432 Class 01

https://thomaselove.github.io/432-2023/

2023-01-17

Today's Agenda

1. Mechanics of the course
2. Why I write dates the way I do
3. Data organization in spreadsheets
4. Naming Things and Getting Organized
5. Switching from R Markdown to Quarto
6. Building and Validating small models for Penguin Bill Length

Section 1

Course Mechanics

Welcome to 432.

Just about everything is linked at https://thomaselove.github.io/432-2023

- Calendar
  - final word on all deadlines, and links to each class and TA office hours.
- Syllabus (can download as PDF)
- Course Notes work in progress: only HTML
- Software
  - Updating / Installing R and RStudio, necessary R Packages
- Get Data (Code, Quarto templates) at our 432-data page
- Assignments (Labs, Projects, Quizzes - see next slide)
- Sources (books, articles, videos, etc.)
- Key Links (Canvas, Campuswire, Shared Drive, Minute Papers)
- Contact Us (Campuswire + TA office hours + My email)

Assignments

Every deliverable for the entire semester is listed in the Calendar.

- First thing is the Welcome to 432 Survey at https://bit.ly/432-2023-welcome-survey which you should complete by tomorrow (Wednesday 2023-01-18) at Noon.
  - Also, please sign up for or accept your invitation to Campuswire and then answer my little poll question as soon as you can. Thanks.
- Two projects (complete instructions now available for each)
  - Project A (use publicly available data for linear & logistic models)
    1. Plan due in mid-February (data selection, cleaning, exploration)
    2. Final Portfolio & (recorded) Presentation right after Spring Break
  - Project B (use almost any data and build specific models)
    1. Proposal Form in early April
    2. Presentation (in-person or Zoom) in May
    3. Portfolio (prepared using Quarto) also in May

Assignments

Every deliverable for the entire semester is listed in the Calendar.

- Eight labs, meant to be (generally) shorter than 431 Labs
  - Lab 1 is due Monday 2023-01-23 at 9 PM.
  - Lab 2 is due Monday 2023-01-30 at 9 PM.
  - Instructions are available now for all 8 labs. All due Mondays 9 PM.
- Two Quizzes
  - Quiz 1 in late February, Quiz 2 in late April
  - Receive Quiz on Thursday at 5 PM, due Monday at 9 PM.
  - Multiple choice and short answer, mostly, taken via a Google Form
- Many Minute Papers (due most Wednesdays at Noon.)
  - First is after Class 3 due 2023-01-25.
  - These actually take about 5 minutes each.

Syllabus and Instructions provide information on grading/feedback.

Spring 2023 Teaching Assistants for 432

- Stephanie Merlino Barr, PhD candidate in Clinical Translational Science
- Shiying Liu, PhD candidate in Epidemiology & Biostatistics
- Ali Elsharkawi, MS student in Clinical Research
- Monika Strah, MS student in Epidemiology & Biostatistics
- Ria Tilve, MPH student in Population Health Research
- Kyaw Hla, MS student in Clinical Research
- Zhengxi Chen, PhD student in Epidemiology & Biostatistics
- Lindsay Petrenchik, MS graduate in Epidemiology & Biostatistics

All return from working with students in 431 this past Fall, and I couldn't be more grateful for their energy and effort. Learn more about the TAs in the Syllabus.

TA Zoom Office Hours begin this Friday 2023-01-20. Details coming soon to Canvas, our website, and our Shared Drive.

