Advanced data visualization with ggplot2

Wenbin Guo
Bioinformatics IDP, UCLA
wbguo@ucla.edu

2024 Fall

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 

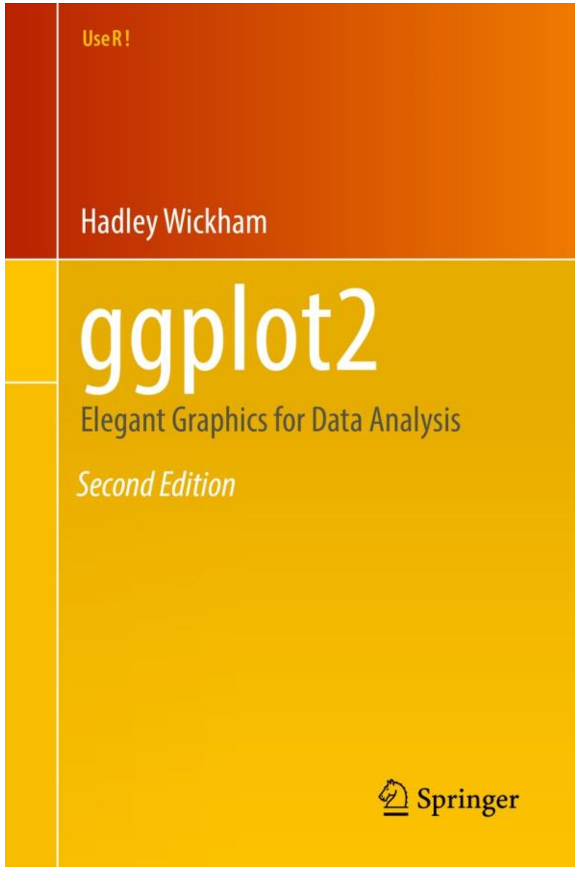
Workshop goals

- 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

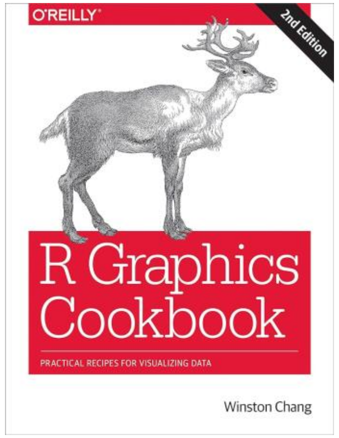
- Day 1: Data visualization basics
  - Getting started with ggplot2
  - Recap of data wrangling functions
- Day 2: Building a plot layer by layer
  - Exploring different plot types
  - Getting more control on the plots
- Day 3: Examples and useful packages
  - Practical examples and principles
  - Introducing some useful packages

Reference

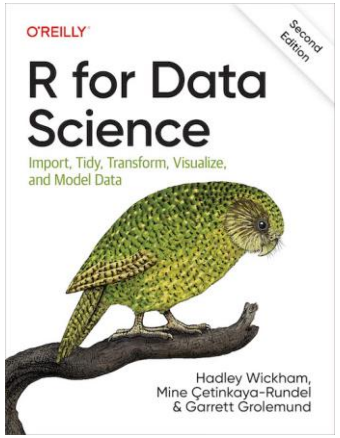


link

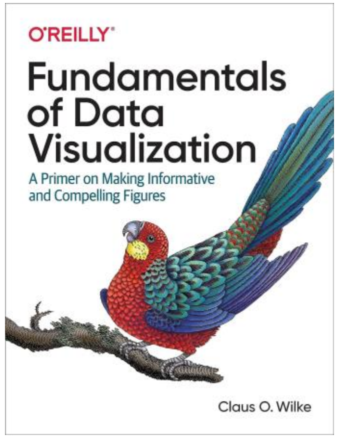
- Other useful references



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."*

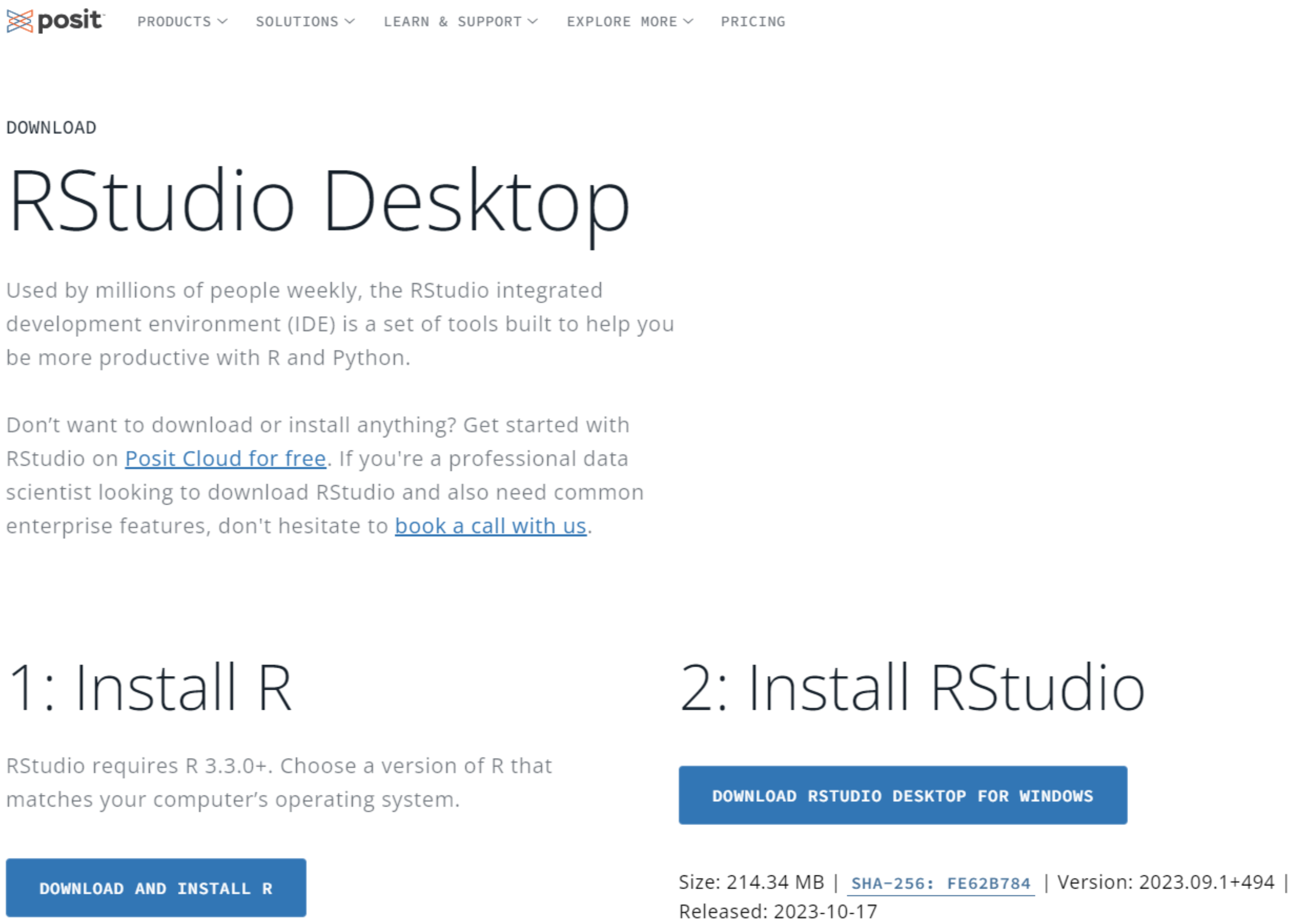
—— 2019 COPSS President's Award

Hadley Wickham
Chief Scientist, Rstudio/posit

Image from Committee of Presidents of Statistical Societies

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")`

UCLA QCBio Collaboratory

Day 1: Data visualization basics

Wenbin Guo
Bioinformatics IDP, UCLA
wbguo@ucla.edu
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Overview

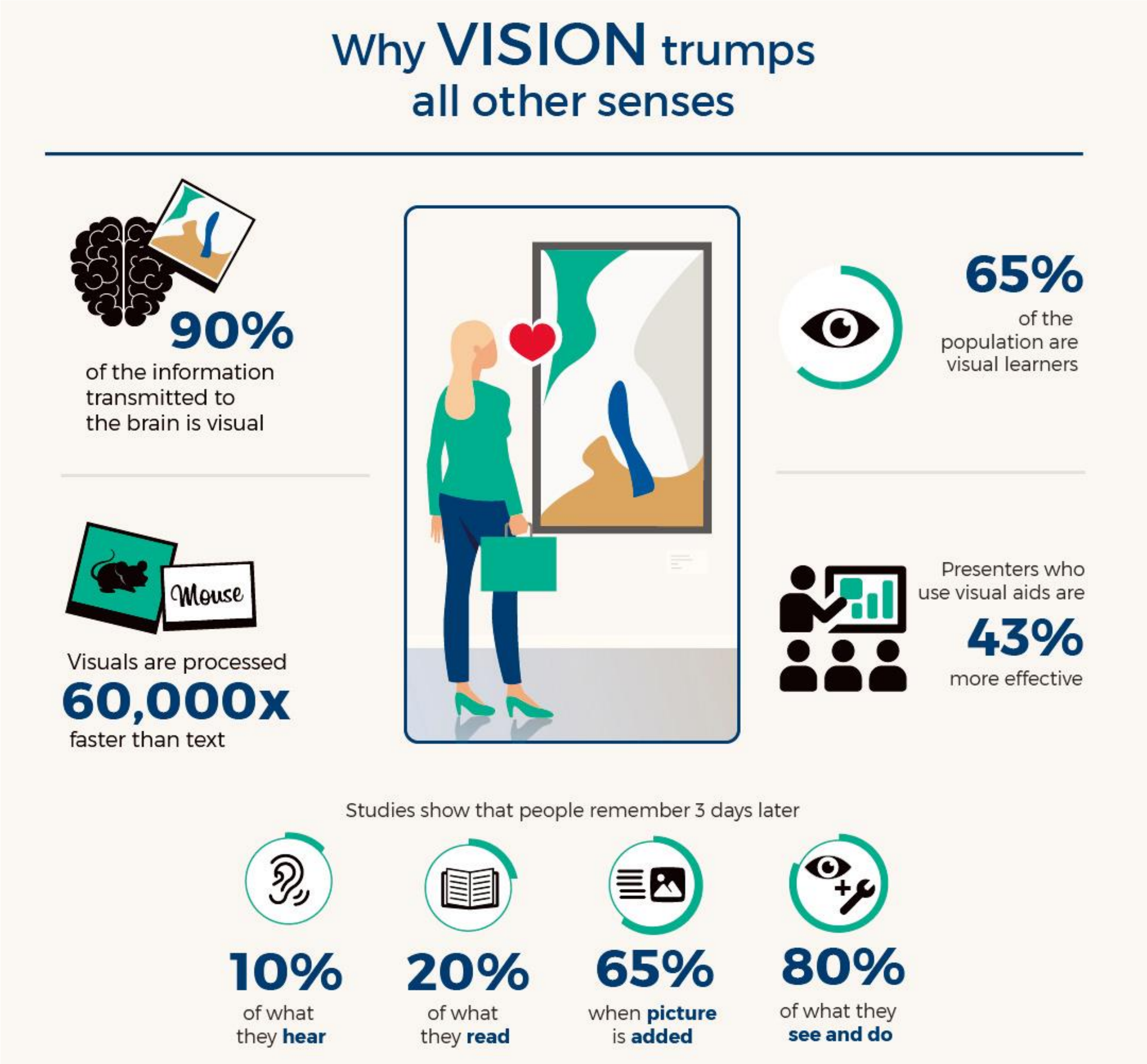
Time

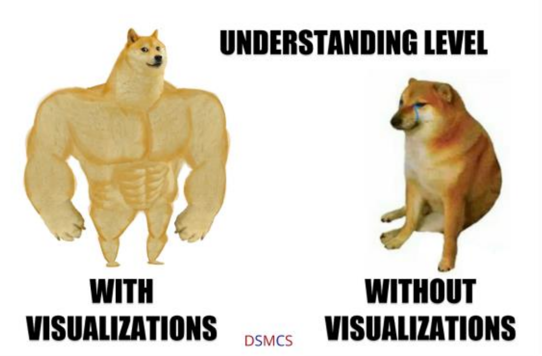
- 3-hour workshop (45min + 45min + 30min + practice/Q&A)

