R Exposure 3

Unit 1: Loops

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Overview of the Day

- Part 3, Unit 1
 - for() and while() loops¹
 - Flow control with if() and else
- Part 3, Unit 2
 - Vectorization
 - Writing functions

[1] Note one short portion of the loops lecture makes use of a directory of .csv files. To run this easily, <u>download the repository .zip file</u>, unzip anywhere on your computer, then double-click the .Rproj file to open in RStudio.

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Repetition

Repetition

Repetition

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swiss Data

Consider the swiss data.

head(swiss, 20)

##		Fertility	Agriculture	Examination	Education	Catholic	Infant.Mortality
##	Courtelary	80.2	17.0	15	12	9.96	22.2
##	Delemont	83.1	45.1	6	9	84.84	22.2
##	Franches-Mnt	92.5	39.7	5	5	93.40	20.2
##	Moutier	85.8	36.5	12	7	33.77	20.3
##	Neuveville	76.9	43.5	17	15	5.16	20.6
##	Porrentruy	76.1	35.3	9	7	90.57	26.6
##	Broye	83.8	70.2	16	7	92.85	23.6
##	Glane	92.4	67.8	14	8	97.16	24.9
##	Gruyere	82.4	53.3	12	7	97.67	21.0
##	Sarine	82.9	45.2	16	13	91.38	24.4
##	Veveyse	87.1	64.5	14	6	98.61	24.5
##	Aigle	64.1	62.0	21	12	8.52	16.5
##	Aubonne	66.9	67.5	14	7	2.27	19.1
##	Avenches	68.9	60.7	19	12	4.43	22.7
##	Cossonay	61.7	69.3	22	5	2.82	18.7
##	Echallens	68.3	72.6	18	2	24.20	21.2
##	Grandson	71.7	34.0	17	8	3.30	20.0
##	Lausanne	55.7	19.4	26	28	12.11	20.2
##	La Vallee	54.3	15.2	31	20	2.15	10.8
##	Lavaux	65.1	73.0	19	9	2.84	20.0

Bad Repetition

If someone doesn't know better, they might find the means of variables in the swiss data by typing in a line of code for each column:

```
mean1 <- mean(swiss$Fertility)
mean2 <- mean(swiss$Agriculture)
mean3 <- mean(swissExamination)
mean4 <- mean(swiss$Fertility)
mean5 <- mean(swiss$Catholic)
mean5 <- mean(swiss$Infant.Mortality)
c(mean1, mean2 mean3, mean4, mean5, man6)</pre>
```

Can you spot the problems?

How upset would they be if the swiss data had 200 columns instead of 6?

Good Repetition

You learned some techniques specific to dataframes last time. Today you will learn general solutions, such as loops:

```
swiss_means <- setNames(numeric(ncol(swiss)), colnames(swiss))
for(i in seq_along(swiss)) {
    swiss_means[i] <- mean(swiss[[i]])
}
swiss_means</pre>
```

```
## Fertility Agriculture Examination Education
## 70.1 50.7 16.5 11.0
## Catholic Infant.Mortality
## 41.1 19.9
```

```
setNames() adds names (second argument) to its first argument.
numeric() creates a numeric vector of length equal to its first argument.
```

Don't Repeat Yourself (DRY)!

The **DRY** idea: Computers are much better at doing the same thing over and over again than we are.

Writing code to repeat tasks for us reduces the most common human coding mistakes.

It also *substantially* reduces the time and effort involved in processing large volumes of data.

Lastly, compact code is more readable and easier to troubleshoot.

What is a Loop?

I'll be bad and cite Wikipedia:

A loop is a sequence of statements which is specified once but which may be carried out several times in succession. The code "inside" the loop is obeyed a specified number of times, or once for each of a collection of items, or until some condition is met, or indefinitely." (Wikipedia)

for() Loops

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The for() Loop

for() loops are the most general kind of *loop*, found in pretty much every programming language.

