



70th Conference on Mass Spectrometry and Allied topics

Getting Started with R for Mass Spectrometry Data Analysis

SHORT COURSES

ASMS 2022: R Short Course
June 4 - 5 Saturday/Sunday June 4-5, 2022

#ASMS2022

The Team

Ryan Benz
Seer, Inc.



Jeffrey Jones
Caltech



N. Heath Patterson
Vanderbilt School of Medicine



Ryan Benz

Education

Chapman University

BS Chemistry, BS Mathematics

UC Irvine PhD

Computational Chemistry & Bioinformatics

UC Irvine

Post-Doc Inst. of Genomics and Bioinformatics



... discovered that lab work was not for me, data was going to be big!

Experience

Applied Proteomics Inc

Bioinformatics Scientist, Director

SoCal Bioinformatics Inc

Bioinformatics consulting, biotech & pharma

Seer, Inc.

Principal Scientist, Director of Data Science

Feel free to connect with me on LinkedIn: <https://www.linkedin.com/in/ryan-benz/>

Jeff Jones

Education

Cal Poly SLO	BA Microbiology, BA Biochemistry
Univ Arkansas PhD	Analytical Chemistry (FTMS)
UC Irvine	Post-Doc Inst. of Genomics and Bioinformatics



... learned programming and stats (bioinformatics) out of a need to analyze large data sets generated by mass spectrometry...

Experience

Applied Proteomics Inc	blood based biomarkers, colorectal cancer
SoCal Bioinformatics Inc	bioinformatics consulting
Caltech Proteome Exp Lab	bespoke proteomics and bioinformatics

Useful Code

Quantitative Proteomics Analysis Pipeline: github.com/jeffsocal/keystone

Nathan “Heath” Patterson

Education

Univ Wyoming
U de Montréal
Vanderbilt

BS Chemistry
Analytical Chemistry (Imaging Mass Spectrometry)
Post-Doc MS Research Center (Caprioli Group)



Took an interest in programming when vendor solutions no longer solved the problem

Experience

Vanderbilt University

Current: Faculty in Biochemistry - Research Instructor

Some of my code

github.com/nhpatterson

Goals for the Short Course

- Learn basic fundamentals of the R programming language
- Learn how to use to the RStudio integrated development environment (IDE)
- Learn about tidy data, what it is, and why it's important for data analysis
- Learn basic fundamentals of the tidyverse ecosystem of R packages and how they can be used to streamline the data analysis process
- Learn how to make data visualizations using the ggplot2 R package

We'll Cover 3 Main Topics

1. Gettings started with R and RStudio
2. Introduction to tidy data and the tidyverse
3. Introduction to data visualization in R with ggplot2

R is a great language for data analysis!

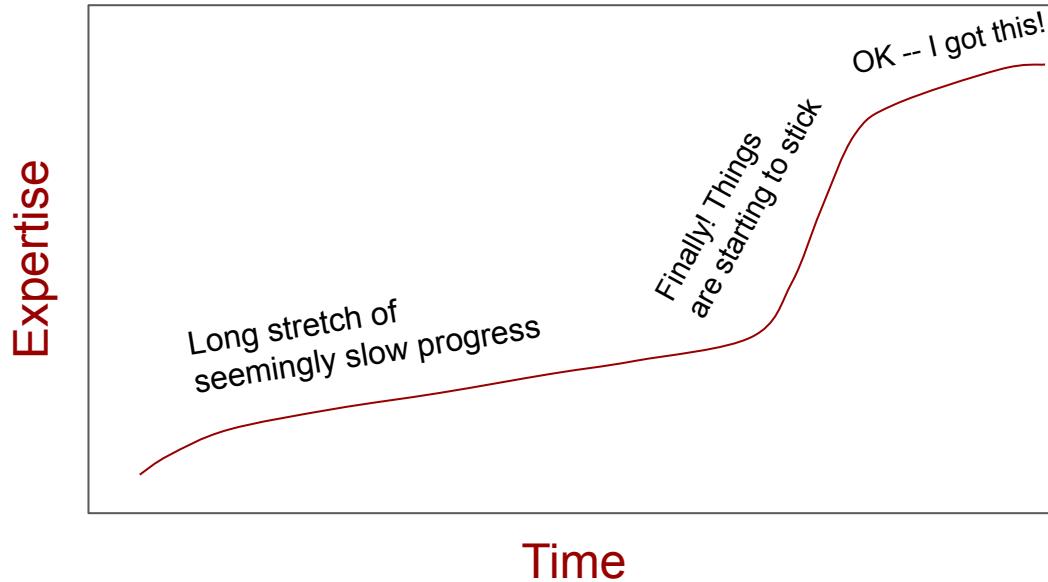
- Many programming languages are general purpose (can be used in any domain), e.g. C/C++, Java, Python
- R is *not* a general purpose programming language, it's a language specifically designed for working with data (that's what scientists do!)
- Because R is geared toward data, its design, structure and continued development is focused on making it easier to work with data
- R has become one of the top languages for data science, and its popularity and usage continues to grow
- For scientists, R is a great tool to learn

But what about Python?

- Python is a great language, and is another top language for data science
- If you want to become a data scientist or work heavily with data, learning both R and Python is a great idea – both have pros and cons
- But, if you choose Python over R, that's not a bad choice either
- R might work better for some, Python for others
- If R just isn't working for you, give Python a shot

The R Learning Curve

10 years ago...

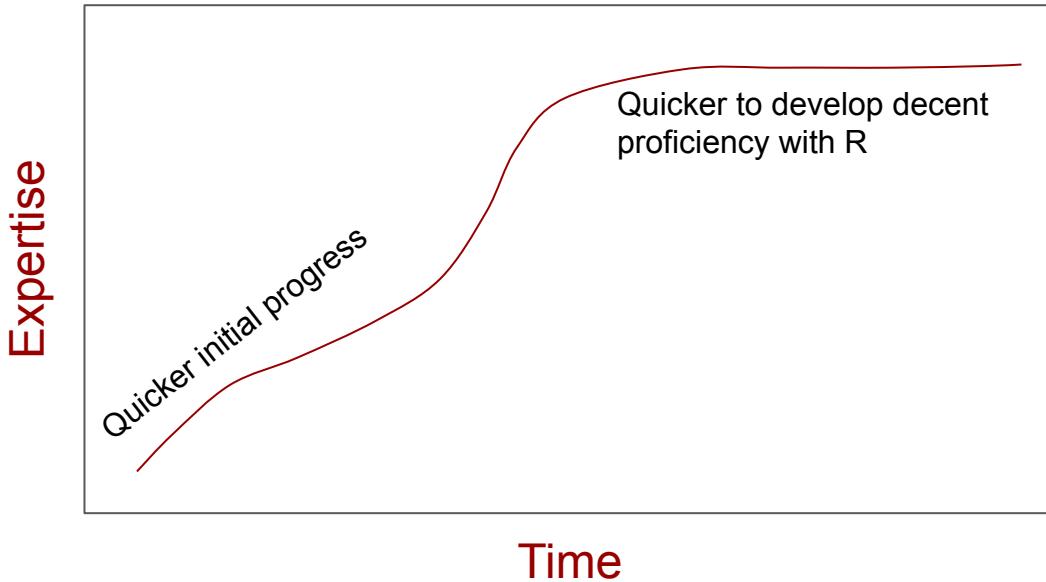


What made R challenging to learn 10 year ago?

- Fewer R resources
- Less mature
- Less interest
- Fewer people in the community
- Data science wasn't "a thing" yet

The R Learning Curve

Today...



Why is R easier to learn today?

- More (high quality) R resources
- Very mature, lots of amazing tools in R
- Lots of interest
- Lots of people in the community, and the community is great
- The data science “revolution” has pushed R to develop and evolve, become more user-centric

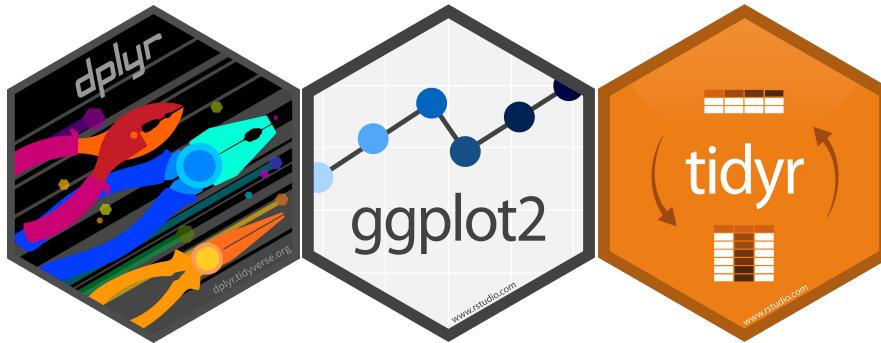
R is still challenging to learn – but it's worth it!

- R is a quirky language, but the quirks are often there for a reason (to make working with data easier)
- R can be frustrating for beginners, and the quirks don't help
- For many, R might be initially harder to learn than other languages (e.g. Python)
- But, once R starts to stick, its data-centric capabilities and tools really shine!

Thoughts about learning R and how to code

- The first step to learning a programming language is to learn its *syntax* (the set of rules and symbols that make up structurally correct code)
- Computers are *really* picky, and even the smallest violations of the syntax rules will result in code that doesn't run:
typos, incorrect names, missing spaces or too many spaces, wrong brackets, ...
- Syntax errors are frustrating, and unfortunately, the most common mistake for beginners
- Hang in there, start simple, try to understand very simple cases first, then build and expand on them

The R ecosystem is vast and awesome!



Shiny

Interactive web apps for data

RMarkdown, Blogdown, Bookdown
Reproducible reporting, blogs & books

At the end of the course, are you able to...

- start-up RStudio and make an RStudio project?
- read a formatted text file (e.g. csv file) into R?
- understand basic properties about the data (e.g. # rows, cols)?
- tell someone what tidy data is and why it's important?
- perform some basic data manipulations and operations on the data?
- make a simple plot from the data?

Schedule

Saturday – Learning the Fundamentals

Start Time	End Time	Durration	Session
9:00 AM	9:15 AM	15 min	Short course introduction
9:15 AM	10:15 AM	1 hr	Getting Set-up
10:15 AM	10:45 AM	30 min	Coffee Break
10:45 AM	11:00 AM	15 min	Introduction to R and R Studio
11:00 AM	11:15 AM	15 min	Practice: Working with RStudio Projects
11:15 AM	12:00 PM	45 min	Essential R Basics & Reading Data into R
12:00 PM	1:00 PM	1 hr	Lunch
1:00 PM	1:15 PM	15 min	Introduction to Tidy Data & the Tidyverse
1:15 PM	2:00 PM	30 min	Data Manipulation with dplyr
2:15 PM	2:30 PM	15 min	Practice: dplyr Examples
2:30 PM	3:00 PM	30 min	Coffee Break
3:00 PM	3:45 PM	45 min	Introduction to ggplot2
3:45 PM	4:00 PM	15 min	Practice: Basic ggplot2 Plots
4:00 PM	5:00 PM	1 hr	Day 1 Recap & Practice: MS Data Examples

Schedule

Sunday – Practice with Examples

Start Time	End Time	Durration	Session
9:00 AM	9:30 AM	30 min	Day 2 Overview, Review of MS Data Exercises
9:30 AM	10:15 AM	45 min	Pivoting & Merging Data Frames
10:15 AM	10:45 AM	30 min	Coffee Break
10:45 AM	11:30 AM	45 min	Preparing Example Data
11:30 AM	12:00 PM	30 min	Exploratory Data Review
12:00 PM	1:00 PM	1 hr	Lunch
1:00 PM	1:15 PM	15 min	Intro to R Functions
1:15 PM	2:00 PM	45 min	Plotting Calibration Curves
2:00 PM	2:30 PM	30 min	Reproducing Skyline Tutorial Plots
2:30 PM	3:00 PM	30 min	Coffee Break
3:00 PM	4:00 PM	1 hr	Multiple Calibration Curves
4:00 PM	4:30 PM	30 min	Wrap-up & Next Steps
4:30 PM	5:00 PM	30 hr	General Questions, Office Hours

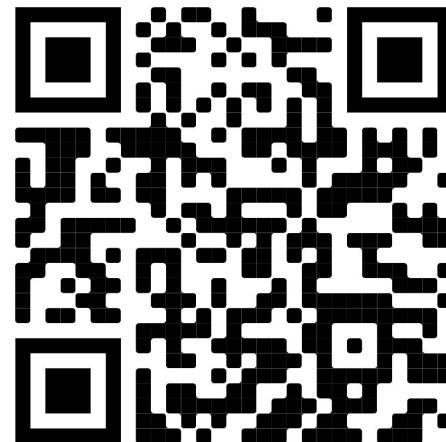
Logistics

- Feel free to ask questions any time, or grab us at breaks
- As the presenter is presenting, the other team members will be circulating to help with questions or problems
- We'll save the end section of each day for practice exercises and to help with specific questions you might have
- We'll provide ways to follow-up with us after the course in case your questions aren't answered during the course, or you have new ones afterwards

Logistics

- Course materials (slides, code, additional info) are on GitHub

<https://github.com/ZenBrayn/asms-2022-r-shortcourse>





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Getting Set-up: Installing R & RStudio

SHORT COURSES

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Overview: Installing R & RStudio

1. Install R: <https://www.r-project.org/>
 - a. Installers available for Windows, Mac, Linux
 - b. (optional): install RTools (Windows) or XCode (Mac)
2. Install RStudio: <https://www.rstudio.com/>
 - a. RStudio Desktop, free version
3. Install R Packages

We'll cover this live during the course

What are R Packages?

- R packages wrap-up code written by others so you can use it in your own projects
- Most R packages provide new functions to deal with specific problems, e.g.
 - ggplot2: helps you make plots
 - mzR: read mass spectrometry data files
 - twitteR: access twitter data
- Packages can be written by anyone, and quality can vary widely
- There are lots of high quality packages, but also be wary of random packages you come across on the internet

Where to get R packages

- CRAN (Comprehensive R Archive Network)
 - Main (and default) repository for R packages
 - Maintainers review packages for basic structure and utility before they are approved
(is the package structured properly? can it build and load without problems?)
 - Don't assume that just because a package is on CRAN that it "does the right/correct thing"
- Bioconductor
 - Alternative R package repository for bioinformatics related packages
 - Lots of MS related packages
 - Uses a different installation procedure than CRAN
- GitHub
 - Anyone can host an R package from GitHub -- this is a Pro and a Con
 - Faster way to get your code out to others (no review or submission process)
 - Newer package versions are often on GitHub before they make it to CRAN

Notes on RTools and Command Line Tools

- Most R packages have binary versions that can be directly installed with no additional steps
- If binary versions are not available (e.g. the package is new or just been updated), it may need to be compiled before it can be installed
- RTools (Windows) and Command Line Tools (Mac) provide the necessary programs and libraries you'll need to compile packages
- But... package compilation sometimes doesn't work (for a variety of reasons) and can be frustrating!
- In general, stick with using binary packages

RStudio Cloud - cloud hosted RStudio in a browser

- A cloud hosted version of RStudio, runs in a web browser
 - Same RStudio interface
 - Can run on any device with a modern web browser
- Sign-up for a free account at: <https://rstudio.cloud/>
 - 25 hrs/month
 - Paid plans with more CPU hours available
- We'll use this as a back-up if anyone has issues getting set-up on their own computer



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Introduction to R and RStudio

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June 4 - 5

ASMS 2022: R Short Course

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Goals for this module

- Find out where to download R and RStudio
- Become familiar with the RStudio layout
- Learn how to execute lines of code in RStudio from the editor or the console
- Learn about projects and code organization

Why use R to analyze your data?

- Current software solutions do not do exactly what you would like
- Reproducibility
- Control over all aspects of the analysis

Why RStudio?

- Built for purpose R IDE
(interactive development environment)
 1. Great for interactive data reading, analysis and plotting
 2. Can help you organize your project and workflow
 3. Also great for developing advanced R programs and packages



<https://www.r-project.org/>



<https://rstudio.com/>

Download and installation

- **Download and install R**

- The engine of the R language
- <https://www.r-project.org/>



<https://www.r-project.org/>

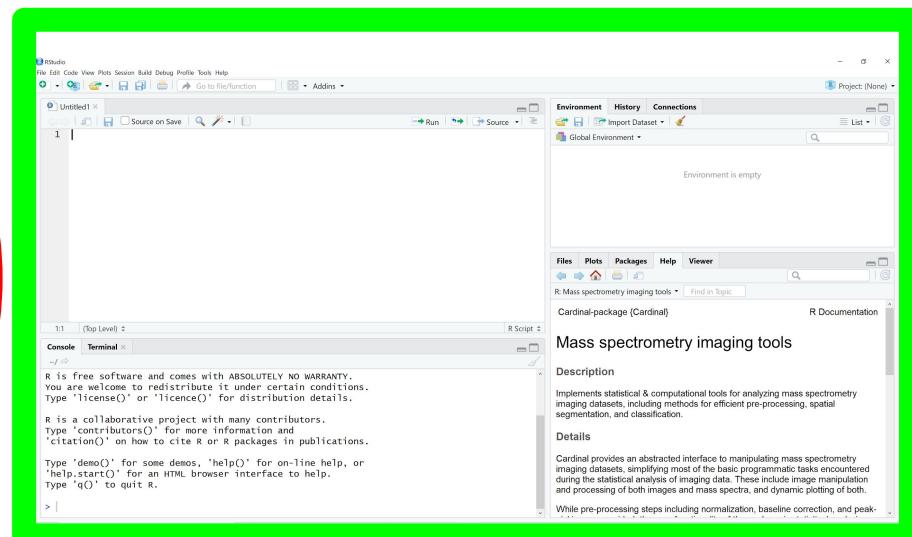
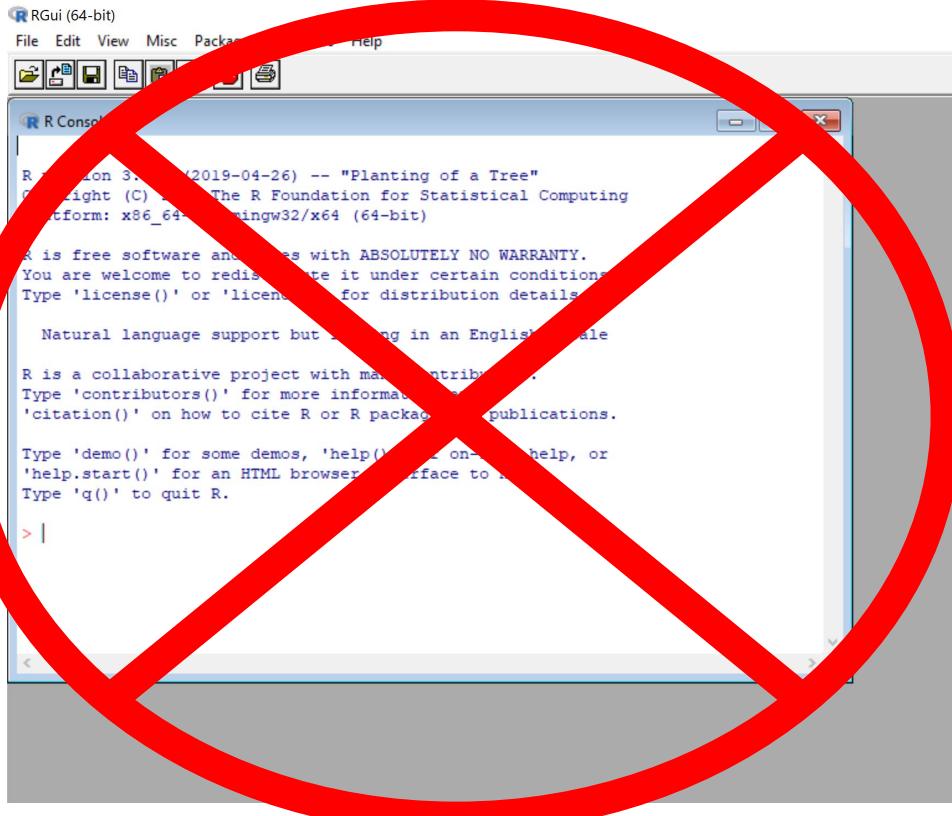
- **Download RStudio**

- The best solution to editing, managing, and running your code
- <https://rstudio.com/>

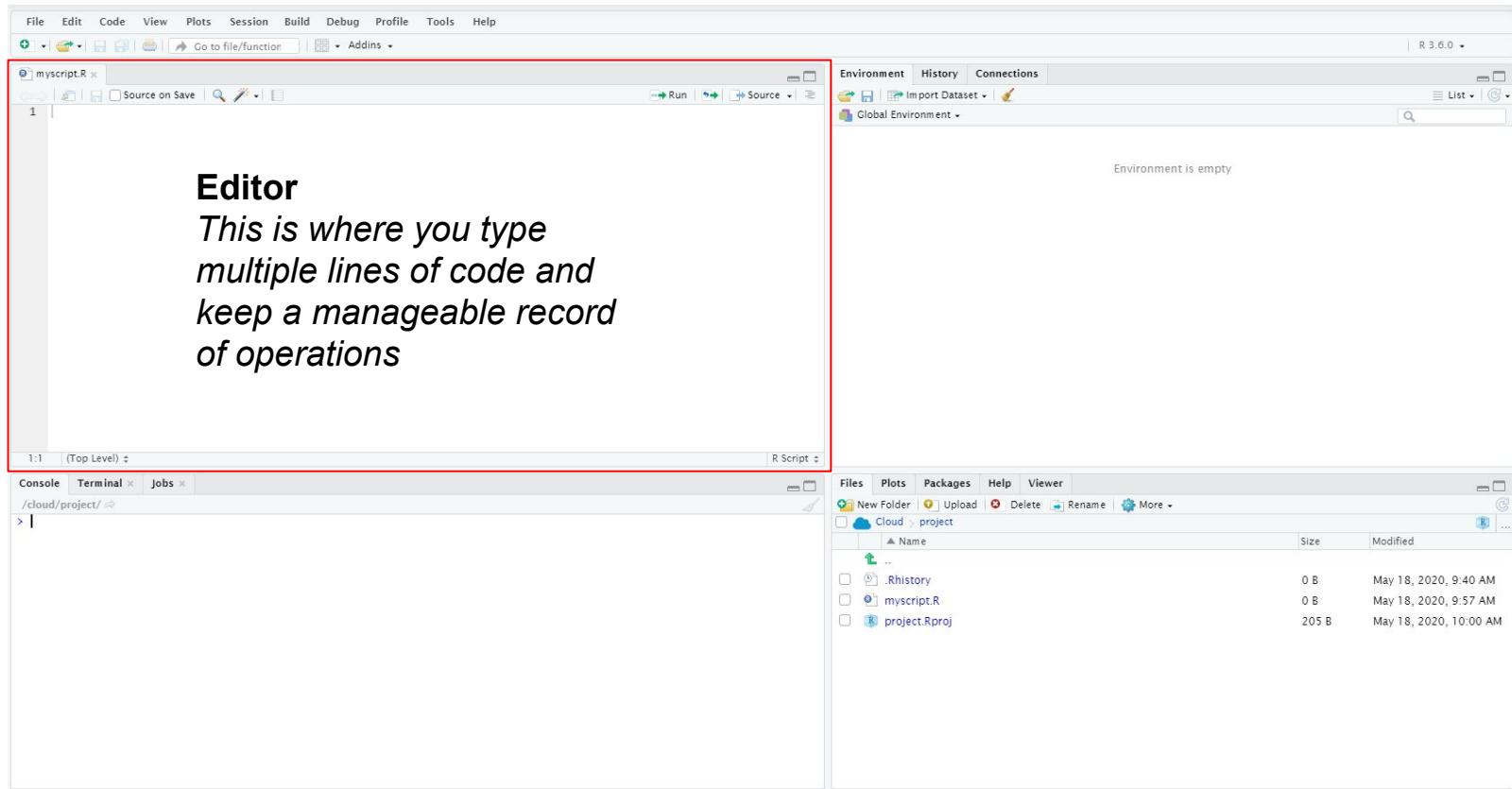


<https://rstudio.com/>

Opening R vs. opening RStudio IDE



The RStudio pane layout



The RStudio pane layout

The screenshot shows the RStudio interface with the following layout:

- Editor pane (top-left):** Contains a script editor window titled "myscript.R".
- Environment pane (top-right):** Shows the Global Environment with the message "Environment is empty".
- Cloud Project browser pane (bottom-right):** Displays a file tree for a project named "project" in a cloud storage location. The tree includes ".Rhistory", "myscript.R", and "project.Rproj".
- Terminal pane (bottom-left):** Contains the text:

Console area
*This is where lines of code
will be run from the editor
You can also run code here*

*Also gives access to the
computer's terminal*

The RStudio pane layout

The screenshot displays the RStudio interface with several panes:

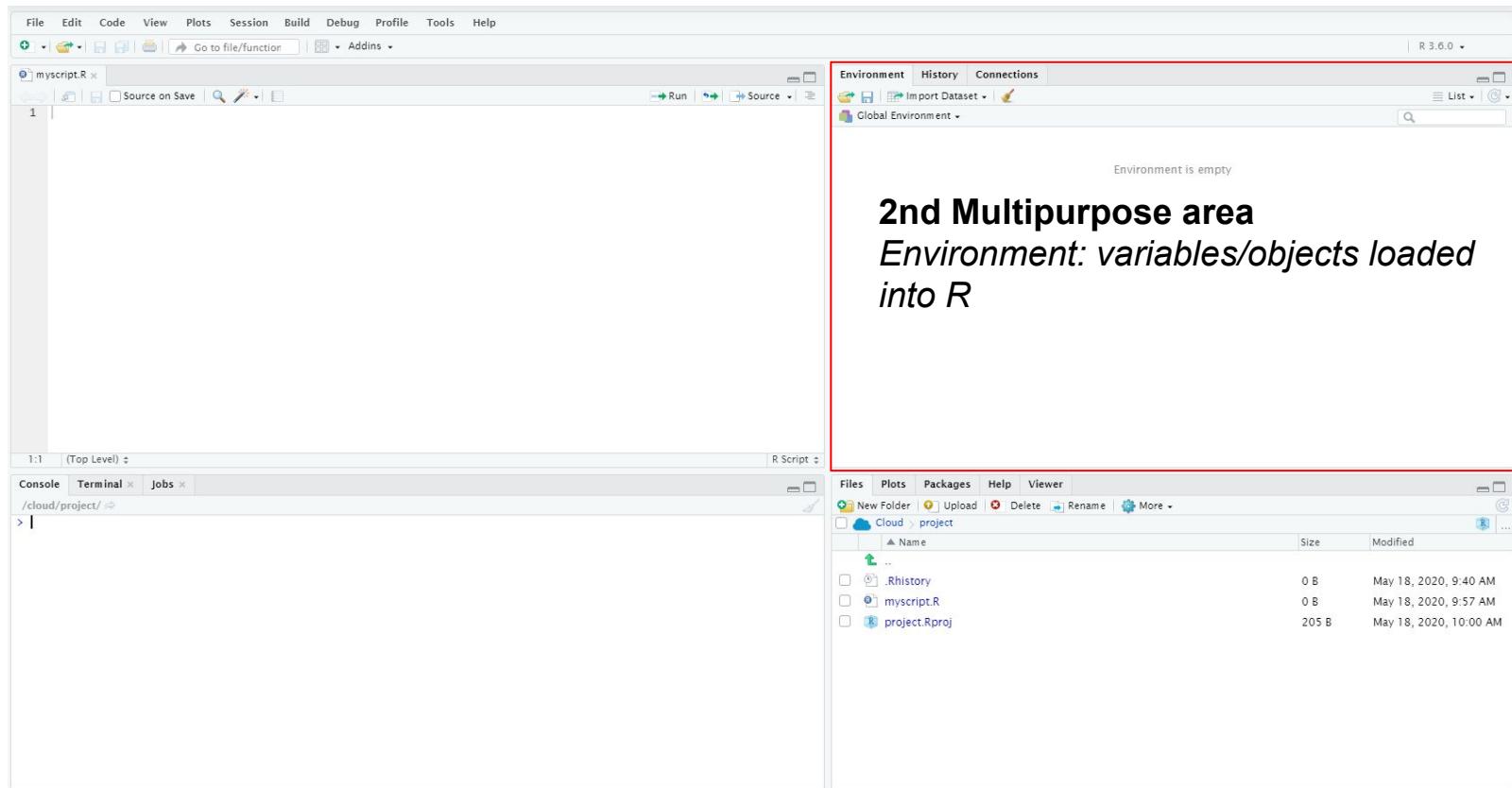
- Top Left Pane (Code Editor):** Shows a file named "myscript.R" with one line of code: "1".
- Top Right Pane (Environment):** Shows the Global Environment tab with the message "Environment is empty".
- Bottom Left Pane (Console):** Shows the command "/cloud/project/" followed by a prompt ">".
- Bottom Right Pane (Files/Plots multipurpose area):** A red box highlights this pane, which contains a file browser for the project directory. The contents are:

Name	Size	Modified
.Rhistory	0 B	May 18, 2020, 9:40 AM
myscript.R	0 B	May 18, 2020, 9:57 AM
project.Rproj	205 B	May 18, 2020, 10:00 AM

Text overlay:

Files/plots multipurpose area
File explorer, plots, help are displayed here

The RStudio pane layout



Running lines of code in RStudio

- **Run from the editor (*recommended*)**

1. Type in the code in the top-left pane

```
print("Hello world from the editor!")
```

2. Put editor cursor anywhere on that line
3. Press **Ctrl/CMD+Enter**.
4. Multiple lines: highlight multiple lines then press **Ctrl/CMD+Enter**

- **Run from the console (*occasionally*)**

1. Type code into console after the '**>**'

```
print("Hello world from the console!")
```

2. Press **Enter**.
3. Multiple lines, not advised, but copy and paste multiple lines into console then press **Enter**.

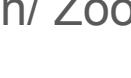
Important things to know...

The screenshot shows the RStudio IDE interface. The main area displays an R script with numbered lines from 1 to 11. The code includes comments, strings, numbers, and logical values. The RStudio toolbar at the top features icons for back, forward, save, search, and run. The status bar at the bottom indicates the current file is 'R Script'.

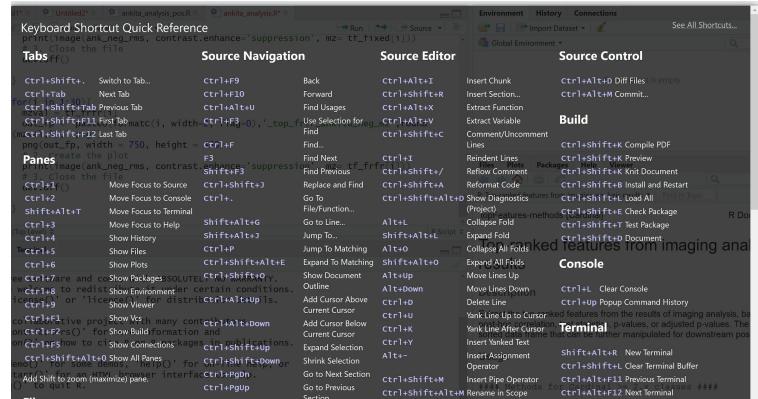
```
1 # this is a comment
2
3 "R formatted text"
4
5 # a number
6 2
7
8 # TRUE/FALSE
9 TRUE
10 FALSE
11 |
```

11:1 (Top Level) R Script

Getting RStudio the way you like...

- Set Theme: Tools → Global options → Appearance
 - Text size (on local RStudio): View → Zoom in/ Zoom out
 - Keyboard shortcut cheat sheet: alt+shift+k

The screenshot shows a portion of the RStudio keyboard shortcut guide. The title is "Keyboard Shortcut Quick Reference". Under the "Tabs" section, it lists several keyboard shortcuts for navigating tabs, such as Ctrl+Shift+T for Switch to Tab, Ctrl+Tab for Next Tab, and Ctrl+Shift+F13 for First Tab. The "Source" tab is selected at the top right.



RStudio Cheat Sheet

Setting up your working directory (where files will go when you save, by default)

- This determines the default output for where files will go
 - `getwd() # print the current working directory`
 - `setwd("/directory") # file path to the where you'd like the working directory to be`
- Acceptable file path formatting:
 - iOS/Linux/Windows : “/data/myfolder/”
 - Windows: “C:\\data\\myfolder\\”
- **WARNING:** Windows style file paths with “\” separating directories will not work in R!
- Unacceptable file path formatting:
 - Windows: “C:\\data\\myfolder\\”

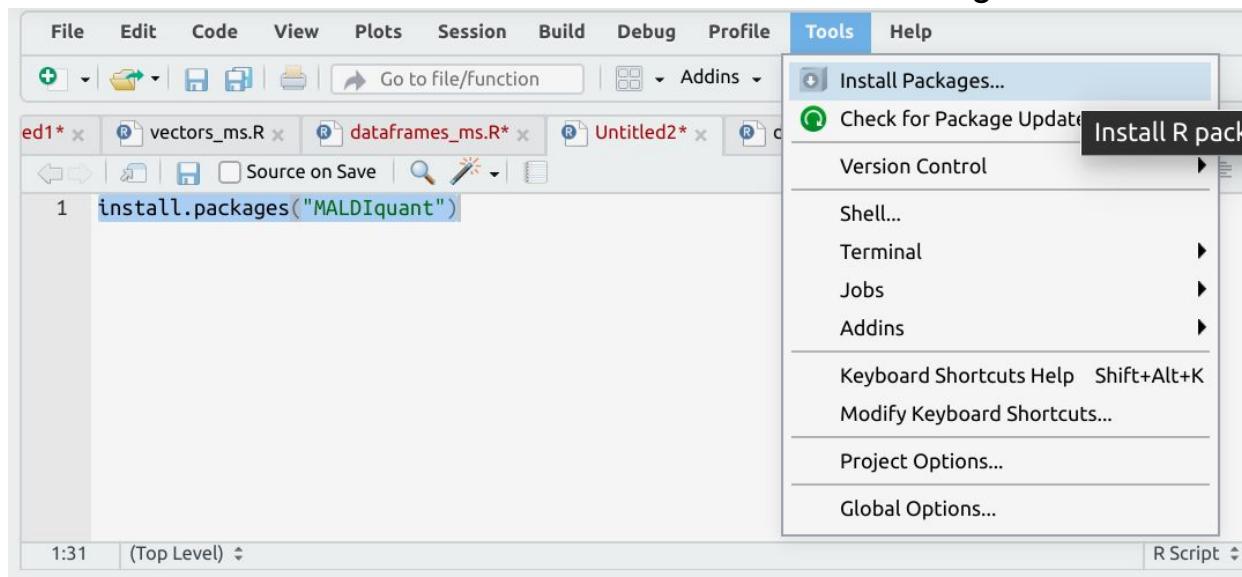
R packages: “fundamental unit of shareable code”

- Most packages are stored and downloaded from CRAN
(Comprehensive R Archive Network)

From Editor/Console

```
install.packages("MALDIquant")
```

From RStudio Tools → Install Packages...



R packages: loading/using installed packages

- When you load a package, all of its functionality is available without explicit reference to the package...
- Example: `library(MALDIquant)` RStudio will auto-complete functions in MALDIquant

```
3 library(MALDIquant)
4
5 align
6 alignSpectra {MALDIquant}
```

alignSpectra(spectra, halfWindowSize = 20, noiseMethod = "MAD",
 SNR = 2, reference, tolerance = 0.002, warpingMethod =
 "lowess", allowNoMatches = FALSE, emptyNoMatches = FALSE,
 ...)

This function aligns a list of MassSpectrum objects (spectra alignment is also known as *warping/phase correction*).

Managing your R code with RStudio Projects

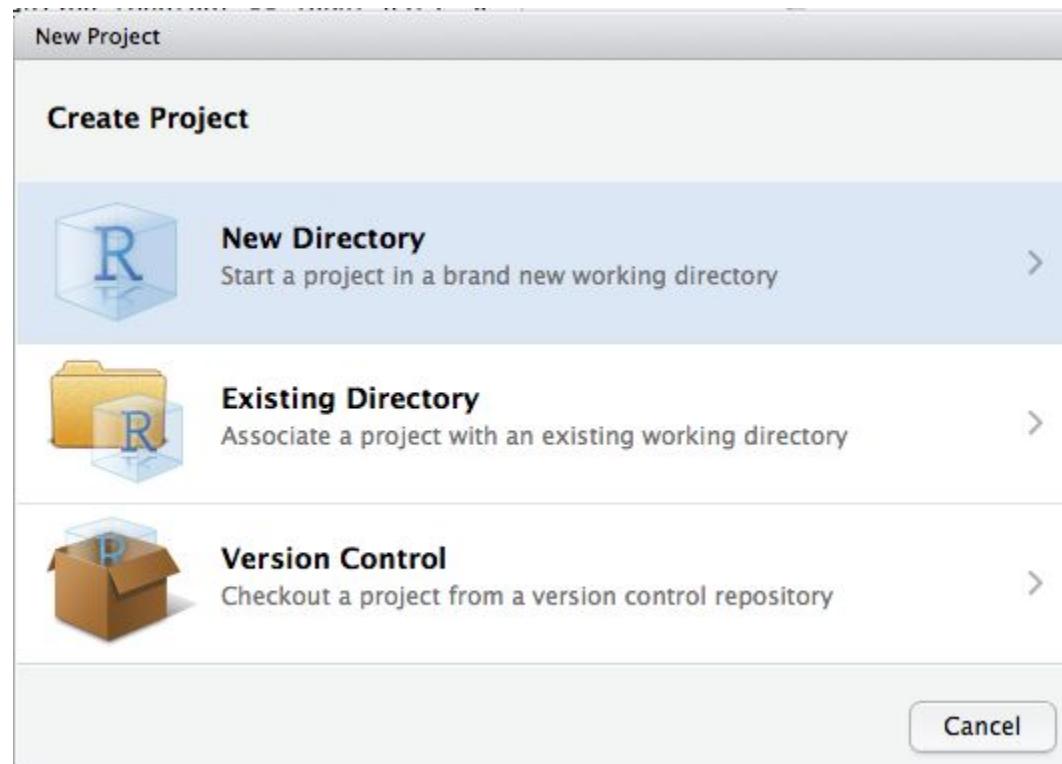
- Projects are highly recommended as they aid to organize and store your R scripts and data
- Starting a project *File* → *New project...* → *New directory* → *New project* then name the project and a directory will be created and RStudio will start working from this directory
- **Tip:** In a project you may want separate subfolders and plan to have a structure to all of the data

Managing your R code with RStudio Projects

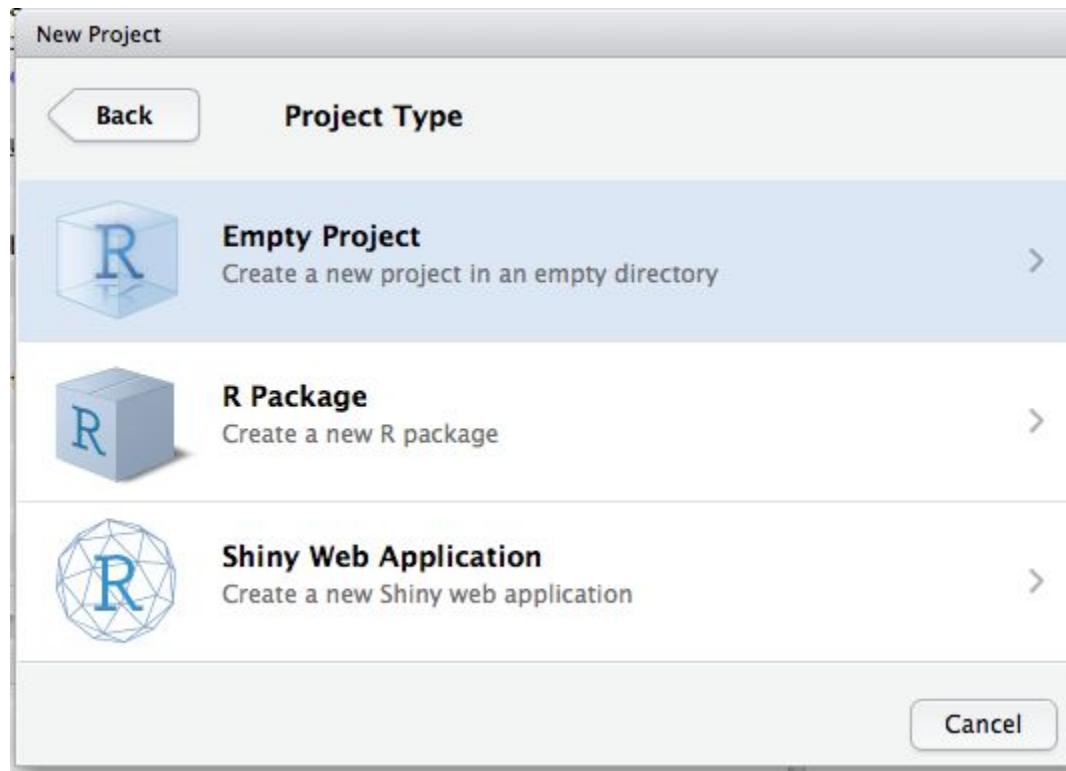
1. Create a new RStudio Project
2. Assemble the required input data & info you need, put them inside the project directory*
3. Write analysis scripts that do the work; consider naming them with a numeric prefix (e.g. 01_..., 02_...) indicating the order they should be executed in
4. Write, test, write test, write, test...
5. Double click the .Rproj file when you want to get back to work

* can depend on how you store data (e.g. networked storage)

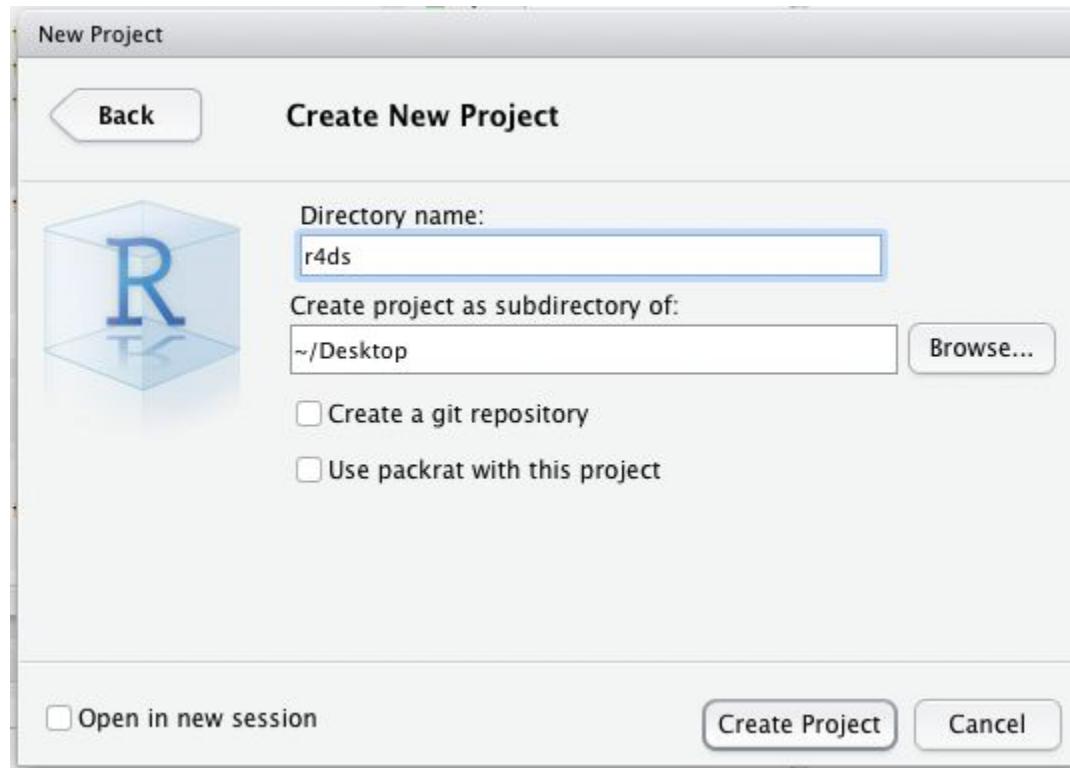
Setting up a project in RStudio



Setting up a project in RStudio



Setting up a project in RStudio



Basics: R as a calculator

- Certain symbols, called operators, do math in R

```
# Addition  
10 + 2  
  
# Subtraction  
10 - 2  
  
# Multiplication  
10 * 2  
  
# Division  
10 / 2  
  
#Exponential  
10 ^ 2
```

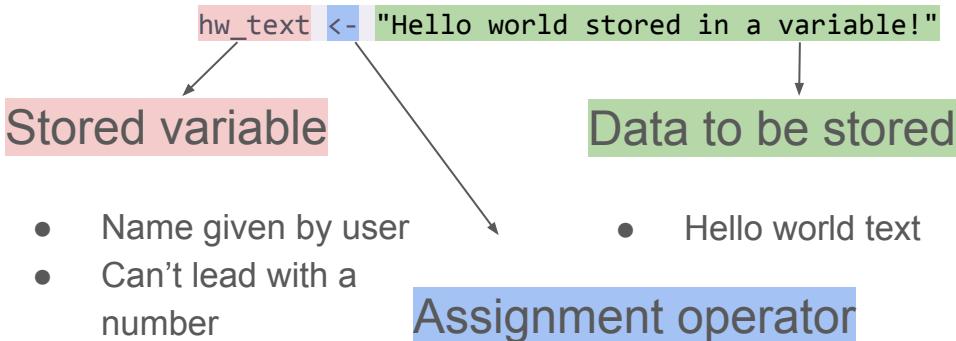


```
# Addition  
10 + 2  
[1] 12  
  
# Subtraction  
10 - 2  
[1] 8  
  
# Multiplication  
10 * 2  
[1] 20  
  
# Division  
10 / 2  
[1] 5  
  
#Exponential  
10 ^ 2  
[1] 100
```

Defining a variable

- **Define and use a variable**

1. Type in and run code in the editor



- Name given by user
- Can't lead with a number

- Hello world text

Assignment operator

- Assigns text to object,
can also be `=`

2. Run previous print function on variable

```
print(hw_text)
```



Where to get help when you are stuck...a primer

- *First and foremost...don't worry...*a lot or most of the questions you have that are specific to the R programming language or it's packages have been answered.
- The most important part of getting help is asking the right question... This is why it is important to understand the basics we will overview in the next two sections as well as the terms.
- Once you have these in mind, you can google your issue!

Getting help: [RStudio Community](#)

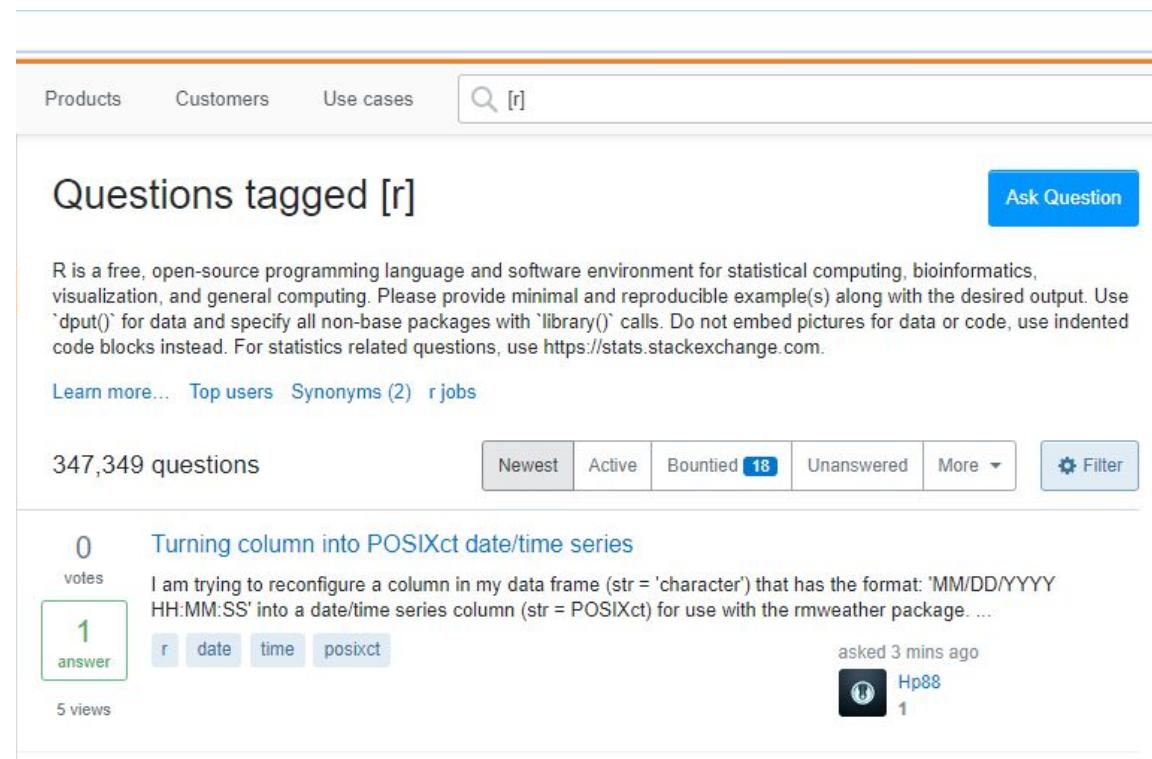
- RStudio community is forum with many many users and questions answered, it is especially friendly to new users

The screenshot shows the RStudio Community forum homepage. At the top, there's a navigation bar with links for "Sign Up", "Log In", and a search icon. Below the header, a blue banner announces the "Public RStudio Package Manager". The main content area has a light blue header with buttons for "all categories", "all tags", "Latest Activity", "Categories", and "Top". A table lists 15 recent posts, each with a thumbnail, title, tags, and engagement metrics (Replies, Views, Activity). The posts cover various topics like package management, RStudio IDE issues, and general R programming.

