UCLA QCBio

Collaboratory

Advanced data visualization with ggplot2

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2024 Fall

UCLA Bioinformatics

Notation of the slides

- `Code or Pseudo-Code` chunk starts with " ➢ ", e.g.
  - ➢ `print("Hello world!")`

- [Link](#) is underlined

- Important terminology is in **bold** font

- Practice comes with

Workshop goals

- Master the syntax and grammar of ggplot2

- Use online resources to to generate publication-quality figures

- Develop a mindset and taste for better data visualizations

Agenda

- Day 1: Data visualization basics
  - Getting started with ggplot2
  - Recap of data wrangling functions

- Day 2: Building a plot layer by layer
  - Exploring different plot types
  - Getting more control on the plots

- Day 3: Examples and useful packages
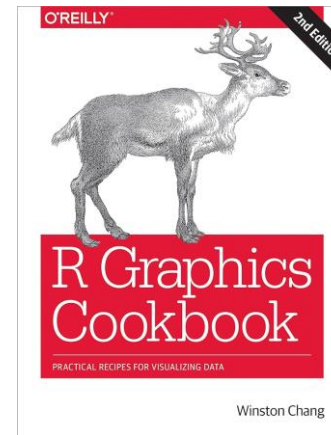 - Practical examples and principles
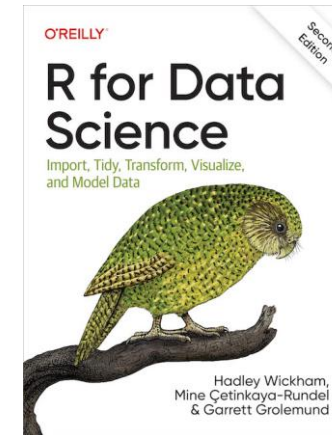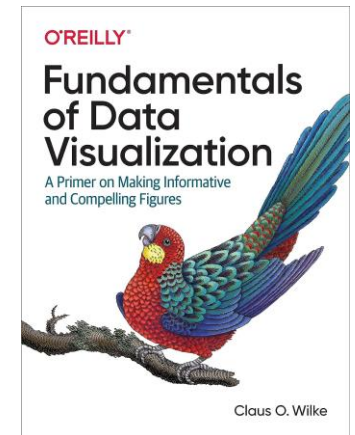 - Introducing some useful packages
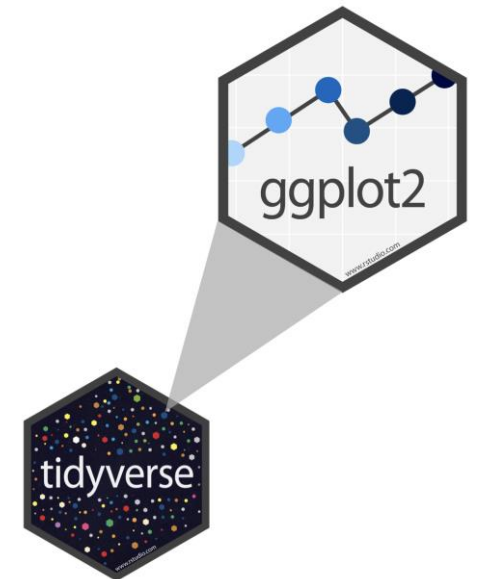
Reference
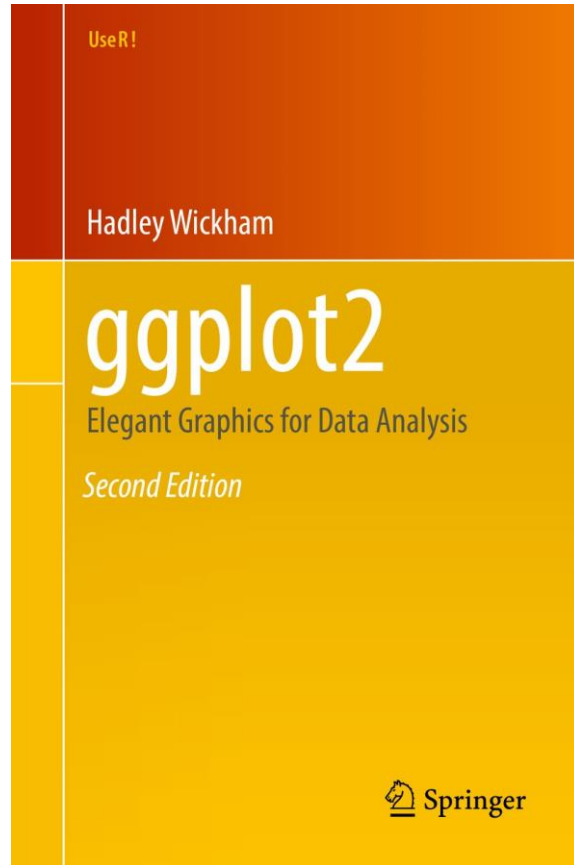
link

- Other useful references

link

link

link

The creator

*"**for influential work in statistical computing, visualization, graphics, and data analysis**; for developing and implementing an impressively comprehensive **computational infrastructure for data analysis through R** software; for making statistical thinking and computing accessible to large audience; and for enhancing an appreciation for the important role of statistics among data scientists."*

—— 2019 COPSS President's Award

Hadley Wickham
Chief Scientist, Rstudio/posit

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Environment setup

- Go to the official download website

Environment setup

- Go to the official download [website](#)

- Install R and RStudio desktop based on your operating system

The Comprehensive R Archive Network

Download and Install R

Precompiled binary distributions of the base system and contributed packages, **Windows and Mac** users most likely want one of these versions of R:

- Download R for Linux (Debian, Fedora/Redhat, Ubuntu)
- Download R for macOS
- Download R for Windows

R is part of many Linux distributions, you should check with your Linux package management system in addition to the link above.

Source Code for all Platforms

Windows and Mac users most likely want to download the precompiled binaries listed in the upper box, not the source code. The sources have to be compiled before you can use them. If you do not know what this means, you probably do not want to do it!

- The latest release (2023-10-31, Eye Holes) R-4.3.2.tar.gz, read what's new in the latest version.

- Sources of R alpha and beta releases (daily snapshots, created only in time periods before a planned release).

- Daily snapshots of current patched and development versions are available here. Please read about new features and bug fixes before filing corresponding feature requests or bug reports.

- Source code of older versions of R is available here.

- Contributed extension packages

Questions About R

- If you have questions about R like how to download and install the software, or what the license terms are, please read our answers to frequently asked questions before you send an email.

Environment setup

- Go to the official download website

- Install R and RStudio desktop based on your operating system

- Install the necessary package(s) in RStudio Console
  - ➢ `install.packages("tidyverse")`

Day 1: Data visualization basics

Wenbin Guo
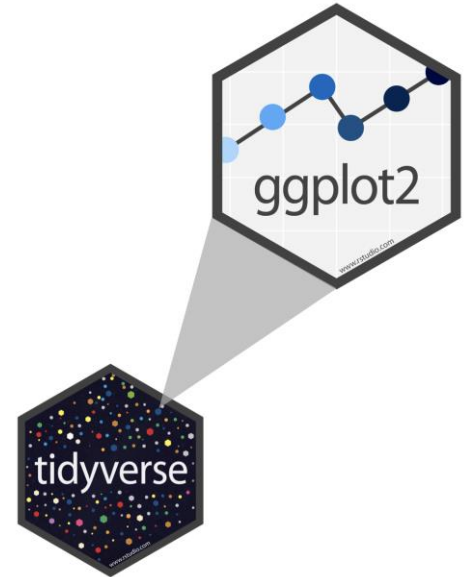
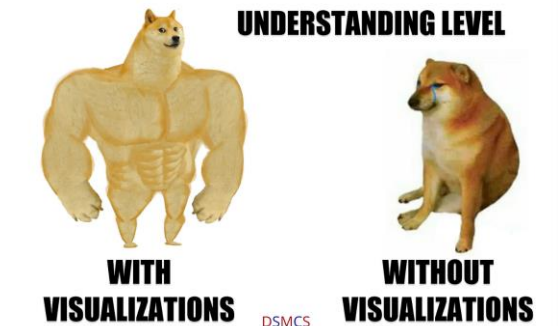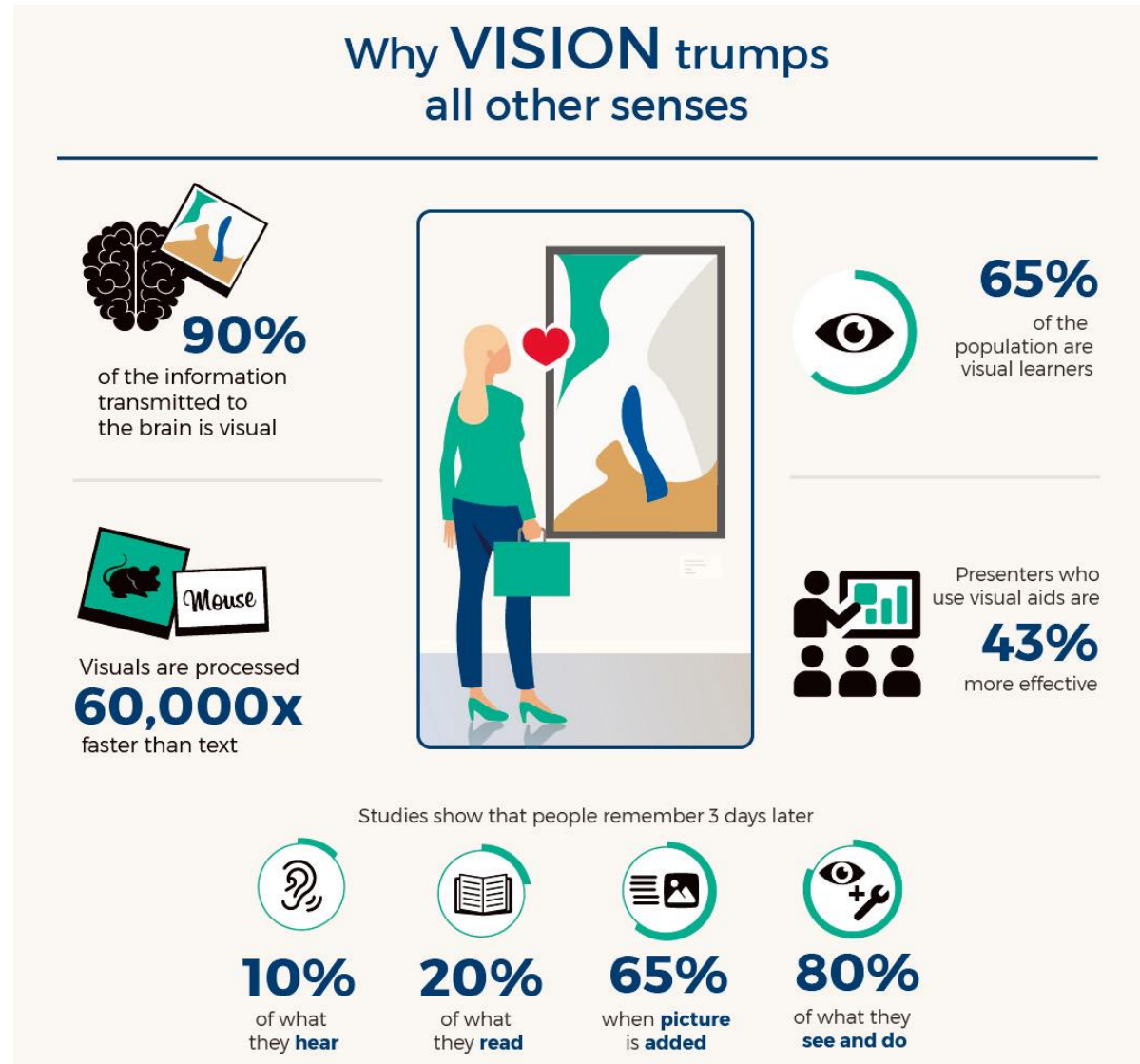Bioinformatics IDP, UCLA