"For each of these values—in order—do this"

Conceptually:

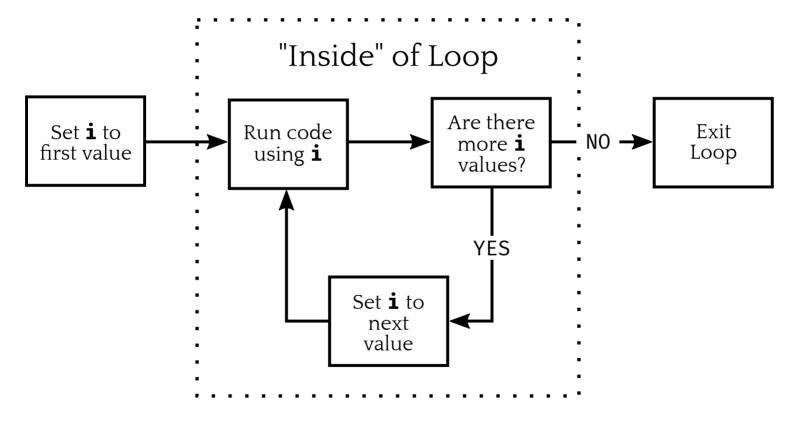
Given a set of values...

- 1. You set an index variable (often i) equal to the first value
- 2. Do some set of things (usually depending on current value)
- 3. Is there a next value?
 - YES: Update to next value, go back to 2.
 - NO: Exit loop

We are *looping* through values and repeating some actions.

for() Loop: Diagram

Given a set of values...



for() Loop: Example

```
for(i in 1:10) {
    # inside for, output won't show up without print()
    print(i^2)
}
```

```
## [1] 1
## [1] 4
## [1] 9
## [1] 16
## [1] 25
## [1] 36
## [1] 49
## [1] 64
## [1] 81
## [1] 100
```

Note this runs 10 separate print commands, which is why each line starts with [1].

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These Do the Same Thing

```
for(i in 1:3) {
   print(i^2)
}

## [1] 1
## [1] 4
## [1] 9
```

```
i <- 1
print(i^2)
i <- 2
print(i^2)
i <- 3
print(i^2)</pre>
```

[1] 1 ## [1] 4 ## [1] 9

Iteration Conventions

- We call what happens in the loop for a particular value one **iteration**.
- Iterating over indices 1:n is *very* common. n might be the length of a vector, the number of rows or columns in a matrix or data frame, or the length of a list.
- Common notation: i is the object that holds the current value inside the loop.
 - If loops are nested, you will often see j and k used for the inner loops.
 - This notation is similar to indexing in mathematical symbols (e.g $\sum_{i=1}^{n}$)
- Note i (and j,k, etc) are just normal objects. You can use any other names you want.
 - Ex: When iterating over rows and/or columns, I often use row and/or col!

Iterate Over Characters

What we iterate over doesn't have to be numbers 1:n or numbers at all! You can also iterate over a character vector in R:

```
some_letters <- letters[4:6] # Vector of letters d,e,f
for(i in some_letters) {
    print(i)
}

## [1] "d"
## [1] "e"
## [1] "f"

i # in R, this will exist outside of the loop!

## [1] "f"</pre>
```

seq_along() and Messages

 $seq_along(x)$ creates an integer vector equal to 1:length(x).

When you want to loop over something that isn't numeric but want to use a numeric index of where you are in the loop, seq_along is useful:

```
for(a in seq_along(some_letters)) {
   print(paste0("Letter ", a, ": ", some_letters[a]))

## [1] "Letter 1: d"

## [1] "Letter 2: e"

## [1] "Letter 3: f"

a # The object `a` contains the number of the last iteration

## [1] 3
```

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Pre-Allocation

Usually in a for() loop, you aren't just printing output, but want to store results from calculations in each iteration somewhere.

To do that, figure out what you want to store, and **pre-allocate** an object of the right size as a placeholder (typically with missing values as placeholders).