Topic	Replies	Views	Activity
Welcome to the RStudio Community!	0	10.5K	2018-07-22
Creation of a chronological series with the * ts () * function	0	1	4m
Using filter() with across() to keep all rows of a data frame that include a missing value for any variable	3	77	14m
PCRE Pattern Compilation Error	0	12	15m
Problems importing dataset	15	70	25m
How to match patterns between different datasets.	2	30	34m
Mac cannot install any package requires compilation ('stdio.h' file not found)	1	24	1h
pkgdown and pre-compiled html articles	4	87	1h
saving gmail attachments	0	33	2h
RStudio v1.3.1004-1 Preview: Cannot Insert Tilde	0	12	2h
Problem: rstudio-server installed in ubuntu20.04	0	25	3h
Using haven to label data for STATA: Error: If any elements of `data` are named, all must be named	1	50	3h
Clarification of using models	17	142	3h

Getting help: >347,000 R questions on '[R](#)' stackoverflow.com

- Stackoverflow.com, more extensive but possibly less friendly to newcomers



The screenshot shows the 'Questions tagged [r]' page on Stack Overflow. At the top, there are navigation links for 'Products', 'Customers', and 'Use cases', followed by a search bar containing '[r]'. A blue 'Ask Question' button is located on the right. Below the header, the title 'Questions tagged [r]' is displayed, along with a brief instruction about asking R-related questions. There are links for 'Learn more...', 'Top users', 'Synonyms (2)', and 'r jobs'. The main statistics are shown as '347,349 questions'. Below this, a specific question is listed: 'Turning column into POSIXct date/time series'. The question has 0 votes and 1 answer. The answer was posted 3 mins ago by user Hp88, who has 1 reputation. The question is tagged with 'r', 'date', 'time', and 'posixct'.

Products Customers Use cases Ask Question

Questions tagged [r]

R is a free, open-source programming language and software environment for statistical computing, bioinformatics, visualization, and general computing. Please provide minimal and reproducible example(s) along with the desired output. Use `dput()` for data and specify all non-base packages with `library()` calls. Do not embed pictures for data or code, use indented code blocks instead. For statistics related questions, use <https://stats.stackexchange.com>.

Learn more... Top users Synonyms (2) r jobs

347,349 questions

Newest Active Bountied 18 Unanswered More Filter

0 votes 1 answer 5 views asked 3 mins ago by  Hp88 1

Turning column into POSIXct date/time series

I am trying to reconfigure a column in my data frame (str = 'character') that has the format: 'MM/DD/YYYY HH:MM:SS' into a date/time series column (str = POSIXct) for use with the rmweather package. ...

r date time posixct

Helpful RStudio tips: stopping code execution

Situation: I've made a mistake in my code but I have already started executing it

Solution: Use the stop button



This will stop the execution.

Warning: sometimes this will require a restart of the R console

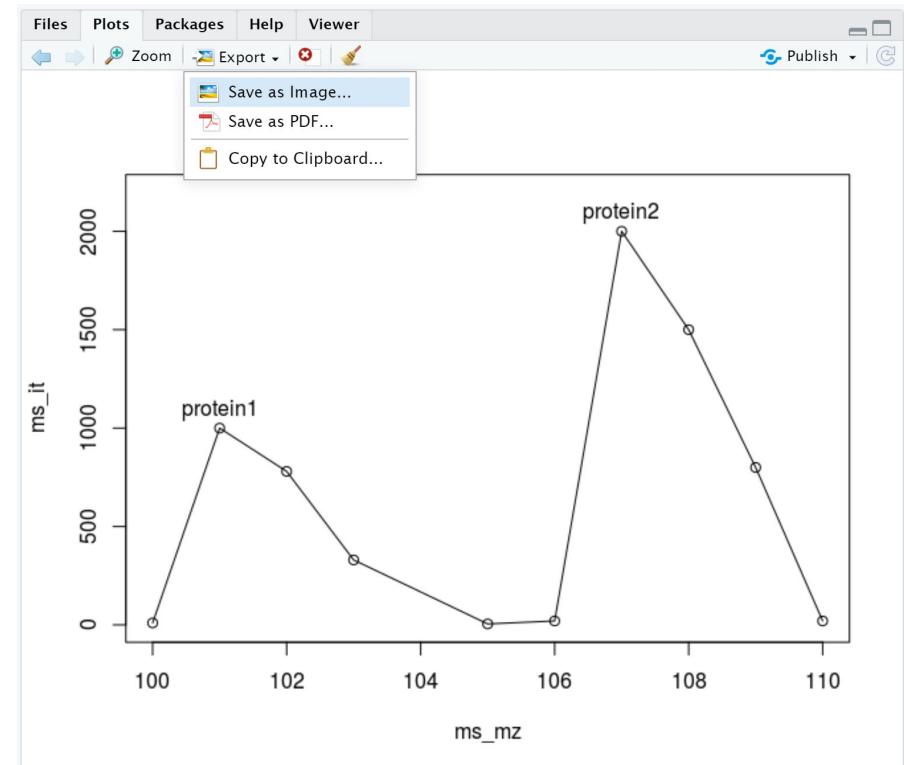
Helpful RStudio tips: exporting plots

Situation: Need high quality figure for publication

Solution: Use the Plot pane's *Export* button

You will have options to export as PDF, image files, vector graphics, etc.

Tip: Check journal specifications on figures and export them at EXACTLY the right size/resolution and you may mitigate submission issues! (maybe, definitely maybe, no guarantees...)





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Basic R data structures

SHORT COURSES

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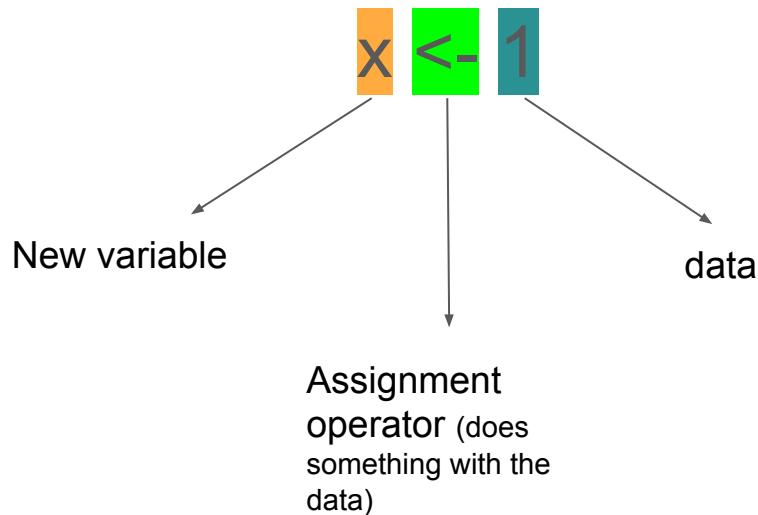
ASMS 2022: R Short Course

#ASMS2022

Goals for this module

- Learn fundamentals of R
 - variable assignment
 - reading in tabular data
 - data.frames
 - vectors
 - subsetting/filtering
- Learn why these data structures are so useful and how they permeate more advanced R functionality in the tidyverse

Adding variables in R



- Simple concept but is very important, without assignment the actions the code performs are not **SAVED**
- Not just for saving bits of data like numbers, but also complex data structures from analyses, plots, etc. Anything that creates an **R object**

Reading in tabular data example

```
peak_data <- read.csv("bacteria-peak-data.csv")
```

New variable
containing data from
what is read with `read.csv`

Assignment operator
taking what is
returned by `read.csv`
and putting it in
“peak_data”

Function that takes a file
“high-res-peak-data.csv”,
reads it, and creates a
data.frame

data.frames : accessing variables

- In the previous example we saw the '\$' operator, this allows us to access data.frame columns by name
- You may not always need to subset, you may be after a piece of information from a single column in your data.frame

```
# print highest m/z value in peak data
max(peak_data$mz)
# or get m/z range
range(peak_data$mz)
```

Working with vectors : data.frames are organized vectors!

- Multiplying a vector by a scalar multiples all elements in a vector by the scalar
- Some basic math on vectors, some examples

```
# multiply FWHM values by 1.3, expanding window
peak_data$fhwm * 1.3
```

- Vector - Vector interaction

```
# adding two vectors
# vectors are operated on element by element
# make sure they are the same length!
peak_data$mz + peak_data$fhwm
peak_data$mz * mass_error
```

```
# common math functions
length(peak_data$mz)
min(peak_data$snr)
max(peak_data$snr)
mean(peak_data$snr)
sd(peak_data$snr)
```

- Modifying vectors

```
# index vector and replace values
peak_data$fhwm * 1.3
peak_data$fhwm <- peak_data$fhwm * 1.3
peak_data$fhwm_expanded <- peak_data$fhwm * 1.3
```

Working with vectors : subsetting and indexing

R indexing starts at 1, not 0 like many other languages

- Index with integer

```
# simple indexing  
# grabs first m/z value  
mzs[1]  
  
[1] 100
```

- Subset indexing

```
# subset indexing  
# grabs first five m/z values  
# ':' operator  
mzs[1:5]
```

- Conditional indexing

```
# indexing based on a condition  
mzs_above_103 <- mzs > 103  
  
# print indexed mzs as sanity check  
mzs[mzs_above_103]
```

- Non-continuous indexing

```
# indexing odd-indexed m/z using integer  
vector  
mzs[c(1,3,5,7,9)]
```

data.frame subsetting: indexing with integer index

R indexing starts at 1, not 0 like many other languages

- The index is the **address** of the data
- data.frames are indexed using [] with [row index, col index]

```
peak_data[2,]
```

- Above get the 2nd row, and all the columns. Leaving an index area blank gets all of the values

```
peak_data[1:10,3]
```

- Above get the first 2 rows (using ':'), and all the columns, the ':' operator creates a sequence between the two numbers, i.e., 1:5 creates [1,2,3,4,5]

data.frame subsetting: conditional indexing

- This uses the advantage that multiple vectors are linked in the data table and indexing by a condition based on one vector slices all the rest the same way

```
# conditional indexing  
peak_data[peak_data$mz > 650, ]
```

	peak_index	mz	mass_resolution	snr	intensity	base_peak_ratio	fwhm
1523	1523	650.2489	13766	12.6	181	0.1	0.0472
1524	1524	650.2932	14641	12.4	178	0.1	0.0444
1525	1525	650.3727	14642	9.2	132	0.1	0.0444
1526	1526	650.4107	24887	15.9	228	0.2	0.0261
1527	1527	651.2916	9714	14.9	216	0.2	0.0670
1528	1528	651.3520	17247	14.8	215	0.2	0.0378

- One operation to slice the data.frame, while keeping all adjoined information

Data types for vectors

- *numeric* : `c(1.1, 2.1, 3.1)` # no quotes must be a number
- *integer* : `c(1,2,3,4)` # numeric but all numbers are WHOLE numbers
- *character* : `c("a", "b", "c", "d")` # always surrounded by QUOTES
- *logical* : `c(TRUE, FALSE, TRUE)` # boolean logic, T/TRUE, F/FALSE
- *factors* : nominal variable (can be any type) that can be used for sorting

data.frames/vectors : more conditional operators!

- `>`, `<`, `>=` and `<=` (see previous slides), compares numerical values
- Exact search: `==`

```
vec_data <- c("p1","p1","p2","p2","p4","p4")
p2_pro <- vec_data == "p2"
```
- Exact NOT search: `!=`

```
not_p2_pro <- vec_data != "p2"
```
- Condition multiple values: `%in%` → `p1p4_pro <- vec_data %in% c("p1","p2")`

data.frames : add a variable using \$

- Let's imagine we had a new piece of information from a second source or from an analysis. We may want to append it as a new column...

```
# adding a variable (Length should match number of rows)
peak_data$background <- c(TRUE, FALSE, FALSE, FALSE, TRUE, ...)
```

- We can assigned a new column to the data.frame simply by using the \$ at the end of the object name and adding a new vector
- N.B.:* The length of the new column must match the dimension of the data.frame

Data.frame subsetting exercise: make a mass defect filter!

- **Background:** In MALDI-MS, many matrix peaks are detected simultaneously with biologically relevant peaks due to the lack of separation. However, in some examples, like in phospholipid analysis, lipids don't have unusual mass defects
- Peak at m/z 734.5534 – mass defect is 0.5534
- **TASK:** Find mass defect for all peaks in `peak_data`, add it to data.frame, then filter to find peaks with a mass defect between 0.4 and 0.7, find number of peaks with this

data.frames conclusion

- These structures are very critical and when we discuss the tidyverse you will see how they can be streamlined and manipulated for analysis
- The **tibble** is the data.frame analogue in the *tidyverse* and has all the same features of the data.frame and more: different printing, subtly different subsetting, and easily embedding lists as columns in tibble

Additional resources (some are more advanced)

- [Data structures](#)
- [Data Structures | Introduction to R](#)
- [6 Inbuilt Data Structures in R with practical examples](#)

data.frames : organizing vectors into tables

- In this example, we create psuedo processed protein dataset where we have protein IDs and some values statistics associated
- Let's put all these vectors into a data.frame which is a table view of all this information that enables better analysis through

```
# as vectors
proteins <- c("protein1", "protein2", "protein3", "protein4", "protein5")
retention_times <- c(10.2, 15.2, 12.2, 9.1, 17.3)
sum_ms1_intensities <- c(20000, 50000, 1000, 2000, 30000)
n_ms2_transitions <- c(2L, 4L, 3L, 1L, 1L)
fdr <- c(0.11, 0.03, 0.02, 0.15, 0.06)
seq_coverage <- c(0.63, 0.65, 0.55, 0.90, 0.82)
in_ds2 <- c(TRUE, TRUE, FALSE, FALSE, TRUE)
```

```
# write a data.frame from vectors
protein_id_df <-
data.frame(proteins=c("protein1", "protein2", "protein3", "protein4",
", "protein5"),
retention_times = c(10.2, 15.2, 12.2, 9.1, 17.3),
sum_ms1_intensities = c(20000, 50000, 1000, 2000, 30000),
n_ms2_transitions = c(2L, 4L, 3L, 1L, 1L),
fdr = c(0.11, 0.03, 0.02, 0.15, 0.06),
seq_coverage = c(0.63, 0.65, 0.55, 0.90, 0.82),
in_ds2 <- c(TRUE, TRUE, FALSE, FALSE, TRUE))
```

data.frames : conditional indexing

- Let's do that same thing with vectors

```
# with vectors
low_fdr_idx <- fdr < 0.05

proteins[low_fdr_idx]
retention_time[low_fdr_idx]
sum_ms1_intensities[low_fdr_idx]
n_ms2_transitions[low_fdr_idx]
fdr[low_fdr_idx]
seq_coverage[low_fdr_idx]
in_ds2[low_fdr_idx]
```

- Interact with 1 object vs interacting with 7 objects. Now imagine you have a data.frame with 100 or even 1000 columns

data.frames : add a variable using cbind

```
# new variables (cols) to add
pathway_result <- data.frame(pathway = c("apoptosis","immune response","regulation","immune
response","apoptosis"),
                               database = c("in-house","in-house","in-house","reactome","reactome"))

cbind(protein_id_df, pathway_result)
```

```
> cbind(protein_id_df, pathway_result)
   proteins retention_times sum_ms1_intensities n_ms2_transitions   fdr seq_coverage in_ds2      pathway database
1 protein1          10.2              20000                2 0.11        0.63    TRUE apoptosis in-house
2 protein2          15.2              50000                4 0.03        0.65    TRUE immune response in-house
3 protein3          12.2               1000                3 0.02        0.55   FALSE regulation in-house
4 protein4           9.1               2000                1 0.15        0.90   FALSE immune response reactome
5 protein5          17.3              30000                1 0.06        0.82    TRUE apoptosis reactome
```

data.frames : add a new observation (row) with rbind

```
# new variables (cols) to add
protein6_df <- data.frame(proteins = "protein6",
                           retention_times = 15.1,
                           sum_ms1_intensities = 20000,
                           n_ms2_transitions = 4,
                           fdr = 0.01,
                           seq_coverage = 0.22,
                           in_ds2 = FALSE,
                           pathway = "regulation",
                           database = "reactome")

rbind(protein_id_df_pw, protein6_df)
```

	proteins	retention_times	sum_ms1_intensities	n_ms2_transitions	fdr	seq_coverage	in_ds2	pathway	database
1	protein1	10.2	20000	2	0.11	0.63	TRUE	apoptosis	in-house
2	protein2	15.2	50000	4	0.03	0.65	TRUE	immune response	in-house
3	protein3	12.2	1000	3	0.02	0.55	FALSE	regulation	in-house
4	protein4	9.1	2000	1	0.15	0.90	FALSE	immune response	reactome
5	protein5	17.3	30000	1	0.06	0.82	TRUE	apoptosis	reactome
6	protein6	15.1	20000	4	0.01	0.22	FALSE	regulation	reactome



70th Conference on Mass Spectrometry and Allied topics

JUNE 5 - 9, 2022
Minneapolis, Minnesota, USA

Reading Data Files into R

SHORT COURSES

June 4 - 5

ASMS 2022: R Short Course

#ASMS2022

Goals for this module

- Learn how to read data files into R
 - .csv
 - Excel
- Practice with file paths and how RStudio projects help
- Important things to keep in mind when working with .csv files

Getting data into R

- Before you can work with a data set, you need to get it into your R session
- R can handle a large variety of file formats, including
 - Formatted text files (e.g. .csv, .tsv)
 - Most standard open formats (e.g. web formats, json, markup formats)
 - Open and some proprietary binary formats
 - Open and some MS data formats (e.g. mzML)
- You can read data into R using “reader” functions
- Formatted text files and Excel are workhorse formats, will focus on them here

Reading formatted text files

- R has several built-in functions for reading text files
 - `read.csv` - comma separated files
 - `read.delim` - tab separated files
 - `read.fwf` - fixed width column files
- The `readr` package (part of the `tidyverse`) has similar functions, but take a more modern approach
 - `read_csv` - comma separated files
 - `read_delim` - tab separated files
 - `read_fwf` - fixed width column files

Example: reading a .csv file

```
# load the tidyverse package  
# will also load the readr package  
library(tidyverse)  
  
# Read an example data file  
# and store it in a variable  
dat <- read_csv("example_data.csv")
```

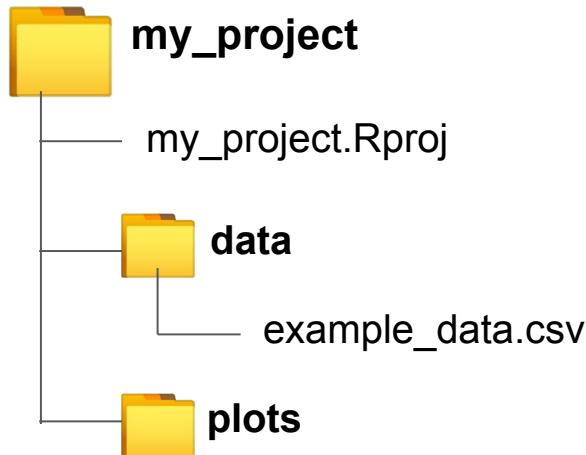


example.csv needs to be in your R working directory

If you're using an RStudio project, example.csv should be in the (main) project directory

For RStudio projects, file paths start at the base directory

Project Directory Structure



R Code

```
read_csv("data/example_data.csv")
```

This is a relative file path to example.csv,
relative to where it exists in the project directory

csv Files: important things to keep in mind

- The first row should be the header row
 - Lists the names of the columns
 - Can contain spaces in the name, but better if not
- Following rows contain the data, each value separated by a column
- Values can contain commas if the entire value is quoted
- The number of values in each row must be the same and match the number of values in the header row

*Deviations from the above can result in errors when trying to read a file
If you run into problems, you can open the file in a text editor and diagnose*

Reading data from Excel files

- Reading data from Excel files is very common, but a bit more complex due to the additional flexibility Excel provides
 - Data tables can coexist with other data tables, free text, plots, etc.
 - A single Excel file can contain multiple sheets
- Need to be aware of 3 main items
 - Name of the Excel file (and it's file path)
 - Name of the Sheet
 - Cell range of the data table you want to read

Example: reading data from an Excel file

The screenshot shows a Microsoft Excel window with the title bar "example_data". The ribbon menu is visible with tabs like Home, Insert, Draw, Page Layout, Formulas, Data, Review, View, and Tell me. The Home tab is selected. The main area displays a table of data. Row 1 contains column headers: "file_name", "ms_instr", and 10 columns labeled "MCL_001" through "MCL_010". Rows 2 through 14 contain data points for two samples (Samp01 and Samp02) across two mass spectrometer runs (MS01 and MS02). The data includes numerical values and some missing or zero entries. The bottom of the screen shows the Excel interface with tabs for "Sheet1" and "analyte_data", and a status bar indicating "Ready" and "151%".

file_name	ms_instr	MCL_001	MCL_002	MCL_003	MCL_004	MCL_005	MCL_006	MCL_007	MCL_008	MCL_009	MCL_010
Samp01_Rep01	MS01	104.897862	192.029172	315.32509	384.047518	581.934303	637.276438	714.189301	888.715023	881.439772	962.103496
Samp01_Rep01	MS02	108.587579	203.390259	314.182573	355.503568	564.131875	664.893805	715.300169	836.354925	777.050722	986.005661
Samp01_Rep02	MS01	99.5433671	231.031288	296.347494	388.994298	463.24035	535.679354	750.745854	744.011244	911.990541	901.043255
Samp01_Rep02	MS02	100.719677	219.598041	263.613584	452.155956	448.269134	525.240096	809.353437	835.991785	967.214574	1073.21608
Samp01_Rep03	MS01	105.941549	173.23455	333.547067	423.217268	512.315598	666.16052	654.122401	812.134274	801.238611	875.901148
Samp01_Rep03	MS02	101.851924	216.039868	301.525188	426.723183	556.321497	645.508864	629.51041	728.334783	814.679329	1015.14108
Samp02_Rep01	MS01	99.3850077	218.253608	309.420985	333.011888	476.235734	528.803056	656.573972	714.155843	873.015429	873.898012
Samp02_Rep01	MS02	89.7949898	215.63495	280.673291	325.85331	422.666037	718.829874	649.890336	930.776966	942.308524	1011.18906
Samp02_Rep02	MS01	89.7064734	194.161818	327.852344	433.958994	472.180871	589.616751	683.256884	775.244775	935.863355	954.229473
Samp02_Rep02	MS02	89.7869805	173.982437	311.148771	460.797192	419.053505	506.544589	694.753717	752.92385	899.429511	1049.49375

Example: reading data from an Excel file

The screenshot shows a Microsoft Excel window titled "example_data". The ribbon menu is visible at the top, and the "Home" tab is selected. The worksheet contains the following data:

		file_name	ms_instr	MCL_001	MCL_002	MCL_003	MCL_004	MCL_005	MCL_006	MCL_007	MCL_008	MCL_009	MCL_010
1		Samp01_Rep01	MS01	104.897862	192.029172	315.32509	384.047518	581.934303	637.276438	714.189301	888.715023	881.439772	962.103496
2		Samp01_Rep01	MS02	108.587579	203.390259	314.182573	355.503568	564.131875	664.893805	715.300169	836.354925	777.050722	986.005661
3		Samp01_Rep02	MS01	99.5433671	231.031288	296.347494	388.994298	463.24035	535.679354	750.745854	744.011244	911.990541	901.043255
4		Samp01_Rep02	MS02	100.719677	219.598041	263.613584	452.155956	448.269134	525.240096	809.353437	835.991785	967.214574	1073.21608
5		Samp01_Rep03	MS01	105.941549	173.23455	333.547067	423.217268	512.315598	666.16052	654.122401	812.134274	801.238611	875.901148
6		Samp01_Rep03	MS02	101.851924	216.039868	301.525188	426.723183	556.321497	645.508864	629.51041	728.334783	814.679329	1015.14108
7		Samp02_Rep01	MS01	99.3850077	218.253608	309.420985	333.011888	476.235734	528.803056	656.573972	714.158543	873.015429	873.898012
8		Samp02_Rep01	MS02	89.7949898	215.63495	280.673291	325.85331	422.666037	718.829874	649.890336	930.776966	942.308524	1011.18906
9		Samp02_Rep02	MS01	89.7064734	194.161818	327.852344	433.958994	472.180871	589.616751	683.256884	775.244775	935.863355	954.229473
10		Samp02_Rep02	MS02	89.7869805	173.982437	311.148771	460.797192	419.053505	506.544589	694.753717	752.92385	899.429511	1049.49375

A red box highlights the data starting from row 4. A red arrow points from the text "Sheet name" to the sheet tab bar, which shows "Sheet1" and "analyte_data".