Getting Help

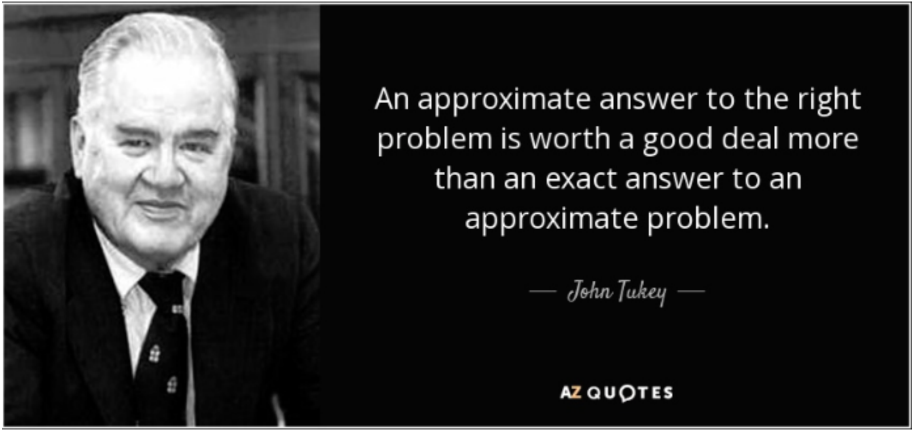
- Campuswire is the location for discussion about the class.
- We have 8 teaching assistants volunteering their time to help you.
- TAs will hold Office Hours beginning Friday 2023-01-20 via Zoom.
  - Details will be available all over the place, soon.
- Dr. Love is available before and (especially) after class to chat.
- Email Dr. Love if you have a matter you need to discuss with him specifically. He's at `Thomas dot Love at case dot edu`.

We WELCOME your questions/comments/corrections/thoughts!

Tools You Will Definitely Use in this Class

- **Course Website** (see the bottom of this slide) especially the Calendar
    - Each class has a README (announcements, etc.) plus slides
- **R, RStudio and Quarto** for, well, everything
- **Canvas** for access to Zoom meetings and 432 recordings, submission of most assignments
- **Google Drive via CWRU** for forms (Minute Papers/Surveys/Quizzes) and for feedback on assignments
- **Campuswire** is our discussion board. It's a moderated place to ask questions, answer questions of your colleagues, and get help fast. Open 24/7.
- **Zoom** for class recordings and TA office hours

Some source materials are **password-protected**. What is the password?



An approximate answer to the right problem is worth a good deal more than an exact answer to an approximate problem.

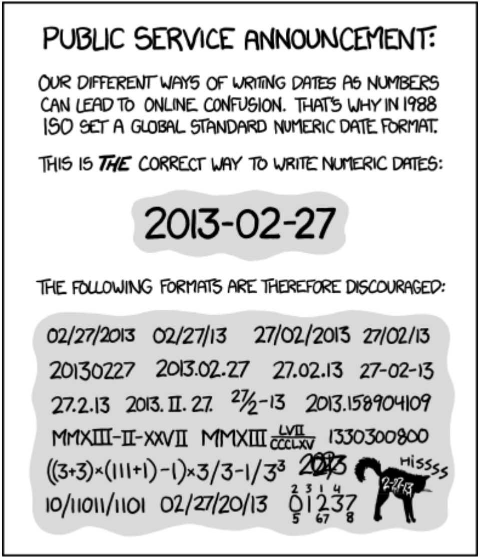
— John Tukey —

AZ QUOTES

Section 2

Why I Write Dates The Way I Do

How To Write Dates (https://xkcd.com/1179/)


PUBLIC SERVICE ANNOUNCEMENT:
OUR DIFFERENT WAYS OF WRITING DATES AS NUMBERS CAN LEAD TO ONLINE CONFUSION. THAT'S WHY IN 1988 ISO SET A GLOBAL STANDARD NUMERIC DATE FORMAT.
THIS IS THE CORRECT WAY TO WRITE NUMERIC DATES:
2013-02-27
THE FOLLOWING FORMATS ARE THEREFORE DISCOURAGED:
02/27/2013 02/27/13 27/02/2013 27/02/13
20130227 2013.02.27 27.02.13 27-02-13
27.2.13 2013. II. 27. 27/2-13 2013.158904109
MMXIII-II-XXVII MMXIII LVII/CCCLXV 1330300800
((3+3)×(111+1)−1)×3/3−1/3³ 2013
HISSsss
2-27-13
10/11011/1101 02/27/20/13 01237
2 3 1 4
5 67 8

Section 3

Data Organization in Spreadsheets

Tidy Data (Wickham)

> *"A huge amount of effort is spent cleaning data to get it ready for analysis, but there has been little research on how to make data cleaning as easy and effective as possible....*

Tidy datasets are easy to manipulate, model and visualize, and have a specific structure: each variable is a column, each observation is a row, and each type of observational unit is a table.