Examples of what to pre-allocate based on what you store:

- Single numeric value per iteration: numeric(num_of_iters)
- Single character value per iteration: character(num_of_iters)
- Single true/false value per iteration: logical(num_of_iters)
- Numeric vector per iteration: matrix(NA, nrow = num_of_iters, ncol = length_of_vector)
- Some complicated object per iteration: vector("list", num of iters)

Pre-Allocation: Numeric

```
iters <- 10 # Set number of interations
output <- numeric(iters) # Pre-allocate numeric vector

for(i in 1:iters) { # Run code below iters times
    output[i] <- (i-1)^2 + (i-2)^2
}
output # Display output</pre>
```

```
## [1] 1 1 5 13 25 41 61 85 113 145
```

Steps:

- 1. Set a number of iterations
- 2. Pre-allocated a numeric vector of that length
- 3. Ran ten iterations where the output is a mathematical function of each iteration number.

setNames()

The function setNames() can be handy for pre-allocating a named vector:

```
(names_to_use <- paste0("iter ", letters[1:5]))</pre>
## [1] "iter a" "iter b" "iter c" "iter d" "iter e"
# without setNames:
a vector <- numeric(5)</pre>
names(a_vector) <- names_to_use</pre>
# with setNames: first arg = values, second = names
 (a_vector <- setNames(numeric(5), names_to_use))</pre>
## iter a iter b iter c iter d iter e
##
```

Extended Regression
Example

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Premise

Suppose we have some data that we want to try fitting several regression models to.

We want to store the results of fitting each regression as elements of a list so that we can compare them.

To do this consistently, we'll write a loop. That way no matter if we had 2 models or 200 models, we could use the same code.

After we do this, we'll try something more advanced with loops: **Cross-validating** regressions to get an estimate of their true accuracy in predicting values out-of-sample.

Simulating Data

Let's simulate some fake data for this using the rnorm() function to generate random values from a normal distribution.

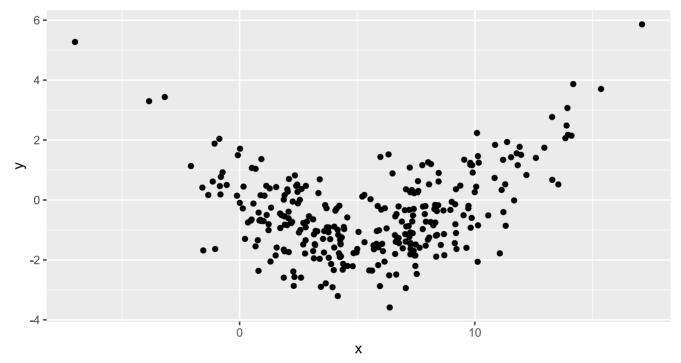
This generates a dataframe of 300 observations where y is dependent on x, with some uncorrelated, normally-distributed residual (from rnorm()).

Aside: If you followed the 2014 scandal in political science when a grad student faked data for a publication in *Science*, it is believed he used the rnorm() function to add noise to an existing dataset to get his values.

Plot of sim_data

```
library(ggplot2)
ggplot(data = sim_data, aes(x = x, y = y)) +
  geom_point() + ggtitle("Simulated Data")
```

Simulated Data



Candidate Regression Models

Let's say we want to consider several different regression models to draw trendlines through these data:

• Intercept Only: draw a horizontal line that best fits the y values.

$$E[y_i|x_i] = \beta_0$$

• Linear Model: draw a line that best fits the y values as a function of x.

$$E[y_i|x_i] = eta_0 + eta_1 \cdot x_i$$

• **Quadratic Model:** draw a quadratic curve that best summarizes the y values as a function of x.

$$E[y_i|x_i] = eta_0 + eta_1 \cdot x_i + eta_2 \cdot x_i^2$$

• **Cubic Model:** draw a cubic curve that best summarizes the y values as a function of x.

$$E[y_i|x_i] = eta_0 + eta_1 \cdot x_i + eta_2 \cdot x_i^2 + eta_3 \cdot x_i^3$$

Preallocating a List

Let's make a *named character vector* for the formulas we'll use in lm():

```
models <- c("intercept only" = "y \sim 1", # Name on left, formula on right

"linear" = "y \sim x",

"quadratic" = "y \sim x + I(x^2)",

"cubic" = "y \sim x + I(x^2) + I(x^3)")
```

Then pre-allocate a list to *store* the fitted models:

```
## $`intercept only`
## NULL
##
## $linear
## NULL
##
## $quadratic
## NULL
##
## $cubic
## NULL
```

Fitting Models in for() Loop

Next, we'll loop over the models vector and fit each one, storing it in the appropriate slot.

The formula() function converts a character string describing a model to a formula object readable by lm():

```
for(mod in names(models)) {
    fitted_lms[[mod]] <- lm(formula(models[mod]), data = sim_data)
}</pre>
```

What this does:

For each model name (which will be referred to as mod)...