Example: reading data from an Excel file

```
# Need to load the readxl package  
library(readxl)  
  
dat <- read_excel("example_data.xlsx",  
                  sheet = "analyte_data",  
                  range = "B4:M14")
```

What do you think will happen if you don't specify the sheet and/or range?

Notes about reading data files into R

- You'll usually want to store the output as a variable
`dat <- read_csv("example_data.csv")`
- For table-like formats, the data will be read as a data frame
- If a data file is large (~100's MBs to GBs), be careful
 - It might take a (really) long time to read
 - You need to have enough RAM (data is usually read into memory)
 - R may start to have issues with files larger than several GBs

Recap

- Reading csv files
 - Load your RStudio project and make sure your data file is inside the project folder
 - Load the tidyverse package

```
library(tidyverse)
```
 - Read the file

```
dat <- read_csv("my_data.csv")
```
- Reading Excel files
 - Note the file path (RStudio project), sheet name, data range
 - Load the readxl package

```
library(readxl)
```
 - Read the file

```
dat <- read_excel("my_data.xlsx", sheet = "My Sheet",  
range = "B2:H26")
```



70th Conference on Mass Spectrometry and Allied topics

JUNE 5 - 9, 2022
Minneapolis Convention Center

Tidy Data & The Tidyverse

SHORT COURSES

June 4 - 5

ASMS 2022: R Short Course

#ASMS2022

Goals for this module

- Understand what tidy data is
 - How is it different from “messy” data?
 - What makes tidy data “tidy”?
 - Why tidy data is useful for doing data analysis in R
- Learn how to recognize messy data and why it’s hard to work with
 - Understand the things you may need to do when tidying-up messy data
 - Be able to communicate to others what tidy data is
- Learn about the tidyverse and why it’s a great ecosystem for working with data in R

Quick note about the terms “messy” & “tidy”

Messy

- Has negative connotations but that's not the intent here
- Messy data is simply data that's not yet in a form suitable for analysis
- Messy data doesn't mean bad data

Tidy

- Has positive connotations but that's not the intent here either
- Tidy data is data in a consistent format that supports the analysis process
- Tidy data doesn't mean good data

In the R ecosystem, the term “tidy data” has a very specific meaning
(that we'll get to soon)

The Anna Karenina principle...

Happy families are all alike;
every unhappy family is unhappy in its own way.

– Leo Tolstoy

... applies to data too

Tidy datasets

~~Happy families~~ are all alike;
every ~~unhappy family~~ is ~~unhappy~~ in its own way.

messy dataset *messy*

– Hadley Wickham

Messy data

Most “real world” data starts out messy...



...which makes it hard to work with.



All tidy data has similar structure...



...making it easier to work with since you know what to expect

Data can be messy in all kinds of ways

Excel spreadsheet with complex formatting

Professor Smith: Data Science Grades Sheet, 1st Trimester 2020						
University of DS, Department of Biology						
Class Date: 1/6/2020 to 3/27/2020						
Quizzes			Tests			
Name	Score 1	Score 2	Score 3	Test 1	Midterm	Final
al-Jafri, Anas	17 / 25	41 / 50	18 / 25	87 / 100	89 / 100	90 / 100
Drum, Anyssa	19 / 25	40 / 50	19 / 25	88 / 100	87 / 100	92 / 100
Gonzales, David	18 / 25	38 / 50	19 / 25	84 / 100	91 / 100	83 / 100
Granger, Shannan	14 / 25	42 / 50	20 / 25	89 / 100	82 / 100	90 / 100
Kwak, Surabhi	16 / 25	41 / 50	21 / 25	85 / 100	88 / 100	93 / 100
Michels, Breana	17 / 25	46 / 50	18 / 25	80 / 100	85 / 100	82 / 100
Reed, Tyler	19 / 25	39 / 50	17 / 25	78 / 100	94 / 100	88 / 100
Smith, Tyler	16 / 25	40 / 50	19 / 25	79 / 100	90 / 100	86 / 100
Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

Proprietary MS data formats 

Data tables in PDF (or even images!)

	John Smith	Jane Doe	Mary Johnson
treatmenta	—	16	3
treatmentb	2	11	1

Tidy Data, H. Wickham, J. Stat. Software

Badly formatted text files

1, 4, 5, 6, 10
10,000, 900, 874
5, 6, 8
7473,134187,1398,17

Data in web pages, plots & figures, ...

Messy data can be hard to work with

- Unclear structure & organization can make it hard to understand what's there
- Data might be optimized for data entry or visual consumption, not computer consumption
- Might be represented in a strange ways (e.g. numbers combined with words, unclear coding variables)
- Might be in multiple places (e.g. in different files)
- Might be in strange formats (html, pdf, png )

Messy data isn't necessarily bad data

- Not all data is created or presented with data analysis in mind
- The people who curate the data might not understand the needs of someone who needs to work with it
- The goals for the data might not align directly with data analysis needs (presenting data on a slide, performance or storage requirements)
- ... but messy data might be a sign of lurking data problems too 

Tidy data in the R ecosystem

Tidy data has consistent structure, arranged in a rectangular table

country	year	cases	population
Afghanistan	1990	45	1980701
Afghanistan	2000	2666	20595360
Brazil	1999	31737	172006362
Brazil	2000	81488	174504898
China	1999	212258	1272915272
China	2000	213766	128042583

Variables (columns)

the “things” you
are measuring

country	year	cases	population
Afghanistan	1990	45	1980701
Afghanistan	2000	2666	20595360
Brazil	1999	31737	172006362
Brazil	2000	81488	174504898
China	1999	212258	1272915272
China	2000	213766	128042583

Observations (rows)

the “things” you
are making
measurements on

country	year	cases	population
Afghanistan	1990	45	1980701
Afghanistan	2000	2666	20595360
Brazil	1999	31737	172006362
Brazil	2000	81488	174504898
China	1999	212258	1272915272
China	2000	213766	128042583

Values (cells)

the values of the
measurements

What is this table about? Variables? Observations?

Last Name	First Name	Age	Major	Graduation Year
Smith	Sally	22	Chemistry	2024
Yamamoto	Akira	24	History	2023
Snow	John	21	Business	2024

(more rows...)

What is this table about? Variables? Observations?

Table of New Students

Last Name	First Name	Age	Major	Graduation Year
Smith	Sally	22	Chemistry	2024
Yamamoto	Akira	24	History	2023
Snow	John	21	Business	2024

(more rows...)

Each **observation** is a **student**

Each **variable** is a piece of **information about the student** (name, age, etc)

Each (individual) **piece of information** is in its own **cell**

A few notes about tidy data

- Tidy data is not the only way
 - Other structures might be needed to optimize for performance or storage
 - Certain fields might follow other data conventions
 - Some types of data might not naturally fit into a rectangular table
- BUT, if your data *can* fit into rectangular structure, tidy data is usually the way to go
- Sometimes the differences between observations and variables is not always clear, and you might swap them depending on the context
- Data tidiness isn't necessarily black & white, different circumstances might require different levels of tidiness

Prof. Smith is recording class grades in a spreadsheet

Professor Smith: Data Science Grades Sheet, 1st Trimester 2020

University of DS, Department of Biology

Class Date: 1/6/2020 to 3/27/2020

Name	Quizzes			Tests		
	Score 1	Score 2	Score 3	Test 1	Midterm	Final
al-Jafri, Anas	17 / 25	41 / 50	18 / 25	87 / 100	89 / 100	90 / 100
Drum, Anyssa	19 / 25	40 / 50	19 / 25	88 / 100	87 / 100	92 / 100
Gonzales, David	18 / 25	38 / 50	19 / 25	84 / 100	91 / 100	83 / 100
Granger, Shannan	14 / 25	42 / 50	20 / 25	89 / 100	82 / 100	90 / 100
Kwak, Surabhi	16 / 25	41 / 50	21 / 25	85 / 100	88 / 100	93 / 100
Michels, Breana	17 / 25	46 / 50	18 / 25	80 / 100	85 / 100	82 / 100
Reed, Tyler	19 / 25	39 / 50	17 / 25	78 / 100	94 / 100	88 / 100
Smith, Tyler	16 / 25	40 / 50	19 / 25	79 / 100	90 / 100	86 / 100
Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

Is this data tidy?

It looks nice and
neat...

No – this data is not tidy for several reasons

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Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

The file contains free form text at the top

Some of this data might be useful but it's not immediately ready for analysis

No – this data is not tidy for several reasons

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Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

First and last names are stored together in the same cell

Might want these two pieces of information separate

No – this data is not tidy for several reasons

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Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

The main data table is not “by itself”

Can't simply read the data into R



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Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100



The “Quizzes” and “Tests” labels exist in merged columns, and link to multiple columns below them

This is visual structure, not well suited for computers

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Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

Column naming is inconsistent

All refer to a specific quiz or test, but quizzes are referred to by “Score”, tests by the type of test

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Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

Each data point for a score is actually two pieces of data:

points received / total points

Also, the data is represented as text since it contains a “/” character



No – this data is not tidy for several reasons

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Smith, Westin	15 / 25	45 / 50	17 / 25	87 / 100	85 / 100	91 / 100
Vang, Seher	19 / 25	43 / 50	19 / 25	79 / 100	82 / 100	87 / 100

Important data points are highlighted in red text

“Information by formatting” is very difficult to deal with

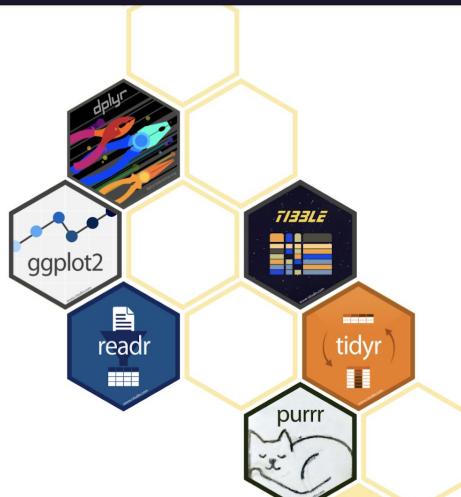


The Tidyverse

An opinionated collection of R packages for data science

Tidyverse

Packages Blog Learn Help Contribute



R packages for data science

The tidyverse is an opinionated collection of R packages designed for data science. All packages share an underlying design philosophy, grammar, and data structures.

Install the complete tidyverse with:

```
install.packages("tidyverse")
```

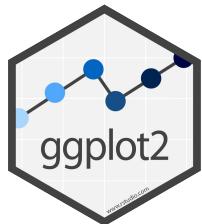
<https://www.tidyverse.org>

Once you know the general structure of the input data (i.e. tidy data), you can build all kinds of tools to work with it

That's the tidyverse!

The tidyverse covers the fundamental components of the data analysis workflow

Core tidyverse Packages



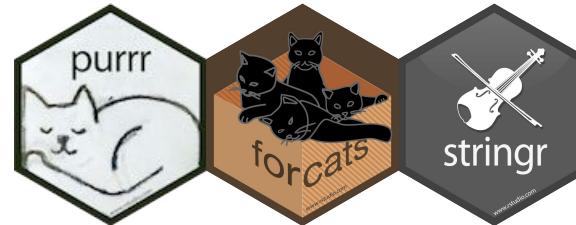
Data Visualization



Read Data
Tidy Data



Fundamental Data
Manipulation &
Pipelines



Manipulate Specific
Types of Data

High-level takeaways

- Real world data is often messy, and we (usually) need to make it tidy before you can start to work with it
- Learning to recognize the how data can be messy is an important first step to understanding how important well structured data is to the data analysis process
- Teaching others (i.e. those that provide data to you) about good "tidy data" practices will make your job easier as a data analyst

Resources

- Paper on tidy data by H. Wickham
<https://vita.had.co.nz/papers/tidy-data.pdf>
- R For Data Science, section on tidy data
<https://r4ds.had.co.nz/tidy-data.html>
- tidyr package website
<https://tidyverse.org>
- Data importing cheat sheet
<https://github.com/rstudio/cheatsheets/blob/master/data-import.pdf>



70th Conference on Mass Spectrometry and Allied topics

Data Manipulation & Pipelines with dplyr

JUNE 5 - 9 2022

Minneapolis Convention Center

SHORT COURSES

June 4 - 5

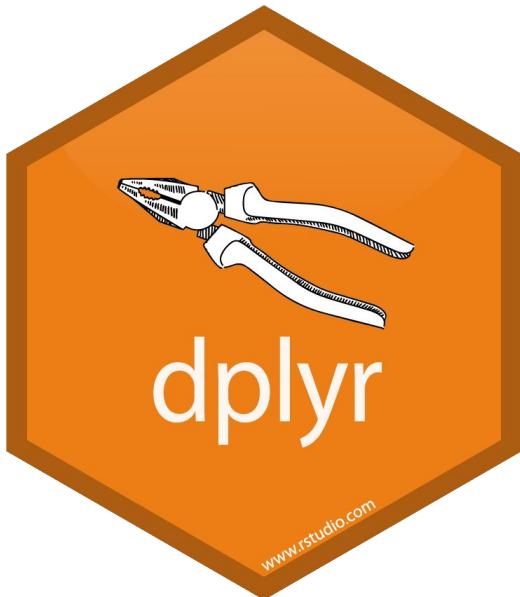
ASMS 2022: R Short Course

#ASMS2022

Goals for this module

- Understand the fundamental operations that underlie most common data manipulation challenges
- Learn about the dplyr R package and how it provides the functionality perform these data manipulation operations
- Learn about the pipe: `%>%`
- Learn how the pipe can be used to combine multiple data manipulation operations together into data pipelines
- Get a basic understanding of how to use dplyr for your own work

dplyr is a tidyverse R package for data manipulation

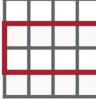
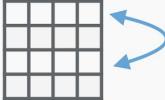
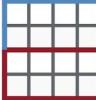
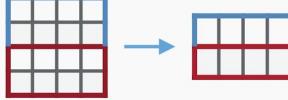


- Defines the fundamental operations that encompass most data analysis tasks
- Assumes you already have tidy data
- Uses a pipeline coding structure to perform complex operations a straight-forward, natural way

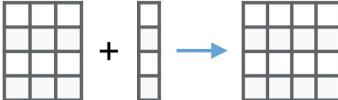
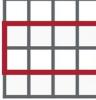
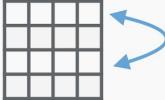
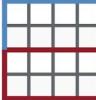
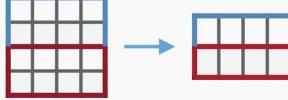
dplyr defines fundamental data manipulation verbs

- dplyr formalizes the **fundamental operations** that occur when working with data **into a set of “verbs”**
- These **verbs are represented as functions** that you can use to manipulate data in R
- There are a **small number of these verbs**, which makes them **easy(er)** to remember and work with
- Helps you to **focus on the question** you want to answer **rather than the mechanics** of how to answer the question

Fundamental data manipulation operations

Operation	Use case
Add a column	
Pick specific columns	
Subset to specific rows	
Reorder/sort rows	
Group subsets	
Summarize rows	

Fundamental data manipulation operations

Operation	Use case	dplyr verb
Add a column		compute new data from existing variables, join new data
Pick specific columns		focus in on specific variables
Subset to specific rows		focus on a specific sub-group in the data
Reorder/sort rows		understand the order of the data, find top/bottom observations
Group subsets		want to analyze sub-groups in your data
Summarize rows		compute summary values across multiple rows, useful with grouping

dplyr verbs represent high-level data manipulation tasks, not the specific “math” operations

- dplyr doesn't perform specific mathematical operations, statistical summaries, statistical tests, machine learning, data visualization, etc., etc..
- Rather it provides a structural framework inside of which all of these things can be accomplished in an organized, streamlined way
- You'll still need to know how to perform these specific operations in R, but can then use them in combination with dplyr to structure your analysis

Practice with verbs

Recall the long form of our student exam grades data that we tidied?

What verb would we use to compute the percentage correct?

```
# A tibble: 60 x 4
  Name          exam    points total
  <chr>        <chr>    <int> <int>
1 al-Jafri, Anas Score 1     17    25
2 al-Jafri, Anas Score 2     41    50
3 al-Jafri, Anas Score 3     18    25
4 al-Jafri, Anas Test 1     87   100
5 al-Jafri, Anas Midterm    89   100
6 al-Jafri, Anas Final      90   100
7 Drum, Anyssa  Score 1     19    25
8 Drum, Anyssa  Score 2     40    50
9 Drum, Anyssa  Score 3     19    25
10 Drum, Anyssa Test 1      88   100
# ... with 50 more rows
```

Practice with verbs

Recall the long form of our student exam grades data

What verb would we use to compute the percentage correct?

```
# A tibble: 60 x 4
  Name      exam  points total
  <chr>     <chr> <int> <int>
1 al-Jafri, Anas Score 1     17    25
2 al-Jafri, Anas Score 2     41    50
3 al-Jafri, Anas Score 3     18    25
4 al-Jafri, Anas Test 1     87   100
5 al-Jafri, Anas Midterm    89   100
6 al-Jafri, Anas Final     90   100
7 Drum, Anyssa Score 1     19    25
8 Drum, Anyssa Score 2     40    50
9 Drum, Anyssa Score 3     19    25
10 Drum, Anyssa Test 1    88   100
# ... with 50 more rows
```



mutate

We need to make a *new* column that has the computed value, *percentage correct*

R Code

```
mutate(dat_tidy,
       pct_correct = points / total)
```

Practice with verbs

dplyr applies this formula to every row in the input data – it's like dragging a formula cell in Excel!

R Code

```
mutate(dat_tidy, pct_correct = points / total)
```

Input (dat_tidy)

```
# A tibble: 60 x 4
  Name      exam  points total
  <chr>     <chr>   <int> <int>
1 al-Jafri, Anas Score 1    17    25
2 al-Jafri, Anas Score 2    41    50
3 al-Jafri, Anas Score 3    18    25
4 al-Jafri, Anas Test 1   87   100
5 al-Jafri, Anas Midterm  89   100
6 al-Jafri, Anas Final   90   100
7 Drum, Anyssa Score 1   19    25
8 Drum, Anyssa Score 2   40    50
9 Drum, Anyssa Score 3   19    25
10 Drum, Anyssa Test 1  88   100
# ... with 50 more rows
```

Output

```
# A tibble: 60 x 5
  Name      exam  points total pct_correct
  <chr>     <chr>   <int> <int>     <dbl>
1 al-Jafri, Anas Score 1    17    25     0.68
2 al-Jafri, Anas Score 2    41    50     0.82
3 al-Jafri, Anas Score 3    18    25     0.72
4 al-Jafri, Anas Test 1   87   100     0.87
5 al-Jafri, Anas Midterm  89   100     0.89
6 al-Jafri, Anas Final   90   100     0.9
7 Drum, Anyssa Score 1   19    25     0.76
8 Drum, Anyssa Score 2   40    50     0.8
9 Drum, Anyssa Score 3   19    25     0.76
10 Drum, Anyssa Test 1  88   100     0.88
# ... with 50 more rows
```

A few notes about writing dplyr code

```
mutate(dat_long,  
       pct_correct = points / total)
```

This second function argument was placed
on its own line!

R doesn't care much about newlines as
long as the other syntax is correct.

Feel free to add new lines to let your code
breathe!

These refer to column names
(i.e. variables) in the input data, or
columns we're going to create

In dplyr code, you don't put quotes ("")
around them

The input data
frame is always
the first argument
to dplyr verbs

The pipe operator: `%>%`

- The pipe operator takes an input data frame and “feeds” it into a function
... the function performs an operation on the input data
- In code, the pipe operator is three characters
- Yes -- you do have to type the three characters (or use a keyboard shortcut)
- Yes -- it looks strange, think of `%>%` as a pipe, funneling the input data into the function to do some work

Template

tidy data frame

`%>%`

dplyr verb

produces a

modified data frame

The pipe operator: `%>%`

Template



Practice with pipes

R Code without pipes

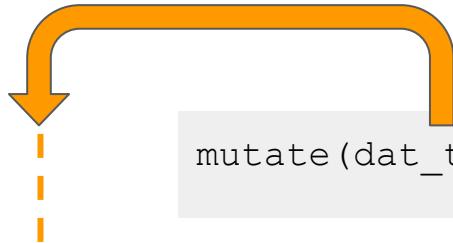
```
mutate(dat_tidy, pct_correct = points / total)
```

R Code *with* pipes

```
dat_tidy %>% mutate(pct_correct = points / total)
```

Both lines of code do exactly the same thing, but are written differently
Can you spot the differences?

Practice with pipes



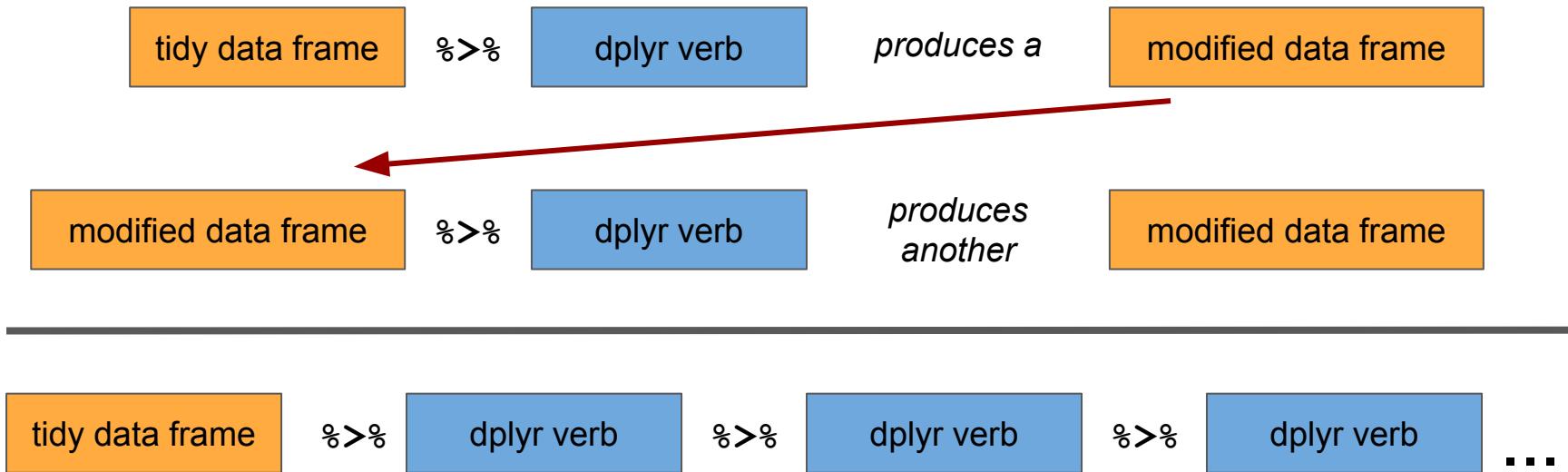
```
mutate(dat_tidy, pct_correct = points / total)
```

```
dat_tidy %>% mutate(pct_correct = points / total)
```

Two different ways to code the same thing

Take the first argument (the input data frame),
move it to the front and add a pipe, `%>%`

The pipe operator can chain multiple verbs (pipeline!)



You can chain (pipe) together dplyr verbs to produce pipelines that embody complex manipulations

Practice with pipes and pipelines

Goal

- compute the fraction correct for each exam
- get only the exams with > 90% correct
- order the results by the percent correct

Input Data

```
# A tibble: 60 x 4
  Name      exam  points total
  <chr>     <chr>   <int> <int>
1 al-Jafri, Anas Score 1     17    25
2 al-Jafri, Anas Score 2     41    50
3 al-Jafri, Anas Score 3     18    25
4 al-Jafri, Anas Test 1     87   100
5 al-Jafri, Anas Midterm    89   100
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7 Drum, Anyssa  Score 1     19    25
8 Drum, Anyssa  Score 2     40    50
9 Drum, Anyssa  Score 3     19    25
10 Drum, Anyssa Test 1     88   100
# ... with 50 more rows
```

Practice with pipes and pipelines

R Code

```
dat_tidy %>%
  mutate(pct_correct = points / total) %>%
  filter(pct_correct > 0.9) %>%
  arrange(pct_correct)
```

Output

# A tibble: 6 x 5					
	Name	exam	points	total	pct_correct
	<chr>	<chr>	<int>	<int>	<dbl>
1	Gonzales, David	Midterm	91	100	0.91
2	Smith, Westin	Final	91	100	0.91
3	Drum, Anyssa	Final	92	100	0.92
4	Michels, Breana	Score 2	46	50	0.92
5	Kwak, Surabhi	Final	93	100	0.93
6	Reed, Tyler	Midterm	94	100	0.94

Practice with pipes and pipelines

The problem statement maps directly to the code
If you can say it, you can code it!