wbguo@ucla.edu

2024 Fall

Overview

Time

- 3-hour workshop (45min + 45min + 30min + practice/Q&A)

Topics

❑ Introduction

❑ Getting started with `ggplot2`

❑ Recap of data wrangling functions

- Variable types, factors, data frame
- `dplyr::filter(), select(), mutate(), left_join(), bind_rows()` …
- `tidyr::pivot_longer(), pivot_wider()` …

❑ Aesthetic mapping

Facts on how our brain reacts to visuals

Why **VISION** trumps all other senses

90% of the information transmitted to the brain is visual

Visuals are processed **60,000x** faster than text

65% of the population are visual learners

Presenters who use visual aids are **43%** more effective

Studies show that people remember 3 days later

10% of what they **hear**

20% of what they **read**

65% when **picture** is **added**

80% of what they **see and do**

UNDERSTANDING LEVEL

WITH VISUALIZATIONS — WITHOUT VISUALIZATIONS

DSMCS

"A picture may be worth a thousand words"

Example

But the visualization can be imprecise   (e.g. the distance between planets)

"A picture may be worth a thousand words"

Remark Whether the traversal is clockwise, is undefined in the case of the degenerate triangle, i.e. a "triangle" with its vertices on a straight line, but in that case its area equals zero and its sign is irrelevant. Also, please note that the theorems
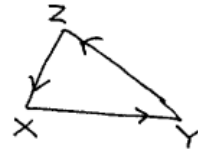
$$\triangle XYZ = -\triangle ZYX$$
$$\triangle XYZ = \triangle YZX$$

hold independently of the sign of $\triangle XYZ$, i.e., for both
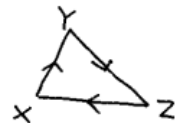
A picture may be worth a thousand words, a formula is worth a thousand pictures. (End of Remark.)

—— *A first exploration of effective reasoning* (1996)

Edsger Dijkstra
(1930-2002)

"A formula is worth a thousand pictures"

A picture may be worth a thousand words,
a formula is worth a thousand pictures.
(End of Remark.)

Newton's law of gravitation:

$$F_1 = F_2 = G \frac{m_1 \times m_2}{r^2}$$

R = radius of Earth

force

R 2R 3R 4R 5R
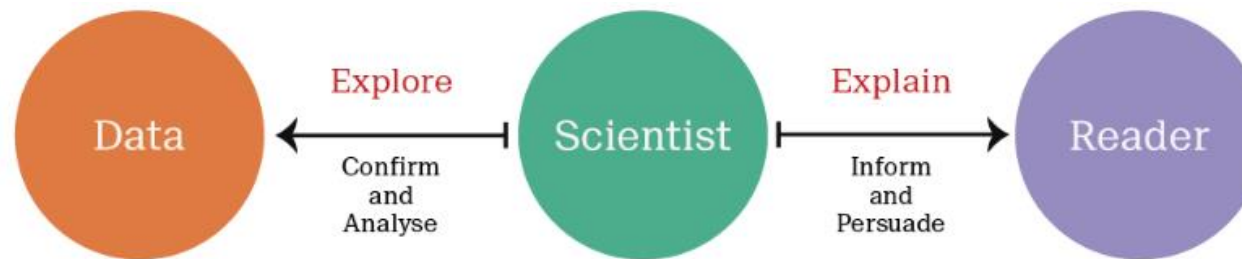distance from centre of Earth
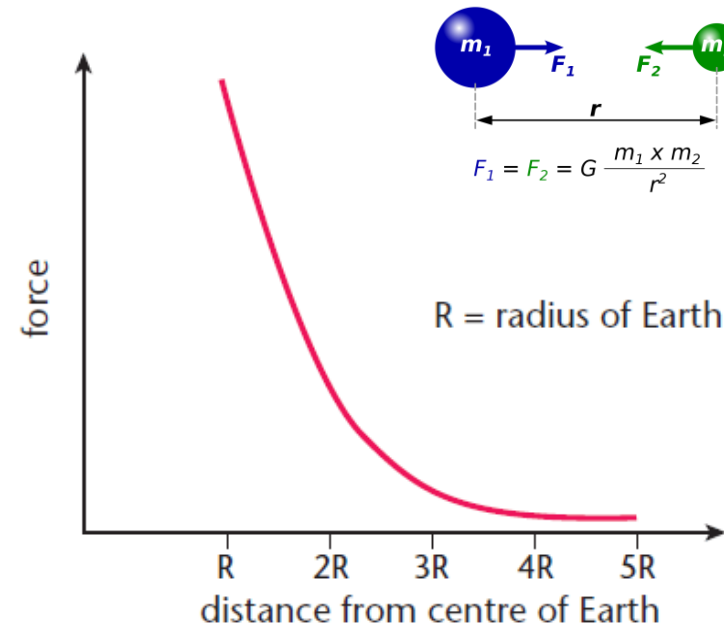
Formula annotation can
make figure more **accurate**

Question: What is worth than a thousand formulas?

The role of data visualization in science
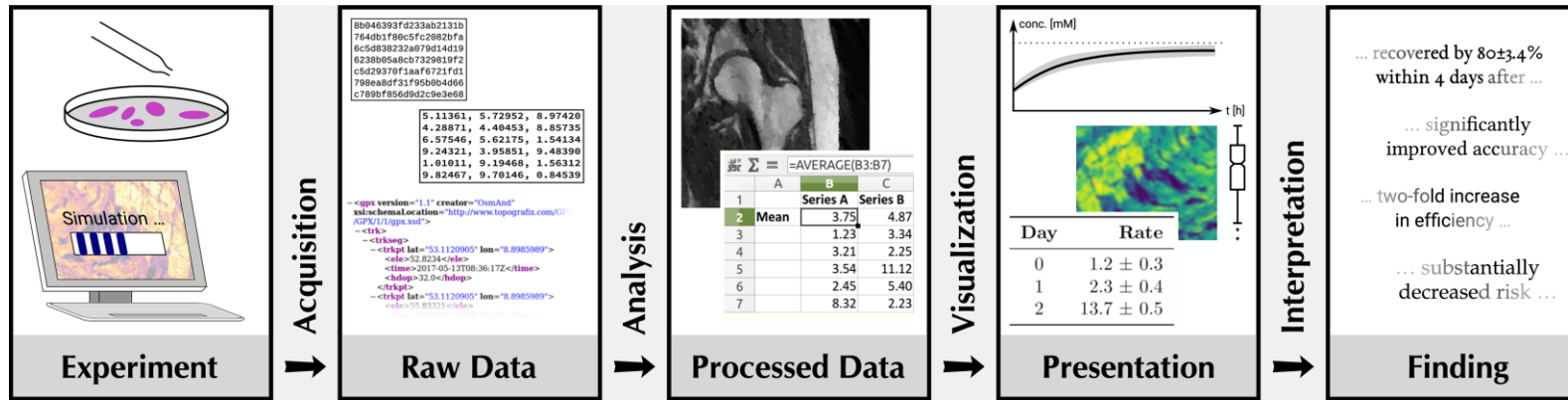
Typical steps in scientific work involving data analysis
(Schwen et al. *Plos Computational Biology*, 2018)

As a scientist, we use data visualization techniques to explore and explain

The role of data visualization in science (example)