- 1. Fit a lm() using the formula with that name (mod).
- 2. Assign the output to the element of the list with the matching name.

Getting Predictions

To plot the fitted models, we can first get predicted y values from each at the x values in our data.

What this does:

For each named lm() model output...

- 1. Get predicted values from the associated model (predict())
- 2. Save each of those predicted values as a *new column* in predicted_data.
 - Values of mod will be the new column names!

Predictions

head(predicted_data, 10)

```
##
                 y intercept only linear quadratic cubic
          Χ
## 1
      6.330 1.521
                           -0.464 -0.4005
                                            -1.117 -1.106
## 2
      5.984 1.437
                           -0.464 -0.4256 -1.155 -1.149
## 3
      6.501 0.887
                           -0.464 -0.3881
                                            -1.093 -1.081
                           -0.464 -0.5851
## 4
      3.788 -1.928
                                            -1.135 -1.153
## 5
     -1.064 1.880
                           -0.464 -0.9375
                                             0.530 0.536
## 6
     7.371 - 0.514
                           -0.464 - 0.3249
                                            -0.932 - 0.911
## 7
    8.393 -1.167
                           -0.464 -0.2506
                                            -0.651 -0.622
## 8 0.886 -0.668
                           -0.464 - 0.7959
                                            -0.408 -0.431
## 9
     11.062 -1.781
                           -0.464 -0.0568
                                             0.550 0.571
## 10 -0.796 0.771
                           -0.464 - 0.9180
                                             0.379 0.380
```

Gathering Predictions

We can use tidyr::pivot_longer() to tidy the predictions, then set the levels of the Model variable.

```
library(dplyr); library(tidyr)
tidy_predicted_data <- predicted_data %>%
    pivot_longer(3:6, names_to="Model", values_to="Prediction") %>%
    mutate(Model = factor(Model, levels = names(models)))
head(tidy_predicted_data) # Displaying some rows
```

```
## # A tibble: 6 x 4
                      Prediction
##
            v Model
##
    <dbl> <dbl> <fct>
                             <dbl>
## 1 6.33 1.52 intercept only -0.464
## 2 6.33 1.52 linear
                     -0.400
## 3 6.33 1.52 quadratic
                              -1.12
## 4 6.33 1.52 cubic
                              -1.11
## 5 5.98 1.44 intercept only -0.464
## 6 5.98 1.44 linear
                           -0.426
```

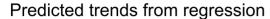
levels = names(models) sets the levels to be in the same order as the models
vector.

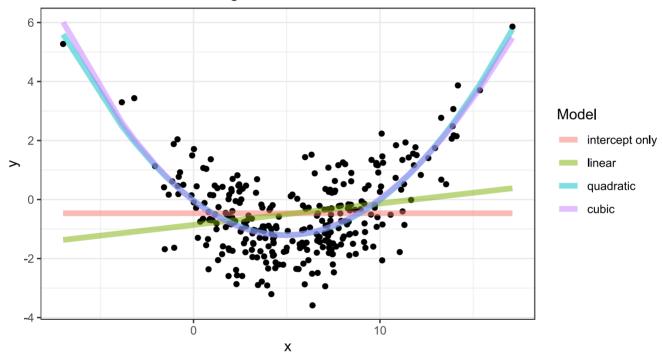
Plotting Predictions

We'll use ggplot2 to plot these tidied up predictions. You'll see us use multiple data sets on the same plot: Look at the geom_line() call.

```
ggplot(data = sim data, # Original data!
      aes(x = x.
          V = V) +
   geom point() + # Original data as points
   geom line(data = tidy_predicted data, # Predicted data!
             aes(x = x,
                 y = Prediction,
                 group = Model,
                 color = Model),
             alpha = 0.5,
             size = 2) +
   ggtitle("Predicted trends from regression") +
   theme bw()
```

Plotted Predictions





Which looks best to you?

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Cross Validation: What is it?

