Data Visualization with R

Gladstone Institutes

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Part 1 Outline

- Introduction
- Hands-on analysis
  1. Explore *Iris* data and save a publication-ready figure.
     - Data: “iris.csv”
     - Result: “Iris.pdf”
     - Script: “1. iris.R”
  2. Brief digression to save a heatmap.
     - Data: “norm_counts.txt”
     - Results: “Heatmap.pdf” and “Heatmap.tiff”
     - Script: “5_Heatmap.R”
- Conclusion

Part 2 Outline

- Introduction
- Hands-on analysis
  3. Plot and annotate nucleotide-resolution data.
     - Data: “nucleotide_resolution.RData”
     - Result: “Nucleotide_resolution.pdf”
     - Script: “2. nucleotide_resolution.R”
  4. Miscellaneous
     - Interactive data visualization
     - Visualization options beyond ggplot2
- Conclusion

R topics covered

- Hands on
  - Plotting with ggplot2.
  - Writing loops.
  - Saving figures in high resolution.
  - Plotting heatmaps.

- Time-permitting
  - Interactive data visualization with Shiny.

Assumed background

- Familiarity with R and RStudio.
- Basic arithmetic operations in R.
- Variables and assignments.
- Commenting in scripts.
- Functions and libraries.
- Read, subset and explore data.
- Basic plotting of data.
- Data structures available in R.
- Troubleshooting.

Reading resources

- ggplot2 cheatsheet. (download link in description)
- *ggplot2: Elegant Graphics for Data Analysis* by Hadley Wickham. (download link in description)
- *The Grammar of Graphics* by Leland Wilkinson. (download link in description)
- Material from *Introduction to R* workshop on GitHub.

Refresher

R:= Calculator with more “buttons” than you'll ever use.

- R can do all that a calculator can.
  - Open R.
  - Try 2+3.
  - Try 2*3.
  - Try (2+3)/5.
- Conclusion: Off with the calculators!

R is a console application.

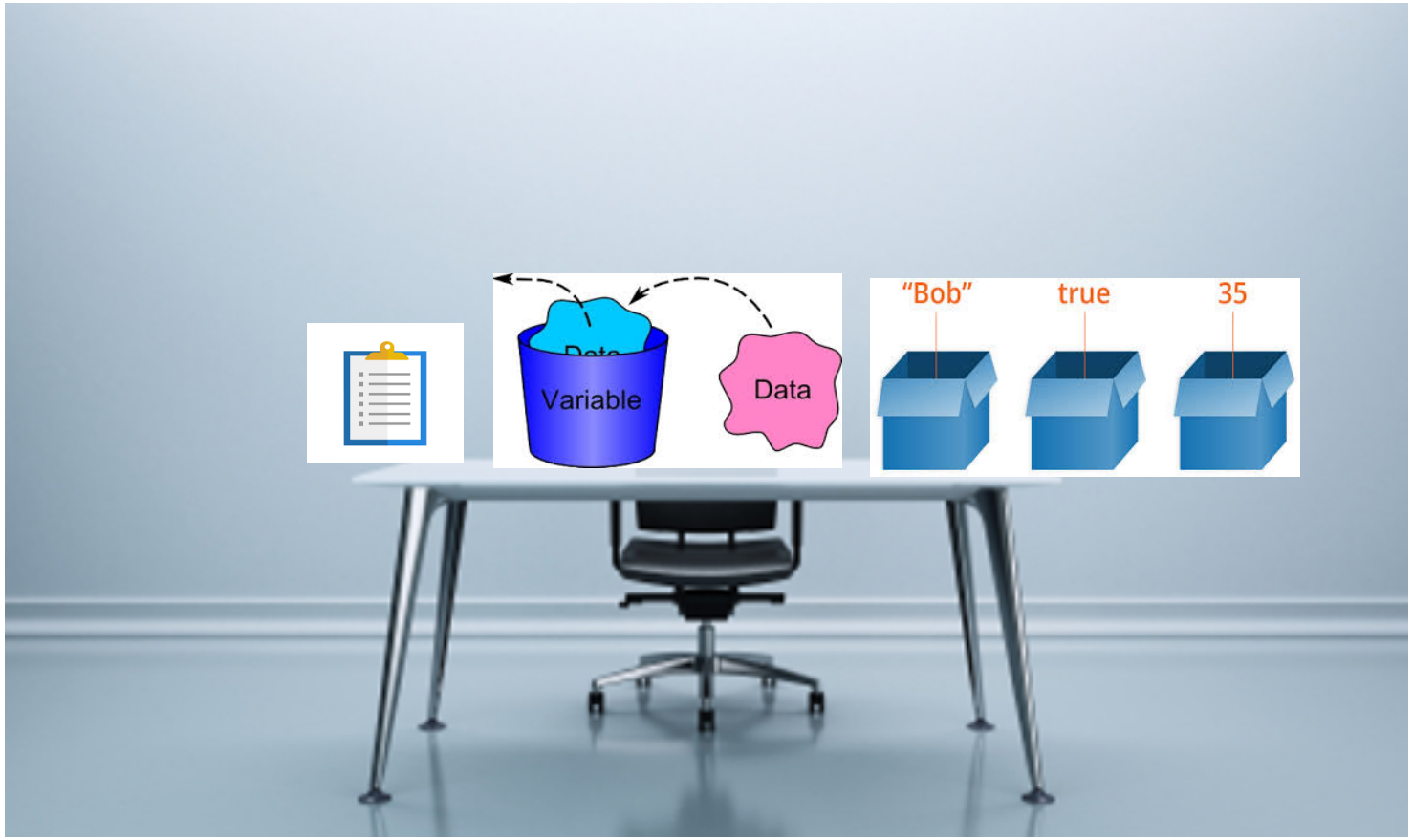
- Text only interface. Inputs and outputs can be images.
- RStudio: Brings more Graphical User Interface (GUI) features to R.
- RStudio is to R as Microsoft Word is to Notepad in Windows or TextEdit in Mac. (~kinda)

Commenting inside a source script

- Looking at an old script, or someone else's script can be scary.
- Speak to machine in code.
- Leave comments in natural language (e.g., English).
  - Anything written after # is interpreted by R as a comment for humans.