> *This framework makes it easy to tidy messy datasets because only a small set of tools are needed to deal with a wide range of un-tidy datasets. This structure also makes it easier to develop tidy tools for data analysis, tools that both input and output tidy datasets. The advantages of a consistent data structure and matching tools are demonstrated with a case study free from mundane data manipulation chores."*

https://www.jstatsoft.org/article/view/v059i10

“Data Tidying” presentation in *R for Data Science, 2e*

- Defines tidy data
- Demonstrates methods for tidying messy data in R

Read Sections 4 (Data transformation) and 6 (Data tidying)

https://r4ds.hadley.nz/

Data Organization in Spreadsheets (Broman & Woo)

- Create a data dictionary.
  - Jeff Leek has good thoughts on this in "How to Share Data with a Statistician" at https://github.com/jtleek/datasharing
  - Shannon Ellis and Jeff Leek's preprint "How to Share data for Collaboration" touches on many of the same points at https://peerj.com/preprints/3139v5.pdf

We want:

1. The raw data.
2. A tidy data set.
3. A codebook describing each variable and its values in the tidy data set.
4. An explicit and exact recipe describing how you went from 1 to 2 and 3.

Data Organization in Spreadsheets: **Be Consistent**

- Consistent codes for categorical variables.
  - Either “M” or “Male” but not both at the same time.
  - Make it clear enough to reduce dependence on a codebook.
  - No spaces or special characters other than _ in category names.
- Consistent fixed codes for missing values.
  - NA is the most convenient R choice.
- Consistent variable names
  - In R, I’ll use `clean_names` from the `janitor` package to turn everything into snake_case.
  - In R, start your variable names with letters. No spaces, no special characters other than _.
- Consistent subject / record identifiers
  - And if you’re building a .csv in Excel, don’t use ID as the name of that identifier.
- Consistent data layouts across multiple files.

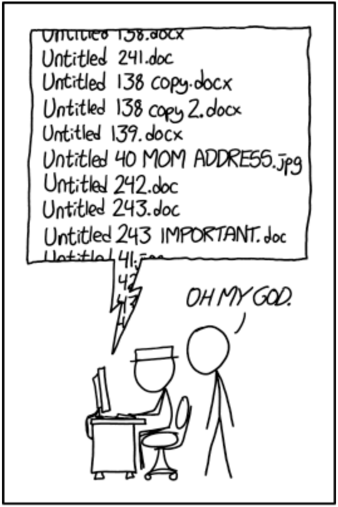
What Goes in a Cell?

- Make your data a rectangle.
    - Each row represents a record (sometimes a subject).
    - Each column represents a variable.
    - First column is a unique identifier for each record.
- No empty cells.
- One Thing in each cell.
- No calculations in the raw data
- No font colors
- No highlighting

Section 4

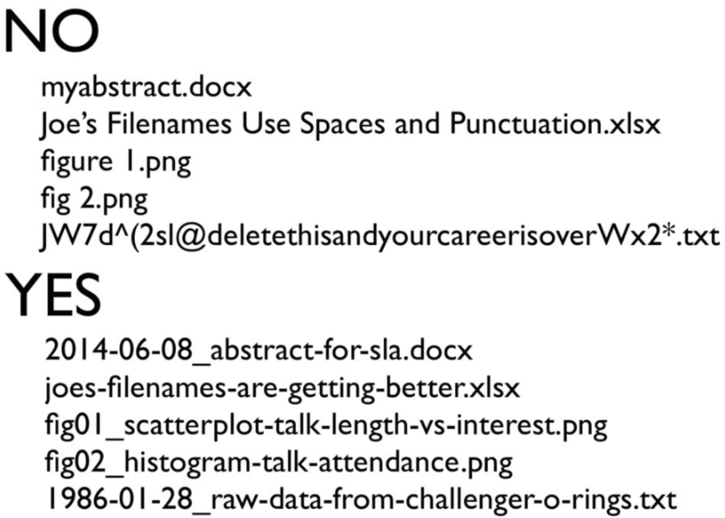
Naming Things and Getting Organized

Naming Files is Hard (https://xkcd.com/1459/)



PROTIP: NEVER LOOK IN SOMEONE ELSE'S DOCUMENTS FOLDER.