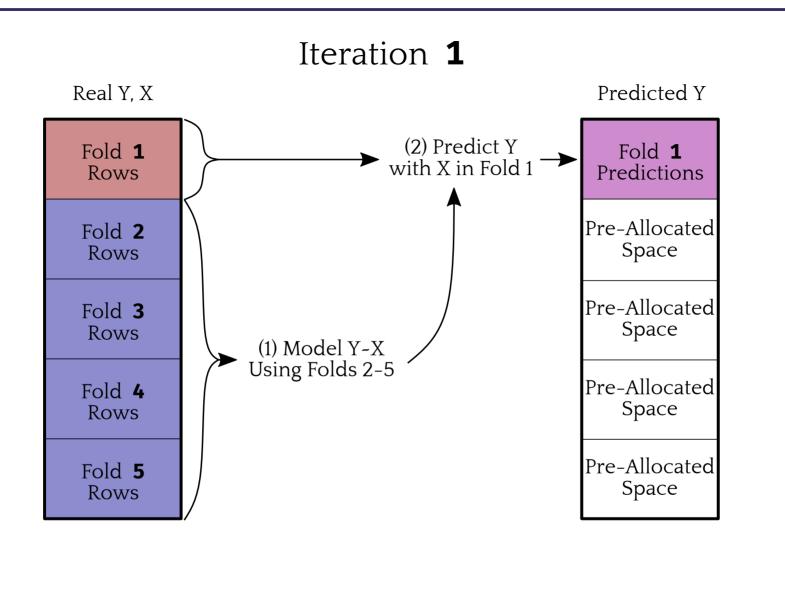
Cross validation is a widely-used method to estimate how well a model makes predictions on unseen data (data not used in fitting the model). The procedure:

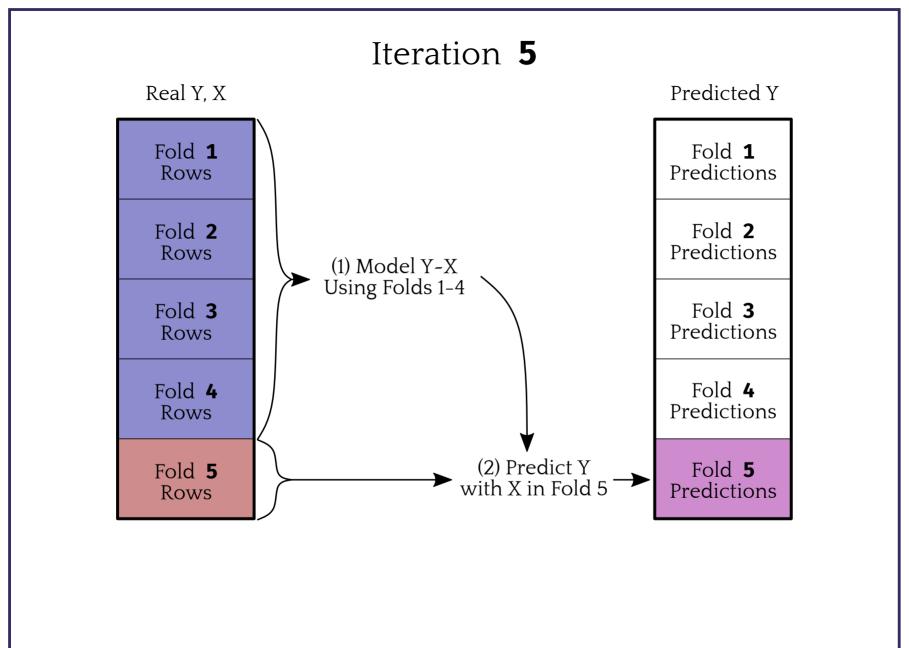
- Split your data into K folds (pieces)
- For each fold $i = 1, \ldots, K$:
 - \circ Fit the model to all the data *except* that in fold i
 - \circ Make predictions for the omitted data in fold i
- Calculate the mean squared error (or your favorite measure of accuracy comparing predictions to actuals):

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (\text{actual } y_i - \text{predicted } y_i)^2$$

A model that fits well will have *low mean squared error*. Models that are either too simple or too complicated will tend to make bad predictions and thus high mean squared error.

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Pre-Allocating for CV

Let's split the data into K=10 folds. We'll make a new data frame to hold the data and sampled fold numbers that we will add predictions to later.