Empty workspace/environment

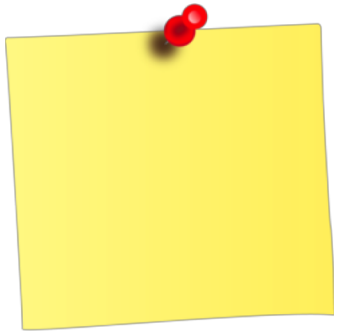
Data analysis creates objects that store data.
(top-right pane in RStudio)



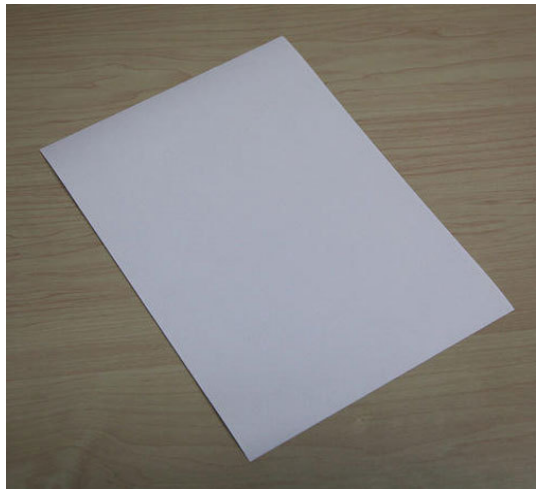
Data structures.

Data structures are data organization/storage formats.

- Storing data physically? Options:



Sticky note



Printer paper

Task pad

Long scroll

Data structures are data organization/storage formats.

- Working with data in R? Options:
  - Numeric vector
    - c(2, 5, 10, 11)
  - Character vector
    - c(“apples”, “oranges”, “butter”, “dry yeast”)
  - Data frames
    - dat from Iris example.
  - Matrix
    - Example counts for genes in several samples.
  - Lists
    - Flexible data structures.
    - mylist <- list(a = c(2, 5, 10, 11),
      b = c(“apples”, “oranges”, “butter”, “dry yeast”)
)

Error!!!


WHAT IF I TOLD YOU
I COME IN PEACE, AND I AM NOT YOUR ENEMY
megenerator.net

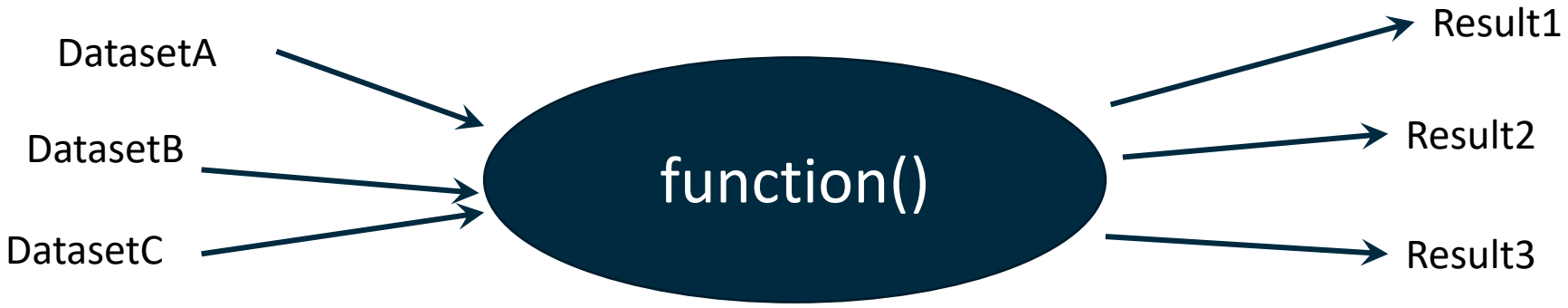
Functions

Working with buttons for modern scientific calculations?

- The best of calculators => 10s of buttons for specific tasks.
- Modern science needs many times more than 10s.

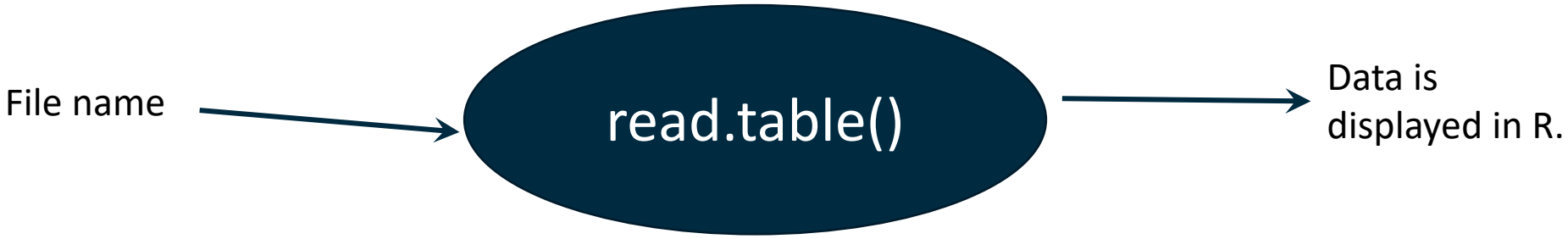
Functions are to R what buttons are to calculators.

- R can perform 100s of 1000s of tasks.
- Tasks are performed by using functions.
  - Examples: sum(), prod(), mean(), t.test().



There are functions for all sorts of things.

- Example to read a table saved in a file:
  - read.table()
  - Usage: read.table(“filename”)



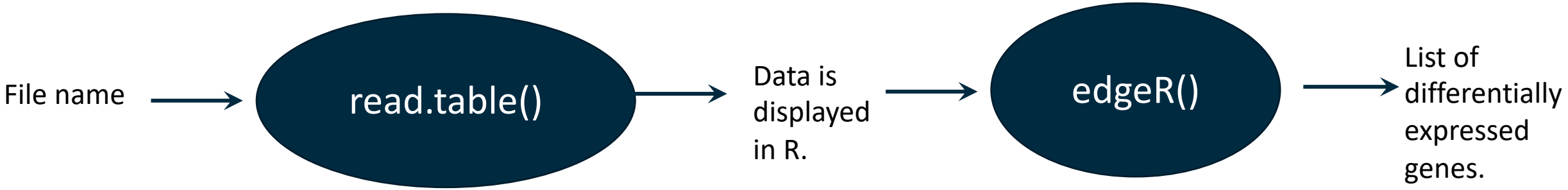
There are functions for all sorts of things.

- Example to find complementary DNA sequence.
  - complement()
  - Usage: complement(sequence)

There are functions for all sorts of things.

- Example to install a package in R.
  - install.packages()
  - Usage: install.packages("ggplot2")

Directing output of one function as input to another.



Library is a collection of functions.

- R works with > 100000 functions.
- More being added everyday.
- If the software were to load (i.e., make available) all of them at startup, it will take a while to launch.
- Solution: Bundle related functions together in a *library.*
  - Example: edgeR.
- Load functions only when needed. (:= Install apps on smartphone as needed)

Functions may need lots of information

- Calculators may take only numbers.
- R functions take variety of things. Numbers, characters, etc.
- Example:
  - Reading a file. Inputs required: File name and address on computer, formatting of file, type of file, etc.
  - Writing a file. Inputs required:
    - what to write?
    - where to write?
    - how to format the file?
    - Include column names, row names?
    - separate with comma?

ggplot2: Package with functions for plotting.

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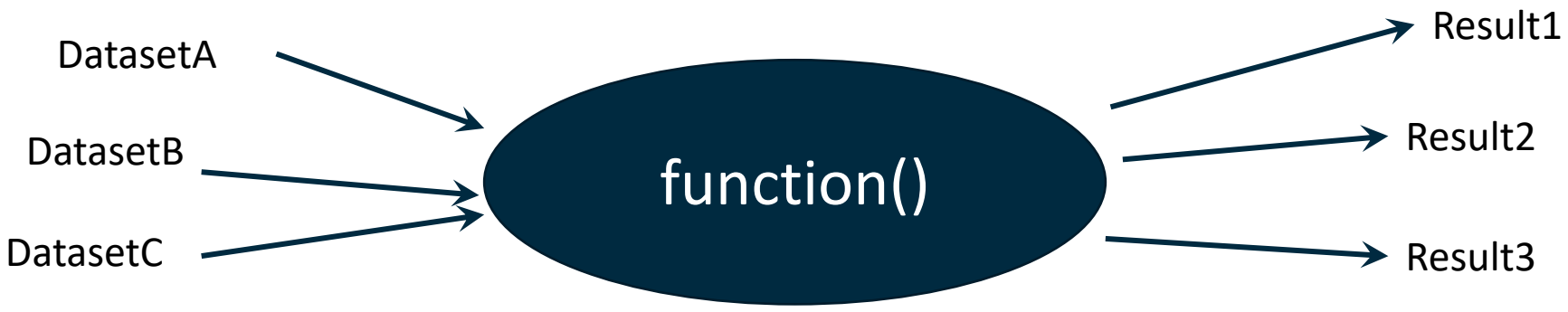
- Tasks are performed by using functions.
  - Examples: sum(), prod(), mean(), t.test().



ggplot2: Package with functions for plotting.