How To Name Files



NO

myabstract.docx
Joe's Filenames Use Spaces and Punctuation.xlsx
figure 1.png
fig 2.png
JW7d^(2sl@deletethisandyourcareerisoverWx2*.txt

YES

2014-06-08_abstract-for-sla.docx
joes-filenames-are-getting-better.xlsx
fig01_scatterplot-talk-length-vs-interest.png
fig02_histogram-talk-attendance.png
1986-01-28_raw-data-from-challenger-o-rings.txt

Data Organization in Spreadsheets: Use consistent, strong file names.

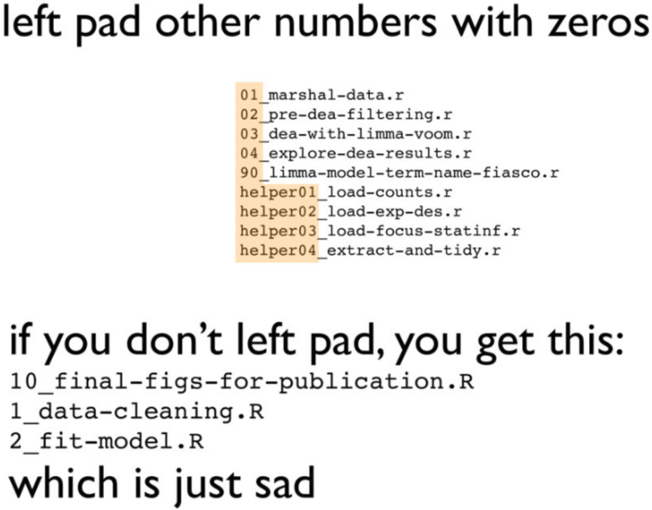
Jenny Bryan's advice on "Naming Things" hold up well. There's a full presentation at SpeakerDeck.

Good file names:

- are machine readable (easy to search, easy to extract info from names)
- are human readable (name contains content information, so it's easy to figure out what something is based on its name)
- play well with default ordering (something numeric first, left padded with zeros as needed, use ISO 8601 standard for dates)

Avoid: spaces, punctuation, accented characters, case sensitivity

from Jenny Bryan's "Naming Things" slides...



left pad other numbers with zeros

```
01_marshal-data.r
02_pre-dea-filtering.r
03_dea-with-limma-voom.r
04_explore-dea-results.r
90_limma-model-term-name-fiasco.r
helper01_load-counts.r
helper02_load-exp-des.r
helper03_load-focus-statinf.r
helper04_extract-and-tidy.r
```

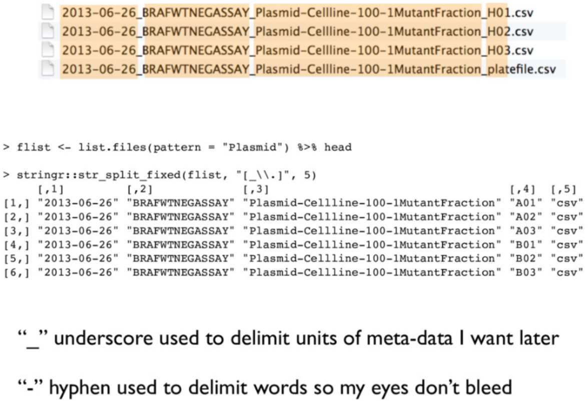
if you don't left pad, you get this:

```
10_final-figs-for-publication.R
1_data-cleaning.R
2_fit-model.R
```

which is just sad

Jenny Bryan: Deliberate Use of Delimiters

Deliberately use delimiters to make things easy to compute on and make it easy to recover meta-data from the filenames.



```
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_H01.csv
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_H02.csv
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_H03.csv
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_platefile.csv
```