Boxplot/Violin plot

Bar plot

Scatter plot

Histogram

Line plot

Heatmap

And more …

Terekhanova, et al. *Nature* (2023)
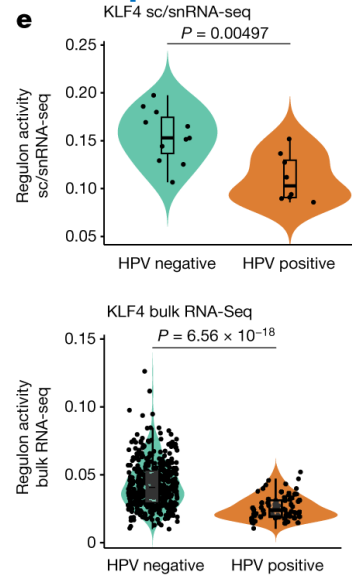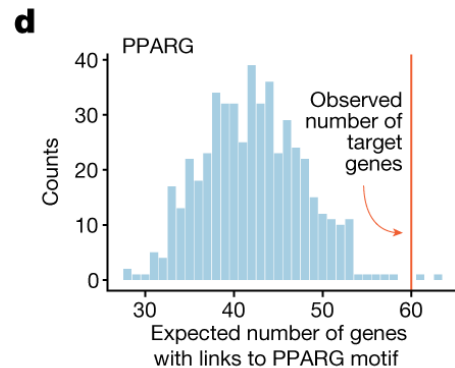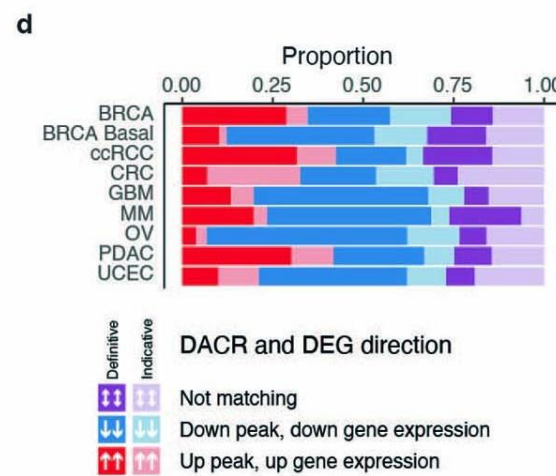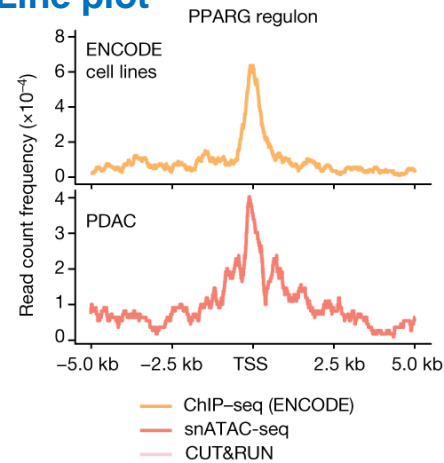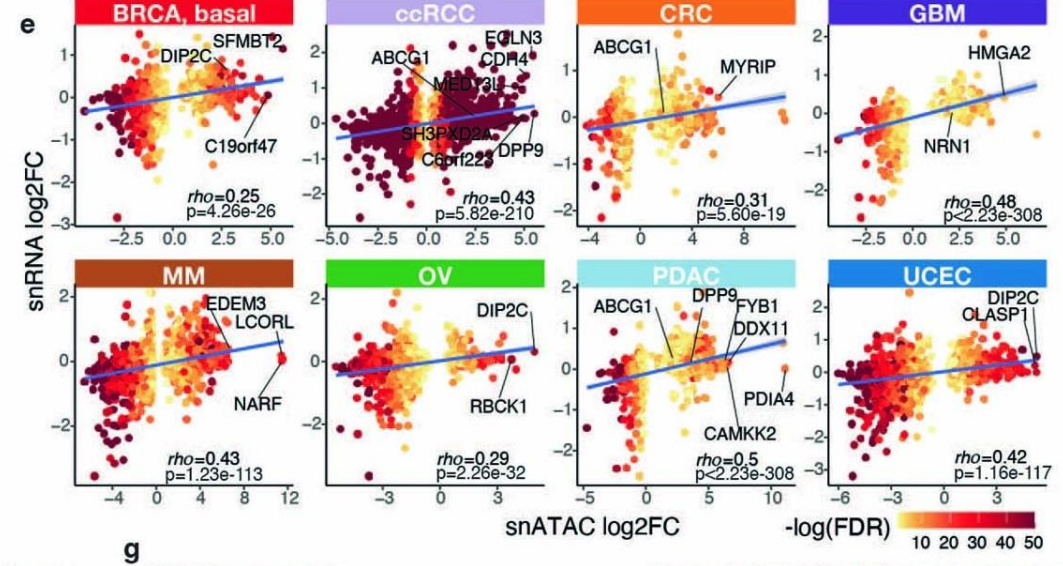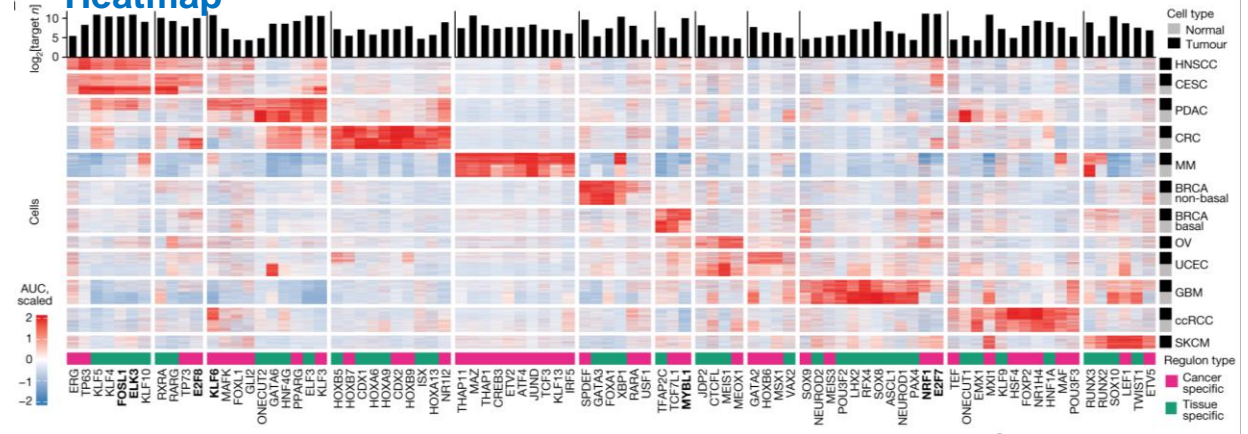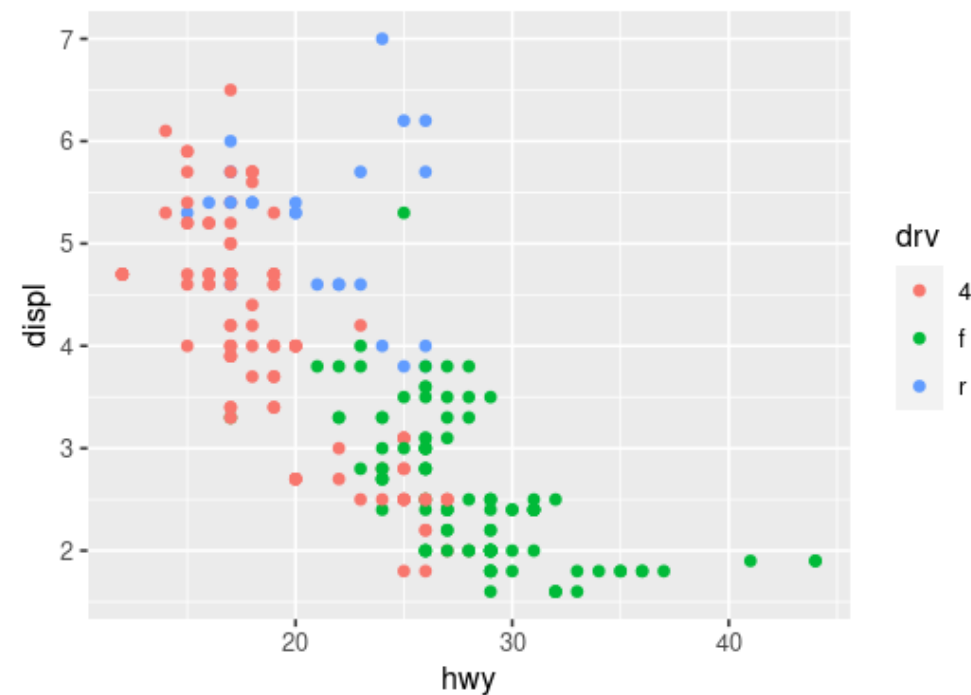
ggplot2: a core member of tidyverse
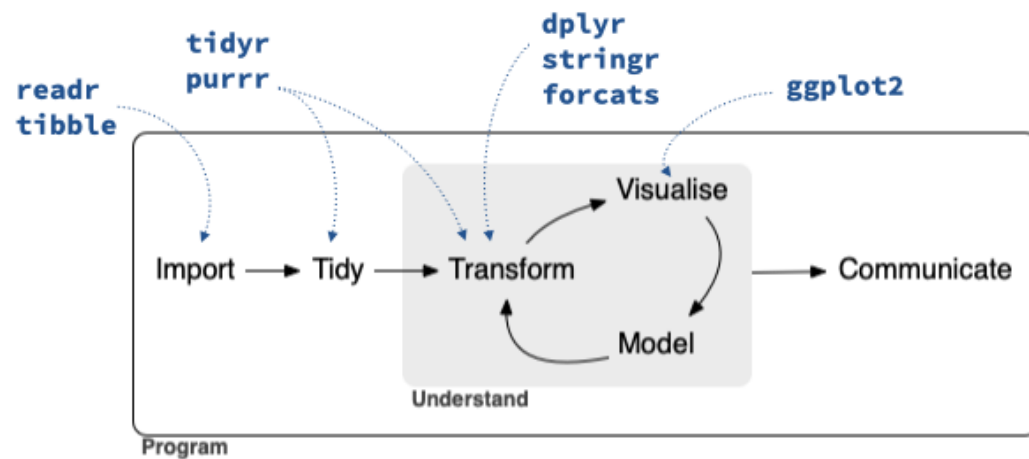
a typical data science project

tidyverse: a collection of R packages for data science

Idea behind ggplot2 visualization

Take scatter plot as an example

Data source: mpg

Idea behind ggplot2 visualization

Take scatter plot as an example

Data source: mpg

Create a ggplot object

Create the initial plot object

➢ ggplot(data = NULL, mapping = aes(), ...)