- Plotting layer-by-layer.
- Function names:
  - qplot
  - ggplot

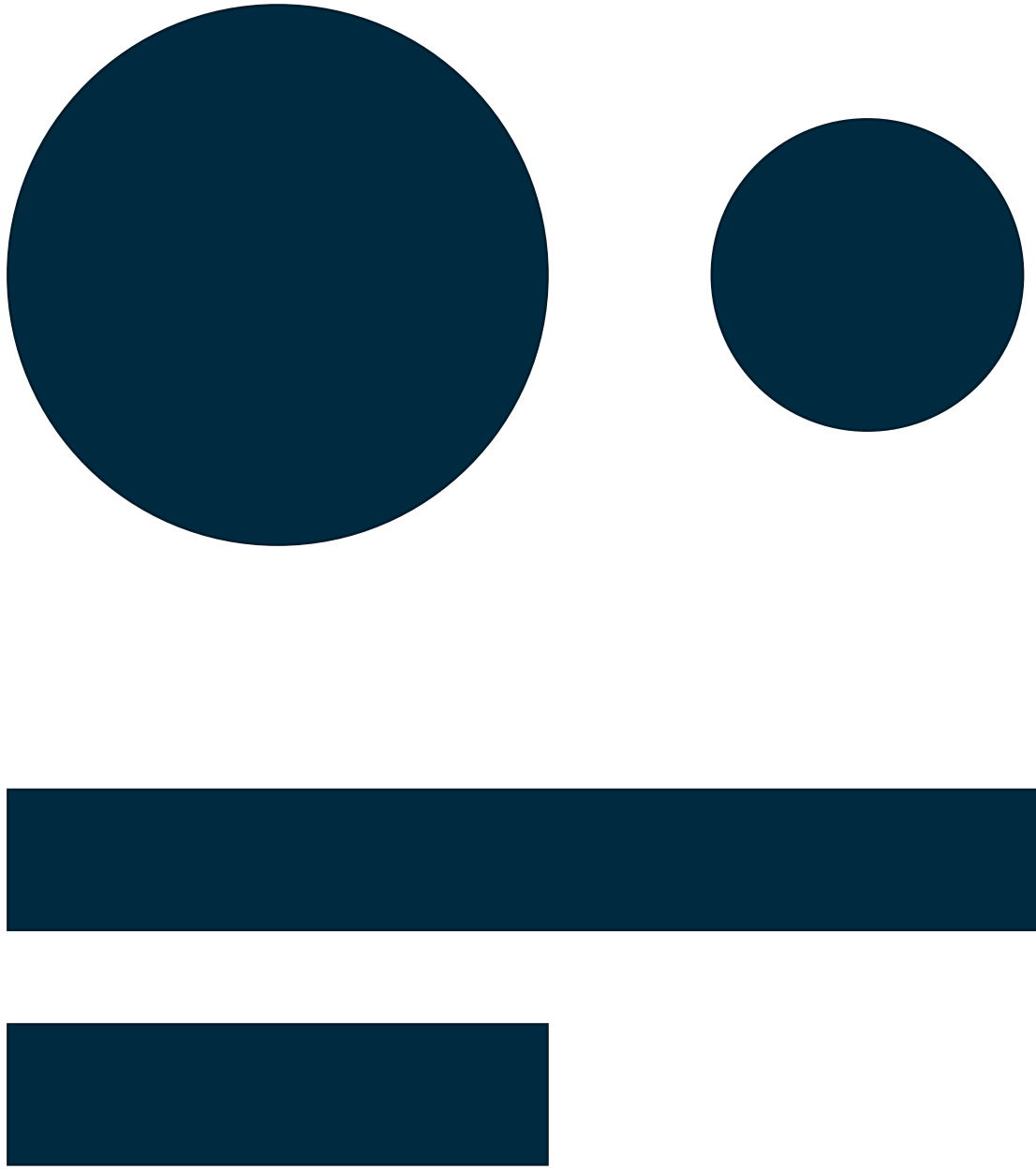
Hands-on: Part 1

Explore *Iris* data and save a publication-ready figure.

- Data: “iris.csv”
  - Iris is a plant genus.
  - Species of this genus may be identified based on the dimensions of petals and sepals of its flowers.
- Result: “Iris.pdf”
- Script: “1. iris.R”

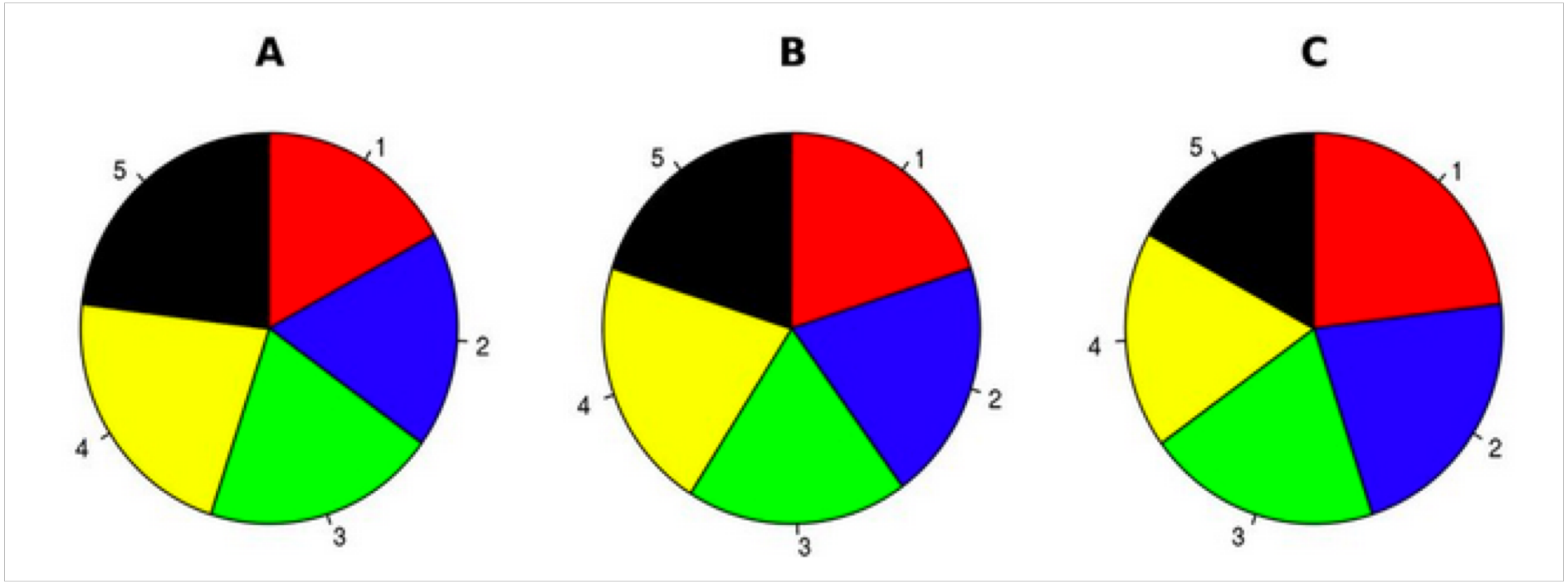
Additional resources

- Q&A: https://stackoverflow.com/
- More on arranging figures for publications.
  - https://cran.r-project.org/web/packages/egg/vignettes/Ecosystem.html