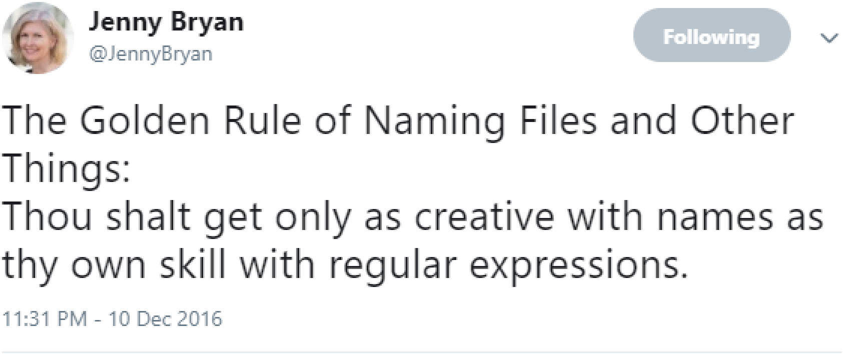
```
> flist <- list.files(pattern = "Plasmid") %>% head

> stringr::str_split_fixed(flist, "[_\\.]", 5)
     [,1]         [,2]            [,3]                                   [,4]  [,5]
[1,] "2013-06-26" "BRAFWTNEGASSAY" "Plasmid-Cellline-100-1MutantFraction" "A01" "csv"
[2,] "2013-06-26" "BRAFWTNEGASSAY" "Plasmid-Cellline-100-1MutantFraction" "A02" "csv"
[3,] "2013-06-26" "BRAFWTNEGASSAY" "Plasmid-Cellline-100-1MutantFraction" "A03" "csv"
[4,] "2013-06-26" "BRAFWTNEGASSAY" "Plasmid-Cellline-100-1MutantFraction" "B01" "csv"
[5,] "2013-06-26" "BRAFWTNEGASSAY" "Plasmid-Cellline-100-1MutantFraction" "B02" "csv"
[6,] "2013-06-26" "BRAFWTNEGASSAY" "Plasmid-Cellline-100-1MutantFraction" "B03" "csv"
```

"_" underscore used to delimit units of meta-data I want later

"-" hyphen used to delimit words so my eyes don't bleed

Don't get too cute.

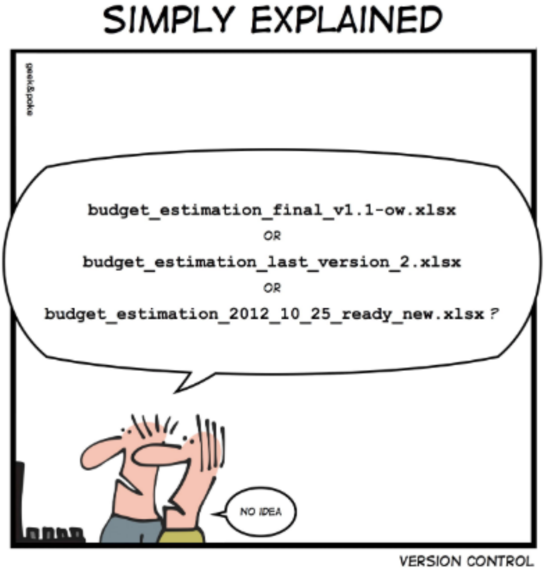


Jenny Bryan
@JennyBryan

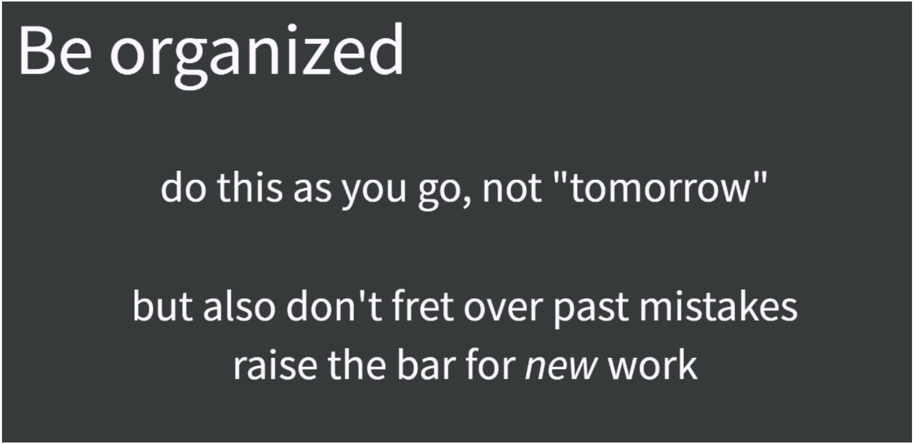
The Golden Rule of Naming Files and Other Things:
Thou shalt get only as creative with names as thy own skill with regular expressions.