❑ data: dataset to use for plot

❑ mapping: list of aesthetic mappings to use for plot

❑ … : other arguments

- The data = and mapping = specifications are optional, so long as the data and mapping are passed into the function in the right order

- ggplot() is usually followed by a plus sign (+) to add additional components/**layers** to the plot
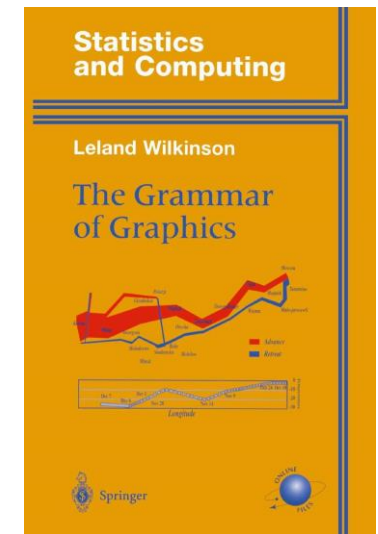
Key components of a ggplot object

- The **data**
- A set of **aesthetic mappings** between *variables* and *visual properties*
- At least one **layer** describing how to render the observations
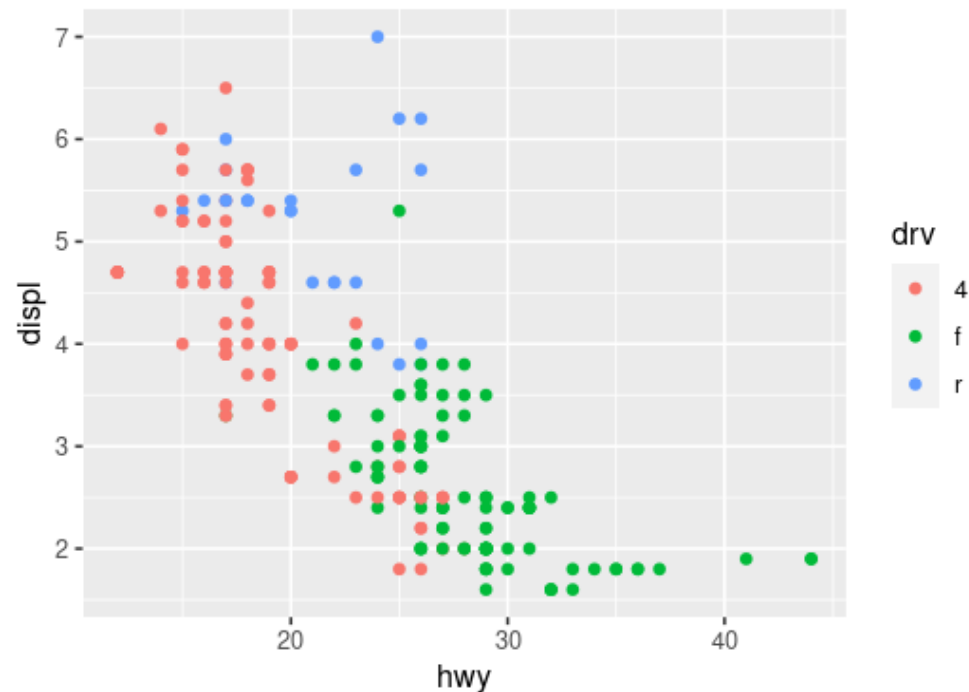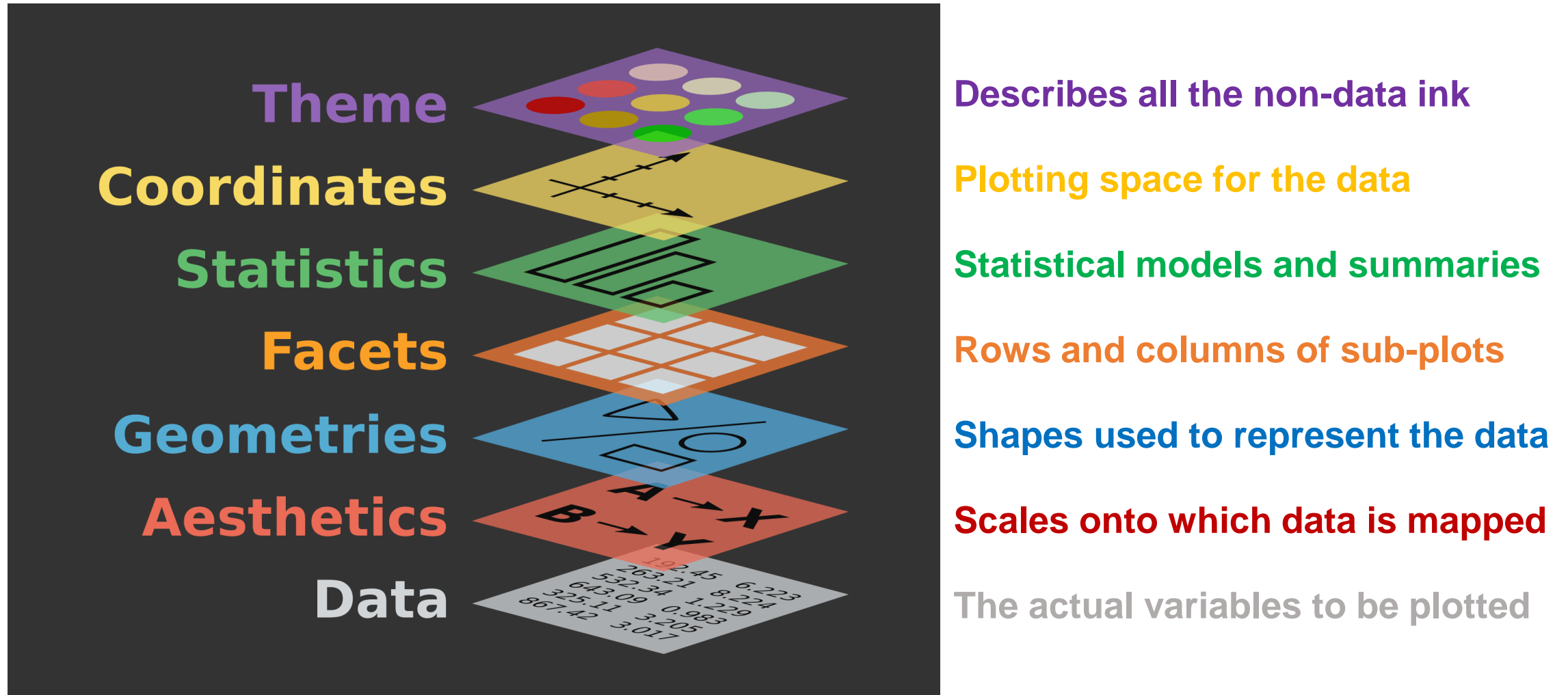
The layered grammar of graphics
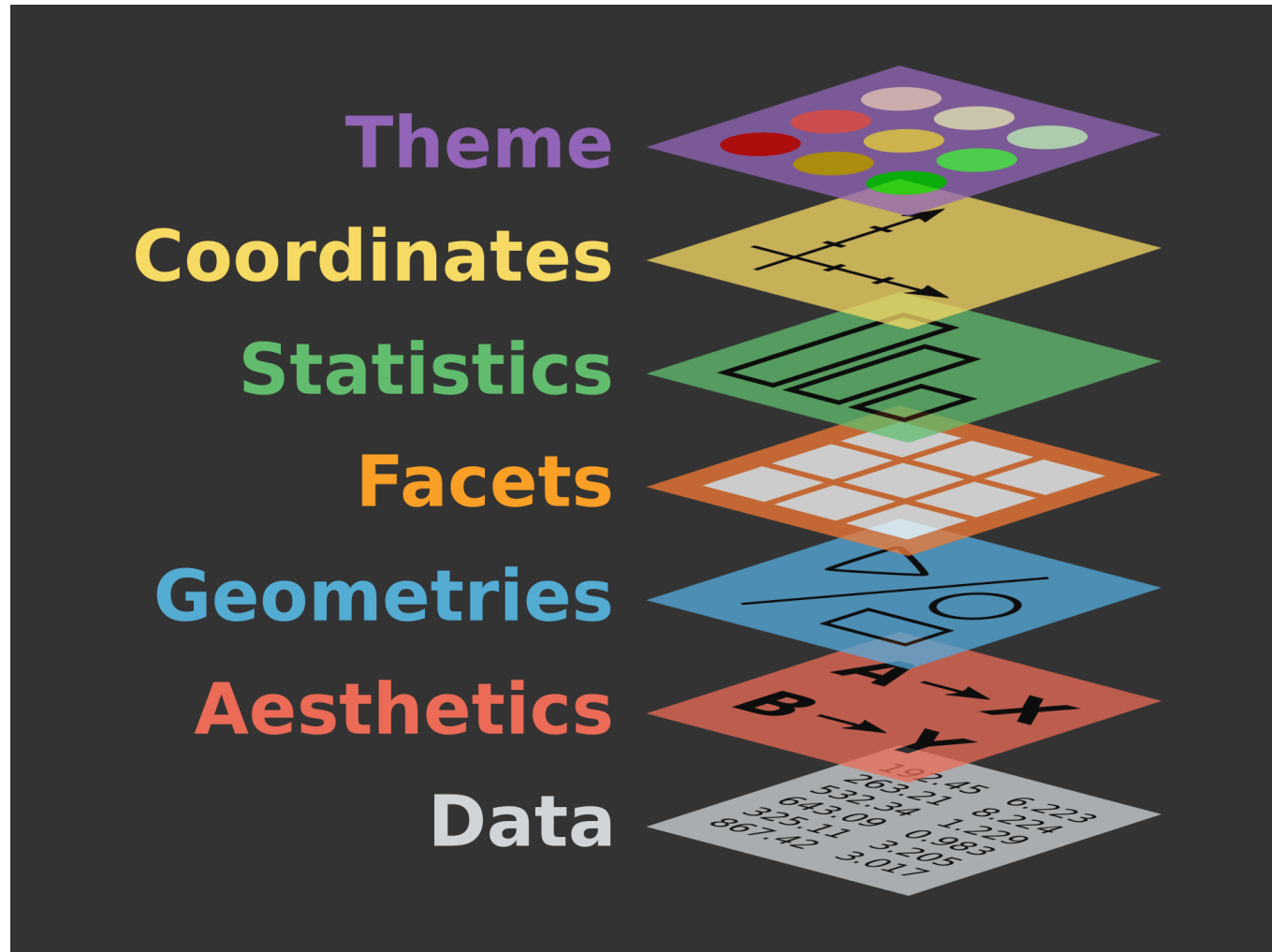
Leland Wilkinson
(1944-2021)

