Getting Started with Tabular Data

Spring R '24

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Agenda

- 1. What are R and RStudio? What can you do with them?
- 2. R as a calculator
- 3. RStudio orientation
- 4. Packages
- 5. Loading data
- 6. R data types and structures
- 7. Saving data

About the trainer

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Services for the Pitt community:

- Consultations
- Training (on-request and via public workshops)
- Talks (on-request and publicly)
- Research collaboration

Support areas and interests:

- Computer programming fundamentals, esp. for data processing and analysis
- Open Science and Data Sharing
- Data stewardship/curation
- Research methods; science and technology studies

Spring R Series

#	Date	Title
1 🏠	2/22	Getting Started with Tabular Data
2	2/29	Working with Data Frames
3	3/7	Data Visualization
4	3/21	Inference and Modeling Intro
5	3/28	Machine Learning Intro

What to expect

- I strongly don't believe in "sink or swim" or the weed-out mentality—reach out if you need help!
- How will we use our time?
 - Some lecturing with slides
 - Practice with hands-on Exercises; work in couples/groups (suggested) or independently
- You/we might not finish all the exercises in the allotted time; that's OK.

Thinking about data

Basic formats of data

- string or character-based data
 - viewable/editable in a text processor
 - may consist of plain text, or specially encoded information (markup languages, tabular formats—"structured data")
- image, audio, video, and sensor data
 - requires additional layers of software for viewing and editing
 - various encoding schemes depending on electronic source and desired use case
 - there is often a processing step to convert some of the information into structured data, for analysis
- compressed data (one of the above types, some bits removed)
 - compression may be "lossy" or "lossless"
 - decompression may occur on-the-fly (playing an MP3) or may need to be accomplished before consuming data (a zip file)

Ways to work with data

- Tabular format quantitative, statistical methods (R's preference)
- Document format (XML) usually qualitative methods
- Computer vision and audition algorithmic processing, deep learning models

Converting from XML or unstructured data to tabular format is popular, because it facilitates statistical analysis. An image containing

In this course, we are working with string data—interpreted as numeric values and pieces of text—in a tabular format.

What are R and RStudio? What can you do with them?

What are R and RStudio?





R is...

- a tool for statistical analysis and visualization dating back to 1993
- a general-purpose programming language
- text-based command interface → it runs on the console/command line
- free, open-source software (FOSS)
 stewarded by the nonprofit, Vienna-based
 R Foundation

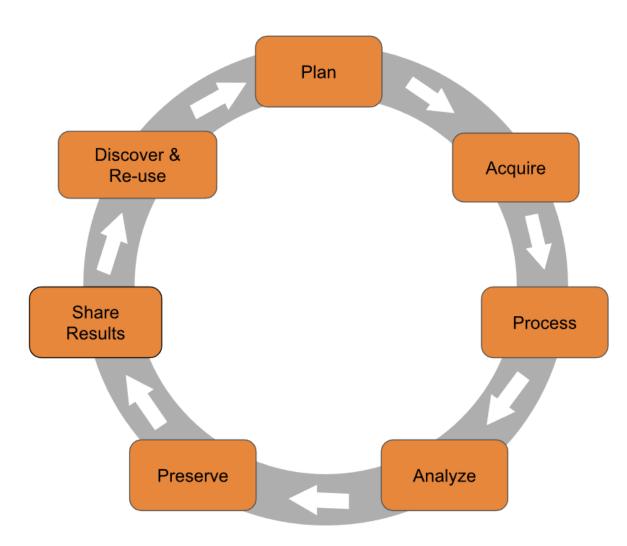
RStudio (Desktop) is...

- an "integrated development environment"—graphical interface with numerous features—for analysis and programming in R and Python
- Posit (until recently, called RStudio) is a Boston-based public benefit corporation, founded 2009; makes both FOSS and commercial software and offers hosted services



What can you do with R and RStudio?

- Import data from file and online sources
- Explore, clean, reformat, and combine data
- Perform calculations and analyses on data, using statistical and/or machine learning (ML) methods
- Visualize data
- Present information in a variety of formats (documents, Web, etc.)
- Build a dashboard or other web app, especially interacting with tabular data



Research Data Lifecycle; source: Princeton Research Data Service

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Example analyses

Here is a (very small) sampling of papers that use analytic methods which are available in R.



Measuring chlorophyll and phosphorus at multiple points in Lake Erie to understand algal bloom patterns; Bayesian network (Rowland et al. 2019)

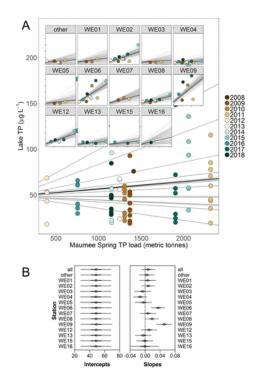
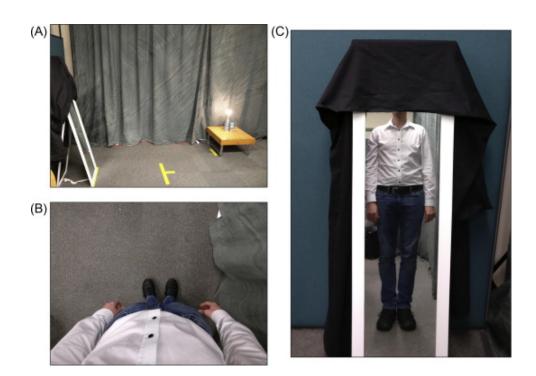


Figure 5. Maumee River spring (1 Mar–30 Jul) loads vs lake concentrations for soluble reactive phosphorus (SRP) 2008–2018 in Lake Erie. ...