11:31 PM - 10 Dec 2016

Goal: Avoid this...


SIMPLY EXPLAINED
geek&poke
budget_estimation_final_v1.1-ow.xlsx
OR
budget_estimation_last_version_2.xlsx
OR
budget_estimation_2012_10_25_ready_new.xlsx ?
NO IDEA
VERSION CONTROL

Get organized



Be organized

do this as you go, not "tomorrow"

but also don't fret over past mistakes
raise the bar for *new* work

Don’t spend a lot of time bemoaning or cleaning up past ills. Strive to improve this sort of thing going forward.

“Good Enough Practices in Scientific Computing”

1. Save the raw data.
2. Ensure that raw data is backed up in more than one location.
3. Create the data you wish to see in the world (the data you wish you had received.)
4. Create analysis-friendly, tidy data.
5. Record all of the steps used to process data.
6. Anticipate the need for multiple tables, and use a unique identifier for every record.

http://bit.ly/good-enuff

Lots of great advice here on software, collaboration and project organization.

Section 5

Switching from R Markdown to Quarto

Switching from R Markdown to Quarto

https://quarto.org/ is the main website for Quarto.

If you can write an R Markdown file, it will also work in Quarto, by switching the extension from `.rmd` to `.qmd`.

- We provide a Quarto template for Lab 1 (due Monday at 9 PM) which should ease your transition a bit.
- Read Chapter 30 (Quarto) in R for Data Science, 2e
- Lots of other suggestions in the Class 01 README and that material is also on our Sources page.

All of Dr. Love's material for this course is written using Quarto now.

Section 6

Building and Validating Linear Prediction Models

R Setup

```r
knitr::opts_chunk$set(comment = NA)

library(broom); library(glue); library(gt)
library(janitor); library(knitr); library(mosaic)
library(patchwork); library(rsample)
library(palmerpenguins); library(tidyverse)

theme_set(theme_bw())
```

Data Load

```
our_tibble <- penguins |>
  select(species, sex, bill_length_mm) |>
  drop_na()

our_tibble |> summary()
```

```
      species        sex      bill_length_mm
 Adelie   :146   female:165   Min.   :32.10
 Chinstrap: 68   male  :168   1st Qu.:39.50
 Gentoo   :119                Median :44.50
                              Mean   :43.99
                              3rd Qu.:48.60
                              Max.   :59.60
```

Partition `our_tibble` into training/test samples

We will place 60% of the penguins in our training sample, and require that similar fractions of each species occur in our training and testing samples. We use functions from the **rsample** package here.

```r
set.seed(20230117)
our_split <- initial_split(our_tibble, prop = 0.6,
                           strata = species)
our_train <- training(our_split)
our_test <- testing(our_split)
```

We could use `slice_sample()` as in the Course Notes if we didn't stratify by species.