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





Martin, K. *Medical Writing* (2020)

"A picture may be worth a thousand words"

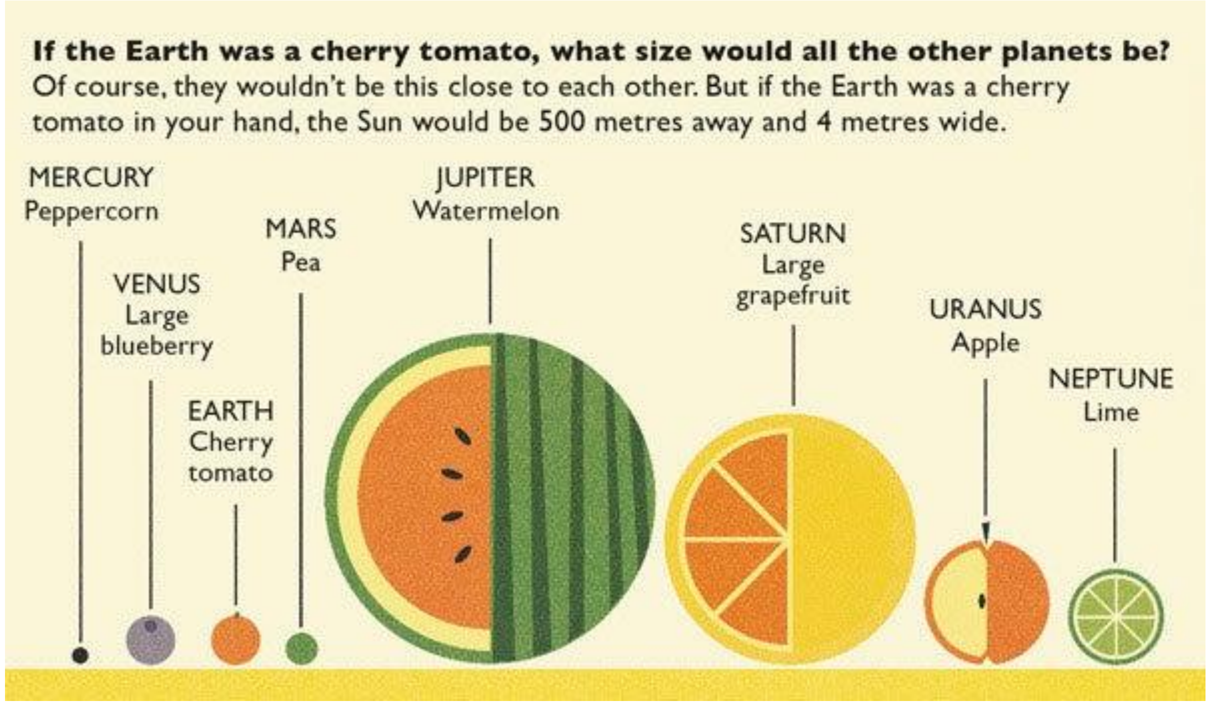
Example

You
list all the planet's diameters in the solar system

ChatGPT
Here are the diameters of the planets in our solar system:

1. **Mercury**: Approximately 4,880 kilometers (3,032 miles).
2. **Venus**: Approximately 12,104 kilometers (7,521 miles).
3. **Earth**: Approximately 12,742 kilometers (7,918 miles).
4. **Mars**: Approximately 6,779 kilometers (4,212 miles).
5. **Jupiter**: Approximately 139,820 kilometers (86,881 miles).
6. **Saturn**: Approximately 116,460 kilometers (72,366 miles).
7. **Uranus**: Approximately 50,724 kilometers (31,518 miles).
8. **Neptune**: Approximately 49,244 kilometers (30,598 miles).

These values represent the equatorial diameters of the planets, which are the most commonly used measurements for planetary diameters.



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

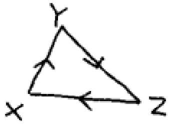
Image from Internet

"A picture may be worth a thousand words"

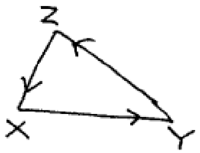
Remark Whether the traversal is clockwise, is undefined in the case of the degenerate triangle, i.e. a "triangle" with its vertices on a straight line, but in that case its area equals zero and its sign is irrelevant. Also, please note that the theorems

$$\triangle XYZ = -\triangle ZYX$$
$$\triangle XYZ = \triangle YZX$$

hold independently of the sign of $\triangle XYZ$, i.e., for both



and



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

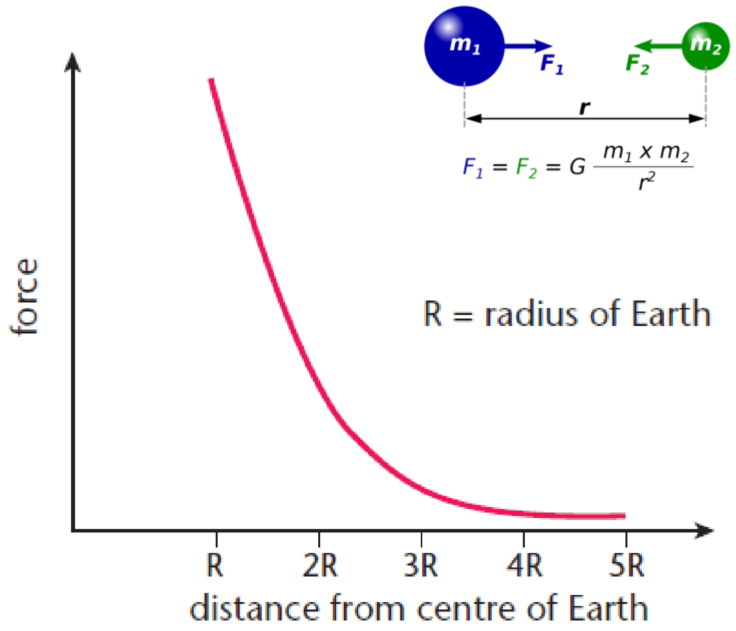
—— *A first exploration of effective reasoning* (1996)

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:

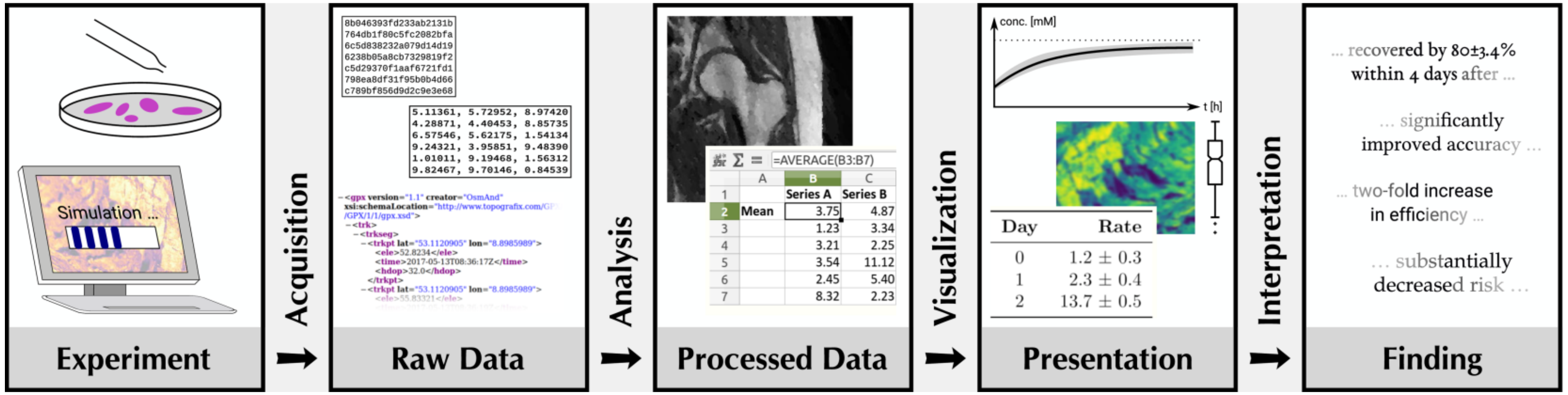


Formula annotation can make figure more **accurate**

Question: What is worth than a thousand formulas?