Characterizing how people perceive themselves in a mirror versus looking at their own body; Principal Components Analysis. Participants answered several questionnaires about mirror-gazing and about their general mental state.

(Jenkinson and Preston 2017)

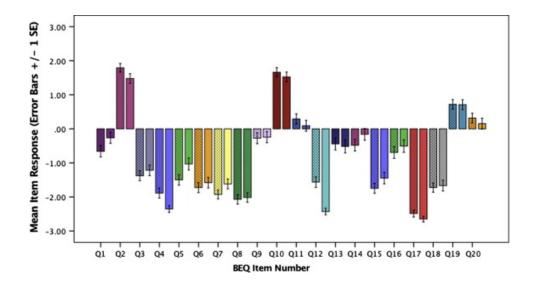


Fig. 2. Mean (SE) responses to BEQ items. Adjacent bars of the same colour represent responses for the direct (left/stippled colour) and mirror (right/solid colour) views. See Table 2 for item labels (Q1-20).

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Paternal age related schizophrenia (PARS): Latent subgroups detected by k-means clustering analysis

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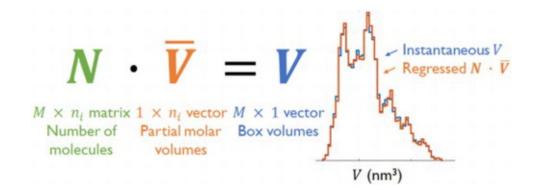
Keywords: Cluster analysis k-Means clustering

ABSTRACT

Background: Paternal age related schizophrenia (PARS) has been proposed as a subgroup of schizophrenia with distinct etiology, pathophysiology and symptoms. This study uses a k-means clustering analysis approach to generate hypotheses about differences between PARS and other cases of schizophrenia. Methods: We studied PARS (operationally defined as not having any family history of schizophrenia among first and second-degree relatives and fathers' age at birth ≥35 years) in a series of schizophrenia cases recruited from a research unit. Data were available on demographic variables, symptoms (Positive and Negative Syndrome Scale- PANSS), cognitive tests (Wechsler Adult Intelligence Scale-Revised; WAIS-R) and olfaction (University of Pennsylvania Smell Identification Test; UPSIT). We conducted a series of k-means clustering analyses to advantise and the property of the

Results: Two analyses generated clusters with high concentrations of PARS cases. The first analysis (N= 136; PARS= 34) revealed a cluster containing 83% PARS cases, in which the patients showed a significant discrepancy between verbal and performance intelligence.... The second analysis (N= 123; PARS= 30) revealed a cluster containing 71% PARS cases, of which 93% were females; the mean age of onset of psychosis, at 17.2, was significantly early.

Conclusions: These results strengthen the evidence that PARS cases differ from other patients with schizophrenia....These findings provide a rationale for separating these phenotypes from others in future clinical, genetic and pathophysiologic studies of schizophrenia and in considering responses to treatment. (Lee et al. 2011)



Modeling chemical properties of constituents in a mixture using molecular simulation; simulation and multiple linear regression (Josephson et al. 2019)

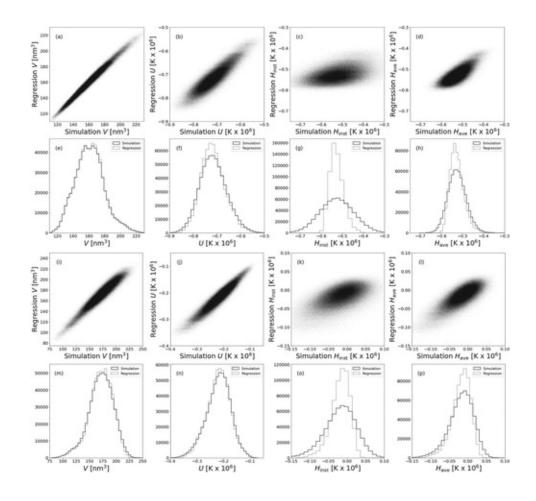


Figure 2. Parity plots and histograms illustrating the quality of the multilinear regression for the EtOH-rich liquid in the LLE system, with .

Why I prefer R

versus Excel:

- ✓ Non-proprietary, open source
- Powerful and fast interactions with data
- Very extensible
- Research-oriented community
- Reproducible and visible interactions with data
- Data viz makes sense to me
- Can handle more data for a given quantity of system resources
- ✓ Less prone to accidental user error
- X R has a steeper learning curve
- R/RStudio doesn't have convenient data entry

versus Python:

- ✓ Purpose-built for stats
- Simpler mental model and syntax (for tabular data work)
- RStudio is better than (free) IDEs for Python
- ✓ I can always call Python from within R if I need to
- R has a smaller (but more focused) community with less published code

Setup

- Recommended: install R and RStudio (Windows, macOS, Linux)
 - R: https://cran.rstudio.com/
 - RStudio Desktop: https://posit.co/download/rstudiodesktop/
- Cloud-based alternative: Posit Cloud (chromeOS)
 - R and RStudio in your web browser—no installation!
 - