]
```

Some actual examples of less-than-ideal code I found on the internet

Original: The problem - Calling a function once, on one dataset, using dataset names in the function

```r
# ORIGINAL
# Remove cols with > 50% missing data
f_lowInfo <- function(data) {
  ncols = ncol(data)
  nrows = nrow(data)
  to_remove = integer(ncols)
  for (i in 1:ncols) {
    if (sum(is.na(data[i])) > .5*nrows) {
      to_remove[i] = 1
    }
  }
  data[to_remove == 1] <- NULL
  return(data)
}
data <- f_lowInfo(data)
```

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Alternative Code - Define a function, apply it multiple times, make it flexible

```r
# ALTERNATIVE
is_col_missing <- function(c.vector){ # create a function to see if a vector is
  return(mean(is.na(c.vector)) > .5)  # over half missing. Use that TRUE = 1, and
}                                     # FALSE = T to our advantage
# Apply across columns of data.frame
data %>% summarize(across(.cols = everything(), is_col_missing)) -> to_remove
data <- data[,to_remove == 0] # remove predominantly empty columns
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Solution explained

- This solution capitalizes on the idea that a function should be portable and should probably be used more than once if it really deserves to be a function.
- Capitalizes on the structure of data frames as just groups of same-length vectors.

Questions?

Code Optimization

Theory of Code Optimization

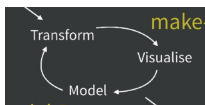- I only optimize code that is essential to my coding process.

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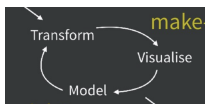

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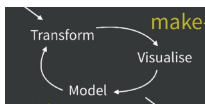
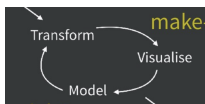- I only optimize code that is essential to my coding process.
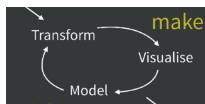
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- Tweaking bottlenecks is often worth it.
- If a bottleneck cannot be fixed or if it's not worth it to fix it, consider removing it from your code.
- Make a separate script for it, that way you're only editing the chunk of code before or after it modularly, and you're not running the bottleneck every time you rerun your script.

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- You have code that runs seems to be running slow but you dont know how to identify the rate-limiting step

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Solution

- RStudio's built-in profiler! (Or bespoke profiling)

Speeding up code

Profiling with rstudio's built-in profiler

- The basic theory of profiling is that it helps you locate bottlenecks in your process.

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- Often times, you can tell what a bottleneck is by simply looking at your code and watching it run.
- However, if you're running a for loop or a function, seeing inside the chunk is much harder.
- You can profile any amount of code, allowing you to optimize within and outside of such chunks.

Speeding up Code

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- Profiling

Here's an example of some code we're going to profile

```r
f <- function() {
  profvis::pause(0.1)
  g()
  h()
}
g <- function() {
  profvis::pause(.1)
  h()
}
h <- function() {
  profvis::pause(0.1)
}
profvis::profvis({f()})
```

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- Profiling
  - Profiling Introduction Link

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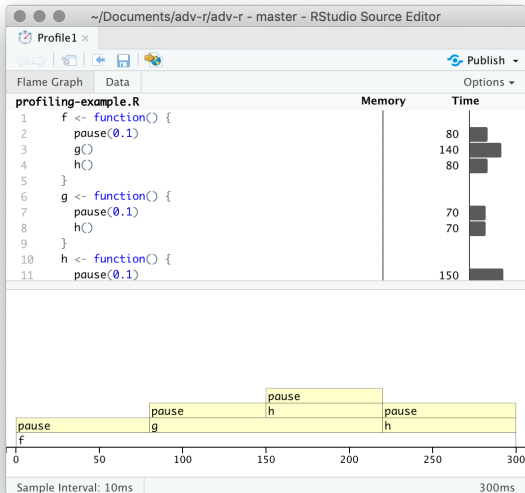
An alternative to profiling

You can also wrap your code in *system.time({})* for a more bespoke analysis.

```
library(data.table)
system.time({Sys.sleep(5)})
```

```
##    user  system elapsed
##   0.000   0.000   5.005
```

```
system.time({Sys.sleep(1)})
```

```
##    user  system elapsed
##   0.000   0.000   1.003
```

Speeding up code, a review

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- Profiling with Rstudio's built-in profiler is very handy!
- Alternatively, use *system.time*.
- If you don't want to make code more efficient, excise the clunky bits from your script so you don't keep running it every time you run your script.

Questions?

Speeding Up Code - Going from bad for-loops to better for-loops to vectorized code (functions + lapply)

Functions

"To become significantly more reliable, code must become more transparent. In particular, nested conditions and loops must be viewed with great suspicion. Complicated control flows confuse programmers. Messy code often hides bugs."

— Bjarne Stroustrup

"A common use of functionals is as an alternative to for loops. For loops have a bad rap in R because many people believe they are slow, but the real downside of for loops is that they're very flexible: a loop conveys that you're iterating, but not what should be done with the results."

— Hadley Wickham https://adv-r.hadley.nz/functionals.html

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- Vectorization here applies to "Array Programming" which simply means applying a function to an array all at once instead of piecewise.

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- They use the syntax *FUN(arg1, arg2, . . .)* to evaluate
- *lapply* (list apply) takes the arguments *X* and *FUN* where *X* is a list or vector of items to iterate the function over, and *FUN* is the function. You can also pass on other arguments but they must stay the same for all evaluations of the function.

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An example of a basic function, how to use lapply

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# Serial replication can be replaced easily!
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z <- 3 + 1
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```

```r
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```

```
## [1] 3
```

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```
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```

```r
add_1(2)
```

```
## [1] 3
```

```r
# Use lapply to run it over a list (or vector)
lapply(3:5, add_1)
```

```
## [[1]]
## [1] 4
##
## [[2]]
## [1] 5
##
## [[3]]
## [1] 6
```

Quick Data Introduction

- For the next few slides, I'll be using data from NLSY 97, a file containing basic demographic information and yearly income numbers for each participant.

```r
source("song.R")
setnames(new_data, c("PUBID", "inc_1997", "sex", "bdate_mo",
                     "bdate_yr", "sample_type", "race",
                     paste0("inc_", 1998:2011),
                     paste0("inc_", seq(2013, 2019, 2))))
new_data <- new_data[,c(1,3,7, 21:25)]
new_data <- data.table(new_data)
new_data <- new_data[complete.cases(new_data)]
head(new_data)
```

```
##    PUBID sex race inc_2011 inc_2013 inc_2015 inc_2017 inc_2019
## 1:     2   1    2    81000    83000    98928   116000   128400
## 2:     4   2    2    51000    29000    45000    45000    27000
## 3:     5   1    2    68000    76000   125000   125000   127000
## 4:     9   1    4    30000    54000    57000    59000    90000
## 5:    11   2    2    17000    33000    36000    36000    38000
## 6:    22   1    2    40000    50000    52000    75000    52000
```

Replacing for-loops with functions > - *Single Iteration Example*

- This task iterates over model designs. Vroom is a package in dplyr made to do a similar task. This might be useful in an exploratory data analysis or in a robustness check in a sensitivity analysis.

Setting up the task, choosing variables to iterate over as dependent variables in a regression.

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c.vars <- regress_vars[c(1,2,3)] # select ind. variables

c.outcome <- regress_vars[7] # select dep. var

print(c.vars)
## [1] "sex"      "race"      "inc_2011"
print(c.outcome)
## [1] "inc_2019"
```

Replacing for-loops with functions - *Single Iteration Example*

Copy data, collapse variables into a formula

```
c.dat <- copy(new_data) # copy data frame for this analysis
                        # This is unnecessary but helps us prepare
                        # to use a function
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form <- as.formula(              # collapse ind. and dep. vars to a formula
  paste0(c.outcome, " ~ ",
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)
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)

print(form)              # Print the formula

## inc_2019 ~ sex + race + inc_2011
```

Questions?

Replacing for-loops with functions - *Single Iteration Example*

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Run the model and collect the results in a data.table

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mod_betas[, ind_vars := paste0(c.vars, collapse = ", ")] # Create an ID variable to know which model I ran

mod_betas[1:4] # display outputs: estimates and SEs for each coefficient, with ID vars to describe model run

##              rn    Estimate Std. Error          ind_vars
## 1: (Intercept) 30633.54723 3785.01125 sex, race, inc_2011
## 2:         sex -9371.84648 1766.57572 sex, race, inc_2011
## 3:        race  2065.22707  696.15427 sex, race, inc_2011
## 4:    inc_2011     1.14018    0.03358 sex, race, inc_2011
```

Questions?

Replacing for-loops with functions - *Bad For-Loop Version (multiple iteration example)*

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- Now we want to do the same thing, using different model specifications.

Replacing for-loops with functions - *For-Loop Version (multiple iteration example)*

- Now we want to do the same thing, using different model specifications.
- In the for loop, I will loop over different combinations of printed variables. In the bad for loop example, I append my data.table to a preexisting data.table, which takes a lot of memory and time. This gets worse as the data.table grows longer (as the for loop keeps going).

Replacing for-loops with functions - *For-Loop Version (multiple iteration example)*

Step 1

- Establish a list of independent variable combinations to run model on. This is a list of vectors.

```
vars_vec <- replicate(3, expr =
                       sample(regress_vars[regress_vars != "inc_2019"], 3), simplify = F)
                       # above, I chose some random independent variables by
                       # sampling from all the possible choices and I assembled
print(vars_vec[1:2])   # them into a list of combinations. Here I print them.
```

```
## [[1]]
## [1] "inc_2013" "inc_2011" "sex"
##
## [[2]]
## [1] "inc_2011" "inc_2013" "inc_2017"
```

Replacing for-loops with functions

Step 2 - Run a model over each combination of independent variables

```r
all_betas <- data.table() # Establish an empty data.table to hold results
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all_betas <- data.table() # Establish an empty data.table to hold results

for(c.vars in vars_vec){  # loop over each combination of independent variables to regress
  form <- as.formula(     # create formula using ind. and dep. variables
    paste0(c.outcome, " ~ ",
           paste0(c.vars, collapse = " + "))
  )
  mod <- lm(formula = form, data = c.dat)  # Run model

  # Accumulate summary stats for each variable in regresssion
  mod_betas <- data.table(round(summary(mod)$coefficients[, 1:2],5), keep.rownames = T)
  mod_betas[, ind_vars := paste0(c.vars, collapse = ", ")] # Create an variable to know which model I ran
  # The below step is the most memory intensive!
  # It rewrites the entire object, growing larger with each iteration.
  all_betas <- rbind(all_betas, mod_betas) # append results to preexisting data table
}
```

Time for this code chunk to run: 0.0190200805664062

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```r
head(all_betas)
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```
##                 rn    Estimate Std. Error                      ind_vars
## 1: (Intercept) 24726.25754 3026.32687       inc_2013, inc_2011, sex
## 2:    inc_2013     0.88260    0.04374       inc_2013, inc_2011, sex
## 3:    inc_2011     0.32410    0.05154       inc_2013, inc_2011, sex
## 4:         sex -6778.72270 1651.90857       inc_2013, inc_2011, sex
## 5: (Intercept)  2328.47001 1121.22181 inc_2011, inc_2013, inc_2017
## 6:    inc_2011     0.05514    0.03903 inc_2011, inc_2013, inc_2017
```

Questions?

Replacing for-loops with functions - *Better For-Loop Version (multiple iteration example)*

Better for-loop version - Write to a list of data.tables

- This version of the same code replaces the object that holds the outcomes of the different models. Instead of appending to one ever-growing data.table, we append each model result (a data.table) to a list of data.tables. This doesn't require removing the list from memory and replacing it.

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```r
all_betas_list <- list() # create an empty list

i <- 0                   # create an index to add to with each iteration

for(c.vars in vars_vec){
  i <- i + 1             # add to iterator
  form <- as.formula(    # create formula, as above
    paste0(c.outcome, " ~ ",
           paste0(c.vars, collapse = " + "))
  )
  mod <- lm(formula = form, data = c.dat) # Run model
  mod_betas <- data.table(round(summary(mod)$coefficients[, 1:2],5), keep.rownames = T)
  mod_betas[, ind_vars := paste0(c.vars, collapse = ", ")]
  # This step saves memory by adding an element to a list
  # It does not copy the list or overwrite it in doing so
  all_betas_list[[i]] <- mod_betas
}
```

Time for this code chunk to run: 0.0203011035919189

Replacing for-loops with functions - *Better For-Loop Version (multiple iteration example)*

*The results are identical!)

Better for-loop version - Write to a list of data.tables

```
all_betas_list[1] # show what a list of data.tables looks like

## [[1]]
##              rn   Estimate Std. Error                    ind_vars
## 1: (Intercept) 24726.2575 3026.32687 inc_2013, inc_2011, sex
## 2:    inc_2013     0.8826    0.04374 inc_2013, inc_2011, sex
## 3:    inc_2011     0.3241    0.05154 inc_2013, inc_2011, sex
## 4:         sex -6778.7227 1651.90857 inc_2013, inc_2011, sex
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all_betas <- rbindlist(all_betas_list) # you can collapse the list of data.tables
                                       # to one large data.table
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head(all_betas)
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Replacing for-loops with functions - *Functions and Vectorization! (multiple iteration example)*

Replacing for-loops with functions - *Better For-Loop Version (multiple iteration example)*

Functions + lapply (list apply)

```r
modr <- function(c.dat, c.vars, c.outcome){ # write a function that takes in 3 arguments
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  mod <- lm(form, data = c.dat)
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  return(mod_betas) # return the data.table
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lapply(vars_vec, modr, c.outcome = "inc_2019", c.dat = new_data) %>%
  rbindlist() -> all_betas
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- Dplyr is more commonly used in learning applications, data.table is more common in industry applications.
- dtplyr uses data.table backend with dplyr syntax!!

Data.table-specific benefits

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- Many processes in data.table are more memory efficient
  - ▶ Shallow copies vs. deep copies of data are made when performing certain tasks
- Really only necessary if your data is above 1 GB

data.table, dplyr, base R cognates

- We can time each using "system.time()" to evaluate performance!

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replicate(new_data, n = 5000, simplify = F) %>% rbindlist() -> new_data2
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##    PUBID sex race inc_2011 inc_2013 inc_2015 inc_2017 inc_2019
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dim(new_data)
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# Perform the same task using three different methods
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```
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```

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data.table/tidyverse tricks

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- dcast/melt in data.table pivot_wider/pivot_longer for efficient reshaping (to be covered later)
- Don't use the $ operator ever with data.frames/data.tables!

Questions?

Data Management and Reshaping Efficiently

Data Storage Tricks

Be cognizant of what kinds of storage your data frame uses

- Long strings are memory intensive.

```r
object.size("Hello") # a character string containing "Hello"
## 112 bytes
object.size(paste0(rep("Hello", 20), collapse = " ")) # Hello Repeated 20 times
## 232 bytes
object.size(numeric(1000)) # Float64
## 8048 bytes
object.size(integer(1000)) # Integers take up less space
## 4048 bytes
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- data.table was first to the scene with optimized versions of reshape2's functions
- data.table::melt() and data.table::dcast()
- tidyr::pivot_longer was inspired by data.table's melt(), and usually performs faster than base R, but I think data.table's reshpaing tools are generally faster.

Data storage considerations

Wide data is often more space efficient, up to a point.

```r
df <- data.frame(Hunter = c(1,2,3),
                 Wade = c(2,4,6),
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head(df) #wide
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```

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df_long <- melt(df, id.vars = "multiplier")

head(df_long) #long
```

```
##   multiplier variable value
## 1          1   Hunter     1
## 2          2   Hunter     2
## 3          3   Hunter     3
## 4          1     Wade     2
## 5          2     Wade     4
## 6          3     Wade     6
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## 3          3   Hunter     3
## 4          1     Wade     2
## 5          2     Wade     4
## 6          3     Wade     6
```

```r
object.size(df)
```

```
## 1224 bytes
```

```r
object.size(df_long)
```

```
## 1888 bytes
```

Questions?

Parallelization

Parallelization

- A related concept to vectorization is parallelization. Just as you can take an operation and apply it to an entire array instead of each item of an array, you can have multiple chunks of code run simultaneously if your machine is capable of this.

Parallelization

- My computer has "1.4GHz quad-core Intel Core i5, Turbo Boost up to 3.9GHz, with 128MB of eDRAM"

```
parallel::detectCores()
```

```
## [1] 8
```

Parallelization

- My computer has "1.4GHz quad-core Intel Core i5, Turbo Boost up to 3.9GHz, with 128MB of eDRAM"
- Parallelization using R is actually a little funky, and so it will allow parameters that shouldn't work, and language gets slippery (cores vs. threads).

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- Parallelization using R is actually a little funky, and so it will allow parameters that shouldn't work, and language gets slippery (cores vs. threads).
- Disclaimer: I don't understand computers! With parallelization, profile to make sure your code is actually faster, because confusing things happen.

```
parallel::detectCores()
```

```
## [1] 8
```

Parallelization

Define your function

```r
modr <- function(c.dat, c.vars, c.outcome){
  form <- as.formula(
    paste0(c.outcome, " ~ (1|",
           paste0(c.vars, collapse = ") + (1|"),
           ")")
  )
  mod <- lme4::lmer(form, data = c.dat)
  mod_betas <- data.table(summary(mod)$coefficients[, 1:2], keep.rownames = T)
  mod_betas[, ind_vars := paste0(c.vars, collapse = ", ")]
  return(mod_betas)
}
```

This is a computationally expensive function. I've changed the model to a random effects model to use more computation power.

Get a longer vector of variables to iterate over.

```r
vars_vec <- replicate(20, expr =
                      sample(regress_vars[regress_vars != "inc_2019"], 3), simplify = F)
```

Parallelization

Serial - 1 Iteration

```
modr(vars_vec[[1]], c.dat = new_data, c.outcome = "inc_2019")
```
Time for this code chunk to run: 1.22157001495361

Serial - 20 Iterations

```
lapply(vars_vec, modr, c.outcome = "inc_2019", c.dat = new_data) %>%
  rbindlist() -> all_betas
```
Time for this code chunk to run: 2.96767401695251

Parallel - 20 Iterations

```
parallel::mclapply(vars_vec, modr, c.outcome = "inc_2019",
                   c.dat = new_data, mc.cores = 4) %>%
  rbindlist() -> all_betas
```
Time for this code chunk to run: 1.28939604759216

Parallelization

Serial - 1 Iteration

```
modr(vars_vec[[1]], c.dat = new_data, c.outcome = "inc_2019")
```
Time for this code chunk to run: 0.142056941986084

Parallel - 2 Iterations

```
parallel::mclapply(vars_vec[1:2], modr, c.outcome = "inc_2019",
                   c.dat = new_data, mc.cores = 4) %>%
  rbindlist() -> all_betas
```
Time for this code chunk to run: 0.197876930236816

Serial - 2 Iterations

```
lapply(vars_vec[1:2], modr, c.outcome = "inc_2019",
                 c.dat = new_data) %>%
  rbindlist() -> all_betas
```
Time for this code chunk to run: 0.231724977493286
There is overhead associated with despatching and receiving each task, resulting in a tradeoff that you have to manage!

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- Model-fitting, loading data, etc.
- This is a handy tool to learn if you need to use cluster-based supercomputing since there are similar concepts.

Questions, comments?