Image from Internet

The role of data visualization in science



Typical steps in scientific work involving data analysis

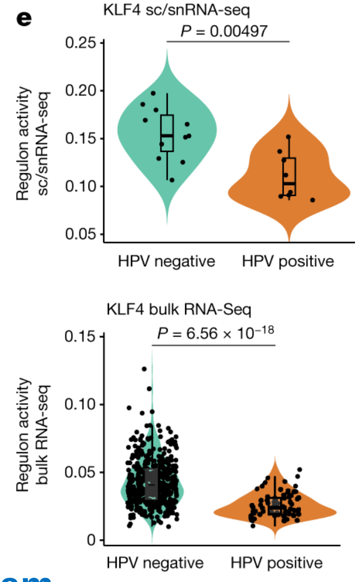
(Schwen et al. *Plos Computational Biology*, 2018)

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

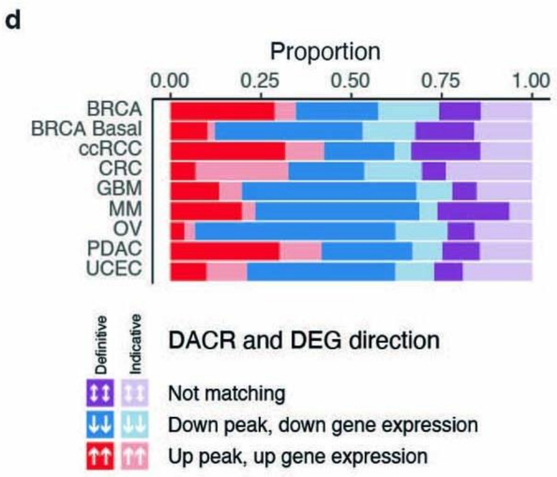
Image from Internet

The role of data visualization in science (example)

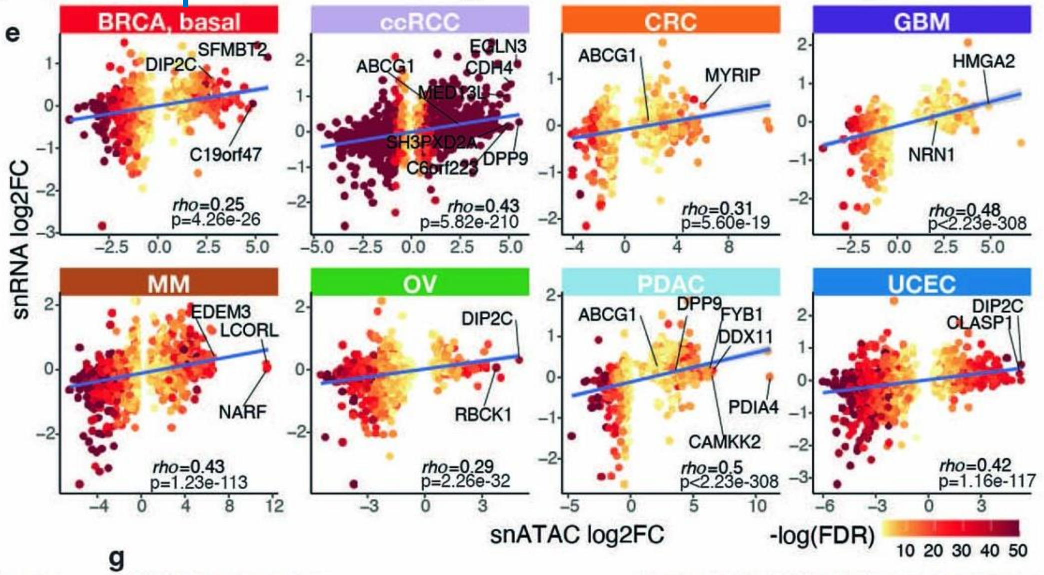
Boxplot/Violin plot



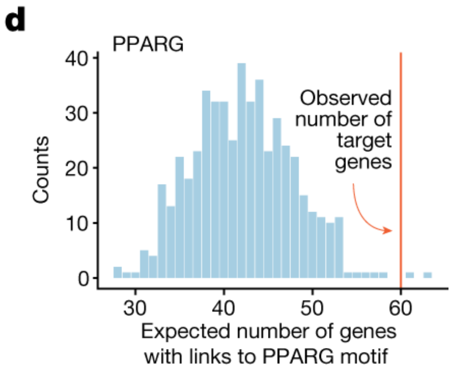
Bar plot



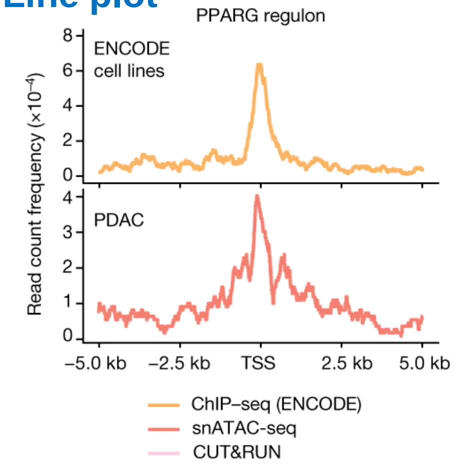
Scatter plot



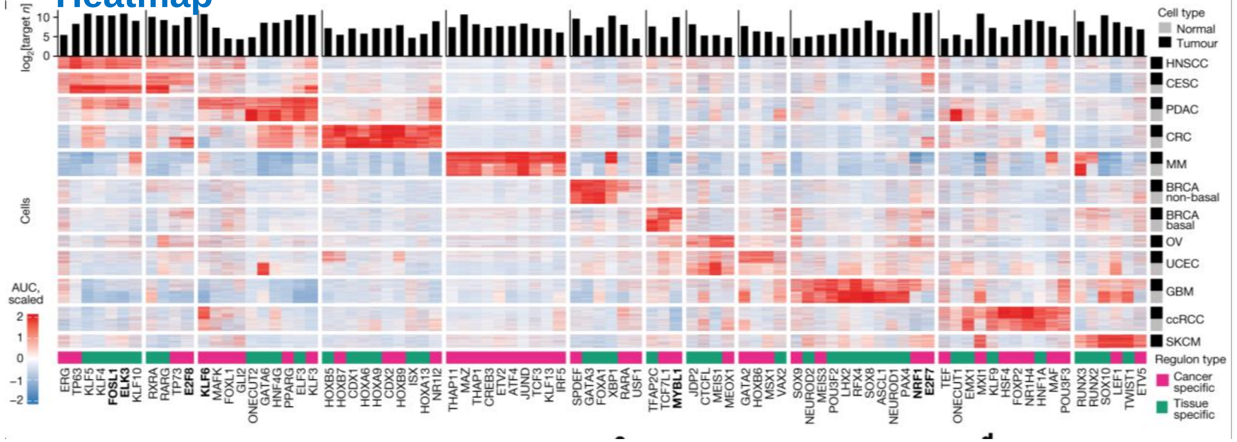
Histogram



Line plot



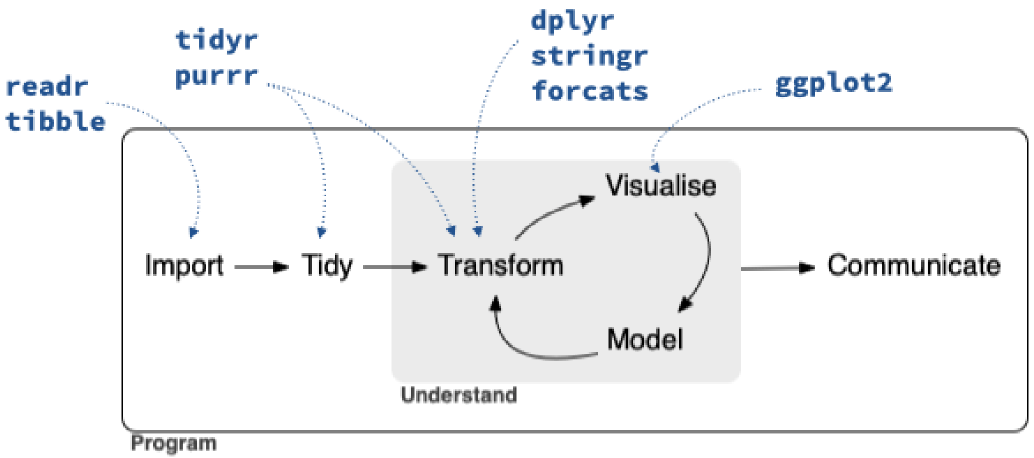
Heatmap



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

Cetinkaya-Rundel et al. *arXiv* (2021)

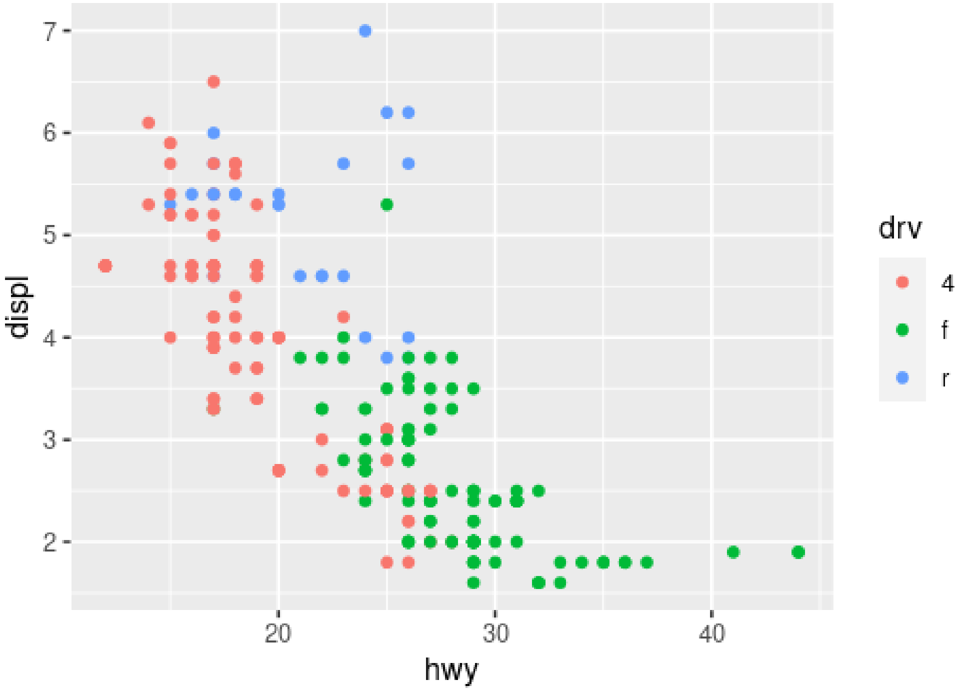
Idea behind ggplot2 visualization

Take scatter plot as an example

Filter

	manufacturer	model	displ	year	cyl	trans	drv	cty	hwy	fl	class
1	audi	a4	1.8	1999	4	auto(l5)	f	18	29	p	compact
2	audi	a4	1.8	1999	4	manual(m5)	f	21	29	p	compact
3	audi	a4	2.0	2008	4	manual(m6)	f	20	31	p	compact
4	audi	a4	2.0	2008	4	auto(av)	f	21	30	p	compact
5	audi	a4	2.8	1999	6	auto(l5)	f	16	26	p	compact
6	audi	a4	2.8	1999	6	manual(m5)	f	18	26	p	compact
7	audi	a4	3.1	2008	6	auto(av)	f	18	27	p	compact
8	audi	a4 quattro	1.8	1999	4	manual(m5)	4	18	26	p	compact
9	audi	a4 quattro	1.8	1999	4	auto(l5)	4	16	25	p	compact
10	audi	a4 quattro	2.0	2008	4	manual(m6)	4	20	28	p	compact
11	audi	a4 quattro	2.0	2008	4	auto(s6)	4	19	27	p	compact
12	audi	a4 quattro	2.8	1999	6	auto(l5)	4	15	25	p	compact
13	audi	a4 quattro	2.8	1999	6	manual(m5)	4	17	25	p	compact
14	audi	a4 quattro	3.1	2008	6	auto(s6)	4	17	25	p	compact
15	audi	a4 quattro	3.1	2008	6	manual(m6)	4	15	25	p	compact