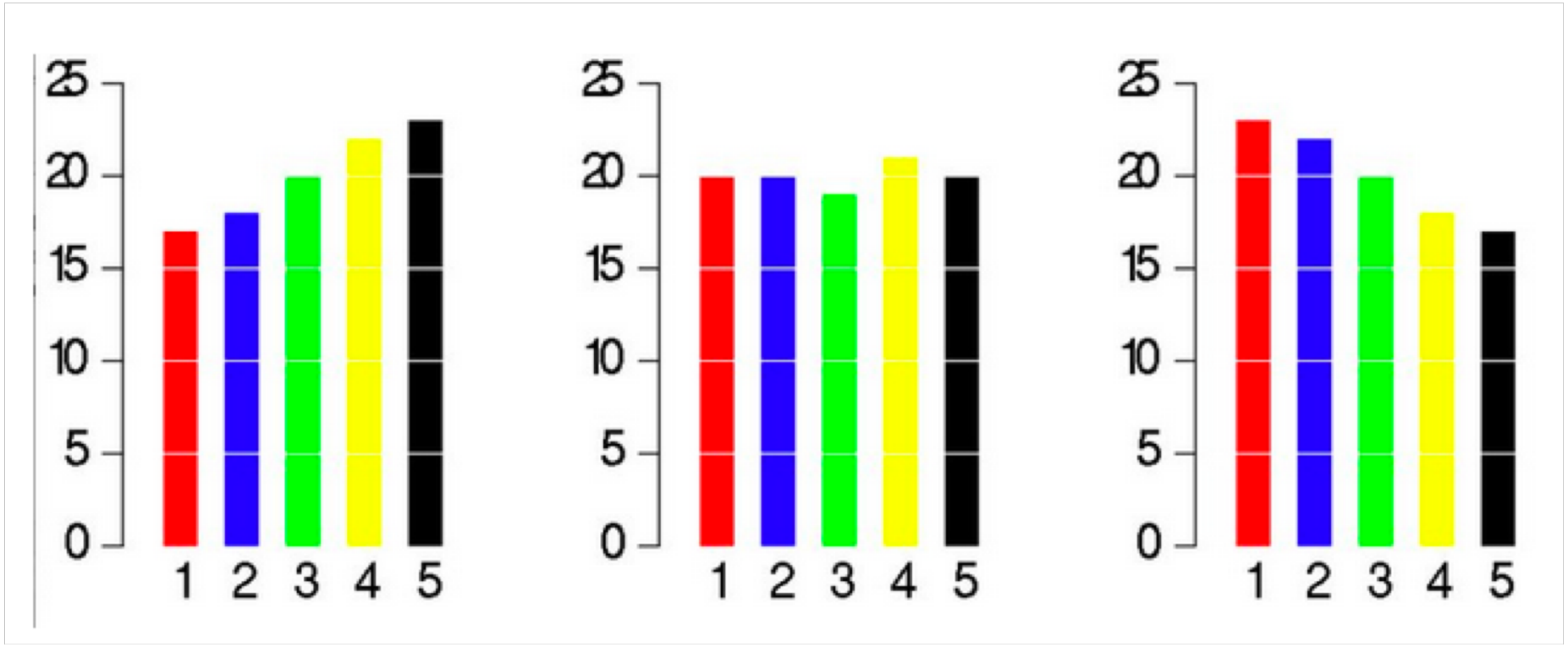


Notes on geometrical attributes of data.

Which color occupies third largest area?



We are better at comparing lengths than areas.



“The purpose of data visualization is insight, not pictures.”

- See link in description.

Brief digression to heatmaps

Save a heatmap for *counts* of genes.

- Data: “norm_counts.txt”
- Results: “Heatmap.pdf” and “Heatmap.tiff”
- Script: “5_Heatmap.R”

Your feedback is important to us!

- https://bioinformatics-course-feedback.questionpro.com/
- ~3 min.

Conclusion (Part 1)

- Need good grammar for effective communication.
  - Grammar of Graphics for plotting data.
- Scripts for high-resolution graphics.
  - Reproducible research.
- Fine control over all of plotting area.
  - Easily change/reproduce figures with alternate themes/annotations.

Part 2:

- Exploring large-scale data enabled by automated plotting.
  - Integrate information from multiple sources on same plot.

Hands-on: Part 2

Plot and annotate nucleotide-resolution data.

- Data: “nucleotide_resolution.RData”
  - One value for six replicates of each nucleotide of > 10000 genes.
  - Need to plot specific regions of 10 genes and annotate motifs.
  - …
- Result: “Nucleotide_resolution.pdf”
- Script: “2. nucleotide_resolution.R”

Hands-on: Additional

Flip book type animation for characteristics of Hill equation.

- Data: To generate using Hill equation.
  - Hill equation gives reaction velocity in terms of substrate concentration.
  - https://en.wikipedia.org/wiki/Hill_equation_(biochemistry)
- Result: “Hill_equation.pdf”
- Script: “3. Hill_equation_static.R”

Interactive visualization for characteristics of Hill equation using Shiny.

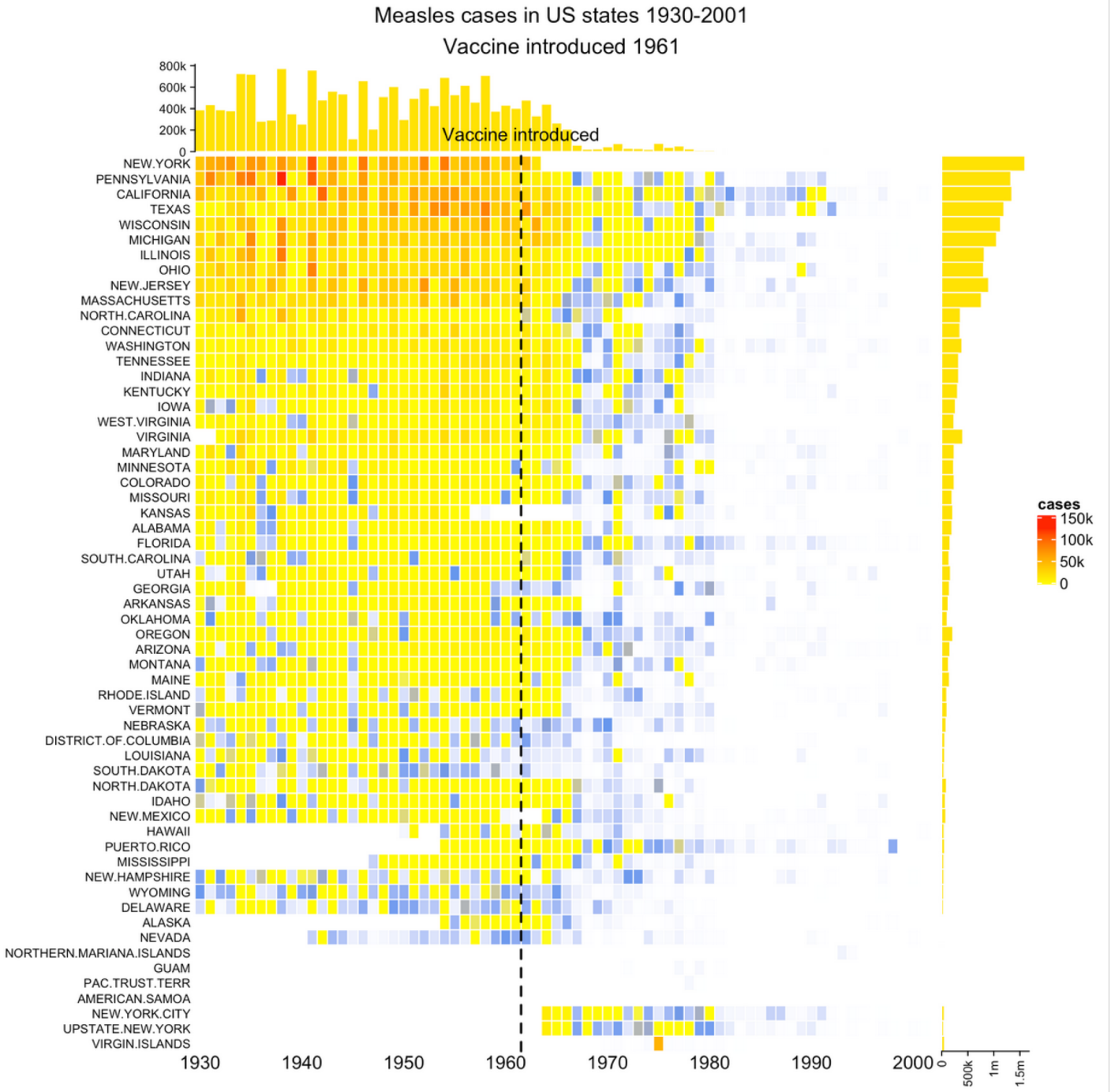
- Data: To generate using Hill equation.
  - Hill equation gives reaction velocity in terms of substrate concentration.
  - https://en.wikipedia.org/wiki/Hill_equation_(biochemistry)
- Result: Interactive application is launched.
- Script: “4. Hill_equation_interactive.R”

Interactive visualization with Shiny.

- Need to define user interface (UI).
- Need to serve data/figures to UI and communicate input values.