- compute the fraction correct for each exam
 - get only the exams with > 90% correct
 - order the results by the percent correct
- ```
dat_tidy %>%
 mutate(pct_correct = points / total) %>%

 filter(pct_correct > 0.9) %>%

 arrange(pct_correct)
```

# group\_by + summarize is extremely powerful!

A common analysis task it to compute summaries by groups

- Compute the average test score for each student
- Count the number of analytes detected in each experimental run
- Compute the coefficient of variation for each analyte in a given run

In a dplyr pipeline, group\_by followed by summarize first groups the data by a specified variable, then summarizes the data within those groups

# Practice with group\_by + summarize

## Goal

- compute the fraction correct for each exam
- compute min, mean and max fraction correct for each student

## Input Data

```
A tibble: 60 x 4
 Name exam points total
 <chr> <chr> <int> <int>
1 al-Jafri, Anas Score 1 17 25
2 al-Jafri, Anas Score 2 41 50
3 al-Jafri, Anas Score 3 18 25
4 al-Jafri, Anas Test 1 87 100
5 al-Jafri, Anas Midterm 89 100
6 al-Jafri, Anas Final 90 100
7 Drum, Anyssa Score 1 19 25
8 Drum, Anyssa Score 2 40 50
9 Drum, Anyssa Score 3 19 25
10 Drum, Anyssa Test 1 88 100
... with 50 more rows
```

## What should we group by?

# Practice with group\_by + summarize

## Goal

- compute the fraction correct for each exam
- compute min, mean and max fraction correct for each student

## Input Data

```
A tibble: 60 x 4
 Name exam points total
 <chr> <chr> <int> <int>
1 al-Jafri, Anas Score 1 17 25
2 al-Jafri, Anas Score 2 41 50
3 al-Jafri, Anas Score 3 18 25
4 al-Jafri, Anas Test 1 87 100
5 al-Jafri, Anas Midterm 89 100
6 al-Jafri, Anas Final 90 100
7 Drum, Anyssa Score 1 19 25
8 Drum, Anyssa Score 2 40 50
9 Drum, Anyssa Score 3 19 25
10 Drum, Anyssa Test 1 88 100
... with 50 more rows
```

Name is the variable that specifies each student

# Practice with pipes and pipelines

## R Code

```
dat_tidy %>%
 mutate(pct_correct = points / total) %>%
 group_by(Name) %>% ←
 summarize(min_score = min(pct_correct),
 max_score = max(pct_correct),
 mean_score = mean(pct_correct))
```

these are just the names  
of new variables  
(columns) that will be  
created -- you can name  
them whatever you want

these are the calculations  
that will be performed on  
each group (student) --  
you can add as many as  
you need

all of the calculations after the  
group\_by will occur separately  
for each student

## Output

| # A tibble: 10 x 4 | Name             | min_score | max_score | mean_score |
|--------------------|------------------|-----------|-----------|------------|
|                    | <chr>            | <dbl>     | <dbl>     | <dbl>      |
| 1                  | al-Jafri, Anas   | 0.68      | 0.9       | 0.813      |
| 2                  | Drum, Anyssa     | 0.76      | 0.92      | 0.832      |
| 3                  | Gonzales, David  | 0.72      | 0.91      | 0.803      |
| 4                  | Granger, Shannan | 0.56      | 0.9       | 0.802      |
| 5                  | Kwak, Surabhi    | 0.64      | 0.93      | 0.827      |
| 6                  | Michels, Breana  | 0.68      | 0.92      | 0.798      |
| 7                  | Reed, Tyler      | 0.68      | 0.94      | 0.803      |
| 8                  | Smith, Tyler     | 0.64      | 0.9       | 0.792      |
| 9                  | Smith, Westin    | 0.6       | 0.91      | 0.802      |
| 10                 | Vang, Seher      | 0.76      | 0.87      | 0.81       |

# Review of the dplyr verbs and common use cases

## `mutate`

- adds a new column to your data table
- often used when you need to transform/combine with existing data in the table
- example: ratio of two variables, log transform a variable, add variables together

## `select`

- subsets your data to a specific set of columns (variables)
- used to focus in on the variables you want, remove ones you don't need
- mainly an “organizational” task

# Review of the dplyr verbs and common use cases

## `filter`

- subset your data to a specific set of observations (rows)
- used to filter data, subset based on conditions within the data
- example: filter to values > than a threshold, exclude data from a specific run

## `arrange`

- reorders the observations (rows) based on values in the data
- often used to put important data at the top of the table, or to rank observations

# Review of the dplyr verbs and common use cases

## `group_by`

- groups your data based upon a variable
- usually the variable is categorical-like (a string or a factor)
- doesn't do anything by itself -- need to combine with another verb to do something, often with `summarize`

## `summarize`

- summarizes all of the observations to a single value, if used with `group_by`, you get one value per group
- you specify how the observation will be summarized, usually with a function
- does not require `group_by` (but you'll typically want to use it)

# High-level takeaways

- dplyr provides a general framework for manipulating tidy data
- The fundamental manipulations are specified as verbs (functions)
- These verbs can be combined (piped) together to create data processing pipelines
- Often, these pipelines can often be translated from “human-form” to R code in a straight-forward, natural way
- dplyr helps you to focus on answering the question rather than the mechanics of how to answer the question

# Resources

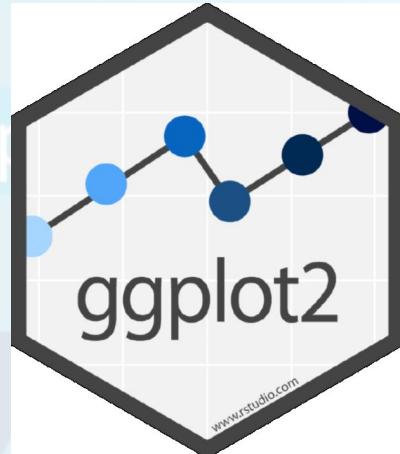
- R for Data Science  
<https://r4ds.had.co.nz>
- dplyr package website  
<https://dplyr.tidyverse.org>
- Data transformation with dplyr cheat sheet  
<https://github.com/rstudio/cheatsheets/blob/master/data-transformation.pdf>



70<sup>th</sup> Conference on Mass S

Applied topics

JUNE 5 - 9, 2022  
Minneapolis Convention Center



# R::ggplot

## Visualization Basics

SHORT COURSES  
June 4 - 5

#ASMS2022 ASMS 2022: R Short Course

# Goals for this module

- Introduction to data visualization using R package **ggplot2**
  - organizational structure
  - coding syntax
- Demonstrated Application
  - basic plotting
- Practical Application
  - plotting a regression line with  $R^2$  stats



# ggplot on the web

The screenshot shows the official ggplot2 website at <https://ggplot2.tidyverse.org>. The main navigation bar includes links for Reference, News, Articles, and Extensions. The 'Overview' section describes ggplot2 as a system for declaratively creating graphics, based on The Grammar of Graphics. It provides examples of how to map variables to aesthetics and use graphical primitives. The 'Installation' section contains R code for installing ggplot2 or the full tidyverse package.

```
The easiest way to get ggplot2 is to install the whole tidyverse:
install.packages("tidyverse")

Alternatively, install just ggplot2:
install.packages("ggplot2")

Or the development version from GitHub:
install.packages("devtools")
devtools::install_github("tidyverse/ggplot2")
```

<https://ggplot2.tidyverse.org/>

The screenshot shows the 'Points' reference page for the geom\_point layer at [https://ggplot2.tidyverse.org/reference/geom\\_point.html](https://ggplot2.tidyverse.org/reference/geom_point.html). The page includes a header with the ggplot2 logo and version 3.3.0, and a navigation bar with Reference, News, Articles, and Extensions. The main content area is titled 'Points' and includes a code example for geom\_point, a 'Source' link to R/geom\_point.r, and a detailed description of the geom\_point layer. Below the description, there are sections for 'Arguments' and detailed explanations for 'mapping', 'data', and 'inherit.aes'.

```
geom_point(
 mapping = NULL,
 data = NULL,
 stat = "identity",
 position = "identity",
 ...,
 na.rm = FALSE,
 show.legend = NA,
 inherit.aes = TRUE
)
```

**mapping** Set of aesthetic mappings created by `aes()` or `aes_()`. If specified and `inherit.aes = TRUE` (the default), it is combined with the default mapping at the top level of the plot. You must supply `mapping` if there is no plot mapping.

**data** The data to be displayed in this layer. There are three options:

If `NULL`, the default, the data is inherited from the plot data as specified in the call to `ggplot()`.

[https://ggplot2.tidyverse.org/reference/geom\\_point.html](https://ggplot2.tidyverse.org/reference/geom_point.html)

# ggplot help on the web

Points — geom\_point + ggplot > [ggplot plot regression line and formula](https://www.google.com/search?client=firefox-b-1-d&q=ggplot+plus+geom_point)

All Images Videos News Shopping More Settings Tools

About 188,000 results (0.63 seconds)

[rpkg.sdatanovia.com](#) > ggpubr > reference > stat\_regline... ▾

**Add Regression Line Equation and R-Square to a GGPlot ...**

Add Regression Line Equation and R-Square to a GGPlot. Add regression line equation and R<sup>2</sup> to a ggplot. Regression model is fitted using the function lm. stat\_regline\_equation(mapping = NULL, data = NULL, formula = y ~ x, label = "label", arguments = Computed variables

[stackoverflow.com](#) > questions > add-regression-line-ed... ▾

**Add regression line equation and R<sup>2</sup> on graph - Stack Overflow**

Oct 11, 2019 - Here is one solution # GET EQUATION AND R-SQUARED AS STRING # SOURCE: [https://groups.google.com/forum/#topic/ggplot2/t1gH-KG5XMA/lm\\_eqn](https://groups.google.com/forum/#topic/ggplot2/t1gH-KG5XMA/lm_eqn) ...

[ggplot2](#) add regression equations and R2 and adjust their ... Jun 11, 2016

Adding Regression Line Equation and R2 on SEPARATE ... Mar 22, 2018

[ggplot](#) Adding Regression Line Equation and R2 with Facet ... May 14, 2017

Plotting regression line on scatter plot using ggplot - Stack ... Sep 4, 2017

More results from stackoverflow.com

8 answers

[community.rstudio.com](#) > annotate-ggplot2-with-regres... ▾

**Annotate ggplot2 with regression equation and r squared ...**

Mar 11, 2018 - HI there, I would like to annotate ggplot2 with a regression equation and r ...

Having the option to display model coefficients and R2 as plot ...

1 answer

[intellipaat.com](#) > Community > R Programming ▾

**Adding Regression Line Equation and R2 on graph - Intellipaat**

Jul 10, 2019 - I wonder how to add a regression line equation and R<sup>2</sup> on the ggplot. My code is library(..., geom\_point()) p Any help will be highly ...

1 answer

[sejohnston.com](#) > 2012/08/09 > a-quick-and-easy-funct... ▾

**A quick and easy function to print lm() results with annotate2 in R**

Points - geom\_point + ggplot2 x ggplot2 - Add regression line e + https://stackoverflow.com/questions/7549694/add-regression-line-equation-and-r-squared-on-graph

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## Add regression line equation and R^2 on graph

Asked 8 years, 8 months ago Active 1 month ago Viewed 254k times

I wonder how to add regression line equation and R<sup>2</sup> on the ggplot. My code is:

library(ggplot2)

```
df <- data.frame(x = c(1:100))
df$y <- 2 + 3 * df$x + rnorm(100, sd = 40)
p <- ggplot(data = df, aes(x = x, y = y)) +
 geom_smooth(method = "lm", se = FALSE, color = "black", formula = y ~ x) +
 geom_point()
```

Any help will be highly appreciated.

share improve this question follow edited Mar 23 at 12:37 Tjebu 7,825 ● 2 ● 24 ● 46 asked Sep 26 '11 at 0:52 MYaseen208 17.5k ● 31 ● 118 ● 241

1 For lattice graphics, see [latticeExtra::lmlineq\(\)](#). – Josh O'Brien Oct 13 '13 at 2:23 add a comment

### 8 Answers

Active Oldest Votes

Here is one solution

# GET EQUATION AND R-SQUARED AS STRING  
# SOURCE: https://groups.google.com/forum/#topic/ggplot2/1Tgh-kG5XVA

```
lm_eqn <- function(df){
 m <- lm(y ~ x, df);
 eq <- substitute((italic(y) == a + b %.% italic(x)^n, ~~italic(r)^2 == r^2),
 list(a = format(unname(coef(m)[1]), digits = 2),
 b = format(unname(coef(m)[2]), digits = 2),
 r^2 = format(summary(m)$r.squared, digits = 3)))
```

# ggplot in print (or also on the web)

Points — geom\_point + ggplot

ggplot plot regression line and

Amazon.com : ggplot

Hello, Sign In

Account & Lists

Returns & Orders

Try Prime

Select your address

All ggplot

Sort by: Featured

48 results for "ggplot"

Amazon Prime

Eligible for Free Shipping

FREE Shipping by Amazon

All customers get FREE Shipping on orders over \$25 shipped by Amazon

Department

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- Computer Science
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★ ★ ★ ★ ★ & Up

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International Shipping Eligible

ggplot2: Elegant Graphics for Data Analysis (Use R!)

Part of: Use R! (63 Books)

★★★★★ 49

Paperback \$48<sup>49</sup> \$59.99

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Best Seller

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★★★★★ 13

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\$47.83 to buy

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More Buying Choices \$38.43 (27 used & new offers)

Other format: Kindle

Data Visualization: A Practical Introduction

by Kieran Healy

★★★★★ 46

Paperback \$36<sup>11</sup> \$40.00

prime Get it as soon as Mon, Jun 1

FREE Shipping by Amazon

More Buying Choices \$28.16 (33 used & new offers)

Other formats: eTextbook, Hardcover

<https://ggplot2-book.org/>

ggplot2: elegant graphics for data analysis

Welcome

Preface to the third edition

Preface to the second edition

I Getting started

- 1 Introduction
- 2 Getting started with ggplot2

3 Frequently asked questions

II Toolbox

- Introduction
- 4 Individual geoms
- 5 Collective geoms
- 6 Statistical summaries
- 7 Maps
- 8 Annotations
- 9 Arranging plots

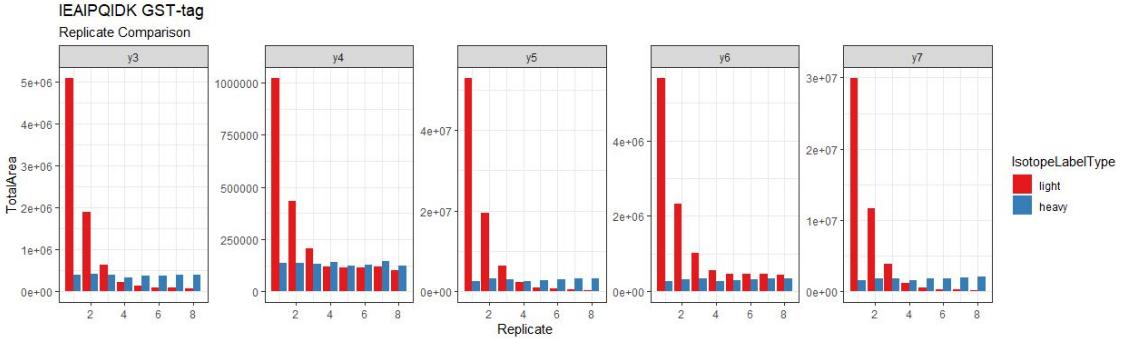
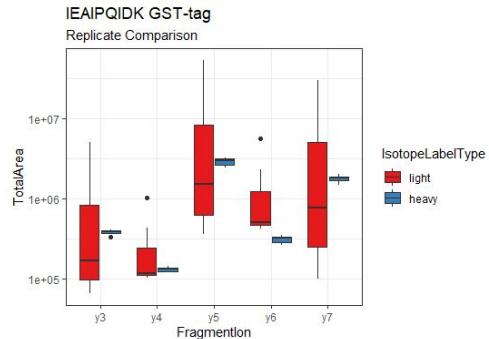
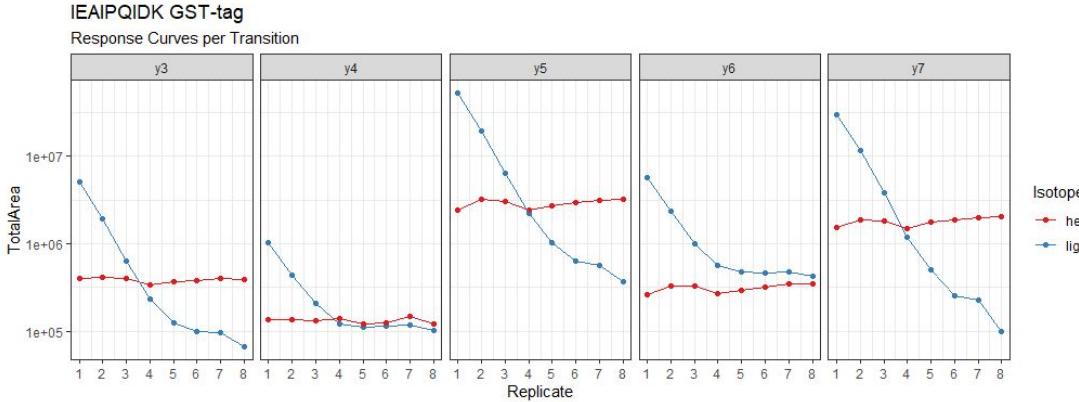
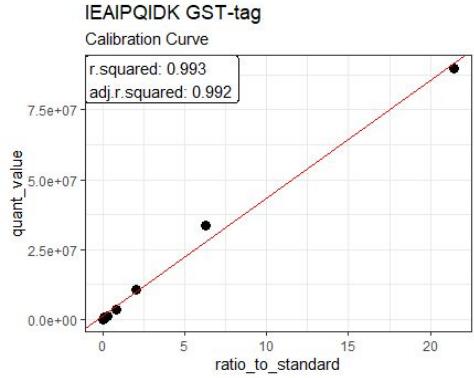
III The Grammar

- 10 Mastering the grammar
- 11 Build a plot layer by layer
- 12 Scales
- 13 Guides: legends and axes
- 14 Coordinate systems
- 15 Facetting
- 16 Themes

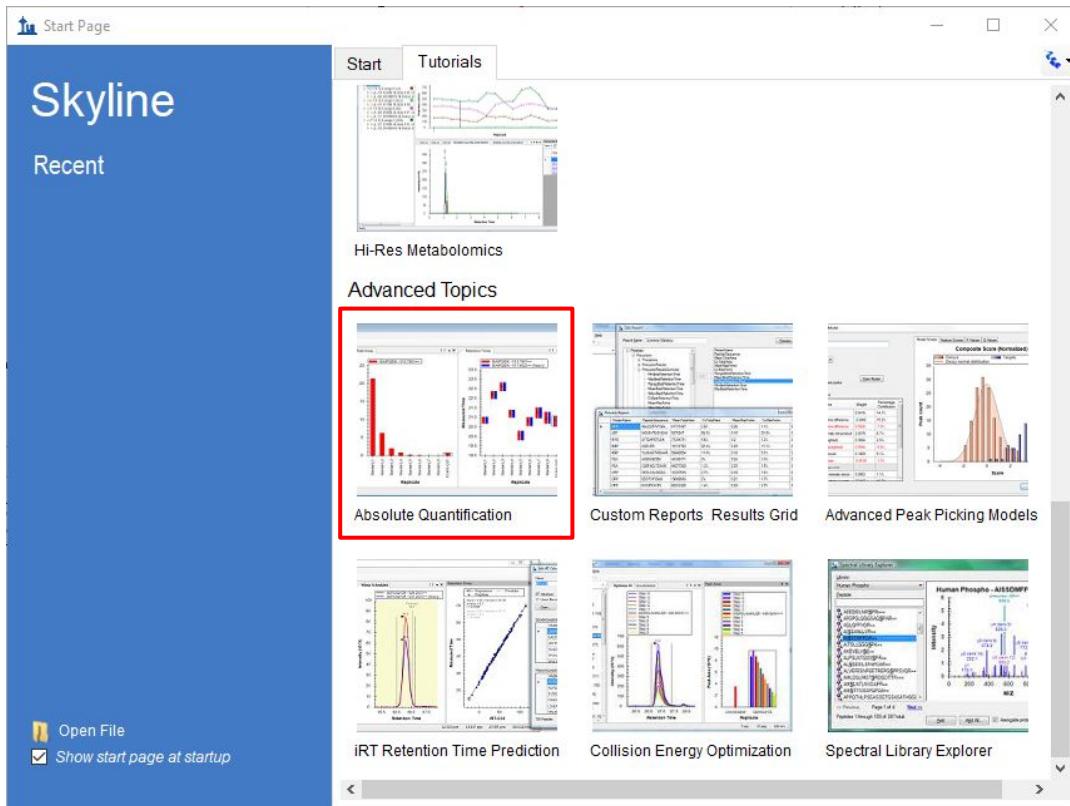
IV Extending ggplot2

17 Programming with ggplot2

# Sample of Plots Covered in this short course



# Data Source: Skyline Tutorial -- Absolute Quantification



Follow the tutorial and export the following data along the way

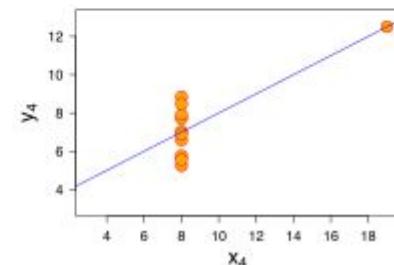
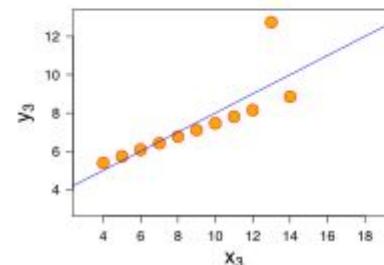
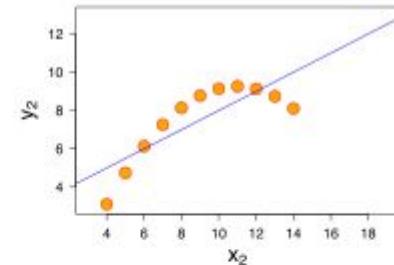
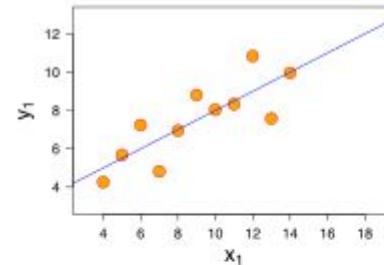
- Transition List
- Report: Calibration Values
- Chromatograms

*Exercise 0 covers the data import from CVS and TSV into a RDS tibble object. There are some advanced aspects such as value separation and nested tables.*

# Why visualize your data

**Anscombe's quartet** is an example that comprises four data sets that have nearly identical simple descriptive statistics, yet have very different distributions and appear very different when graphed.

| Property                        | Value               | Accuracy                                |
|---------------------------------|---------------------|-----------------------------------------|
| Mean of $x$                     | 9                   | exact                                   |
| Sample variance of $x$ :        | 11                  | exact                                   |
| Mean of $y$                     | 7.50                | to 2 decimal places                     |
| Sample variance of $y$ :        | 4.125               | $\pm 0.003$                             |
| Correlation between $x$ and $y$ | 0.816               | to 3 decimal places                     |
| Linear regression line          | $y = 3.00 + 0.500x$ | to 2 and 3 decimal places, respectively |



# Why ggplot

based on the grammar of graphics

*“the idea that you can build every graph from the same few components”*

data

a table of numeric and categorical values (data.frame, tibble)

geoms

a geometric object or visual representation, that can be layered

aesthetics

how variables in the data are mapped to visual properties

coordinate

orientation of the data points (\* optional)

```
1 ggplot(data, aes(x,y)) + geom_point() + coord_cartesian()
2
3 # combined with dplyr makes for a readable process
4 data %>% ggplot(aes(x,y)) + geom_point()
5
```

# The basic ggplot2 plotting template

The variable name of the data table  
you want to create a plot with



```
ggplot (data = <DATA>) +
 <GEOM_FUNCTION>(mapping = aes (<MAPPINGS>))
```

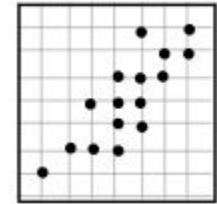
A ggplot2 function  
that defines the  
type of geometric  
representation you  
want to use, e.g.

geom\_point  
geom\_line  
geom\_histogram  
geom\_boxplot

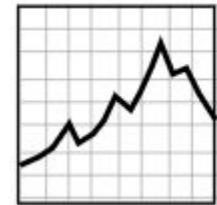
↑  
Expression that link  
columns in <DATA> to  
aesthetic properties

# ggplot geoms: simple

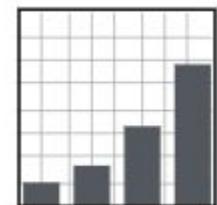
```
1 data %>% ggplot(aes(x, y)) + geom_point()
```



```
1 data %>% ggplot(aes(x, y)) + geom_line()
```

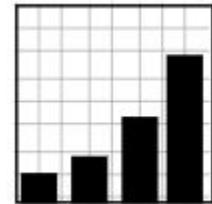


```
1 data %>% ggplot(aes(x)) + geom_bar()
```

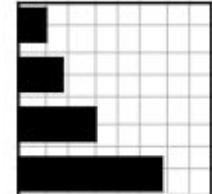


# ggplot coordinates: data projections

```
1 data %>% ggplot(aes(x)) + geom_bar() +
2 coord_cartesian()
```



```
1 data %>% ggplot(aes(x)) + geom_bar() +
2 coord_flip()
```



```
1 data %>% ggplot(aes(x)) + geom_bar() +
2 coord_polar()
```



# dplyr ~ ggplot

Quick note on tidyverse *joiners* ...

**dplyr** → use the **%>%** to join procedural functions in a specific order

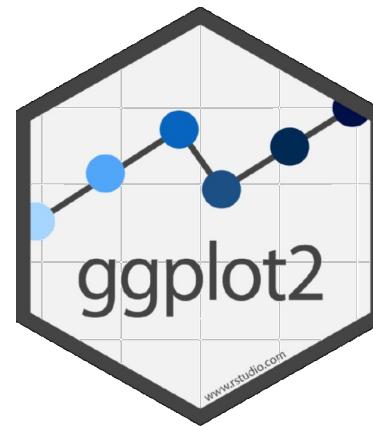
**ggplot** → use the **+** to join layers and customizations, in any order

\* using a **%>%** in a **ggplot** statement results in an error “***Did you use %>% instead of +?***”

# Combining dplyr and ggplot



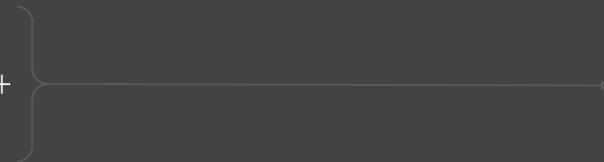
$\%>\%$



**data.frame**  
**tibble**

# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "path" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(x,y)) +
8 geom_point()
9
10 # plot 2 ~ var only exists as a factor here
11 dat %>%
12 mutate(var = as.factor(var)) %>% # wanted discrete colors
13 ggplot(aes(x,y, color=var)) +
14 geom_point() +
15 geom_line()
```



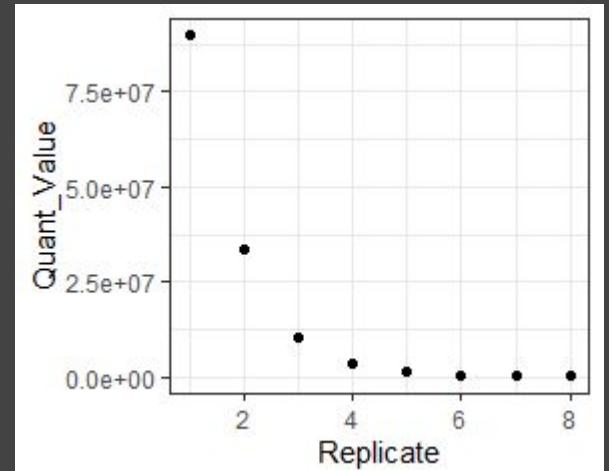
%>%



ggplot2

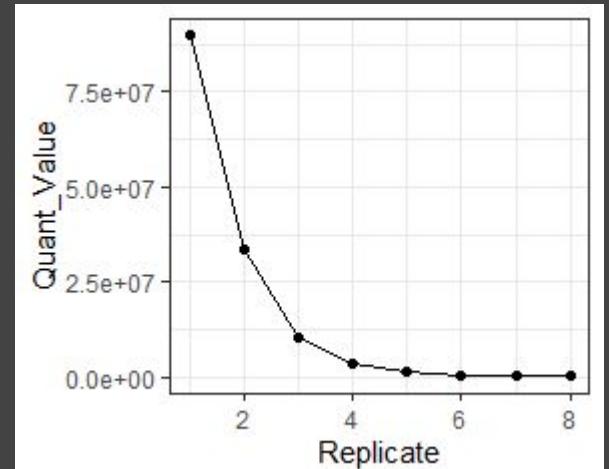
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point()
9
10
11
12
13
14
15
```



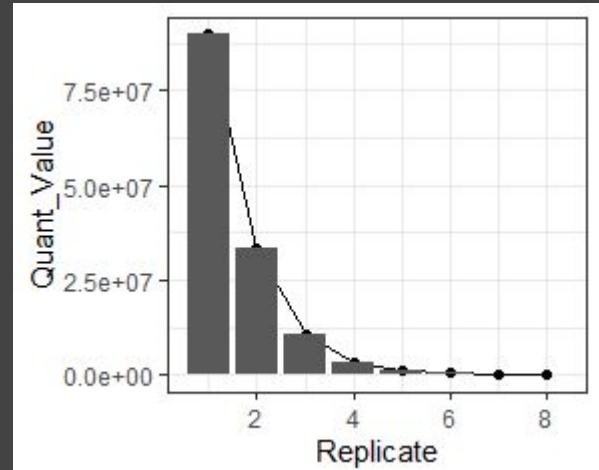
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point() +
9 geom_line()
```



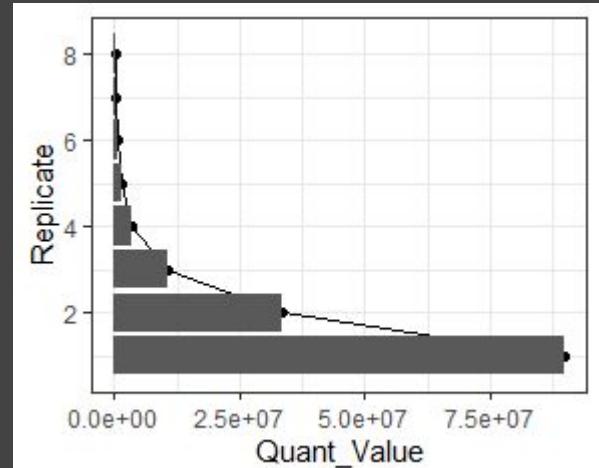
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point() +
9 geom_line() +
10 geom_bar(stat="identity")
11
12
13
14
15
```

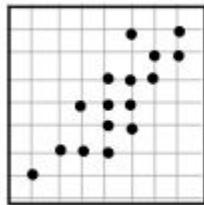


# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point() +
9 geom_line() +
10 geom_bar(stat="identity") +
11 coord_flip()
12
13
14
15
```



# ggplot aesthetics

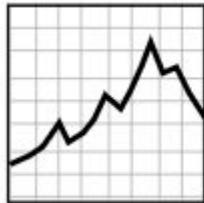


**geom\_point()**

x, y, alpha, color, fill, shape, size

**Position**

x = abscissa  
y = ordinate



**geom\_line()**

x, y, alpha, color, linetype, size

**Appearance**

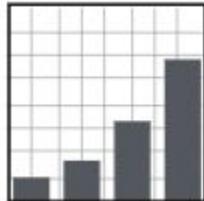
**Color**

alpha = transparency  
color = border / lines  
fill = volume

**Shape**

shape = ie. circle,  
square

size = small to big



**geom\_bar()**

x, alpha, color, fill, linetype, size, weight

# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "path" %>% read_csv()
3
4 # plot 1
5 dat %>%
6 ggplot(aes(var_x, var_y)) +
7 geom_point()
```

```
dat %>%
 ggplot() +
 geom_point(aes(var_x, var_y))
```

ggplot

→ invokes the plotting function → takes the data object and aesthetics

aes

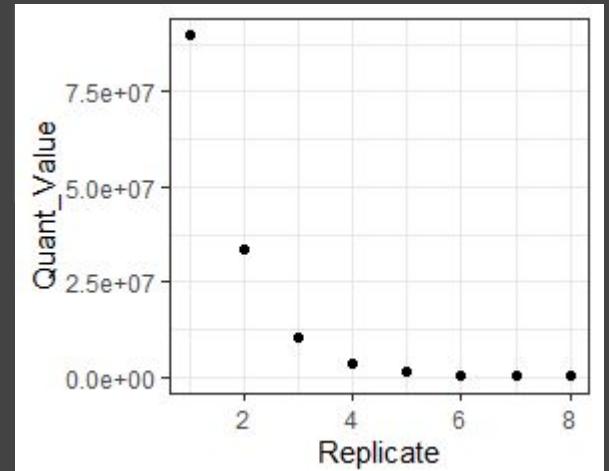
→ aesthetic, or the plot appearance (x,y, color ...)

geom\_point

→ the geometric function

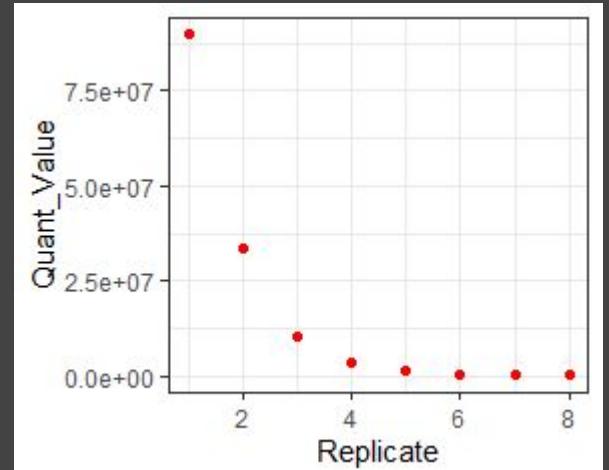
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point()
9
10
11
12
13
14
15
```



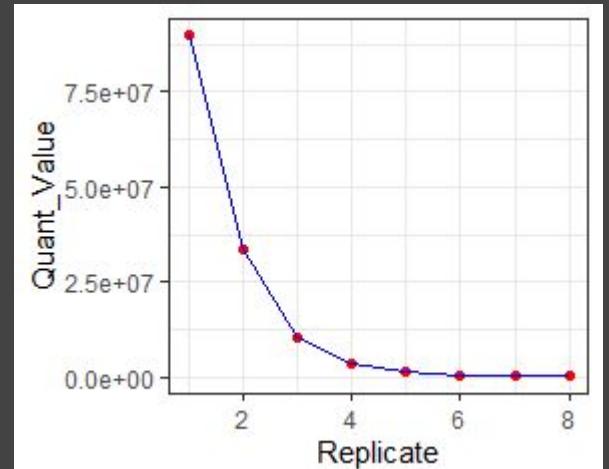
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point(color="red")
9
10
11
12
13
14
15
```



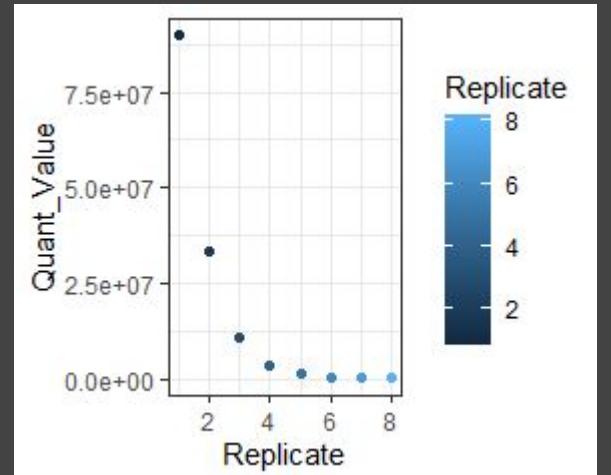
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point(color="red") +
9 geom_line(color="blue")
```



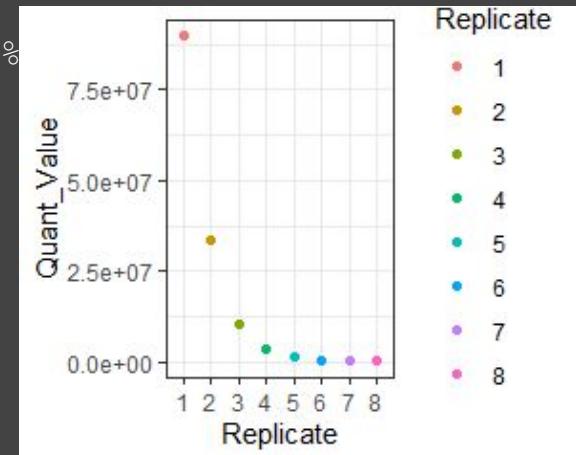
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot(aes(Replicate, Quant_Value)) +
8 geom_point(aes(color = Replicate))
9
10
11
12
13
14
15
```



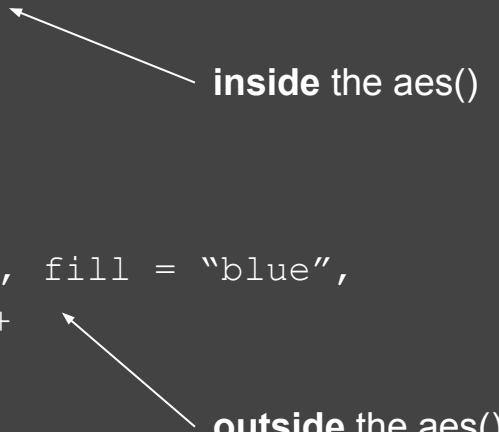
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 mutate(Replicate = as.factor(Replicate)) %>%
8 ggplot(aes(Replicate, Quant_Value)) +
9 geom_point(aes(color = Replicate))
10
11
12
13
14
15
```



# dplyr → ggplot

```
1 # mapping variables to aesthetics
2 dat %>%
3 ggplot(aes(X, Y, color = A, fill = B, size = M, shape = N)) +
4 geom_point()
5
6
7 # custom aesthetics
8 dat %>%
9 ggplot(aes(X, Y), color = "red", fill = "blue",
10 size = 2, shape = 3) +
11 geom_point()
12
13
14
15
```

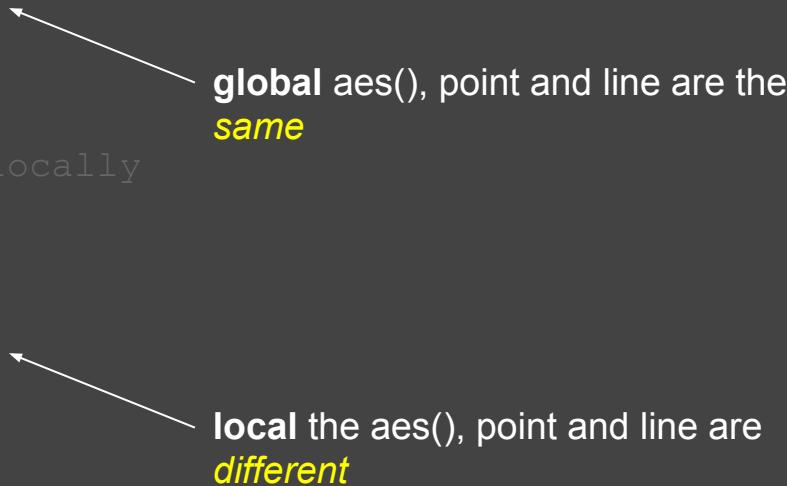


inside the aes()

outside the aes()

# dplyr → ggplot

```
1 # mapping variables to aesthetics, globally
2 dat %>%
3 ggplot(aes(X, Y, color = A, fill = B)) +
4 geom_point() +
5 geom_line()
6
7 # mapping variables to aesthetics, locally
8 dat %>%
9 ggplot(aes(X, Y)) +
10 geom_point(aes(color = A)) +
11 geom_line(aes(color = B))
12
13
14
15
```

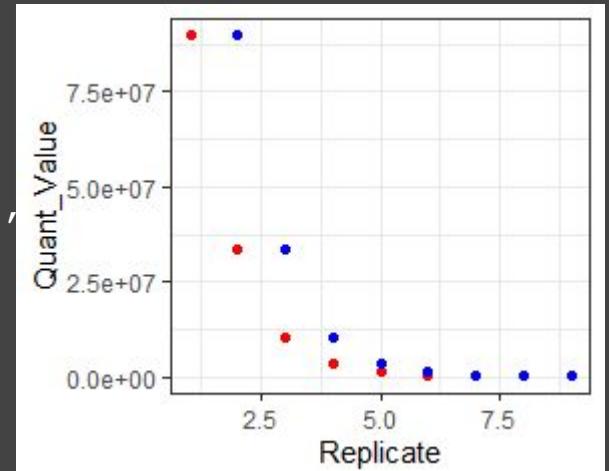


global aes(), point and line are the *same*

local the aes(), point and line are *different*

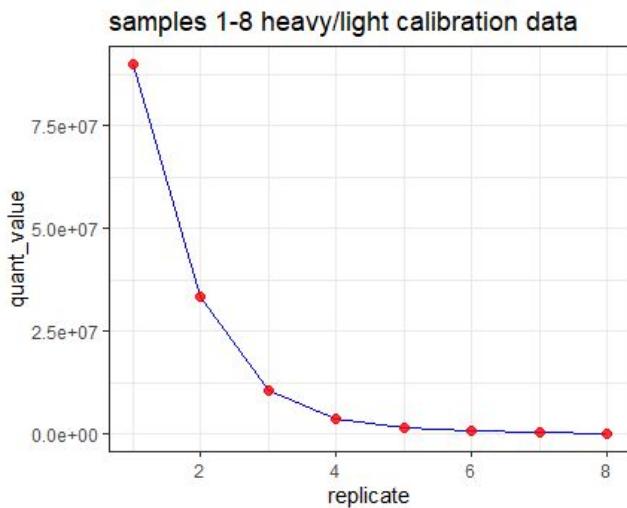
# dplyr → ggplot

```
1 # dat is our original data object
2 dat <- "./data/raw/samples_1-8_heavy-light_calibration.csv" %>%
3 read_csv()
4
5 # plot 1
6 dat %>%
7 ggplot() +
8 geom_point(aes(Replicate, Quant_Value),
9 color="red") +
10 geom_point(aes(Replicate + 1, Quant_Value),
11 color="blue") +
12
13
14
15
```

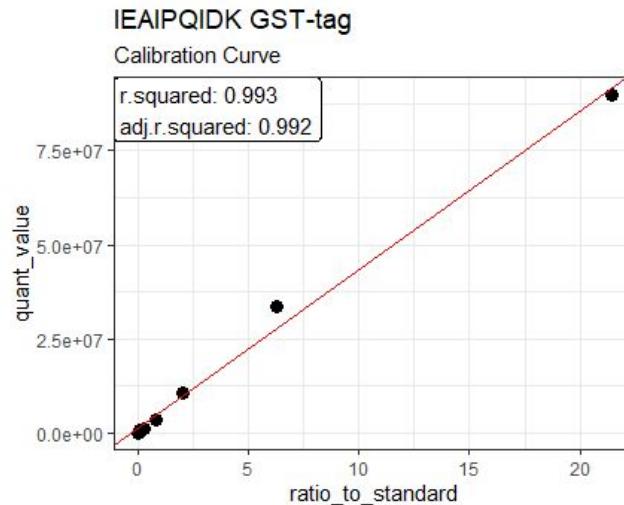


# ggplot exercise 1 & 2

points and lines



calibration plot

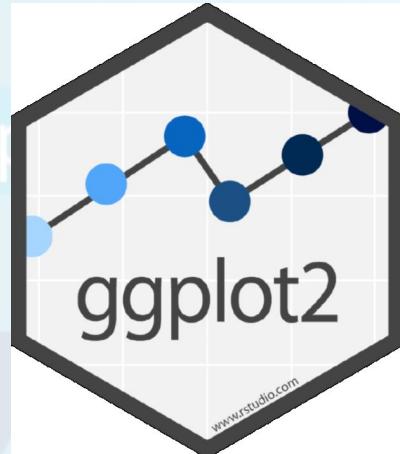




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# R::ggplot

SHORT COURSES

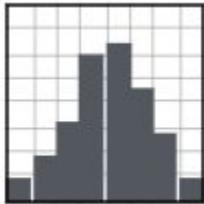
June 4 - Visualization of Stats & Customization

ASMS 2022: R Short Course  
#ASMS2022

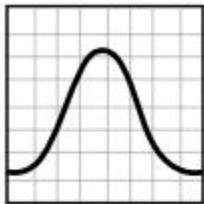
# Goals for this module

- Statistical plotting, advanced **ggplot2** syntax and customization
  - some dplyr tricks
- Demonstrated Application
  - plotting statistical representations of data (distributions)
  - creating multiple comparison plots (facetting)
- Practical Application
  - create a boxplot, histogram and density plot
  - recreating a plot from another application (getting the right look)

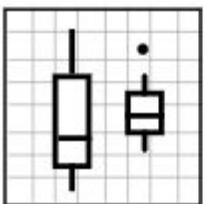
# ggplot geoms: distribution statistics



```
1 data %>% ggplot(aes(x)) + geom_histogram()
```

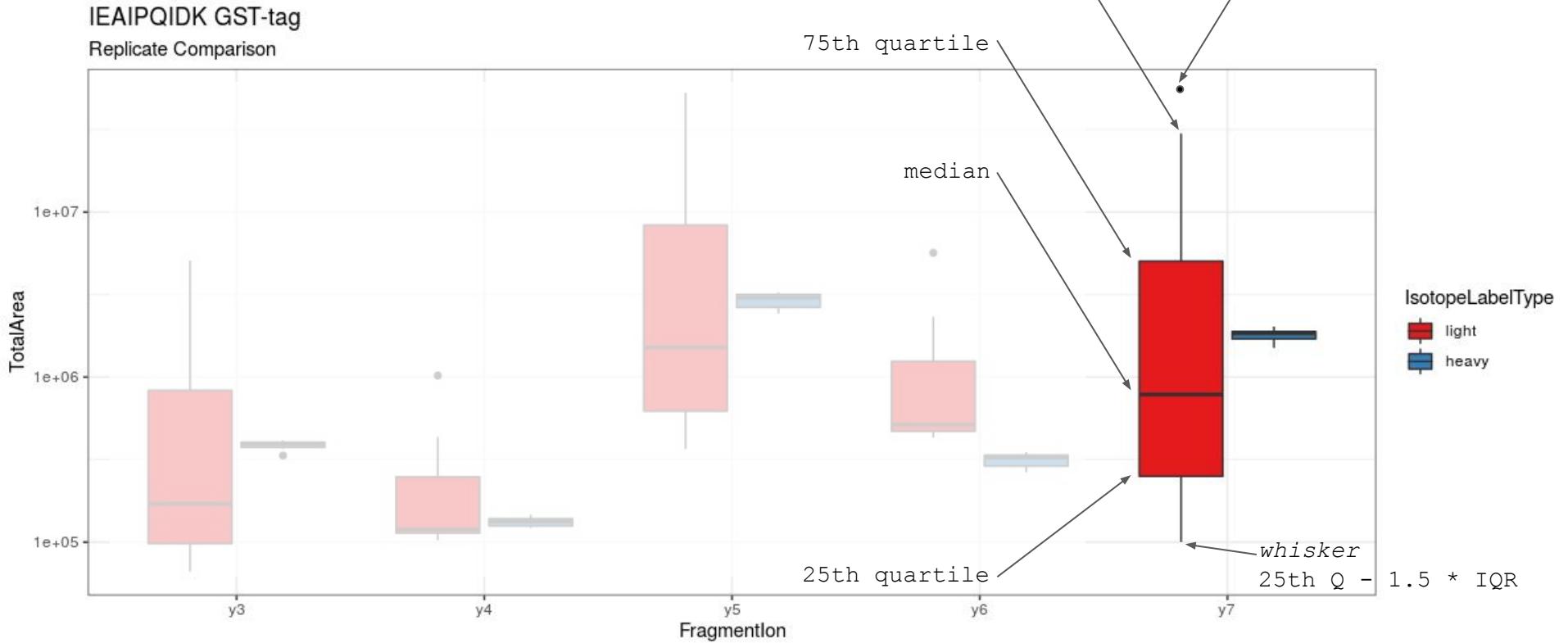