Showing 1 to 16 of 234 entries, 11 total columns



Data source: mpg

Idea behind ggplot2 visualization

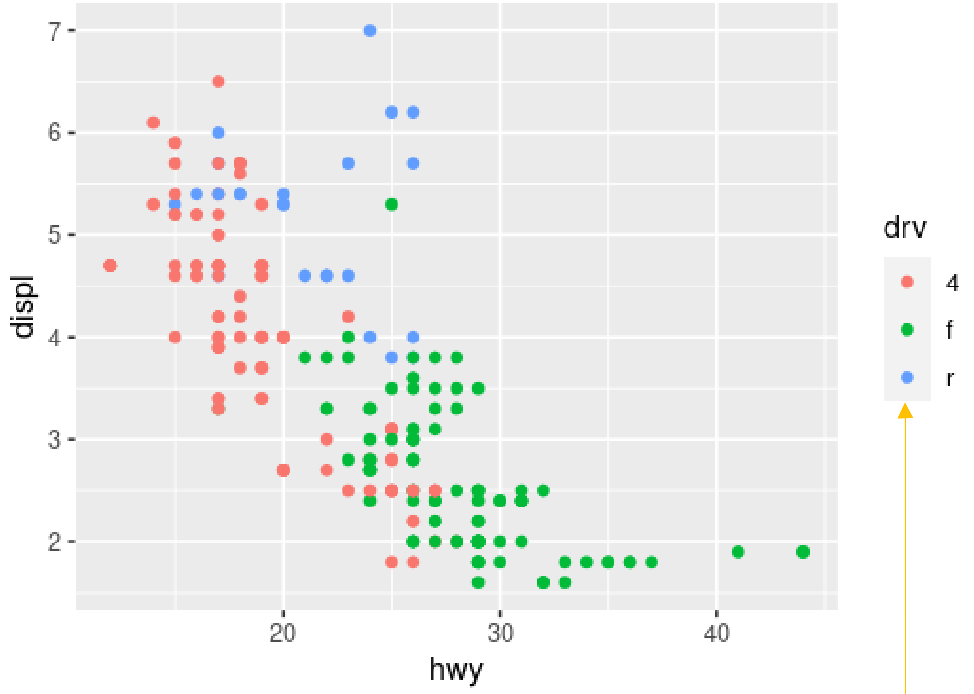
Take scatter plot as an example

hwy → x
displ → y
drv → colour

Filter

	manufacturer	model	displ	year	cyl	trans	drv	cty	hwy	fl	class
1	audi	a4	1.8	1999	4	auto(l5)	f	18	29	p	compact
2	audi	a4	1.8	1999	4	manual(m5)	f	21	29	p	compact
3	audi	a4	2.0	2008	4	manual(m6)	f	20	31	p	compact
4	audi	a4	2.0	2008	4	auto(av)	f	21	30	p	compact
5	audi	a4	2.8	1999	6	auto(l5)	f	16	26	p	compact
6	audi	a4	2.8	1999	6	manual(m5)	f	18	26	p	compact
7	audi	a4	3.1	2008	6	auto(av)	f	18	27	p	compact
8	audi	a4 quattro	1.8	1999	4	manual(m5)	4	18	26	p	compact
9	audi	a4 quattro	1.8	1999	4	auto(l5)	4	16	25	p	compact
10	audi	a4 quattro	2.0	2008	4	manual(m6)	4	20	28	p	compact
11	audi	a4 quattro	2.0	2008	4	auto(s6)	4	19	27	p	compact
12	audi	a4 quattro	2.8	1999	6	auto(l5)	4	15	25	p	compact
13	audi	a4 quattro	2.8	1999	6	manual(m5)	4	17	25	p	compact
14	audi	a4 quattro	3.1	2008	6	auto(s6)	4	17	25	p	compact
15	audi	a4 quattro	3.1	2008	6	manual(m6)	4	15	25	p	compact

Showing 1 to 16 of 234 entries, 11 total columns



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

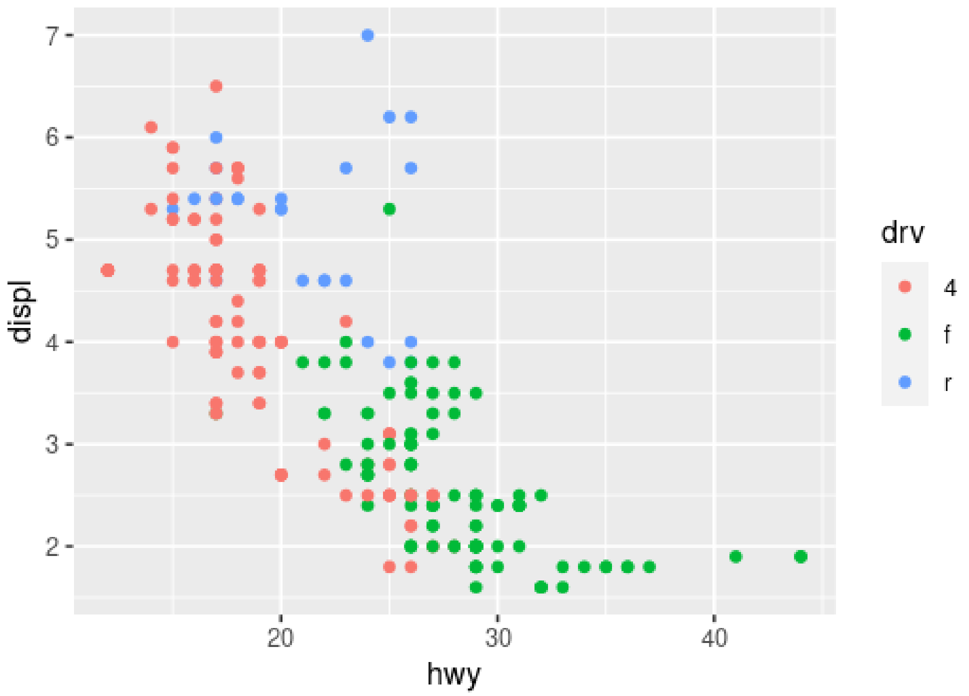
- The `data =` and `mapping =` specifications are optional, so long as the data and mapping are passed into the function in the right order

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

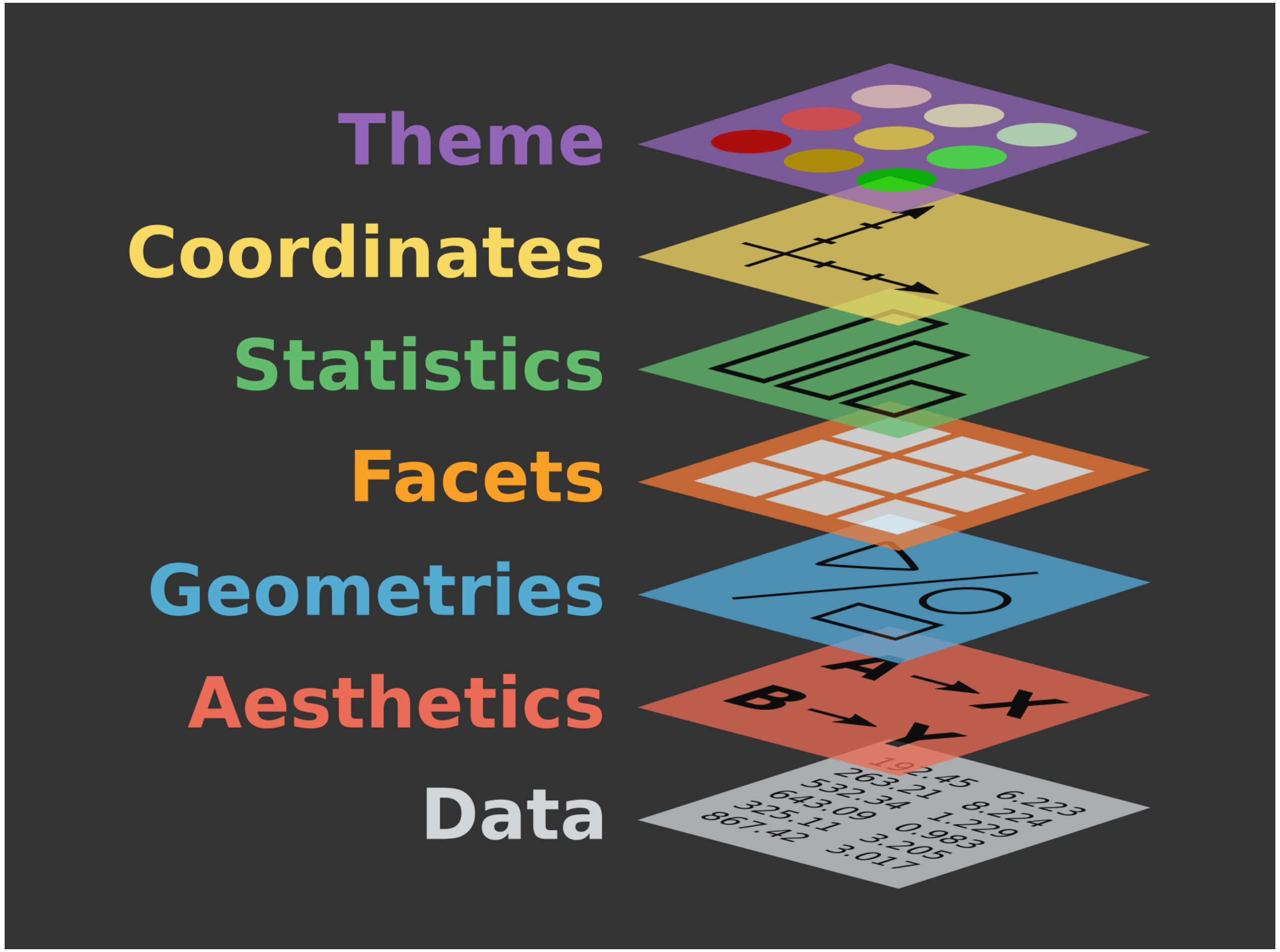
https://ggplot2.tidyverse.org/reference/ggplot.html

Key components of a ggplot object

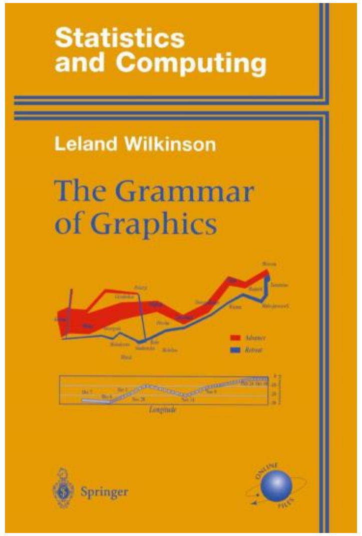
- The **data**
- A set of **aesthetic mappings** between *variables* and *visual properties*
- At least one **layer** describing how to render the observations