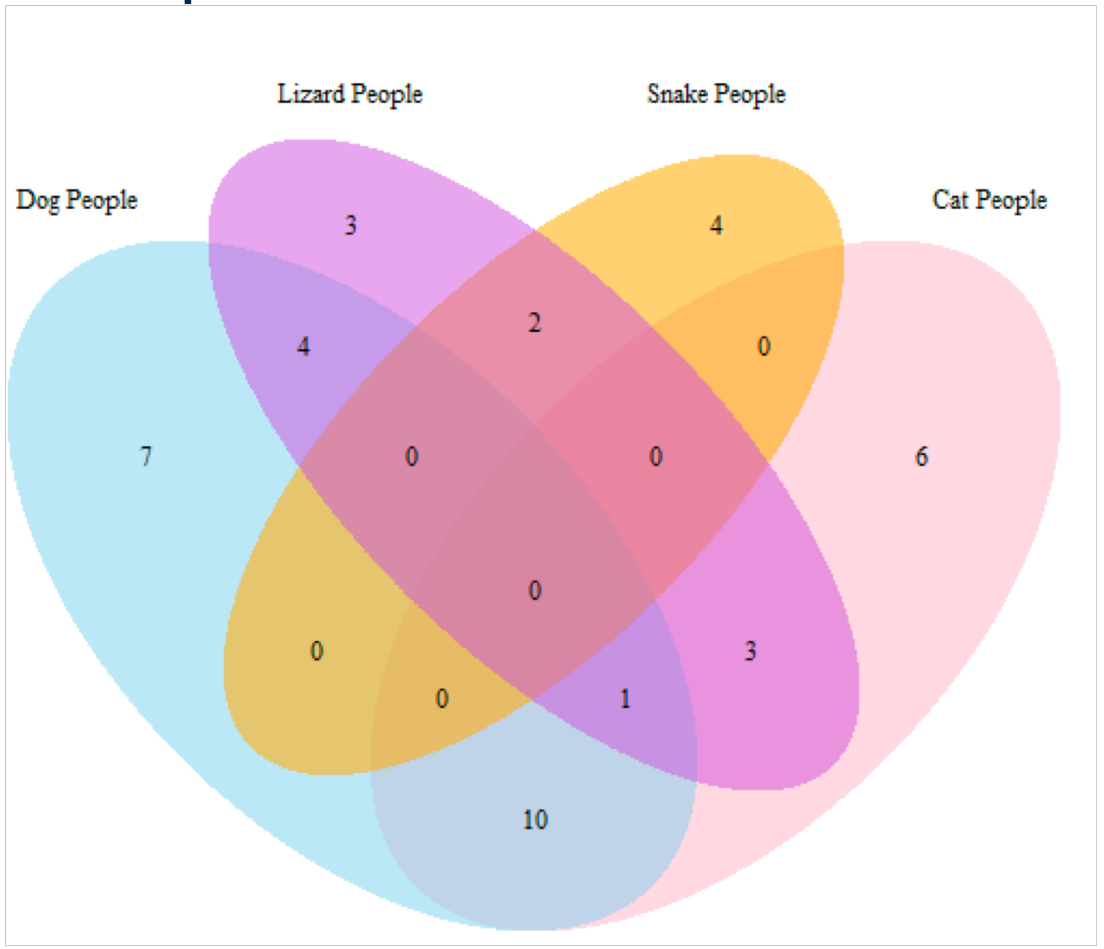
Beyond ggplot2:
1. Heatmap.

- Check out a package called ComplexHeatmap.



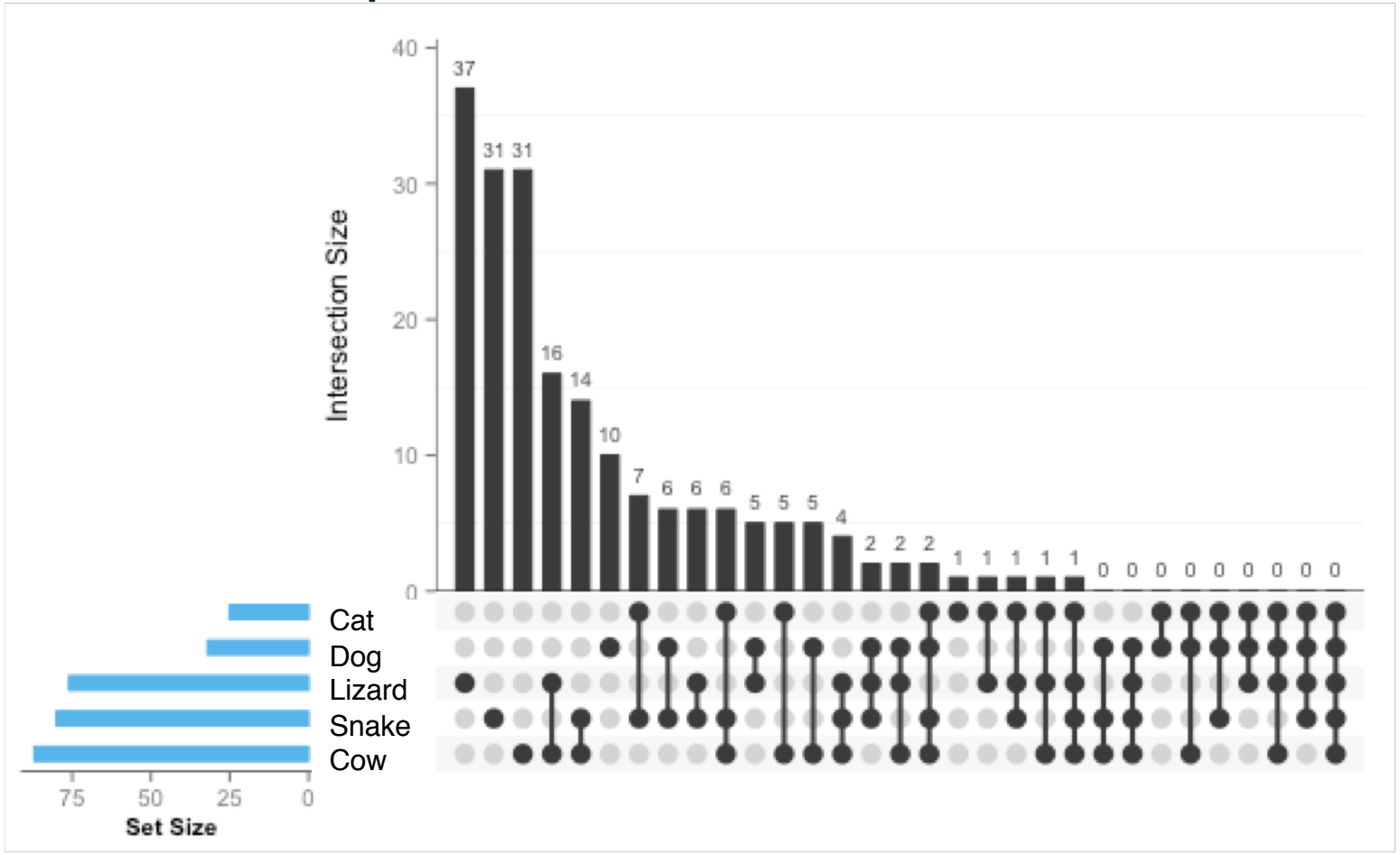
Beyond ggplot2:
2. Venn diagram with multiple sets.