```
1 data %>% ggplot(aes(x)) + geom_density()
```



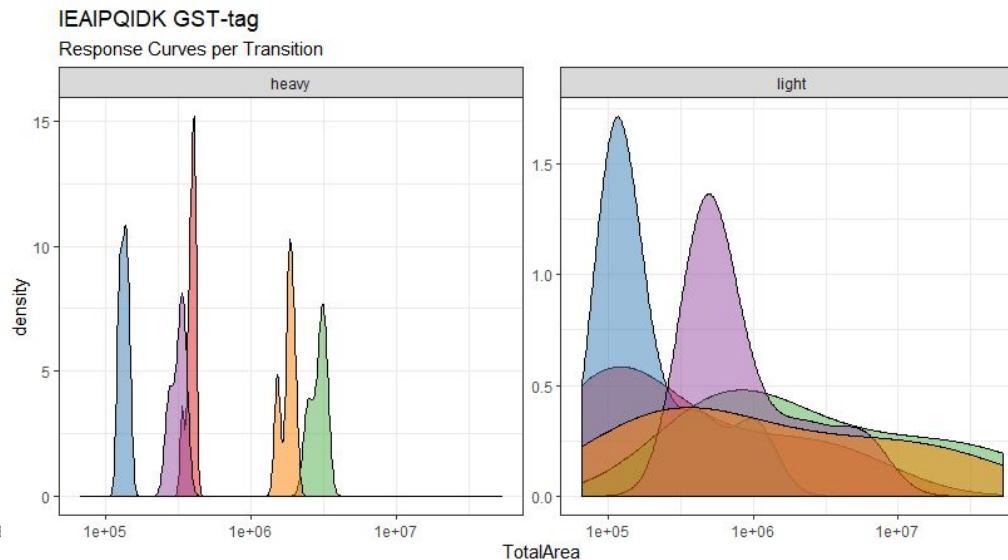
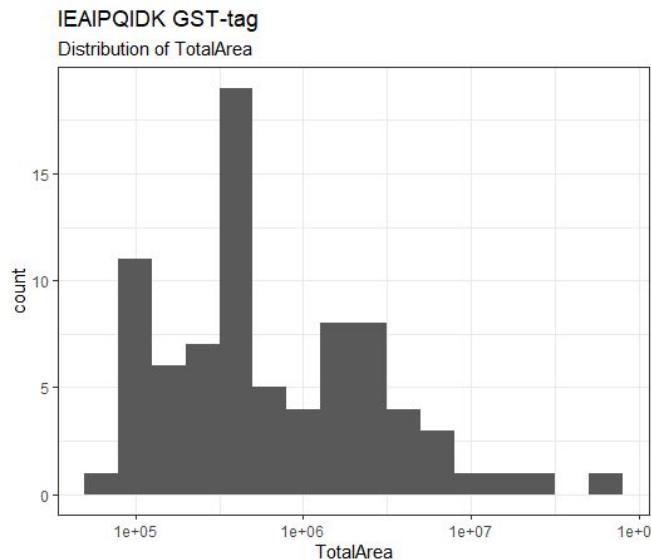
```
1 data %>% ggplot(aes(x, y)) + geom_boxplot()
```

# ggplot exercise 5



# ggplot exercise 6

histograms and density plots



Fragmention

- y3
- y4
- y5
- y6
- y7

*note: these are less informative visualizations, but decent demonstrations*

# ggplot extended syntax

```
1 p <- dat %>% ggplot(aes(x, y, color)) + geom_point() +
2 facet_wrap(~m) +
3 scale_color_brewer(palette="Set1")
4 ggtitle(label, subtitle)
```

**facet\_wrap** → create sub-plots based on a class value

**scale\_color\_brewer** → change the **color** of lines and points

**scale\_fill\_brewer** → change the colors of areas

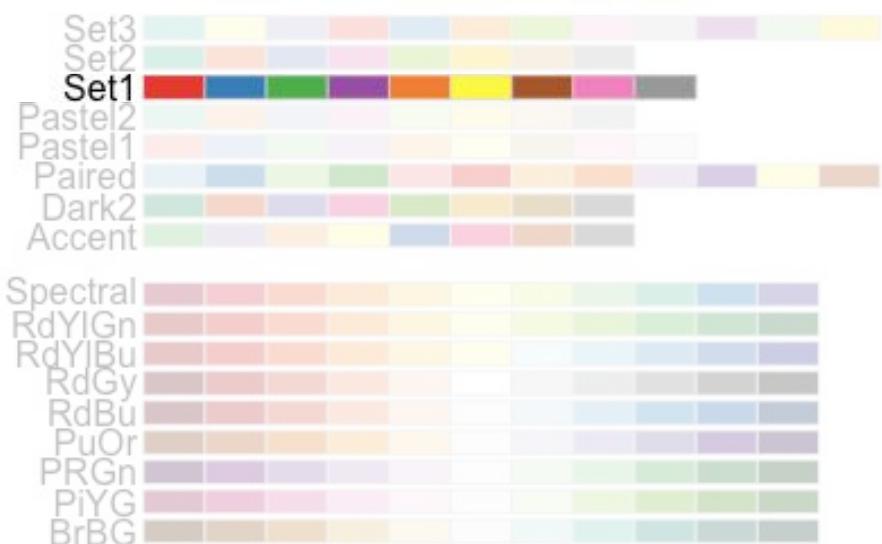
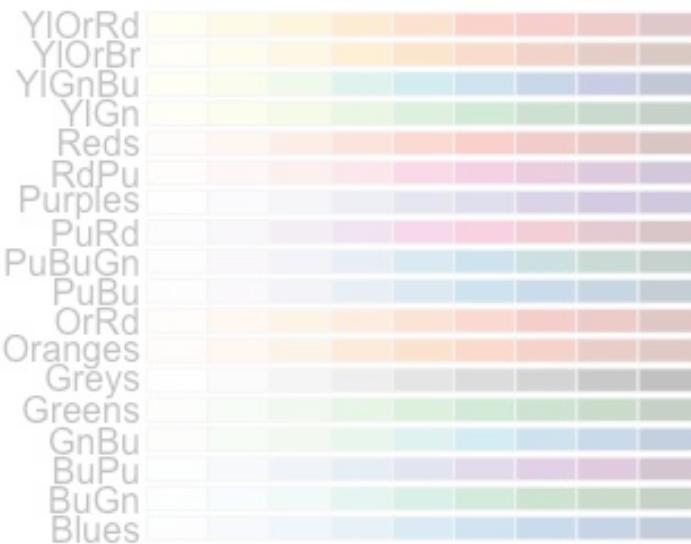
**ggtitle** → add a **main-title** and **subtitle**

**ggsave** → save the plot object

```
5 ggsave("plot.pdf", plot = p, width = 5, height = 3)
```

# ggplot color palettes (*pre-mixed*)

```
1 scale_color_brewer(palette="Set1") # lines and points
1 scale_fill_brewer(palette="Set1") # areas
```



[https://ggplot2.tidyverse.org/reference/scale\\_brewer.html](https://ggplot2.tidyverse.org/reference/scale_brewer.html) for a more indepth discussion

# ggplot facets: data partitioning

a



**facet\_wrap(. ~ a)**

wrap facets into a rectangular layout

b

a



**facet\_grid(b ~ a)**

facet into both rows and columns

a



**facet\_grid(a ~ .)**

a



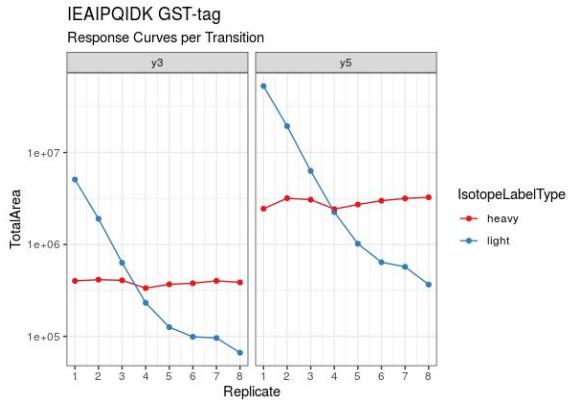
**facet\_grid(. ~ a)**

# ggplot facets: data partitioning

`facet_wrap(~a)  
facet_grid(~a)`

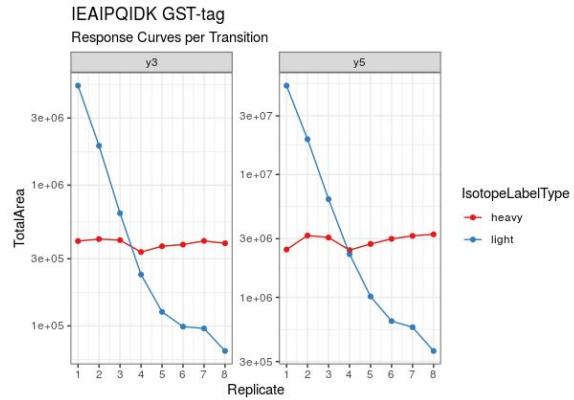
**same scales**

`facet_wrap(~a,  
ncol = 1)  
facet_grid(a~.)`



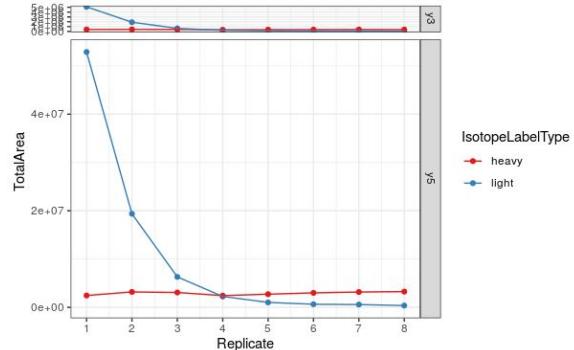
**individual scales**

`facet_wrap(~a,  
scales = "free")`



**proportional scales**

`facet_grid(a~.,  
space = "free")`

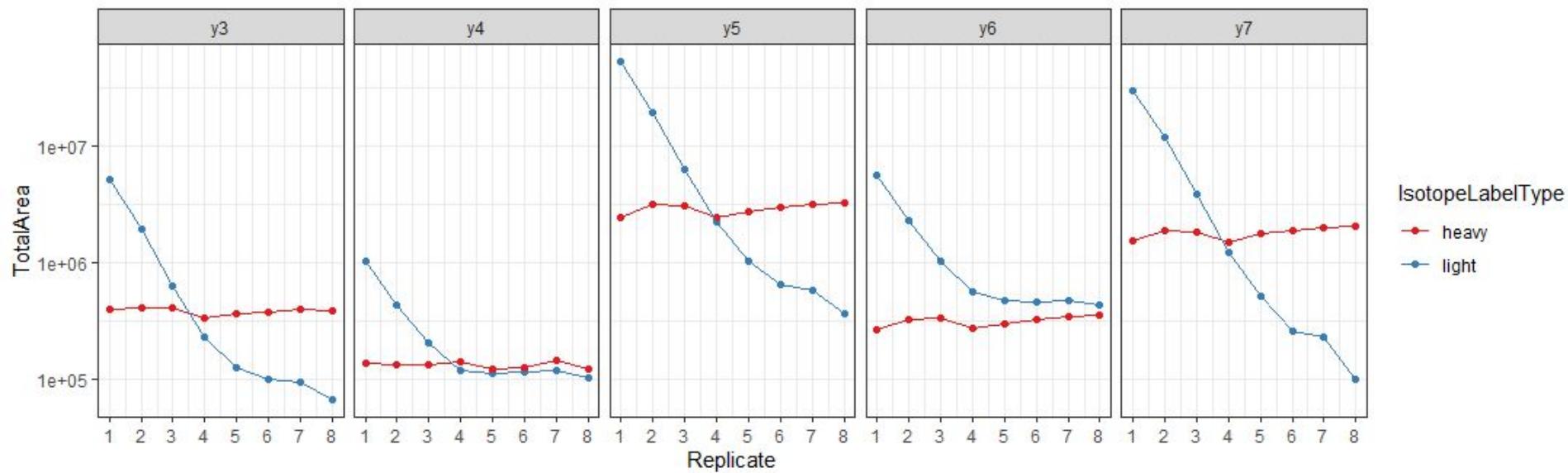


# ggplot exercise 3

faceting and coloring by variable

## IEAIPQIDK GST-tag

Response Curves per Transition



# tidyverse: reorder a variable by another variable

*Factors are the data objects which are used to categorize the data and store it as levels  
... defaults are alphanumeric.*

```
forcats::fct_reorder()
```

reorder by another variable such as rank

```
1 data %>%
 2 mutate(x = fct_reorder(x, y))
```

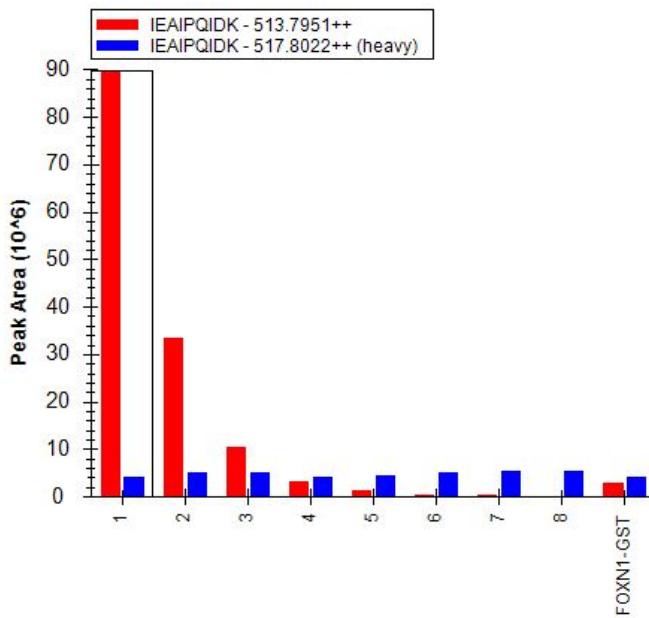
reverse order by alphanumeric sorting

```
1 data %>%
 2 mutate(x = fct_reorder(x, desc(x)))
```

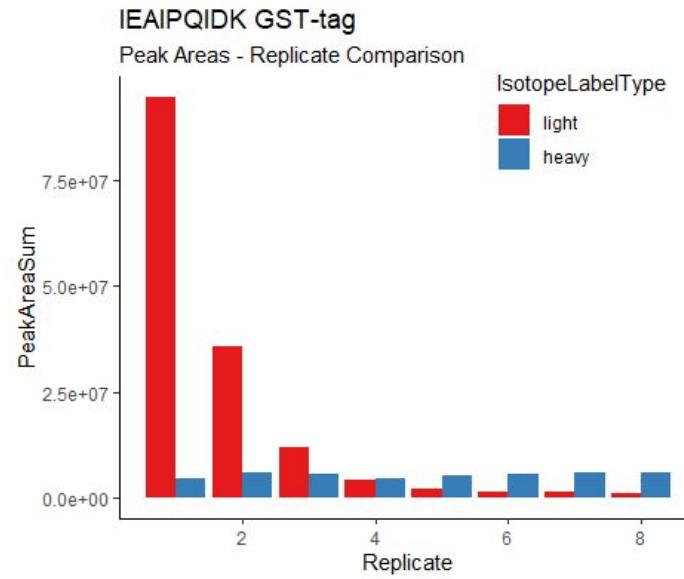
# ggplot exercise 4

replicating standard bar plots

Skyline

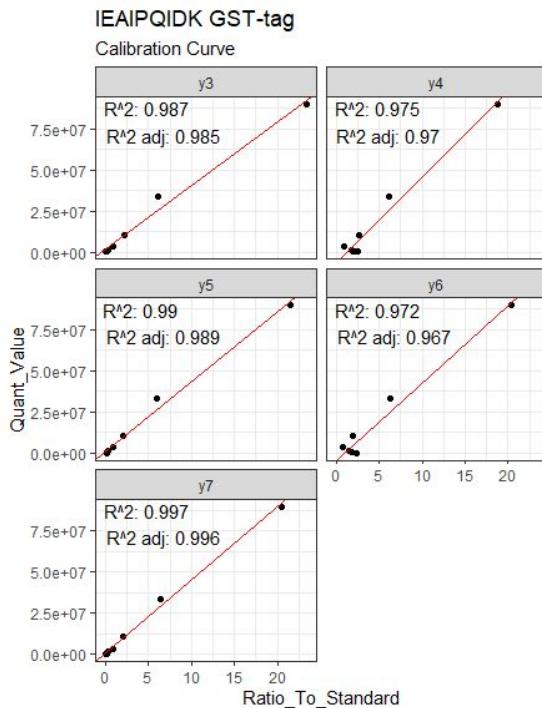


R:::ggplot



# ggplot exercise 8      advanced challenge

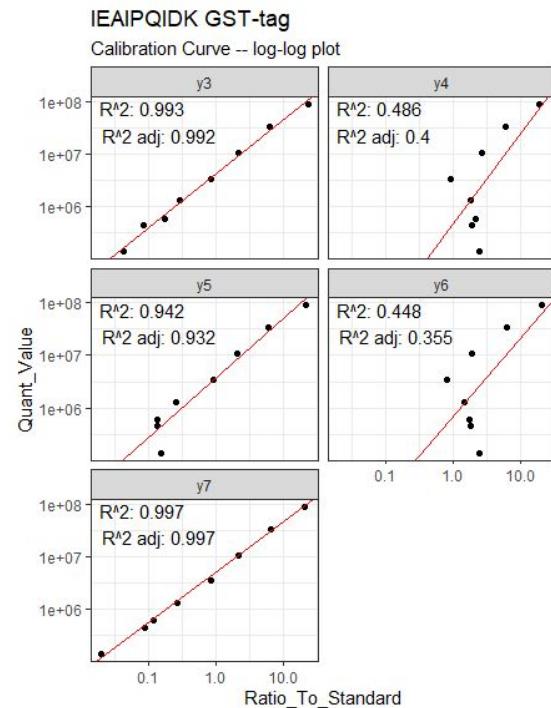
nested calibration model with faceted plot



## Extra Credit

Why do the log-log plots have a different regression correlation estimate ( $R^2$ )?

Note: Refer to Anscombe's quartet set IV for similar regression issues.





70<sup>th</sup> Conference on Mass Spectrometry and Allied topics

# Tidying Data: Pivoting & Separating

JUNE 5 - 9, 2022

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SHORT COURSES

June 4 - 5

ASMS 2022: R Short Course

#ASMS2022

# Goals for this module

- Understand the difference between wide and long forms
- Learn how to pivot data to move between wide and long forms
- Learn how to separate multiple pieces of data that "live" in the same cell

# tidyr is a package in the tidyverse that helps tidy data

- tidyr provides lots of helpful functions for tidying data, but two categories are particularly useful
  - **Pivoting:** long form  $\longleftrightarrow$  wide form
  - **Separating:** extracting pieces of data that are combined in a single cell
- <https://tidyr.tidyverse.org>



# tidy় helps you get to tidy data

tidy় provides many tools, but these are the two most important

## Pivoting

| country | 1999 | 2000 |
|---------|------|------|
| A       | 0.7K | 2K   |
| B       | 37K  | 80K  |
| C       | 212K | 213K |



| country | year | cases |
|---------|------|-------|
| A       | 1999 | 0.7K  |
| B       | 1999 | 37K   |
| C       | 1999 | 212K  |
| A       | 2000 | 2K    |
| B       | 2000 | 80K   |
| C       | 2000 | 213K  |

key      value

*wide(r) form*

*long(er) form*

## Separating

| country | year | rate     |
|---------|------|----------|
| A       | 1999 | 0.7K/19M |
| A       | 2000 | 2K/20M   |
| B       | 1999 | 37K/172M |
| B       | 2000 | 80K/174M |
| C       | 1999 | 212K/1T  |
| C       | 2000 | 213K/1T  |

| country | year | cases | pop |
|---------|------|-------|-----|
| A       | 1999 | 0.7K  | 19M |
| A       | 2000 | 2K    | 20M |
| B       | 1999 | 37K   | 172 |
| B       | 2000 | 80K   | 174 |
| C       | 1999 | 212K  | 1T  |
| C       | 2000 | 213K  | 1T  |

*separate combined data  
into individual columns*

# Pivoting case #1: *a variable is spread across multiple columns*

| Name             | Quizzes |         |         | Tests    |          |          |
|------------------|---------|---------|---------|----------|----------|----------|
|                  | Score 1 | Score 2 | Score 3 | Test 1   | Midterm  | Final    |
| al-Jafri, Anas   | 17 / 25 | 41 / 50 | 18 / 25 | 87 / 100 | 89 / 100 | 90 / 100 |
| Drum, Anyssa     | 19 / 25 | 40 / 50 | 19 / 25 | 88 / 100 | 87 / 100 | 92 / 100 |
| Gonzales, David  | 18 / 25 | 38 / 50 | 19 / 25 | 84 / 100 | 91 / 100 | 83 / 100 |
| Granger, Shannan | 14 / 25 | 42 / 50 | 20 / 25 | 89 / 100 | 82 / 100 | 90 / 100 |
| Kwak, Surabhi    | 16 / 25 | 41 / 50 | 21 / 25 | 85 / 100 | 88 / 100 | 93 / 100 |
| Michels, Breana  | 17 / 25 | 46 / 50 | 18 / 25 | 80 / 100 | 85 / 100 | 82 / 100 |
| Reed, Tyler      | 19 / 25 | 39 / 50 | 17 / 25 | 78 / 100 | 94 / 100 | 88 / 100 |
| Smith, Tyler     | 16 / 25 | 40 / 50 | 19 / 25 | 79 / 100 | 90 / 100 | 86 / 100 |
| Smith, Westin    | 15 / 25 | 45 / 50 | 17 / 25 | 87 / 100 | 85 / 100 | 91 / 100 |
| Vang, Seher      | 19 / 25 | 43 / 50 | 19 / 25 | 79 / 100 | 82 / 100 | 87 / 100 |

← All of these exams (quizzes and test) are in their own columns

We might consider a single variable called “exam” that collects all the different tests & quizzes into a single column

This will make the table longer

# Pivoting case #1: *a variable is spread across multiple columns*

We want to take these columns and put their names into a *new* single column (we'll call it exam), and the scores into a new single column (we'll call it score)

| Name               | `Score 1` | `Score 2` | `Score 3` | `Test 1` | Midterm  | Final    |
|--------------------|-----------|-----------|-----------|----------|----------|----------|
| <chr>              | <chr>     | <chr>     | <chr>     | <chr>    | <chr>    | <chr>    |
| 1 al-Jafri, Anas   | 17 / 25   | 41 / 50   | 18 / 25   | 87 / 100 | 89 / 100 | 90 / 100 |
| 2 Drum, Anyssa     | 19 / 25   | 40 / 50   | 19 / 25   | 88 / 100 | 87 / 100 | 92 / 100 |
| 3 Gonzales, David  | 18 / 25   | 38 / 50   | 19 / 25   | 84 / 100 | 91 / 100 | 83 / 100 |
| 4 Granger, Shannan | 14 / 25   | 42 / 50   | 20 / 25   | 89 / 100 | 82 / 100 | 90 / 100 |
| 5 Kwak, Surabhi    | 16 / 25   | 41 / 50   | 21 / 25   | 85 / 100 | 88 / 100 | 93 / 100 |
| 6 Michels, Breana  | 17 / 25   | 46 / 50   | 18 / 25   | 80 / 100 | 85 / 100 | 82 / 100 |
| 7 Reed, Tyler      | 19 / 25   | 39 / 50   | 17 / 25   | 78 / 100 | 94 / 100 | 88 / 100 |
| 8 Smith, Tyler     | 16 / 25   | 40 / 50   | 19 / 25   | 79 / 100 | 90 / 100 | 86 / 100 |
| 9 Smith, Westin    | 15 / 25   | 45 / 50   | 17 / 25   | 87 / 100 | 85 / 100 | 91 / 100 |
| 10 Vang, Seher     | 19 / 25   | 43 / 50   | 19 / 25   | 79 / 100 | 82 / 100 | 87 / 100 |

Note:  
there are 10 students

Note:  
there are 6 exams

Each row will represent a *single* exam and its score for a given student  
We should get 10 students x 6 exams = 60 rows

# Pivoting case #1: *a variable is spread across multiple columns*

## R Code

```
Load the tidyverse core packages
library(tidyverse)

#
Step 1: Load the data table
#
dat <- read_csv("ex1_tbl.csv")
print(dat)
```

*Load the tidyverse packages  
Read in the data  
Print the data to the screen*

## Output

|    | Name             | `Score 1` | `Score 2` | `Score 3` | `Test 1` | Midterm  | Final    |
|----|------------------|-----------|-----------|-----------|----------|----------|----------|
|    | <chr>            | <chr>     | <chr>     | <chr>     | <chr>    | <chr>    | <chr>    |
| 1  | al-Jafri, Anas   | 17 / 25   | 41 / 50   | 18 / 25   | 87 / 100 | 89 / 100 | 90 / 100 |
| 2  | Drum, Anyssa     | 19 / 25   | 40 / 50   | 19 / 25   | 88 / 100 | 87 / 100 | 92 / 100 |
| 3  | Gonzales, David  | 18 / 25   | 38 / 50   | 19 / 25   | 84 / 100 | 91 / 100 | 83 / 100 |
| 4  | Granger, Shannan | 14 / 25   | 42 / 50   | 20 / 25   | 89 / 100 | 82 / 100 | 90 / 100 |
| 5  | Kwak, Surabhi    | 16 / 25   | 41 / 50   | 21 / 25   | 85 / 100 | 88 / 100 | 93 / 100 |
| 6  | Michels, Breana  | 17 / 25   | 46 / 50   | 18 / 25   | 80 / 100 | 85 / 100 | 82 / 100 |
| 7  | Reed, Tyler      | 19 / 25   | 39 / 50   | 17 / 25   | 78 / 100 | 94 / 100 | 88 / 100 |
| 8  | Smith, Tyler     | 16 / 25   | 40 / 50   | 19 / 25   | 79 / 100 | 90 / 100 | 86 / 100 |
| 9  | Smith, Westin    | 15 / 25   | 45 / 50   | 17 / 25   | 87 / 100 | 85 / 100 | 91 / 100 |
| 10 | Vang, Seher      | 19 / 25   | 43 / 50   | 19 / 25   | 79 / 100 | 82 / 100 | 87 / 100 |

# Pivoting case #1: *a variable is spread across multiple columns*

## R Code