The layered grammar of graphics

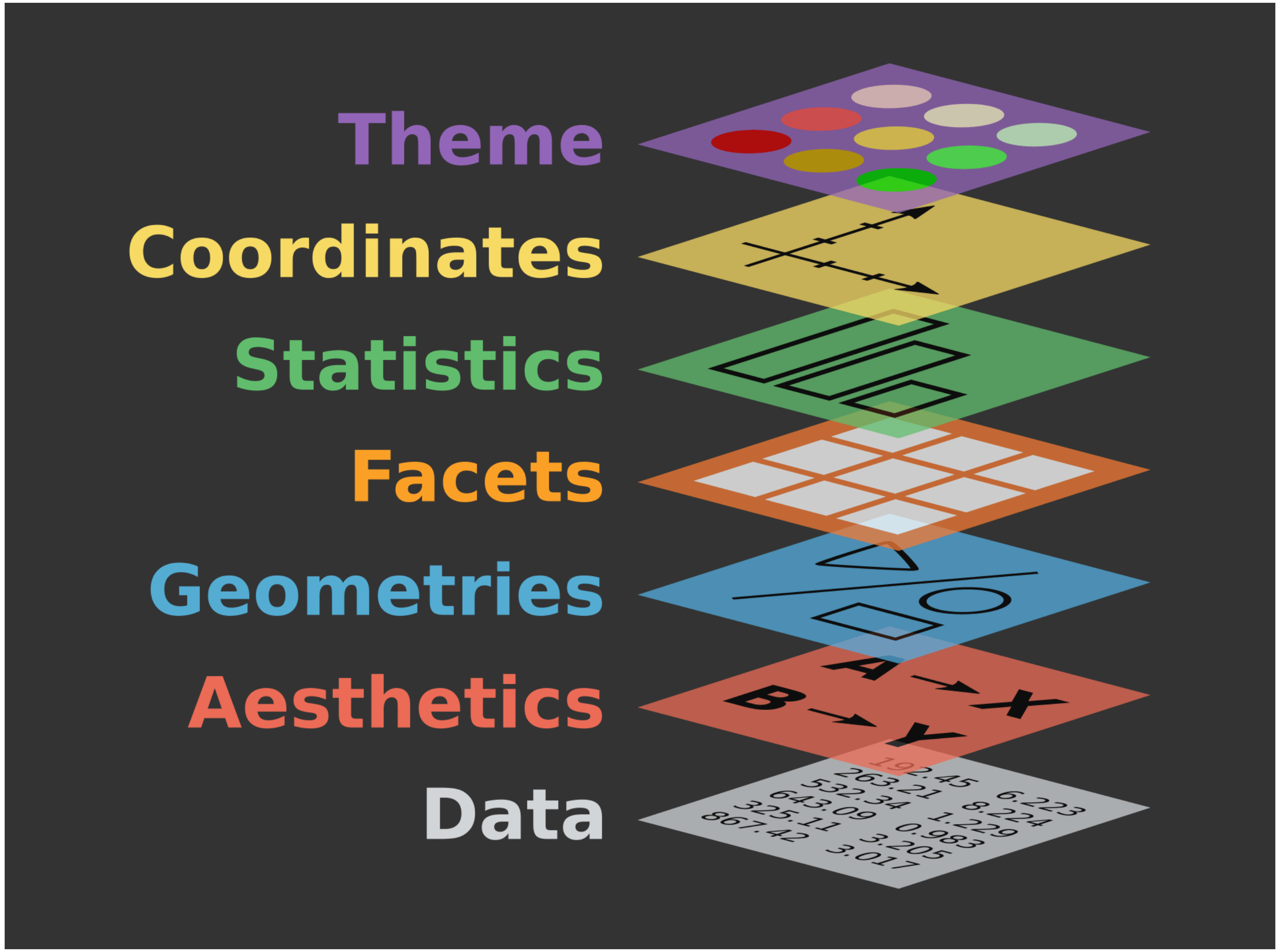


Leland Wilkinson
(1944-2021)



The Grammar of Graphics (1999)

The layered grammar of graphics



Describes all the non-data ink

Plotting space for the data

Statistical models and summaries

Rows and columns of sub-plots

Shapes used to represent the data

Scales onto which data is mapped

The actual variables to be plotted

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()`

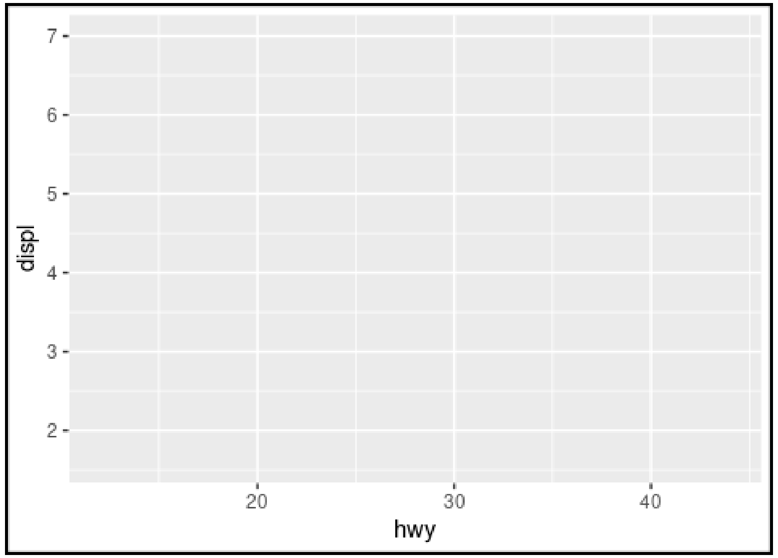
- `ggplot(data = df, mapping = aes(), ...)`
  - when all layers use the same data and the same set of aesthetics

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

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

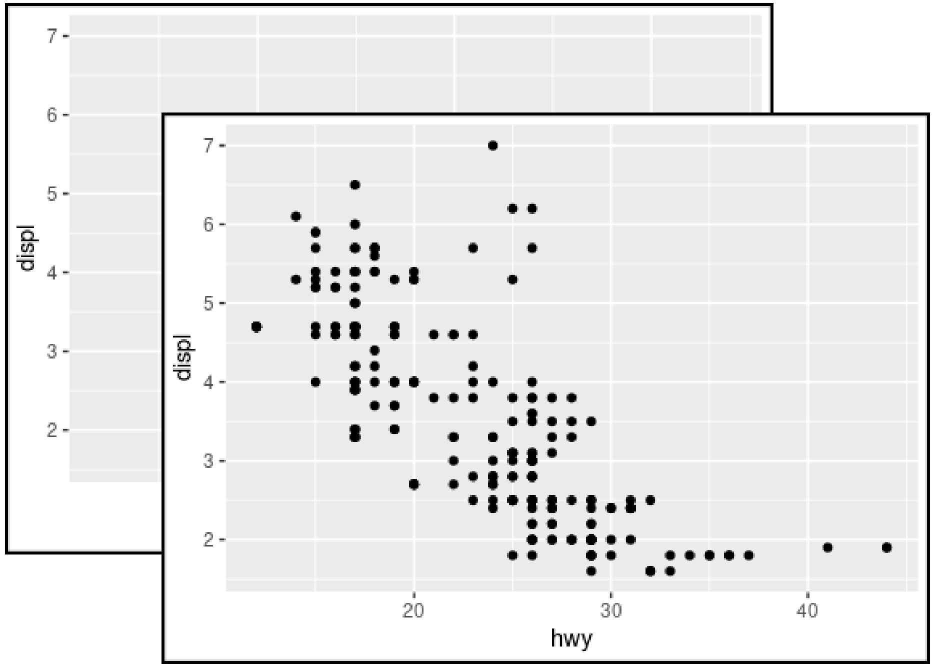
https://ggplot2.tidyverse.org/reference/ggplot.html

Building plots layer by layer (example)



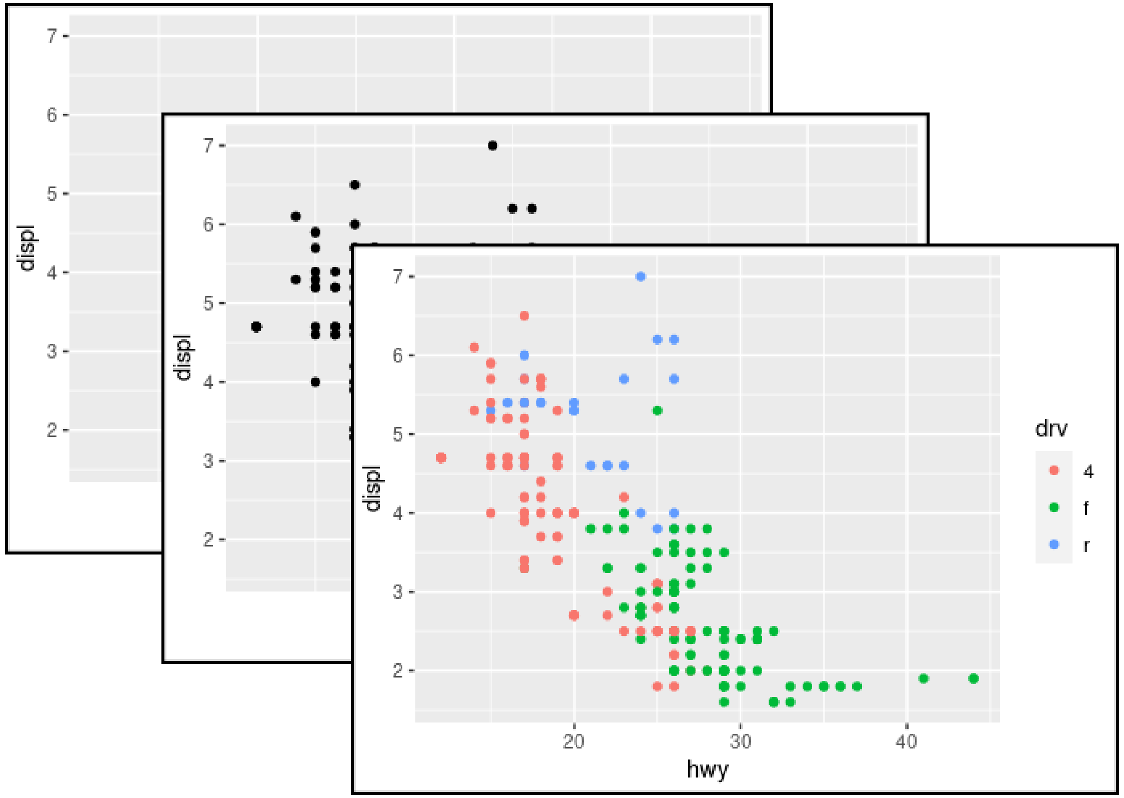

```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base
```

Building plots layer by layer (example)



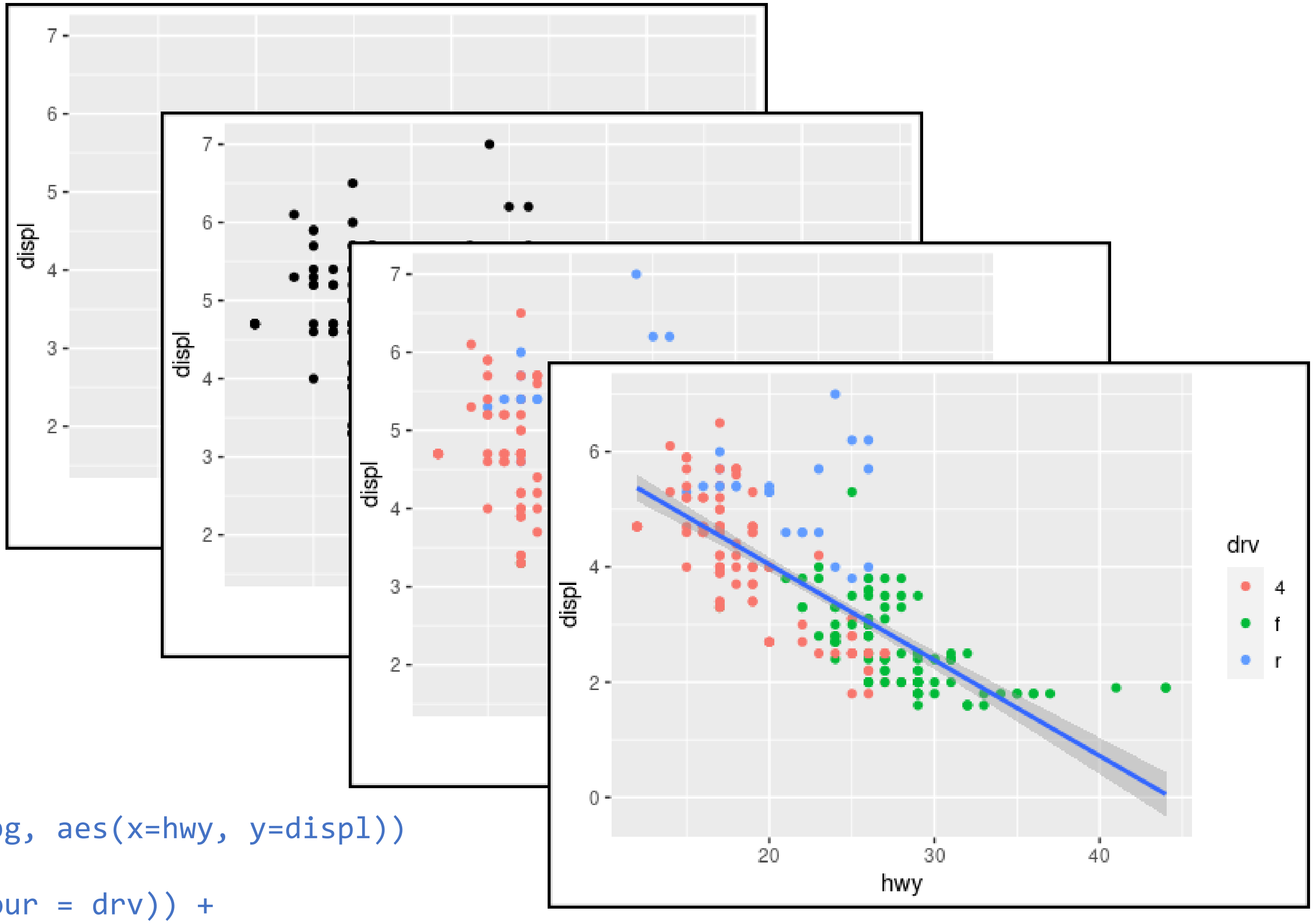

```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base +
  geom_point()
```

Building plots layer by layer (example)



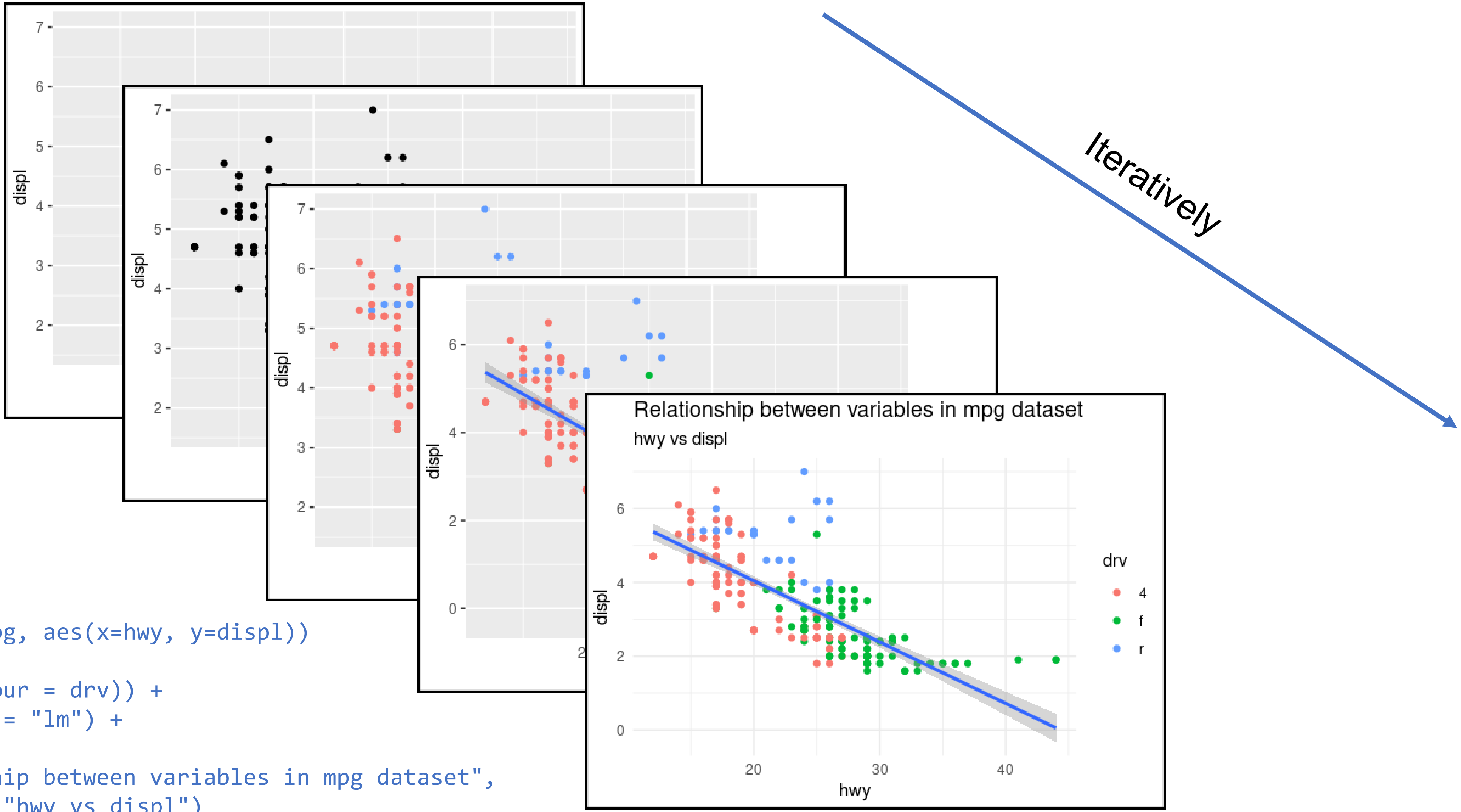

```
base = ggplot(data=mpg, aes(x=hwy, y=displ))
base +
  geom_point(aes(colour = drv))
```

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")
```

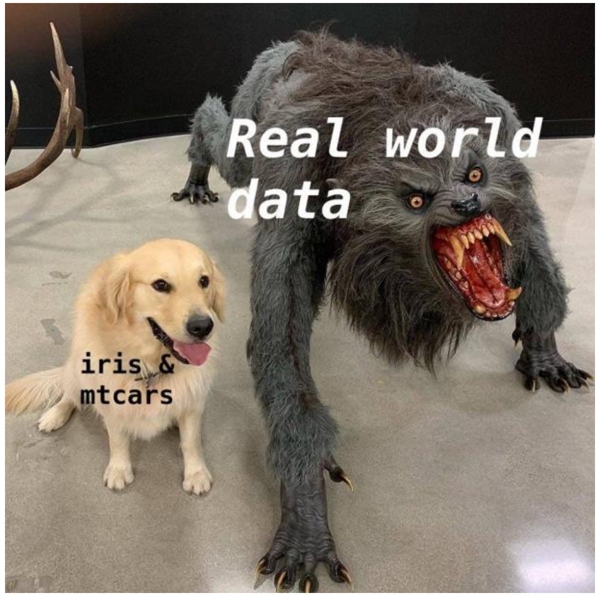
Building plots layer by layer (example)




```
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`



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

- **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)`

Factors: takes the categorical variable and stores data in levels

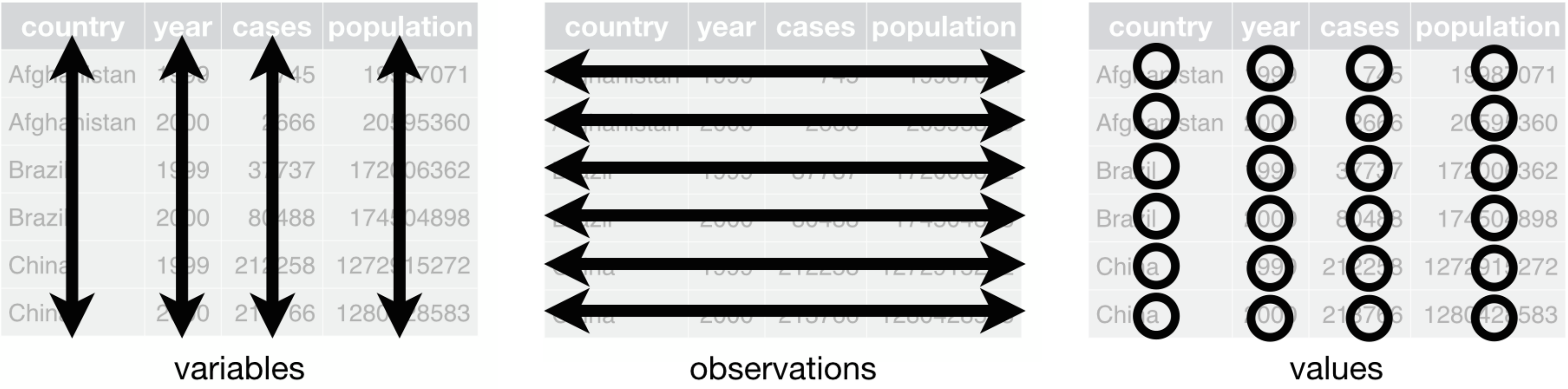
- Use function `factor()` to convert categorical (nominal) and ordered categorical (ordinal) variables to factors