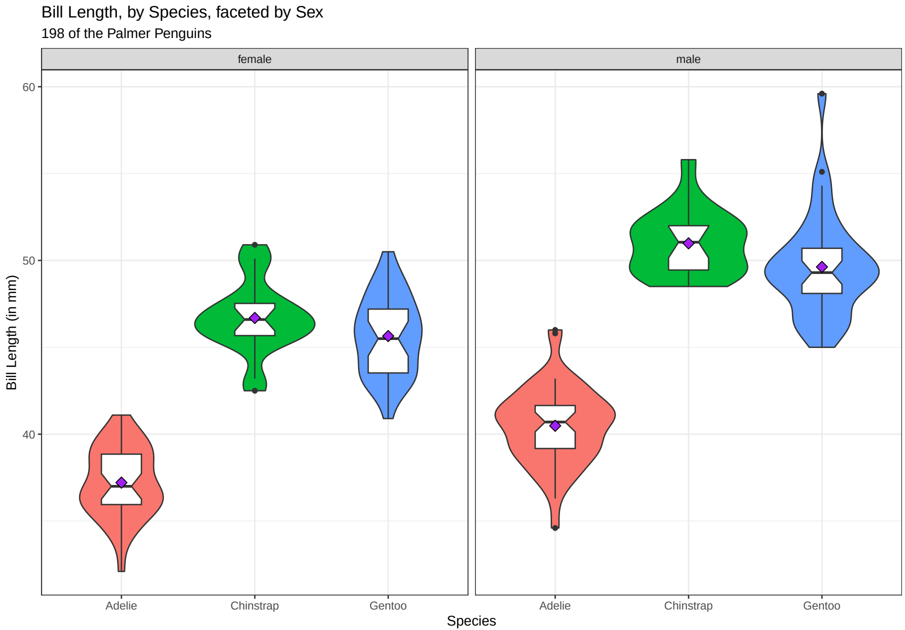
Result of our partitioning

```
our_train |> tabyl(species) |> adorn_totals() |>
  adorn_pct_formatting()
```

```
   species   n percent
    Adelie  87   43.9%
 Chinstrap  40   20.2%
    Gentoo  71   35.9%
     Total 198  100.0%
```

```
our_test |> tabyl(species) |> adorn_totals() |>
  adorn_pct_formatting()
```

```
   species   n percent
    Adelie  59   43.7%
 Chinstrap  28   20.7%
    Gentoo  48   35.6%
     Total 135  100.0%
```


Bill Length, by Species, faceted by Sex
198 of the Palmer Penguins
female
male
60
50
40
Bill Length (in mm)
Adelie
Chinstrap
Gentoo
Adelie
Chinstrap
Gentoo
Species

Code for previous slide

```r
ggplot(data = our_train,
       aes(x = species, y = bill_length_mm)) +
  geom_violin(aes(fill = species)) +
  geom_boxplot(width = 0.3, notch = TRUE) +
  stat_summary(fill = "purple", fun = "mean",
               geom = "point",
               shape = 23, size = 3) +
  facet_wrap(~ sex) +
  guides(fill = "none") +
  labs(title = "Bill Length, by Species, faceted by Sex",
       subtitle =
         glue(nrow(our_train), " of the Palmer Penguins"),
       x = "Species", y = "Bill Length (in mm)")
```

Model m1

```
m1 <- lm(bill_length_mm ~ species + sex, data = our_train)

anova(m1)
```

```
Analysis of Variance Table

Response: bill_length_mm
           Df Sum Sq Mean Sq F value    Pr(>F)
species     2 4076.2 2038.12  395.68 < 2.2e-16 ***
sex         1  686.4  686.44  133.26 < 2.2e-16 ***
Residuals 194  999.3    5.15
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '
```

Model 1 coefficients

```r
tidy(m1, conf.int = TRUE, conf.level = 0.90) |>
  select(term, estimate, conf.low, conf.high) |>
  kable(digits = 1)
```

term	estimate	conf.low	conf.high
(Intercept)	37.0	36.5	37.5
speciesChinstrap	10.0	9.3	10.7
speciesGentoo	8.8	8.2	9.4
sexmale	3.7	3.2	4.3

Model m2

```
m2 <- lm(bill_length_mm ~ species, data = our_train)

## anova(m2) yields p-value < 2.2e-16 (not shown here)

tidy(m2, conf.int = TRUE, conf.level = 0.90) |>
  select(term, estimate, conf.low, conf.high) |>
  kable(digits = 1)
```

term	estimate	conf.low	conf.high
(Intercept)	39.0	38.5	39.5
speciesChinstrap	9.8	8.9	10.7
speciesGentoo	8.7	7.9	9.5

In-Sample Comparison

```r
bind_rows(glance(m1), glance(m2)) |>
  mutate(model = c("m1 (species & sex)",
                   "m2 (species only)")) |>
  select(model, r2 = r.squared, adjr2 = adj.r.squared,
         AIC, BIC, sigma, nobs) |>
  kable(digits = c(0, 3, 3, 1, 1, 2, 0))
```

model	r2	adjr2	AIC	BIC	sigma	nobs
m1 (species & sex)	0.827	0.824	892.4	908.9	2.27	198
m2 (species only)	0.707	0.704	994.0	1007.1	2.94	198

Which model has better in-sample performance?