```
... code continued
Step 2: Pivot the data longer
pull all the exams into a single
column

dat_long <-
 pivot_longer(dat,
 cols = 2:7,
 names_to = "exam",
 values_to = "score")
print(dat_long)
```

`pivot_longer` is the function

`cols` says which columns we want to collect into a single column (we do it here by column number)

`names_to` gives the *new* column name where the cols will go

`values_to` gives the *new* column name where the values will go

## Output

```
A tibble: 60 × 3
 Name exam score
 <chr> <chr> <chr>
1 al-Jafri, Anas Score 1 17 / 25
2 al-Jafri, Anas Score 2 41 / 50
3 al-Jafri, Anas Score 3 18 / 25
4 al-Jafri, Anas Test 1 87 / 100
5 al-Jafri, Anas Midterm 89 / 100
6 al-Jafri, Anas Final 90 / 100
7 Drum, Anyssa Score 1 19 / 25
8 Drum, Anyssa Score 2 40 / 50
9 Drum, Anyssa Score 3 19 / 25
10 Drum, Anyssa Test 1 88 / 100
... with 50 more rows
```

# Pivoting case #1: *a variable is spread across multiple columns*

60 rows just like  
we expected

Each student  
has 6 rows,  
one for each  
exam

```
A tibble: 60 x 3
 Name exam score
 <chr> <chr> <chr>
1 al-Jafri, Anas Score 1 17 / 25
2 al-Jafri, Anas Score 2 41 / 50
3 al-Jafri, Anas Score 3 18 / 25
4 al-Jafri, Anas Test 1 87 / 100
5 al-Jafri, Anas Midterm 89 / 100
6 al-Jafri, Anas Final 90 / 100
7 Drum, Anyssa Score 1 19 / 25
8 Drum, Anyssa Score 2 40 / 50
9 Drum, Anyssa Score 3 19 / 25
10 Drum, Anyssa Test 1 88 / 100
... with 50 more rows
```

exam is a new column

It has the names from  
the old columns

score is a new column

It has the exams score  
for a *single* exam

By default we just see the first 10 rows (but there are 60 total)

# Pivoting case #2: *an observation is scattered across multiple rows*

```
A tibble: 60 x 3
 Name exam score
 <chr> <chr> <chr>
1 al-Jafri, Anas Score 1 17 / 25
2 al-Jafri, Anas Score 2 41 / 50
3 al-Jafri, Anas Score 3 18 / 25
4 al-Jafri, Anas Test 1 87 / 100
5 al-Jafri, Anas Midterm 89 / 100
6 al-Jafri, Anas Final 90 / 100
7 Drum, Anyssa Score 1 19 / 25
8 Drum, Anyssa Score 2 40 / 50
9 Drum, Anyssa Score 3 19 / 25
10 Drum, Anyssa Test 1 88 / 100
... with 50 more rows
```

The long form of the data is **exam-centric**

Each observation (row) represents an exam

Each variable (column) represents something about the exam (student, exam name, score)

What if we want a **student-centric** form of the data?  
That's the wide form  
(students are the observation)

# Pivoting case #2: *an observation is scattered across multiple rows*

## R Code

```
Step 2, in reverse: Pivot the data back
spread the individual tests back into
separate columns
#
dat_wide <-
 pivot_wider(dat_long,
 names_from = exam,
 values_from = score)
print(dat_wide)
```

## Output

|    | Name             | `Score 1` | `Score 2` | `Score 3` | `Test 1` | Midterm  | Final    |
|----|------------------|-----------|-----------|-----------|----------|----------|----------|
|    | <chr>            | <chr>     | <chr>     | <chr>     | <chr>    | <chr>    | <chr>    |
| 1  | al-Jafri, Anas   | 17 / 25   | 41 / 50   | 18 / 25   | 87 / 100 | 89 / 100 | 90 / 100 |
| 2  | Drum, Anyssa     | 19 / 25   | 40 / 50   | 19 / 25   | 88 / 100 | 87 / 100 | 92 / 100 |
| 3  | Gonzales, David  | 18 / 25   | 38 / 50   | 19 / 25   | 84 / 100 | 91 / 100 | 83 / 100 |
| 4  | Granger, Shannan | 14 / 25   | 42 / 50   | 20 / 25   | 89 / 100 | 82 / 100 | 90 / 100 |
| 5  | Kwak, Surabhi    | 16 / 25   | 41 / 50   | 21 / 25   | 85 / 100 | 88 / 100 | 93 / 100 |
| 6  | Michels, Breana  | 17 / 25   | 46 / 50   | 18 / 25   | 80 / 100 | 85 / 100 | 82 / 100 |
| 7  | Reed, Tyler      | 19 / 25   | 39 / 50   | 17 / 25   | 78 / 100 | 94 / 100 | 88 / 100 |
| 8  | Smith, Tyler     | 16 / 25   | 40 / 50   | 19 / 25   | 79 / 100 | 90 / 100 | 86 / 100 |
| 9  | Smith, Westin    | 15 / 25   | 45 / 50   | 17 / 25   | 87 / 100 | 85 / 100 | 91 / 100 |
| 10 | Vang, Seher      | 19 / 25   | 43 / 50   | 19 / 25   | 79 / 100 | 82 / 100 | 87 / 100 |

`pivot_wider` is the function

`names_from` give the *existing* column that contains the *new* columns we want to create

`values_from` gives the *existing* column that contains the values

# Pivoting case #2: *an observation is scattered across multiple rows*

What constitutes a variable and an observation depends on the circumstances  
Pivoting gets you to wide(r) or long(er) forms of the data

```
A tibble: 10 x 7
 Name `Score 1` `Score 2` `Score 3` `Test 1` Midterm Final
 <chr> <chr> <chr> <chr> <chr> <chr> <chr>
1 al-Jafri, Anas 17 / 25 41 / 50 18 / 25 87 / 100 89 / 100 90 / 100
2 Drum, Anyssa 19 / 25 40 / 50 19 / 25 88 / 100 87 / 100 92 / 100
3 Gonzales, David 18 / 25 38 / 50 19 / 25 84 / 100 91 / 100 83 / 100
4 Granger, Shannan 14 / 25 42 / 50 20 / 25 89 / 100 82 / 100 90 / 100
5 Kwak, Surabhi 16 / 25 41 / 50 21 / 25 85 / 100 88 / 100 93 / 100
6 Michels, Breana 17 / 25 46 / 50 18 / 25 80 / 100 85 / 100 82 / 100
7 Reed, Tyler 19 / 25 39 / 50 17 / 25 78 / 100 94 / 100 88 / 100
8 Smith, Tyler 16 / 25 40 / 50 19 / 25 79 / 100 90 / 100 86 / 100
9 Smith, Westin 15 / 25 45 / 50 17 / 25 87 / 100 85 / 100 91 / 100
10 Vang, Seher 19 / 25 43 / 50 19 / 25 79 / 100 82 / 100 87 / 100
```

*back to where we started*

# Separating: a single value consists of multiple pieces of data

| Name             | Quizzes |         |         | Tests    |          |          |
|------------------|---------|---------|---------|----------|----------|----------|
|                  | Score 1 | Score 2 | Score 3 | Test 1   | Midterm  | Final    |
| al-Jafri, Anas   | 17 / 25 | 41 / 50 | 18 / 25 | 87 / 100 | 89 / 100 | 90 / 100 |
| Drum, Anyssa     | 19 / 25 | 40 / 50 | 19 / 25 | 88 / 100 | 87 / 100 | 92 / 100 |
| Gonzales, David  | 18 / 25 | 38 / 50 | 19 / 25 | 84 / 100 | 91 / 100 | 83 / 100 |
| Granger, Shannan | 14 / 25 | 42 / 50 | 20 / 25 | 89 / 100 | 82 / 100 | 90 / 100 |
| Kwak, Surabhi    | 16 / 25 | 41 / 50 | 21 / 25 | 85 / 100 | 88 / 100 | 93 / 100 |
| Michels, Breana  | 17 / 25 | 46 / 50 | 18 / 25 | 80 / 100 | 85 / 100 | 82 / 100 |
| Reed, Tyler      | 19 / 25 | 39 / 50 | 17 / 25 | 78 / 100 | 94 / 100 | 88 / 100 |
| Smith, Tyler     | 16 / 25 | 40 / 50 | 19 / 25 | 79 / 100 | 90 / 100 | 86 / 100 |
| Smith, Westin    | 15 / 25 | 45 / 50 | 17 / 25 | 87 / 100 | 85 / 100 | 91 / 100 |
| Vang, Seher      | 19 / 25 | 43 / 50 | 19 / 25 | 79 / 100 | 82 / 100 | 87 / 100 |

The scores are actually  
two pieces of data

points earned / total points

We can't perform  
calculations on the scores  
in the current form

Need to separate the data

# Separating: *a single value consists of multiple pieces of data*

## R Code

```
.. code continued
Step 3: separate the scores
need to use the long form
#
dat_new <-
 separate(dat_long, score,
 into = c("points", "total"),
 sep = " / ", convert = TRUE)
print(dat_new)
```

## Output

```
A tibble: 60 x 4
 Name exam points total
 <chr> <chr> <int> <int>
 1 al-Jafri, Anas Score 1 17 25
 2 al-Jafri, Anas Score 2 41 50
 3 al-Jafri, Anas Score 3 18 25
 4 al-Jafri, Anas Test 1 87 100
 5 al-Jafri, Anas Midterm 89 100
 6 al-Jafri, Anas Final 90 100
 7 Drum, Anyssa Score 1 19 25
 8 Drum, Anyssa Score 2 40 50
 9 Drum, Anyssa Score 3 19 25
 10 Drum, Anyssa Test 1 88 100
... with 50 more rows
```

separate is the function

score in the column where we want to separate the data

into gives the new column names where the separated data will go

sep gives the part of the value that separates the individual pieces of data

convert say to convert the data into numbers after separating (they are currently “words”)

# Separating: *a single value consists of multiple pieces of data*

```
A tibble: 60 x 4
 Name exam points total
 <chr> <chr> <int> <int>
1 al-Jafri, Anas Score 1 17 25
2 al-Jafri, Anas Score 2 41 50
3 al-Jafri, Anas Score 3 18 25
4 al-Jafri, Anas Test 1 87 100
5 al-Jafri, Anas Midterm 89 100
6 al-Jafri, Anas Final 90 100
7 Drum, Anyssa Score 1 19 25
8 Drum, Anyssa Score 2 40 50
9 Drum, Anyssa Score 3 19 25
10 Drum, Anyssa Test 1 88 100
... with 50 more rows
```

The scores have been converted  
into two new columns:  
points & total

We can now perform calculations  
on these numbers

This wasn't possible before  
because they were "words"

# High-level takeaways

- Real world data is often messy, and we (usually) need to make it tidy before you can start to work with it
- Messiness can occur in different ways
  - A variable is spread across multiple columns → `pivot_longer`
  - An observation is spread across multiple rows → `pivot_wider`
  - Multiple pieces of data exist in a single cell → `separate`
  - ... lots of other (often unexpected) ways...
- As you work with data more, you'll begin to see patterns in messy data and how to fix them to get tidy data

# Resources

- Paper on tidy data by H. Wickham  
<https://vita.had.co.nz/papers/tidy-data.pdf>
- R For Data Science, section on tidy data  
<https://r4ds.had.co.nz/tidy-data.html>
- tidyr package website  
<https://tidyverse.org>
- Data importing cheat sheet  
<https://github.com/rstudio/cheatsheets/blob/master/data-import.pdf>



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# Intro to R Functions

ASMS 2022: R Short Course

SHORT COURSES

June 4 - 5

#ASMS2022

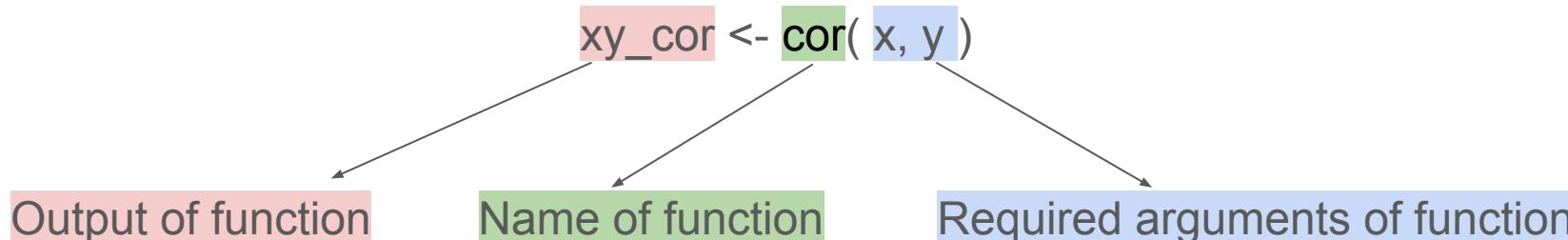
# Goals for this module

- Introduction to using R Functions and getting help to use R functions (using documentation)
- Understand structure of a function (name, arguments, return object)
- Understand that functions described here can be made more effective and concise when used in conjunction with the *tidyverse*

# R functions and why/how to use them

- Many of the important classes tell you something about the *shape* of the data
- Others do very simple but common *statistics*
- There are many other types of useful functions, it's impossible to catalogue them all here

# Using an R function: cor() example (correlation)



- Object defined by function
- Defined in package
- Separated by comma ,

- **Some arguments are optional**

```
correlation function example
x <- c(1,2,3,4)
y <- c(2,4,6,10)

xy_cor <- cor(x,y)
```

```
xy_cor_spearman <- cor(x,y, method="spearman")
```

In arguments  
you use =,  
not <-

Optional argument of function

- Often sets parameters of data but has defaults

# Using an R function: getting help for specific function

```
get docs on cor() function
?cor
```

The screenshot shows the RStudio interface with the 'Viewer' tab selected. The main pane displays the documentation for the `cor` function from the `stats` package. The title is "Correlation, Variance and Covariance (Matrices)". The "Description" section states that `var`, `cov` and `cor` compute the variance of `x` and the covariance or correlation of `x` and `y` if these are vectors. If `x` and `y` are matrices then the covariances (or correlations) between the columns of `x` and the columns of `y` are computed. The "Usage" section shows the function signatures for `var`, `cov`, `cor`, and `cov2cor`. The "Arguments" section defines `x` as a numeric vector, matrix or data frame, and `y` as NULL (default) or a vector, matrix or data frame with compatible dimensions to `x`. The default is equivalent to `y = x` (but more efficient). A green box highlights the command `?cor` at the top of the code input area.

- **Most R packages are well-documented**

We can conveniently view documentation documentation for the package within RStudio.

- **Using the ? and ?? commands**

- `? = find function/package`  
documentation for what has been loaded
- `?? = search installed packages for key words`

# Using an R function: exploring functionality

```
search for functions and package
info about t-testing
??ttest
```

- **Searching with ?? can give a lot of results so check carefully the documentation of a function to make sure it is appropriate**

The screenshot shows the R Help browser interface. At the top, there is a menu bar with tabs: Files, Plots, Packages, Help, and Viewer. Below the menu is a toolbar with icons for back, forward, home, and search. A search bar contains the text "R: Search Results" and a "Find in Topic" button. The main content area has a title "Search Results" next to a large blue R logo. Below the title, there is a section titled "Vignettes:" which lists a single item: [survival::tests](#) Cox models and ``type 3'' Tests. To the right of this item are links for PDF, source, and R code. The next section is "Code demonstrations:" which lists [tcltk::tkttest](#) t-test example of GUI interface to a function call. To the right of this item is a link to run the demo in the console. The final section is "Help pages:" which lists several base functions: [base::all.equal](#) Test if Two Objects are (Nearly) Equal, [base::base-defunct](#) Defunct Functions in Package 'base', [base::gettext](#) Translate Text Messages, [base::identical](#) Test Objects for Exact Equality, [base::is.unsorted](#) Test if an Object is Not Sorted, [base::isS4](#) Test for an S4 object, [base::isSymmetric](#) Test if a Matrix or other Object is Symmetric (Hermitian), [base::sprintf](#) Use C-style String Formatting Commands, and [class::lvqtest](#) Classify Test Set from LVQ Codebook.

# Functions to learn about the shape of data

```
functions to get the shape of a dataset
```

```
with vectors, there is only one shape property,
that is the Length
```

```
length(ms_mz) ←
```

Number of elements in vector

```
with data.frames, there is much more information
to obtain about the shape
```

```
the basics
```

```
nrow(protein_id_df)
```

```
ncol(protein_id_df) ←
```

Number of rows and cols in df

- If we remember the previous data.frame examples, to add columns or rows, we needed to match the existing size of the data.frame, these checks can help us make sure new data is formatted correctly

# Functions to learn about the shape AND type of data

- We have reviewed how R vectors and data.frames have types: numeric, character, logical, etc.
- Sometimes we would like to check and summarize these types in a complex data.frame

```
str(protein_id_df)
```



```
> str(protein_id_df)
'data.frame': 5 obs. of 7 variables:
 $ proteins : Factor w/ 5 levels "protein1","protein2",..: 1 2 3 4 5
 $ retention_times : num 10.2 15.2 12.2 9.1 17.3
 $ sum_ms1_intensities: num 20000 50000 1000 2000 30000
 $ n_ms2_transitions : int 2 4 3 1 1
 $ fdr : num 0.11 0.03 0.02 0.15 0.06
 $ seq_coverage : num 0.63 0.65 0.55 0.9 0.82
 $ in_ds2 : logi TRUE TRUE FALSE FALSE TRUE
```

# Summary statistics

We can use `mean()`, `sd()`, `median()`, `quantile()` for basic statistics on numerical vectors

```
get count information for values in a data.frame vector
table(protein_id_df$in_ds2)
```

```
> table(protein_id_df$in_ds2)
```

```
FALSE TRUE
2 3
```

```
get sumary statistics
summary(protein_id_df$sum_ms1_intensities)
```

```
> summary(protein_id_df$sum_ms1_intensities)
Min. 1st Qu. Median Mean 3rd Qu. Max.
1000 2000 20000 20600 30000 50000
```

# Files and directories functions

```
list.files('directory', pattern='*.csv') ← Find .csv files in 'directory'
```

```
list.files('directory', pattern=".csv", recursive=T, full.names=T) ← Find .csv files
Get full names
Search all subfolders
```

```
read.csv("path_to_csv.csv", header=T) ← Read .csv file
First line is imported as column names
```

```
write.csv(protein_id_df, 'protein_id_df.csv') ← Save a .csv of a data.frame
```

# Bioconductor: package resource for -omics type data

- Need a separate package installation manager : [Bioconductor Install](#)
- Many packages for MS data of all varieties using a common data structure



# Creating an R function: background

- **When:** You have solidified a procedure into R code and will use it repeatedly in your work with future data
- **Advantages:** concise data workflow, repeatability (constant copy and pasted a code snippet and making small edits leads to errors!, feeling like a “real” computer programmer)
- **Things to keep in mind:** Parameters of your function (i.e., arguments), how much optionality will be needed each time a function is run to do what you want it to do

# Creating a simple R function

```
rms_normalization <- function(x){
 # do root mean square calculation of vector
 norm_vec <- x^2
 norm_vec <- mean(norm_vec)
 norm_val <- sqrt(norm_vec)
 x_normalized <- x / norm_val
 return(x_normalized)
}
```

Function name

“function” definition function

“return()”  
Determines the output of the function

# Using the function

```
rms_normalization(peak_data$intensity)
```

```
peak_data$intensity_rms <- rms_normalization(peak_data$intensity)
```

# Saving functions and accessing them later

- **Simple:** You can always define functions at the beginning of your script
- If you start to have a large number of functions, it may be worthwhile saving them in then outside of your current working script and loading them using  
`source("path/to/myscript.R")`
- When you've done something very nice that you believe others may be interested in using then you could create a package, ***forewarning:*** there are some hurdles to get over if you want your package hosted by CRAN

# Function takeaways

- There are many things you can do with R with functions: understand data structure, descriptive and inferential statistics, and much, much more
- Additional packages will need to be installed to access much of this functionality
- You will likely need a MS specific package to load in raw MS data for analysis, resources like Bioconductor provide many great packages specific to MS

# Resources

- [R for Data Science](#) **Essential**
- [R - Functions](#) **Some advanced ideas, exploring making your own functions**
- [A Tutorial on Using Functions in R! \(and their scoping\)](#) **Some advanced ideas, exploring making your own functions**



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# Wrap-up & Next Steps

ASMS 2022: R Short Course

SHORT COURSES

June 4 - 5

#ASMS2022

# High-level Review

- The basics of R and how to start working with R using RStudio
  - The RStudio interface
  - Using RStudio projects to organize your work
  - Basic R syntax
- Some of the fundamental features and structure of the R language
  - Working with data using vectors and data frames
  - Useful functions in R for getting work done
- What tidy data is, why it's important & ways to analyze tidy data
  - How the tidyverse R packages and tidy data help streamline the process of working with data
  - How to use dplyr to perform data analysis tasks
- Data visualization in R using ggplot2
  - Background information about visualization concepts with ggplot2
  - How to put together basic (and even more complex) plots with ggplot2

# Are you now able to...

- start-up RStudio and make an RStudio project?
- read a .csv or Excel file into R?
- understand basic properties about the data (e.g. # rows, cols)?
- tell someone what tidy data is and why it's important?
- perform some basic data manipulations and operations on the data?
- make a simple plot from the data?

# Resources – Websites

- RStudio: <https://rstudio.com/>
- The tidyverse: <https://www.tidyverse.org/>
- ggplot2 documentation: <https://ggplot2.tidyverse.org/reference/>
- Shiny: <https://shiny.rstudio.com/>
- RMarkdown: <https://rmarkdown.rstudio.com/>
- Twitter hash-tags: #rstats, #DataScience

# Resources – Books

- Hands on Programming with R: <https://rstudio-education.github.io/hopr/>
- R for Data Science: <https://r4ds.had.co.nz/>
- ggplot2: <https://ggplot2-book.org/>
- R Markdown: <https://bookdown.org/yihui/rmarkdown/>

# People/Orgs to Follow

- RStudio
- Hadley Wickham (@hadleywickham)
- Jenny Bryan (@JennyBryan)
- Julia Silge (@juliasilge)
- Mara Averick (@dataandme)
- David Robinson (@drob)

# Where to get help

- Google is a good place to start
  - copy error messages and search with quotes: “*error message here*”
  - try to use R specific/centric terms when possible in your search, e.g. data frame, tidyverse, package names, etc.
- Google will often link you to Stack Overflow <https://stackoverflow.com/>, you can often get good help here, but it can be a mixed bag
- RStudio Community <https://community.rstudio.com/> is a great, friendly place to search for help and solutions, but not as extensive as Stack Overflow (yet?); worth it to just browser the topics
- Join a local R Users group (highly recommended!)

# How to ask for help

- It's very easy to ask for help online now, e.g. on Stack Overflow, but it can also be intimidating and sometimes responses might not always be positive (surprise: people can be mean on the internet 😱!)
- Before asking for help
  - Try to do background research on the problem; be sure to use Google first
  - Make it as easy as possible for people to help you, try to state your problem concisely
  - Read about making reproducible examples: <https://www.tidyverse.org/help/>
  - Read a site's rules about posting and asking for help
- If you post a question, be sure to follow-up with anyone who helps; did the suggestions work? Did they help solve the problem? Are you still stuck?

# Proposed plan for next steps

- Try to practice with R a little bit every day, much better than longer sessions spread farther apart
- Take simple R code examples that you understand, and try to re-type them yourself (without looking/copy/pasting) – helps with understanding syntax and debugging syntax errors
- Give yourself small data tasks that apply to your daily work so you can practice things that are also useful to what you do
- Take small steps and slowly build on what you know to expand your expertise

# Homework

1. Choose a simple data task you've already done (maybe in Excel?),  
e.g. a simple plot, a table of summary stats, computing a value from a data set
2. Try to reproduce the task in R using only R code; you can check your results to make sure they match (doesn't have to be *exactly* the same)
3. Think about ways you might change your data analysis workflow for future projects

# We'd love to get your feedback!

What worked for you, what didn't?

What parts were difficult to understand

What else would you like to learn in a intro class like this?

Slower pace? Faster pace?

More examples and practice sessions?

Thank you very much!