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



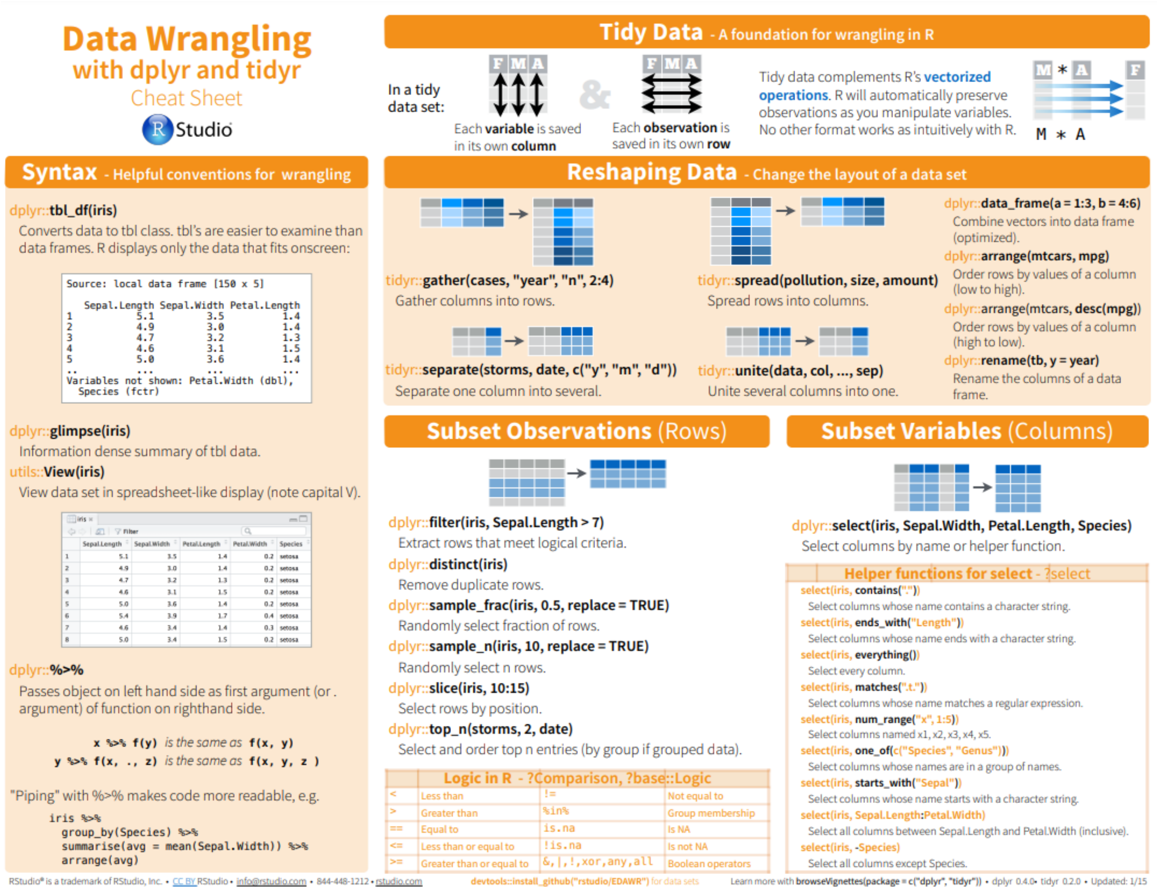
Use function `data.frame()` to create a data frame

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

https://ismayc.github.io/moderndiver-book/4-tidy.html

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()`



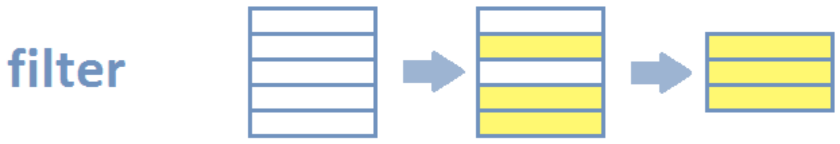
For more information, check the [cheatsheet]()

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:



❑ 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.

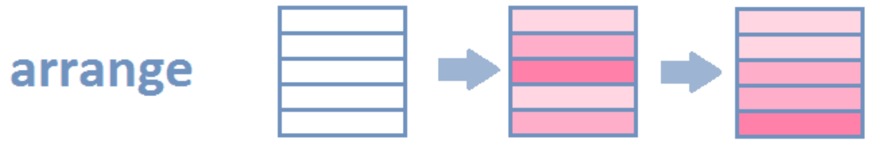
❑ Logical operators

- `!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



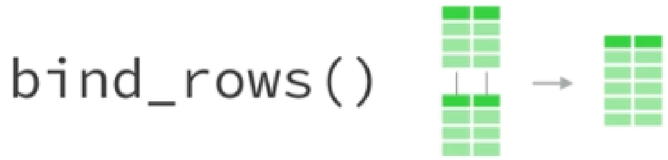
Note:

- 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`

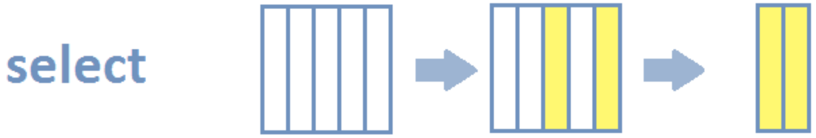


Exercise: let’s do some practice

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



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

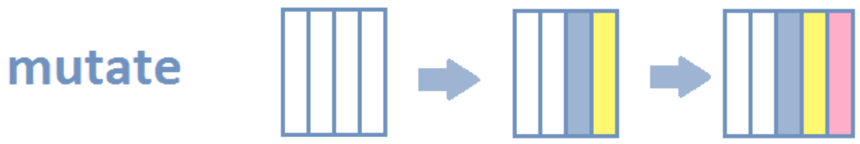
Useful Operators

- `!`: 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)

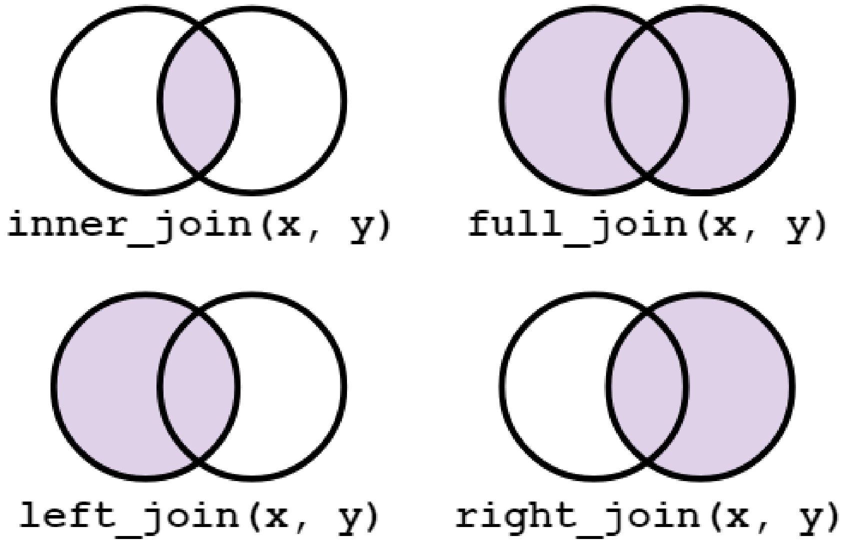


The values can be

- 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()`:



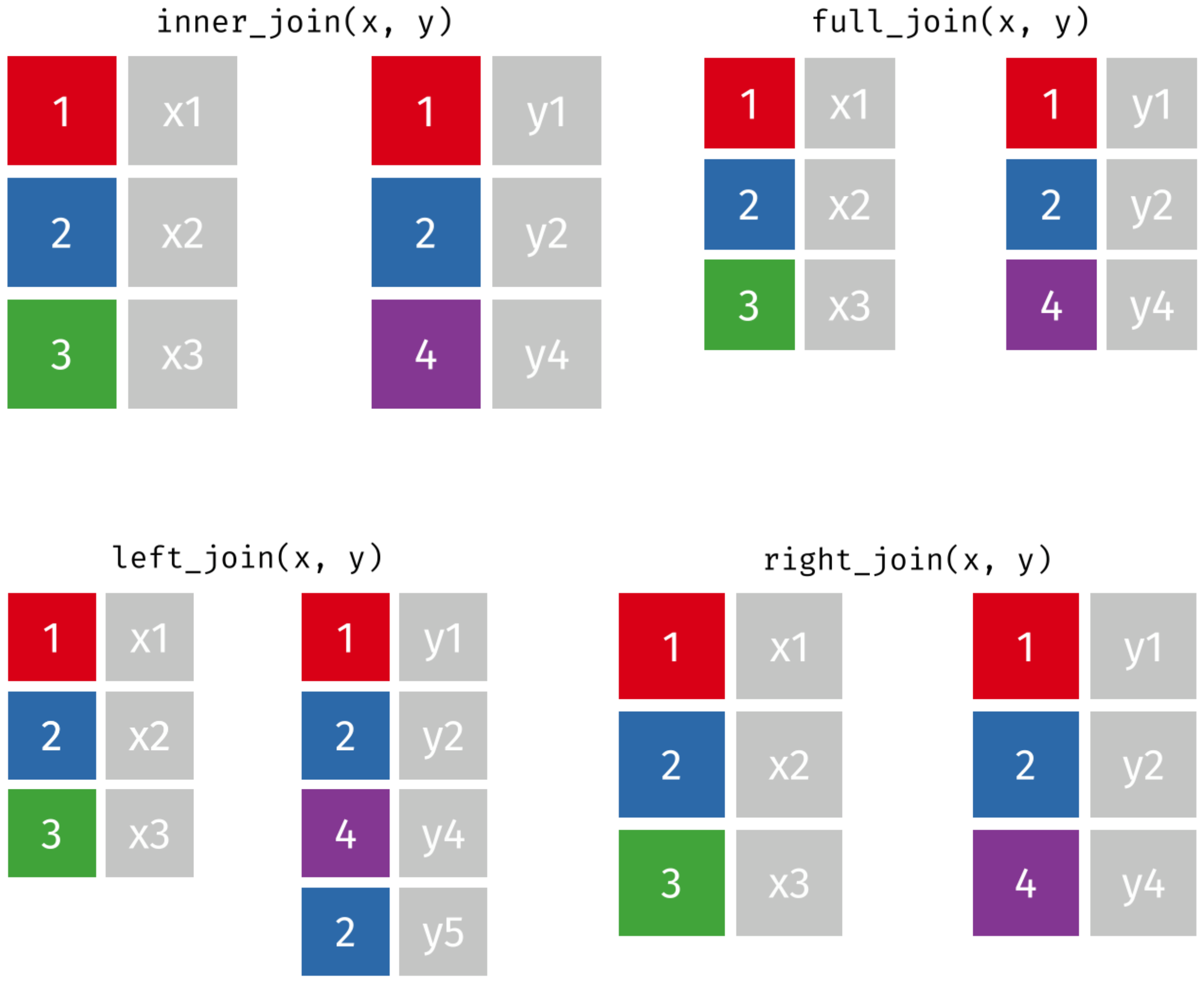
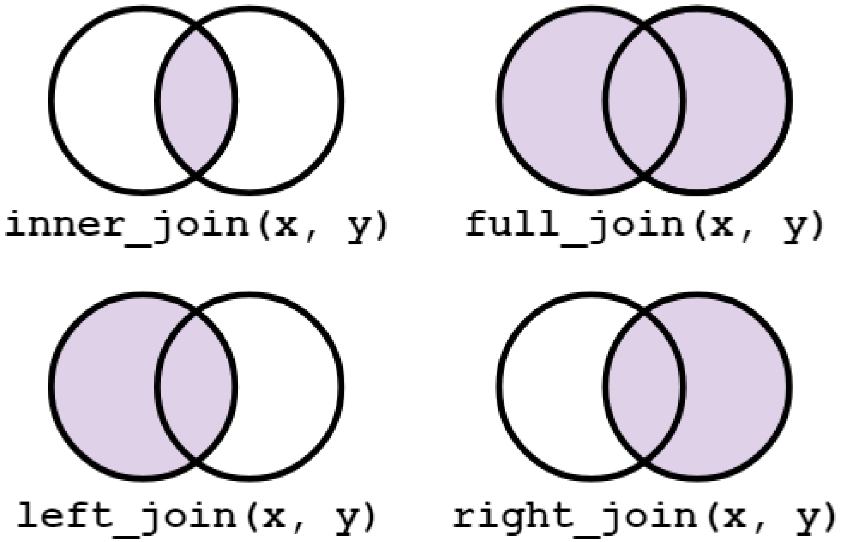
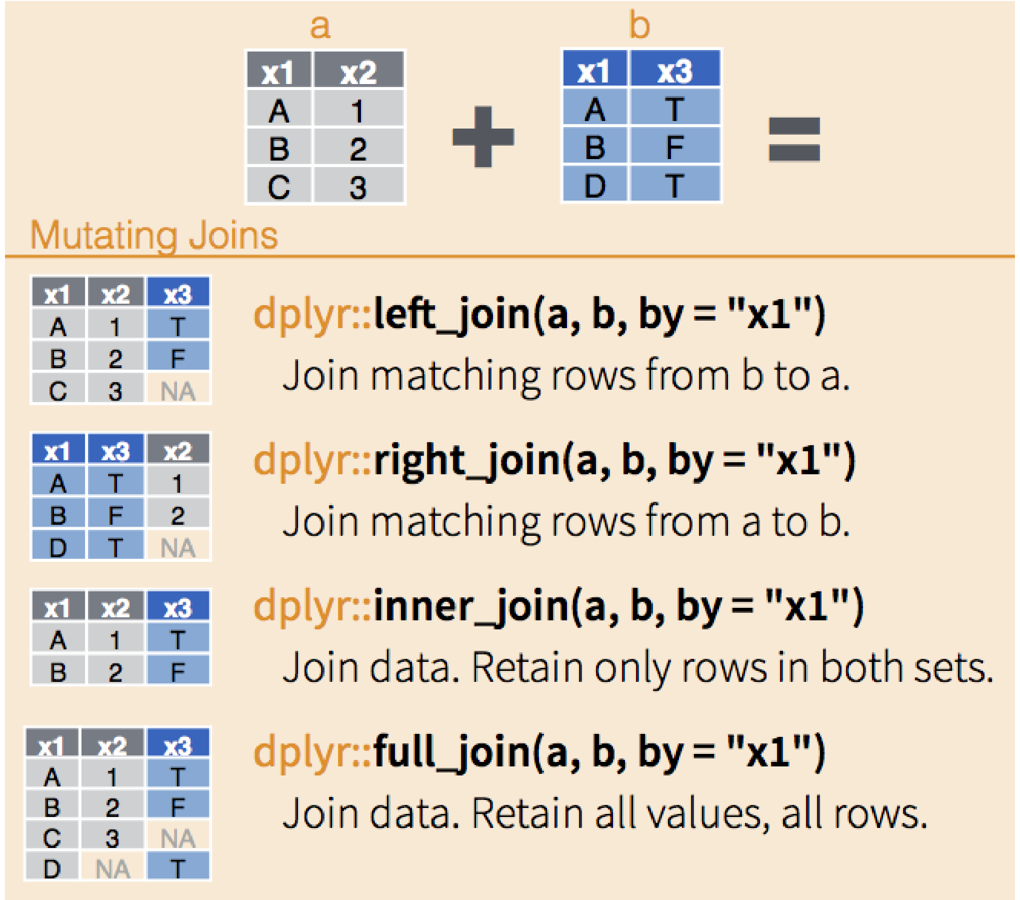