We'll get the folds using the sample() function without replacement on a vector as long as our data that contains the numbers 1 through K repeated:

```
y fold intercept only linear quadratic cubic
##
## 1 6.33 1.521
                    10
                                           NA
                                   NΑ
                                                     NA
                                                           NA
## 2 5.98 1.437
                    10
                                   NA
                                          NA
                                                     NA
                                                           NA
     6.50 0.887
## 3
                                   NA
                                          NA
                                                     NA
                                                           NA
## 4 3.79 -1.928
                    10
                                   NA
                                          NA
                                                     NA
                                                           NΑ
## 5 -1.06 1.880
                                   NA
                                           NA
                                                     NA
                                                           NA
## 6 7.37 -0.514
                                   NA
                                           NA
                                                     NA
                                                           NA
```

Double-Looping for CV

Next, let's loop *over* each model (mod), and *within* each model loop over each fold (k) to fit the model and make predictions.

Note the models are fit *without* the fold rows, but prediction is done on *only the left-out fold rows*.

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Which Did Best?

Let's write another loop to compute the mean squared error of these CV predictions.

The squared error is equal to the difference between the real values and predictions squared. The MSE is the mean of all the squared errors of each prediction.

```
CV_MSE <- setNames(numeric(length(models)), names(models))
for(mod in names(models)) {
   pred_sq_error <- (CV_predictions$y - CV_predictions[[mod]])^2
   CV_MSE[mod] <- mean(pred_sq_error)
}
CV_MSE</pre>
```

```
## intercept only linear quadratic cubic ## 1.946 1.900 0.951 0.960
```

Based on these results, which model would you choose?

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if() then else

You've seen ifelse() before for logical checks on a whole vector. For checking whether a *single* logical statement holds and then conditionally executing a set of actions, use if() and else:

```
for(i in 1:10) {
  if(i %% 2 == 0) { # %% gets remainder after division
    print(paste0("The number ", i, " is even."))
  } else if(i %% 3 == 0) {
    print(paste0("The number ", i, " is divisible by 3."))
  } else {
    print(paste0("The number ", i, " is not divisible by 2 or 3."))
  }
}
```

Warning! else needs to be on same line as the closing brace } of previous if().

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if(), else: Output

The loop from the previous slide produces this output:

```
## [1] "The number 1 is not divisible by 2 or 3."
## [1] "The number 2 is even."
## [1] "The number 3 is divisible by 3."
## [1] "The number 4 is even."
## [1] "The number 5 is not divisible by 2 or 3."
## [1] "The number 6 is even."
## [1] "The number 7 is not divisible by 2 or 3."
## [1] "The number 8 is even."
## [1] "The number 9 is divisible by 3."
## [1] "The number 10 is even."
```

Handling Special Cases

Aside from the previous toy example, if() statements are useful when you have to handle special cases.

if() statements can be used to make a loop ignore or fix problematic cases.

They are also useful for producing error messages, by generating a message *if* an input value is not what is expected.

(file_list <- list.files("./example_data/"))</pre>

One common use of a loop is for loading many individual data files at once—like an entire directory of Excel files—to combine them into one data set.

(1) Let's say we have a folder filled with .csv files. We can get the file names in a folder using list.files().

```
## [1] "ex_dat_1.csv" "ex_dat_10.csv" "ex_dat_2.csv" "ex_dat_3.csv"
```

```
## [5] "ex_dat_4.csv" "ex_dat_5.csv" "ex_dat_6.csv" "ex_dat_7.csv" ## [9] "ex_dat_8.csv" "ex_dat_9.csv"
```

[1] Note you cannot run this example with only the .R script as you will not have the example data. If you want to try this out, download the course repository!

(2) Let's populate an empty list of the same length as our file list:

```
data_list <- vector("list", length(file_list))</pre>
```

(3) For nice object names, we can use stringr to remove the .csv.

```
(data_names <- stringr::str_remove(file_list, ".csv"))

## [1] "ex_dat_1" "ex_dat_10" "ex_dat_2" "ex_dat_3" "ex_dat_4"
## [6] "ex_dat_5" "ex_dat_6" "ex_dat_7" "ex_dat_8" "ex_dat_9"</pre>
```

(4) Then assign those names to the list.

```
names(data list) <- data names</pre>
```

(5) Then, let's run a loop that reads in each data file and writes it to the appropriate element of data_list.

```
library(readr) # readr to load the csv files
for (i in seq_along(file_list)){
   data_list[[ data_names[i] ]] <-
     read_csv(paste0("./example_data/", file_list[i]))
}
head(data_list[[1]], 3)</pre>
```

```
names(data_list[[1]])
```

```
## [1] "id" "x" "z"
```

names(data_list[[2]])

```
## [1] "id" "x" "z"
```

Rows: 10.000

In this case every data frame has the same columns, so we can combine them all into one data frame.

```
complete_data <- bind_rows(data_list)
glimpse(complete_data)</pre>
```

```
## Columns: 3
## $ id <dbl> 44, 49, 50, 60, 62, 76, 81, 91, 113, 114, 116, 156, 157, ~
## $ x <dbl> 0.5156, 2.1673, -0.1216, 1.0551, 0.6660, -0.0213, 1.9835,~
## $ z <dbl> 0.3808, 0.3460, 0.7115, 0.4344, 0.6379, 0.6739, 0.9808, 0~
```

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while() Loops

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while()

A lesser-used looping structure is the while() loop.

Rather than iterating over a predefined vector, the loop keeps going until some condition is no longer true.

Let's see how many times we need to flip a coin to get 4 heads:

```
num_heads <- 0
num_flips <- 0
while(num_heads < 4) {
   coin_flip <- rbinom(n = 1, size = 1, prob = 0.5)
   if (coin_flip == 1) { num_heads <- num_heads + 1 }
      num_flips <- num_flips + 1
}
num_flips # follows negative binomial distribution</pre>
```

[1] 5



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Non-Vectorized Example

We have a vector of numbers, and we want to add 1 to each element.

```
my_vector <- rnorm(100000000) # Length 100 million random vector</pre>
```

A for() loop works but is super slow:

```
for_start <- proc.time() # start the clock
new_vector <- rep(NA, length(my_vector))
for(position in 1:length(my_vector)) {
    new_vector[position] <- my_vector[position] + 1
}
(for_time <- proc.time() - for_start) # time elapsed</pre>
```

```
## user system elapsed
## 91.86 0.06 92.20
```

Vectorization Wins

Recognize that we can instead use R's vector addition (with recycling):

```
vec start <- proc.time()</pre>
new_vector <- my_vector + 1</pre>
 (vec_time <- proc.time() - vec_start)</pre>
      user system elapsed
##
##
      0.12
               0.03
                        0.16
for_time / vec_time
##
      user system elapsed
       765
                  2
                         576
##
```

The vectorized method was 765 times as fast! Vector/matrix arithmetic is implemented using fast, optimized functions that a for() loop can't compete with.

Vectorization Examples

• rowSums(), colSums(), rowMeans(), colMeans() give sums or averages over rows or columns of matrices/data frames

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[1] 22 26 30

More Vectorization Examples

• cumsum(), cumprod(), cummin(), cummax() give back a vector with cumulative quantities (e.g. running totals)

```
cumsum(1:7)
```

[1] 1 3 6 10 15 21 28

• pmax() and pmin() take a matrix or set of vectors, output the min or max for each position (after recycling):

```
pmax(c(0, 2, 4), c(1, 1, 1), c(2, 2, 2))
```

[1] 2 2 4

Vectorized File Loading

vroom is a package with vectorized loading of delimited files like .csv files.

complete data vroom <- vroom::vroom(list.files("./example data/", full.names=T))</pre>

```
## Rows: 10000 Columns: 3

## -- Column specification -----
## Delimiter: ","

## dbl (3): id, x, z

##

## i Use `spec()` to retrieve the full column specification for this data.

## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

glimpse(complete_data_vroom)

```
## Rows: 10,000
## Columns: 3
## $ id <dbl> 44, 49, 50, 60, 62, 76, 81, 91, 113, 114, 116, 156, 157, ~
## $ x <dbl> 0.5156, 2.1673, -0.1216, 1.0551, 0.6660, -0.0213, 1.9835,~
## $ z <dbl> 0.3808, 0.3460, 0.7115, 0.4344, 0.6379, 0.6739, 0.9808, 0~
```

This replaced our entire data loading loop with one line!

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End of R3, Unit 1

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