The Grammar of Graphics (1999)

The layered grammar of graphics

Components of the layered grammar

❑ A default dataset and set of mappings from variables to aesthetics

❑ One or more layers, each composed of
  - a geometric object (visual object in the plot)
  - a statistical transformation
  - a position adjustment
  - optionally, a dataset and aesthetic mappings

```
p + layer(
  mapping = NULL,
  data = NULL,
  geom = "point",
  stat = "identity",
  position = "identity"
)
```

➢ `p + geom_point()`

❑ One scale for each aesthetic mapping
  - maps values in data space to values in aesthetic space

❑ A coordinate system
  - maps data coordinates to the graphic plane

❑ The faceting specification
 - specifies how to display subsets of data

3 ways to invoke `ggplot()`

➢ `ggplot(data = df, mapping = aes(), ...)`
- when all layers use the same data and the same set of aesthetics

➢ `ggplot(data = df)`
- when layers use the same data, but use different aesthetics

➢ `ggplot()`
- when multiple data frames are used to produce different layers

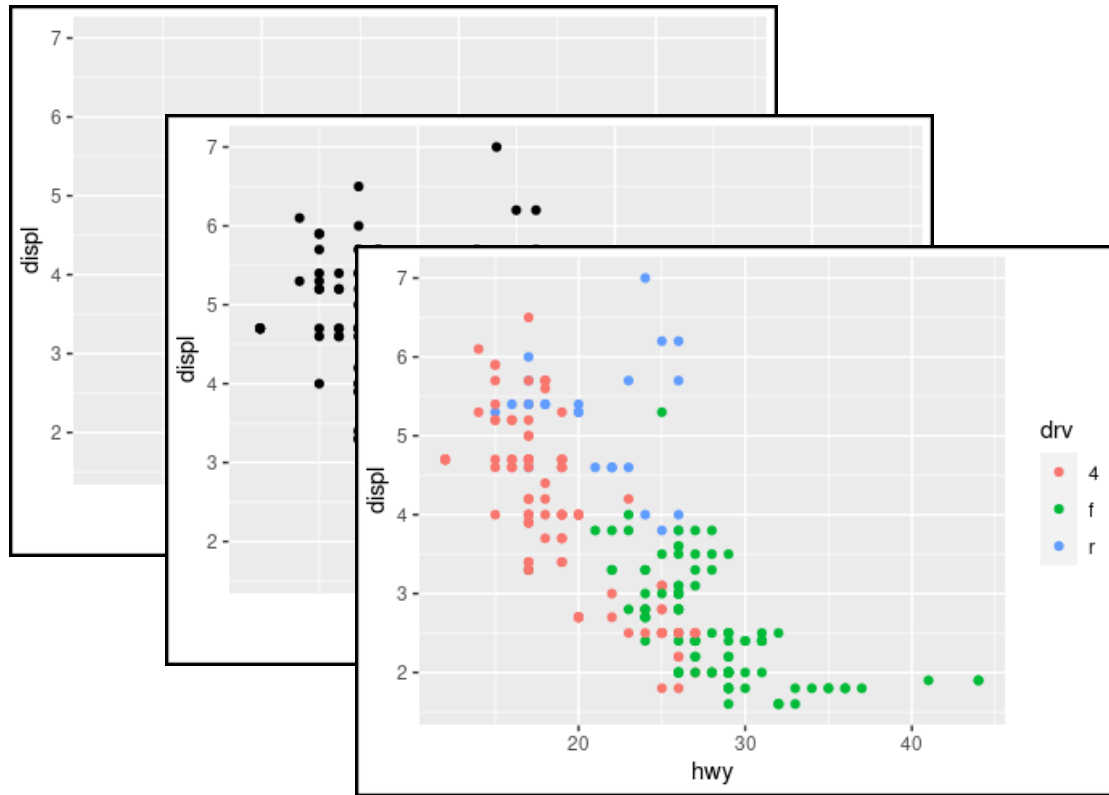# Building plots layer by layer (example)
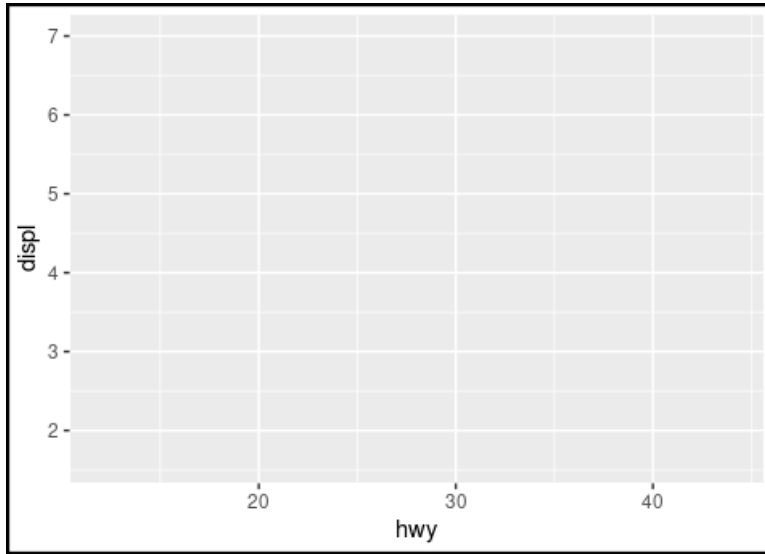

```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base
```

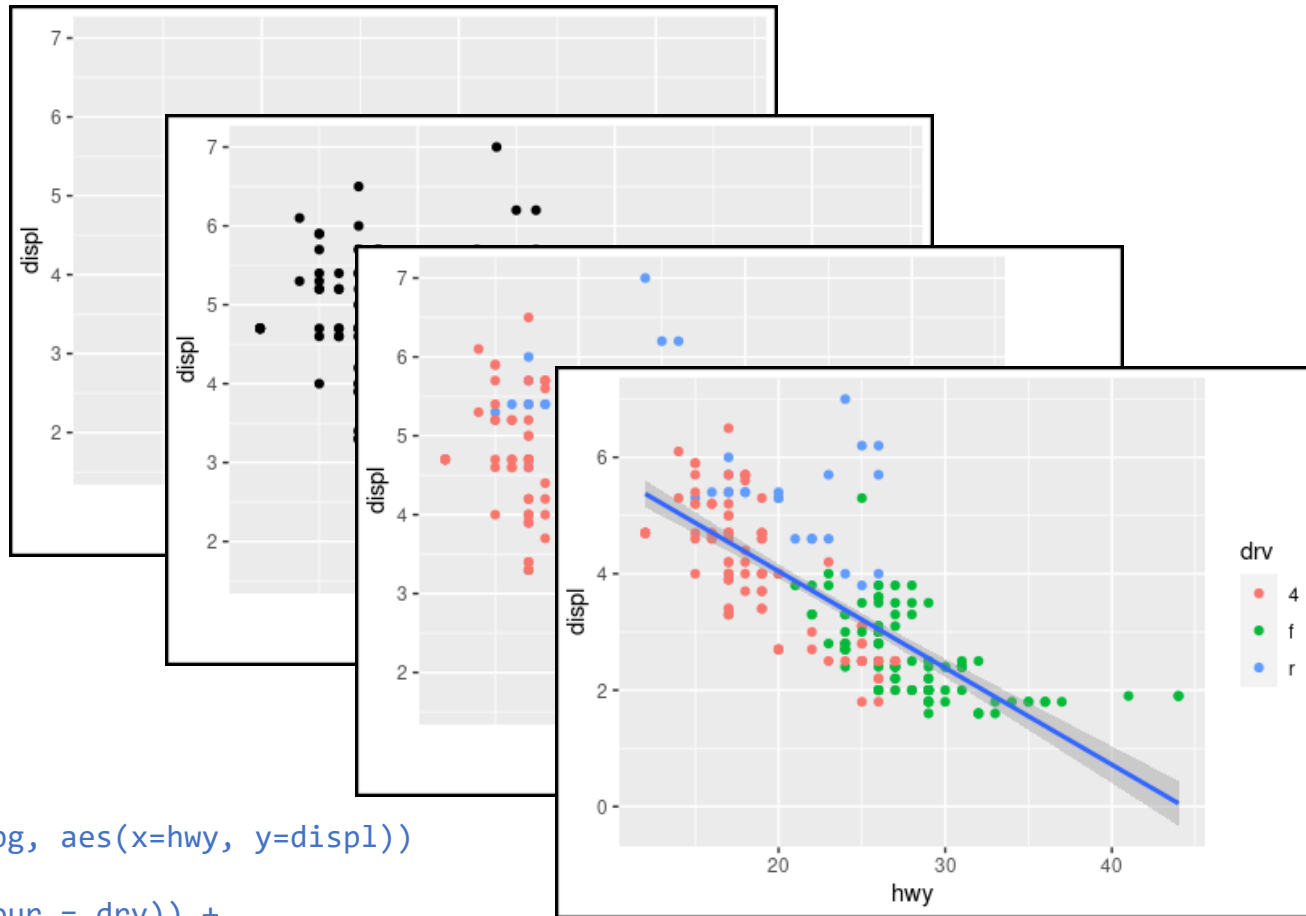# Building plots layer by layer (example)
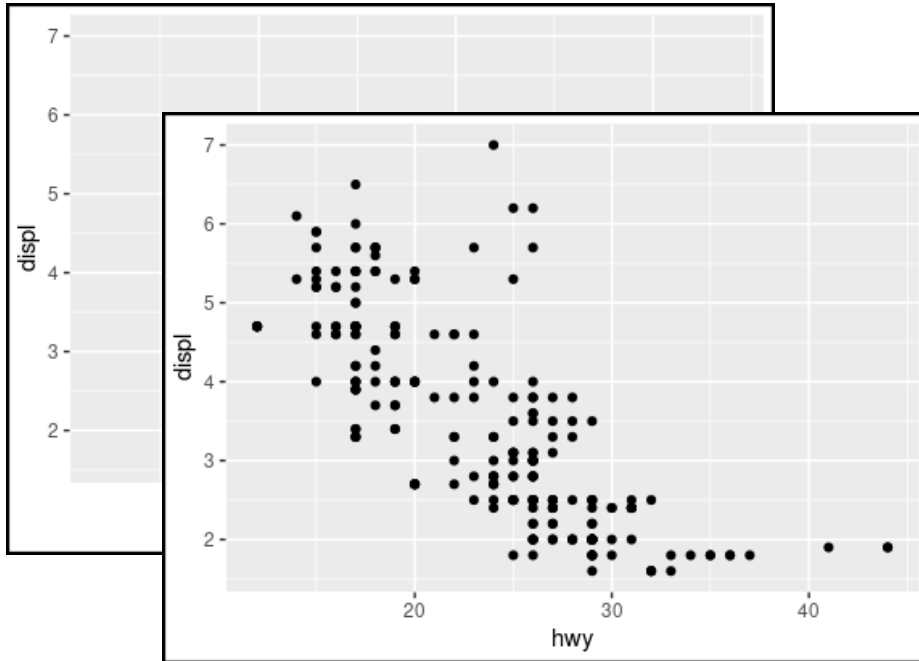

```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base +
  geom_point()
```