- See link in description.



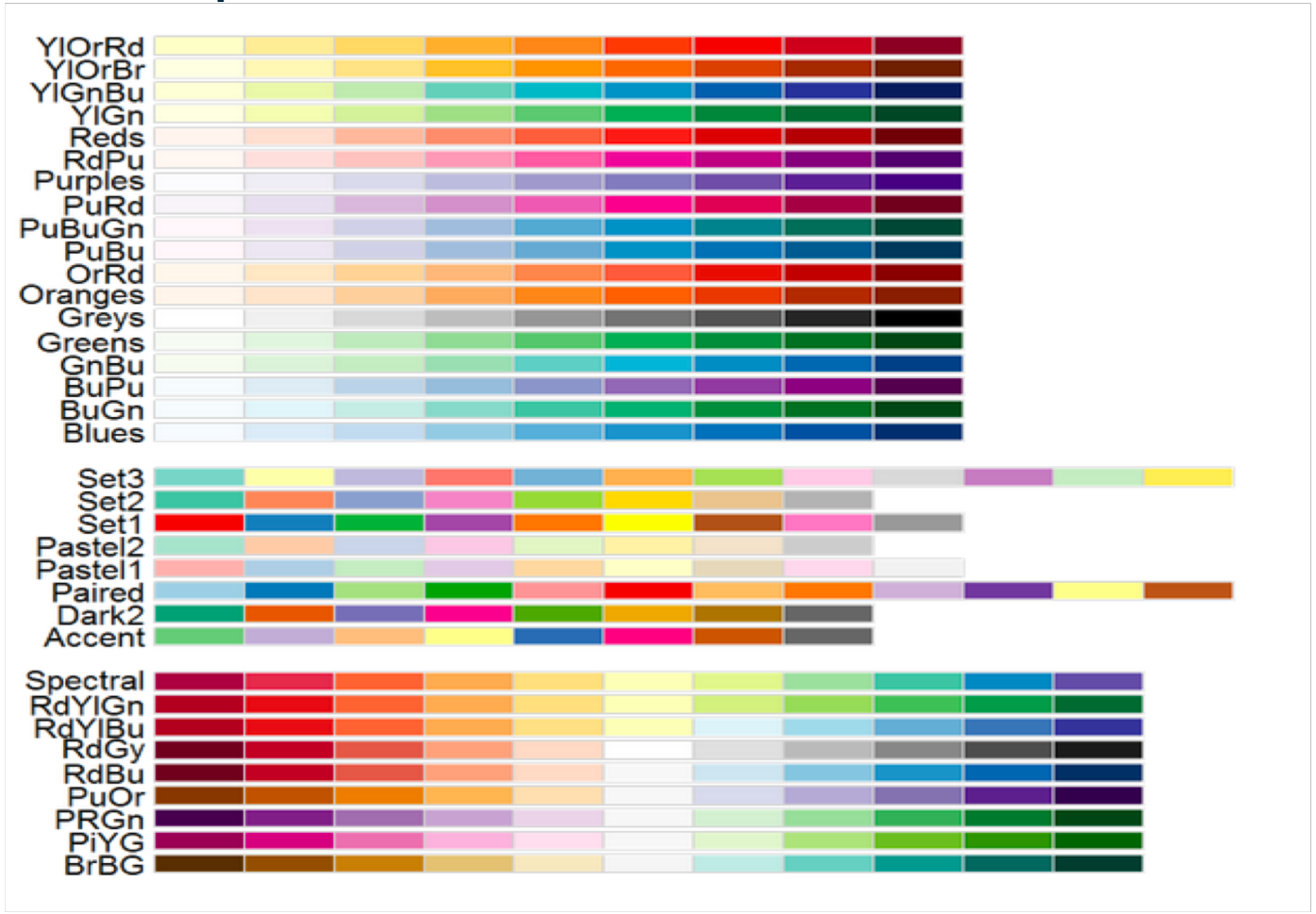
Beyond ggplot2:
2. Venn diagrams with multiple sets (alternative).

- See link in description.



Beyond ggplot2:
3. Select color palettes using RColorBrewer.

- See link in description.



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  - Writing loops.
  - Saving figures in high resolution.
  - Plotting heatmaps.

- Time-permitting
  - Interactive data visualization with Shiny.

Examples of high-resolution graphics

- https://www.r-graph-gallery.com/

Interactive visualization with Shiny

- https://shiny.rstudio.com/gallery/

Conclusion

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