Assessing Performance in Test Sample

```r
m1_aug <- augment(m1, newdata = our_test)

m1_res <- m1_aug |>
  summarize(validated_R_sq = cor(bill_length_mm, .fitted)^2,
            MAPE = mean(abs(.resid)),
            RMSPE = sqrt(mean(.resid^2)),
            max_Error = max(abs(.resid)))

m2_aug <- augment(m2, newdata = our_test)

m2_res <- m2_aug |>
  summarize(validated_R_sq = cor(bill_length_mm, .fitted)^2,
            MAPE = mean(abs(.resid)),
            RMSPE = sqrt(mean(.resid^2)),
            max_Error = max(abs(.resid)))
```

Summarizing Test Sample Performance

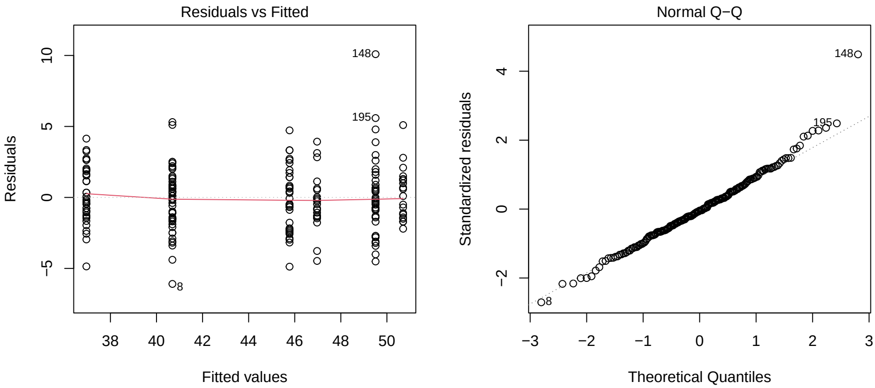
```
bind_rows(m1_res, m2_res) |>
  mutate(model = c("m1 (species & sex)",
                   "m2 (species only)")) |>
  relocate(model) |>
  kable(digits = c(0, 3, 2, 2, 1))
```

model	validated_R_sq	MAPE	RMSPE	max_Error
m1 (species & sex)	0.813	1.73	2.40	11.0
m2 (species only)	0.707	2.50	3.03	9.2

Which model predicts better in the test sample?

Residual Plots for Model m1 (training sample)

```
par(mfrow = c(1,2)); plot(m1, which = c(1,2))
```



```
par(mfrow = c(1,1))
```

What we did in this example...

1. R packages, usual commands, ingest the data.
2. Look at what we have and ensure it makes sense. (DTDP)
3. Partition the data into a training sample and a test sample.
4. Run a two-way ANOVA model (called `m1`) in the training sample; evaluate the quality of fit.
5. Run a one-way ANOVA model (called `m2`) in the training sample; evaluate the quality of fit.
6. Use augment to predict from each model into the test sample; summarize and compare predictive quality.
7. Choose between the models and evaluate assumptions for our choice.

For Next Time...

1. If you're not registered with SIS, do so, for PQHS/CRSP/MPHP 432.
2. Review the website and calendar, and skim the syllabus and Notes.
3. Welcome to 432 Survey at https://bit.ly/432-2023-welcome-survey by noon Wednesday 2023-01-18.
4. Accept the invitation to join the Campuswire Discussion Forum for 432 and answer my little poll there.
5. Buy Jeff Leek's How to be a Modern Scientist and read it by the end of January.
6. Get started installing or updating the software you need for the course.
7. Get started on Lab 1, due Monday 2023-01-23 at 9 PM.