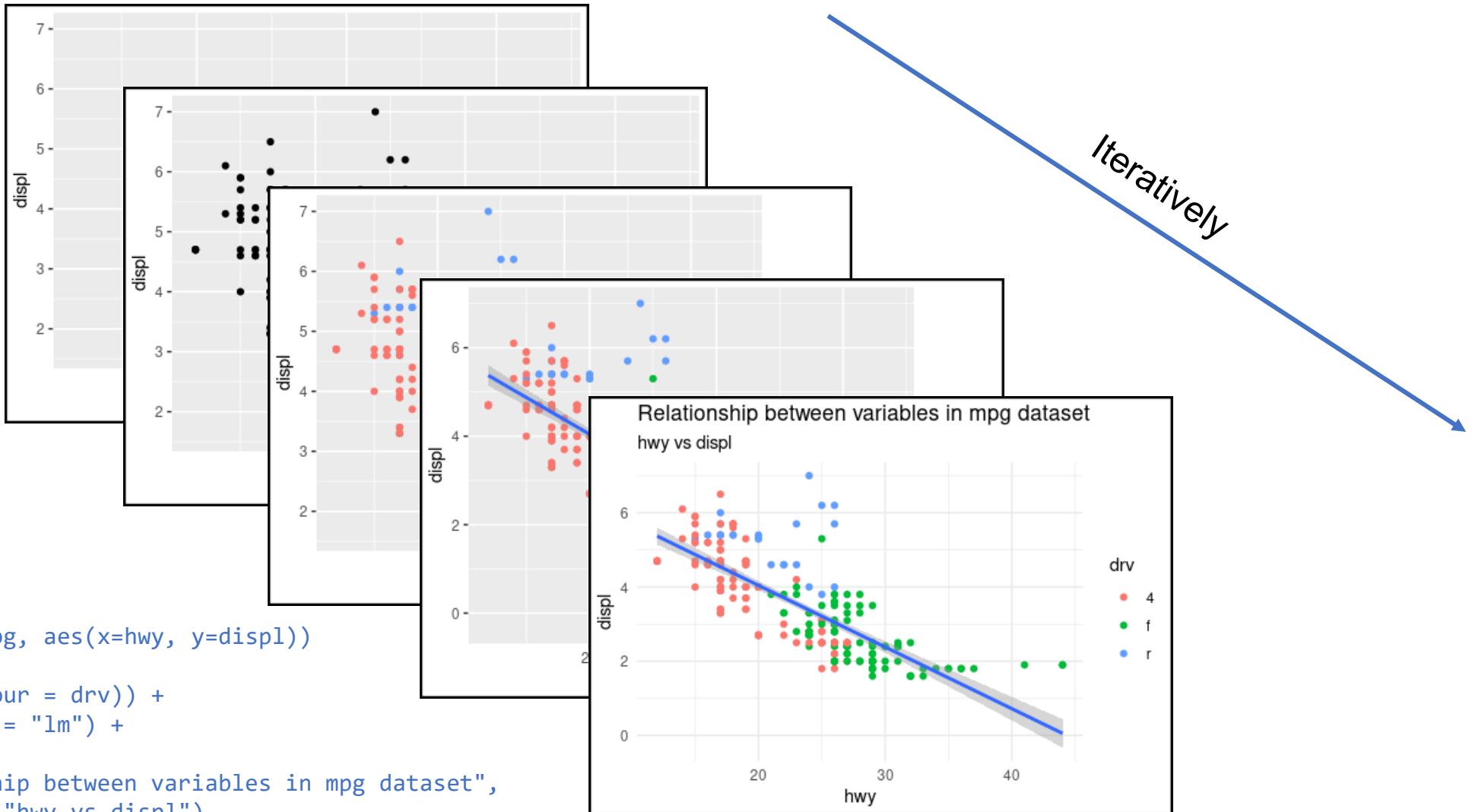# Building plots layer by layer (example)


```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base +
  geom_point(aes(colour = drv))
```

Building plots layer by layer (example)


```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base +
  geom_point(aes(colour = drv)) +
  geom_smooth(method = "lm")
```

Building plots layer by layer (example)

Iteratively

```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base +
  geom_point(aes(colour = drv)) +
  geom_smooth(method = "lm") +
  theme_minimal() +
  ggtitle("Relationship between variables in mpg dataset",
          subtitle = "hwy vs displ")
```

Let's do some practice!

➢ `git clone https://github.com/wbvguo/qcbio-DataViz_w_ggplot2.git`
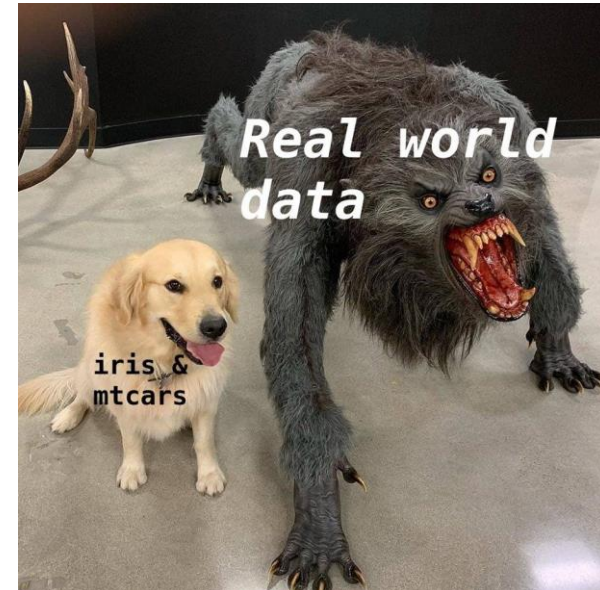
Real world data

iris & mtcars

Data

"Once you have

❑ the right data,

❑ in the right format,

❑ aggregated in the right way,

the right visualization is often obvious"

Variables

The container for storing values

- **Categorical variables**: take discrete values
  - ➤ `x = c("apple", "banana")`   # nominal variables: without an order
  - ➤ `y = c("low", "medium", "high")`# ordinal variables: with an order
- **Continuous variables**: take any values within a range
  - ➤ `z = c(0.05, 1, -2)`

Variables

The container for storing values
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- **Continuous variables**: take any values within a range
  - ➢ `z = c(0.05, 1, -2)`

Factors: takes the categorical variable and stores data in levels
- Use function `factor()` to convert categorical (nominal) and ordered categorical (ordinal) variables to factors
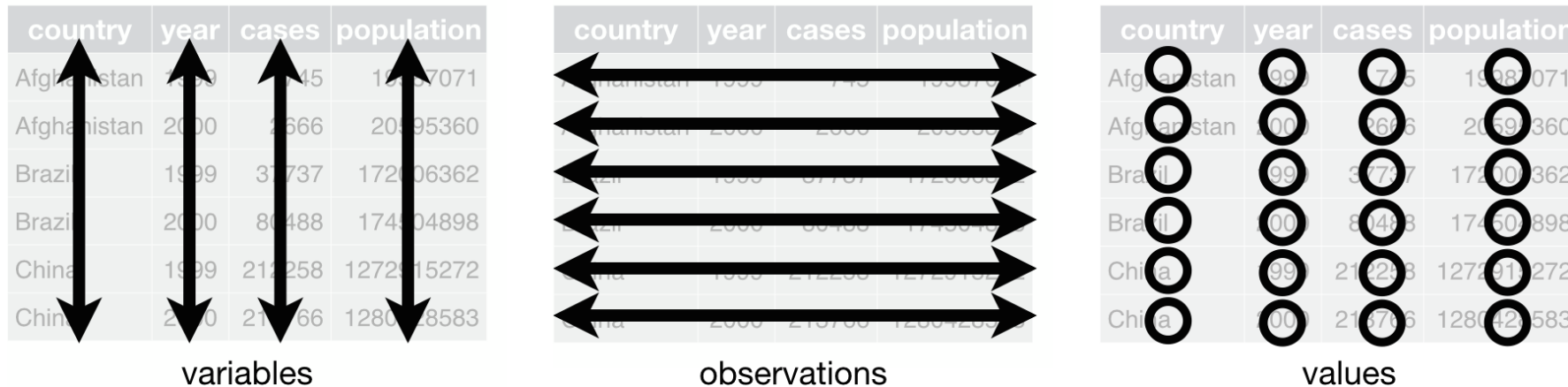
Exercise: compare the following 2 lines' results, what do you find?
- ➢ `y1 = factor(y)`
- ➢ `y2 = factor(y, levels = c("low", "medium", "high"))`

Data frame

A generic data object that are used to store tabular data

variables				observations				values			

Use function `data.frame()` to create a data frame

➢ `df = data.frame(x = c(1,2,3), y = c("low", "medium", "high"))`

Data wrangling functions

- Manipulate observations (rows)
  - `filter()`
  - `arrange()`
  - `bind_rows()`

- Manipulate variables (columns)
  - `select()`
  - `mutate()`
  - `left_join(), right_join()` ...