Image from internet

Manipulate variables

`*_join()`:





Exercise: let’s do some practice

Image from internet

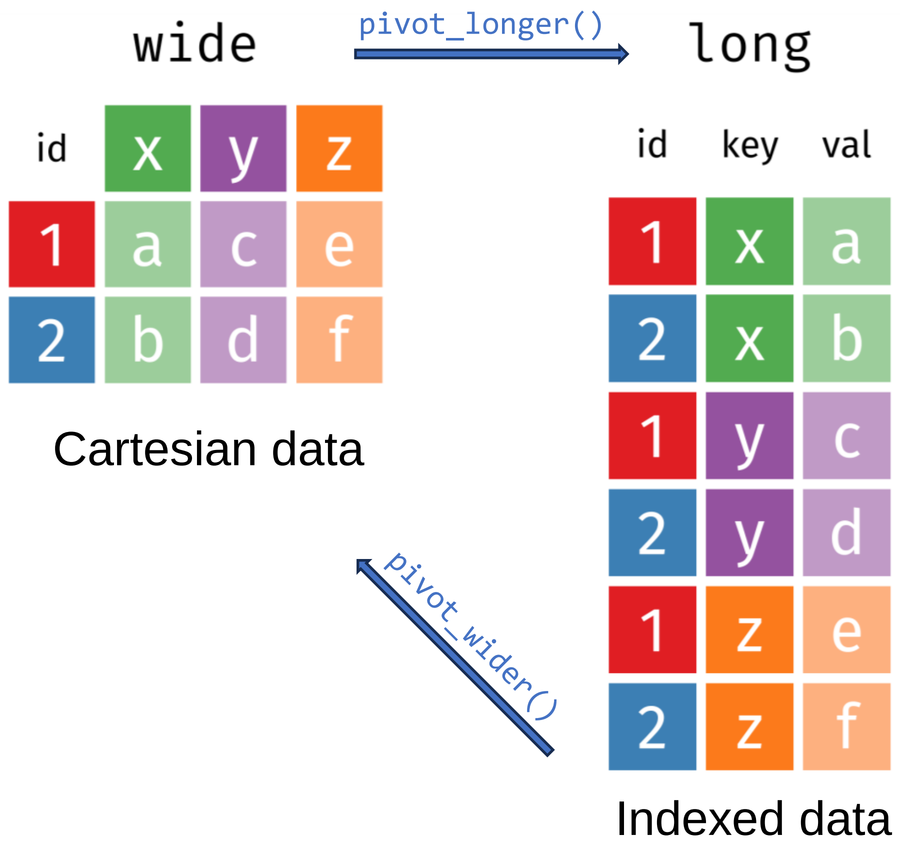
Reshape data frame

`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



https://bookdown.org/Maxine/r4ds/pivoting.html

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

wide

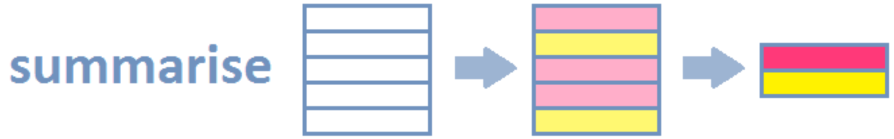
id	x	y	z
1	a	c	e
2	b	d	f

Image from internet

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 (%>%)

```r
# 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))
```

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

```r
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 (%>%)

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

`%>%` 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

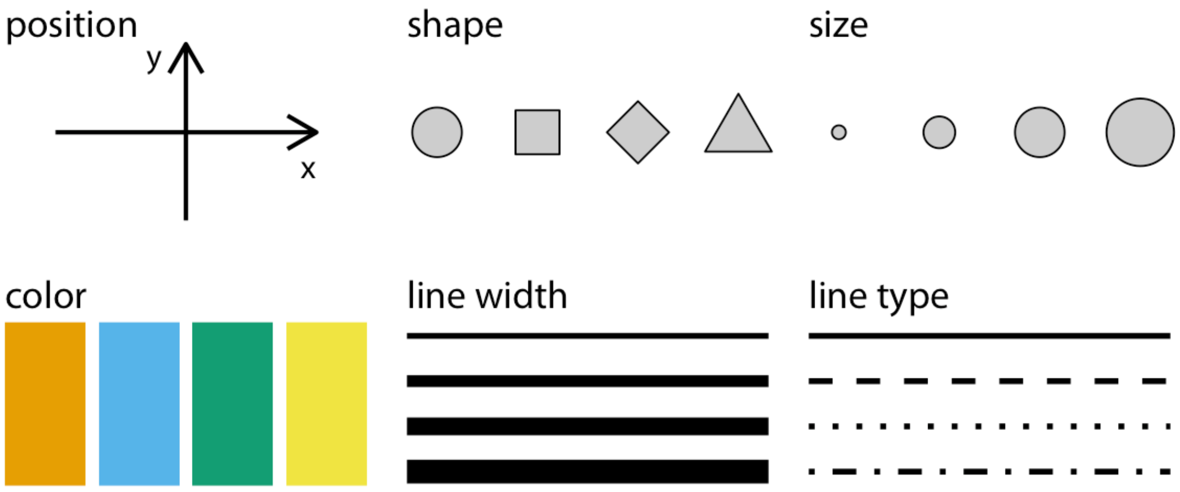

Image from book *Fundamentals of Data Visualization*

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

Image from internet

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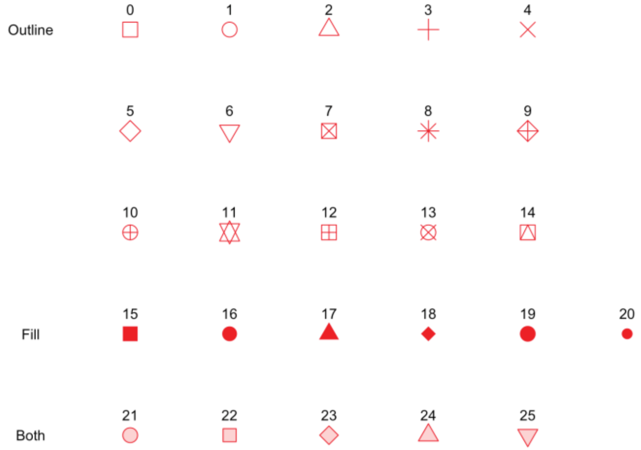
linetype	Line type such a solid, dashed, dotted
labels	Text on the plot
shape	Shape of the geometry

Check available options

- ```
  vignette("ggplot2-specs")
  ```

linetype

shape



Aesthetic mappings and setting

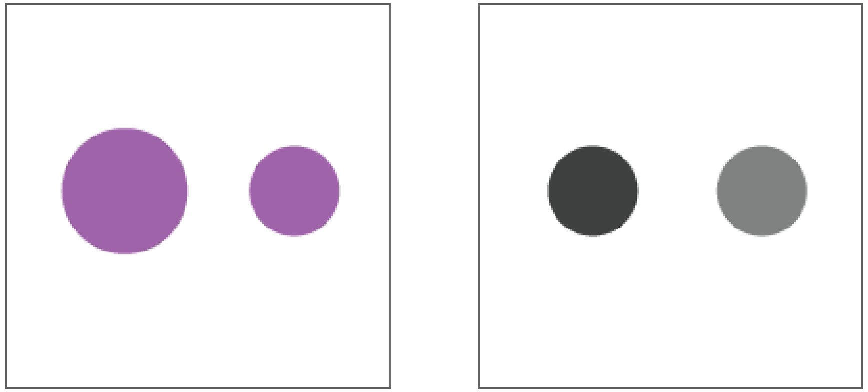
- The function supports some simple transformation (e.g. log(x))
  - ➢ `aes(x = log(displ), y = hwy, colour = class)`

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