- Reshape the data
  - `pivot_longer(), pivot_wider()`

- Group and summarize
  - `group_by()`
  - `summarize()`

For more information, check the cheatsheet

Manipulate observations

`filter()`: keep rows that satisfy certain conditions

- The first argument is a data frame
- The second and subsequent arguments must be logical vectors

Create logical vectors:

filter

❑ Comparison operators

- x == y: x and y are equal.
- x != y: x and y are not equal.
- x %in% c("a", "b", "c"): x is one of the values in the right hand side.
- x > y, x >= y, x < y, x <= y: greater than, greater than or equal to, less than, less than or equal to.

❑ Logical operators

- !x (pronounced "not x"), flips TRUE and FALSE so it keeps all the values where x is FALSE.
- x & y: TRUE if both x and y are TRUE.
- x | y: TRUE if either x or y (or both) are TRUE.
- xor(x, y): TRUE if either x or y are TRUE, but not both (exclusive or).
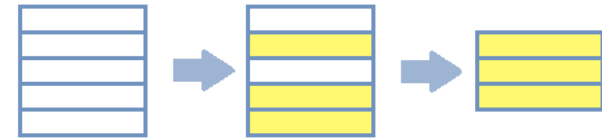
Manipulate observations

`arrange()`: orders observations according to variables

- The first argument is a data frame
- The second and subsequent arguments are variables or function of variables
- `.by_group`: If `TRUE`, will sort first by grouping variable. Applies to grouped data frames only

arrange
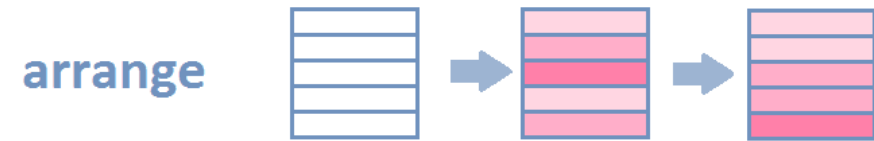
Note:

- the default sorting order is ascending
- use `desc()` to sort a variable in descending order

Manipulate observations

`bind_rows()`: Bind any number of data frames by row
- The first and subsequent arguments are data frames to combine
- Columns are matched by name, and missing columns will be filled with `NA`

`bind_rows()`

Exercise: let's do some practice

Manipulate variables

`select()`: keep or drop variables using their names and types

- The first argument is a data frame
- The second and subsequent arguments are unquoted expressions separated by comma
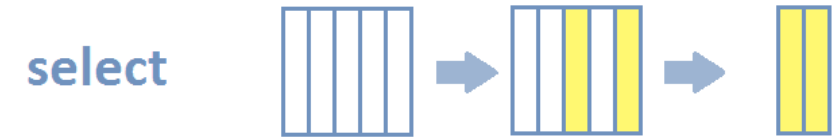
select

Useful functions

- `all_of()`: Matches variable names in a character vector
- `starts_with()/ends_with()`: Starts/ends with a substring
- `where()`: Applies a function to all variables and selects those for which the function returns TRUE

Useful Operators

- `!`: take the complement of a set of variables
- `&` or `|`: select the intersection or union of two sets of variables
- `c()` : combine selections

Manipulate variables

`mutate()`: create new variables
- The first argument is a data frame.
- The second and subsequent arguments are name-value pairs (named expression that generate the new variables)
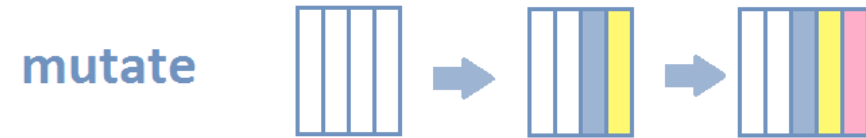
The values can be
- Vector of length 1
- Vector of the same length as whole data frame or current group (for grouped data frame)
- `NULL` to remove the column

Manipulate variables

`*_join()`:

inner_join(x, y)   full_join(x, y)

left_join(x, y)   right_join(x, y)

Manipulate variables

`*_join()`:

inner_join(x, y)   full_join(x, y)
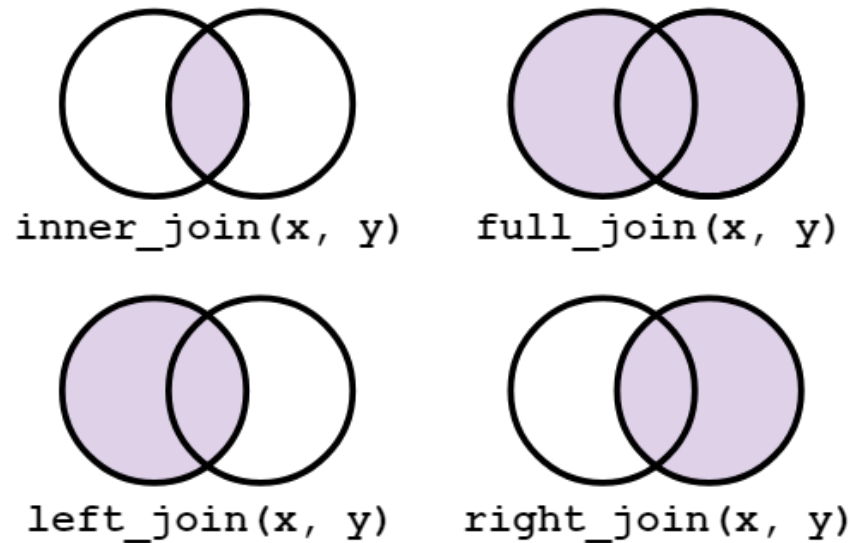
left_join(x, y)   right_join(x, y)

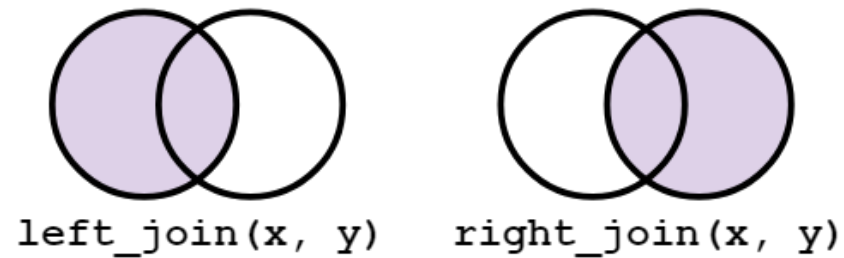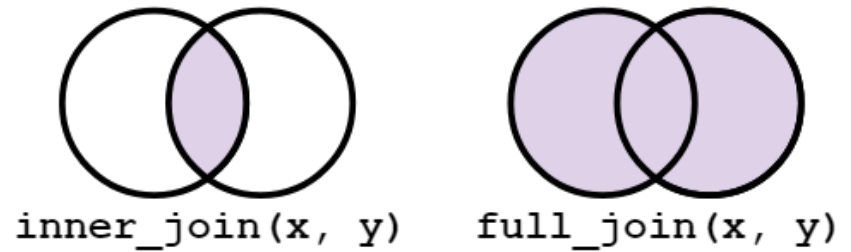| a			b		
x1	**x2**		**x1**	**x3**	
A	1		A	T	
B	2		B	F	
C	3		D	T	

Mutating Joins

x1	**x2**	**x3**
A	1	T
B	2	F
C	3	NA

dplyr::**left_join(a, b, by = "x1")**
Join matching rows from b to a.

x1	**x3**	**x2**
A	T	1
B	F	2
D	T	NA

dplyr::**right_join(a, b, by = "x1")**
Join matching rows from a to b.

x1	**x2**	**x3**
A	1	T
B	2	F

dplyr::**inner_join(a, b, by = "x1")**
Join data. Retain only rows in both sets.

x1	**x2**	**x3**
A	1	T
B	2	F
C	3	NA
D	NA	T

dplyr::**full_join(a, b, by = "x1")**
Join data. Retain all values, all rows.
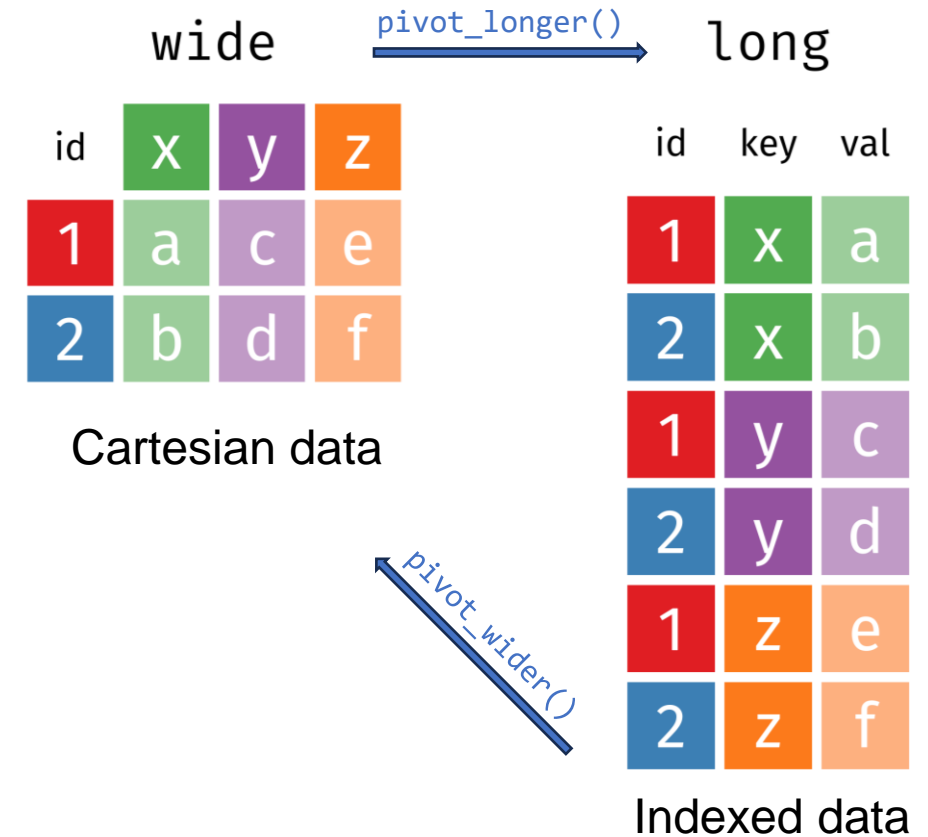
Exercise: let's do some practice

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Reshape data frame

pivot_longer(): pivot into long format

- The first argument is a data frame
- The second argument is columns to pivot into longer format
- names_to: new column name for column names
- values_to: new column name for cell values

pivot_wider(): pivot into wide format

- The first argument is a data frame
- names_from: column to get the names of output column
- values_from: column to get the cell values

Cartesian data

Indexed data

Reshape data frame

wide

id x y z

1 a c e
2 b d f

pivot_longer(): pivot into long format

- The first argument is a data frame
- The second argument is columns to pivot into longer format
- names_to: new column name for column names
- values_to: new column name for cell values

pivot_wider(): pivot into wide format

- The first argument is a data frame
- names_from: column to get the names of output column
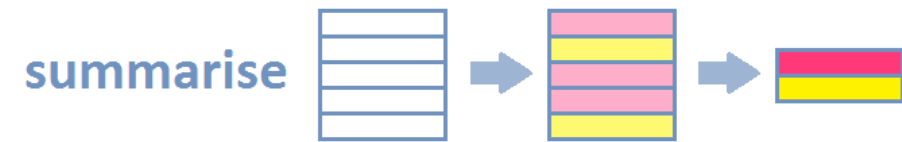- values_from: column to get the cell values

Group and summarize

`group_by()`: Define the grouping variables

- The first argument is a data frame
- The second and subsequent arguments are variables used for grouping

`summarise()`/`summarize()`:

- The first argument is a data frame
- The second and subsequent arguments are name-value pairs for summary function

- Counts: n(), n_distinct(x).
- Middle: mean(x), median(x).
- Spread: sd(x), mad(x), IQR(x).
- Extremes: quartile(x), min(x), max(x).
- Positions: first(x), last(x), nth(x, 2).

`ungroup()`: takes a data frame and removes the grouping

Chain the functions together using pipe (%>%)

```
# By using intermediate values
cut_depth <- group_by(diamonds, cut, depth)
cut_depth <- summarise(cut_depth, n = n())
cut_depth <- filter(cut_depth, depth > 55, depth < 70)
cut_depth <- mutate(cut_depth, prop = n / sum(n))
```

```
# By "composing" functions
mutate(
  filter(
    summarise(
      group_by(
        diamonds,
        cut,
        depth
      ),
      n = n()
    ),
    depth > 55,
    depth < 70
  ),
  prop = n / sum(n)
)
```

```
cut_depth <- diamonds %>%
  group_by(cut, depth) %>%
  summarise(n = n()) %>%
  filter(depth > 55, depth < 70) %>%
  mutate(prop = n / sum(n))
```

Question: Which one do you think is the most elegant?

Chain the functions together using pipe (%>%)

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  summarise(n = n()) %>%
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%>% works by taking the object on the left hand side (LHS) and using it as the first argument to the function on the right hand side (RHS)

➢ `f(x,y)` `<=>` `x %>% f(y)`

Exercise: rewrite `g(f(x, y), z)` using pipe

Aesthetics
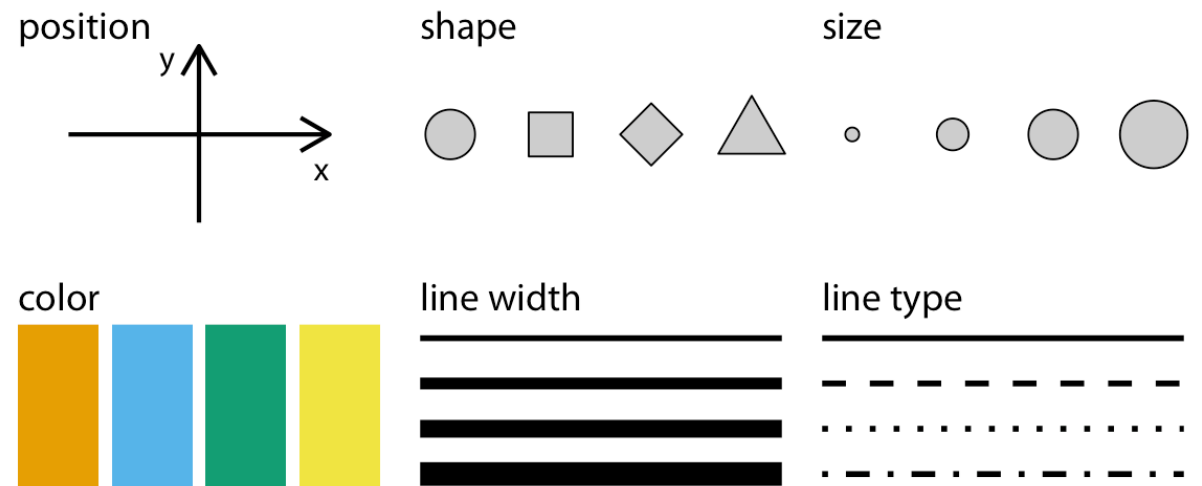
Aesthetic mappings

Aesthetic mappings `aes()` describe how variables are mapped to visual properties or aesthetics. It takes aesthetic-variable pairs

> ➢ `aes(x = displ, y = hwy, colour = class)`

Aesthetic	Description
x	x-axis position
y	y-axis position
colour	Color of points or outlines of other shapes
fill	Fill color
size	size of the point or thickness of line
alpha	Transparency of the shape
linetype	Line type such a solid, dashed, dotted
labels	Text on the plot
shape	Shape of the geometry

Aesthetic mappings

Aesthetic mappings `aes()` describe how variables are mapped to visual properties or aesthetics. It takes aesthetic-variable pairs

> `aes(x = displ, y = hwy, colour = class)`

Check available options
> `vignette("ggplot2-specs")`

Aesthetic	Description
x	x-axis position
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linetype

solid	
dashed	
dotted	
dotdash	
longdash	
twodash	

shape

Aesthetic mappings and setting

- The function supports some simple transformation (e.g. log(x))
  - ➢ `aes(x = log(displ), y = hwy, colour = class)`

- Within each layer, you can add, override, or remove mappings
  - ➢ `base = ggplot(mpg, aes(displ, hwy, colour =class))`
    - o Add: `base + geom_point(aes(shape  = drv))`
    - o Override: `base + geom_point(aes(colour = drv))`
    - o Remove: `base + geom_point(aes(colour = NULL))`

- Aesthetics mapping vs setting
  - Map an aesthetic to a variable when the appearance is governed by a variable
  - Set the aesthetic atrribute to a single value in the layer parameters
    - ➢ `ggplot(mpg) + geom_point(aes(displ, hwy, colour = "blue"))`
    - ➢ `ggplot(mpg) + geom_point(aes(displ, hwy), colour = "blue")`

Things to consider when using `aes()`

- Choose visual aesthetics based on the type of data variables
  - colour and shape work well with categorical variables
  - size works well for continuous variables (bubble plot)
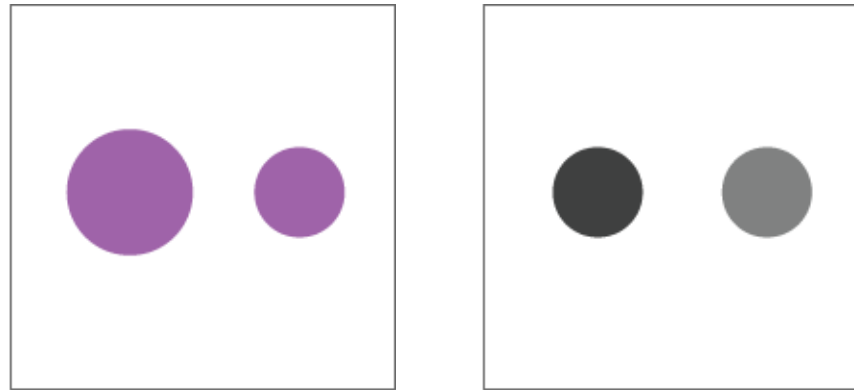
Size works better for quantitative variables than lightness

- Don't make the plot too busy, less is more
  - It's difficult to see the simultaneous relationships among colour, shape and size

Where to get help?

- https://community.rstudio.com/tag/ggplot2

- https://www.google.com

- https://stackoverflow.com

- https://chat.openai.com/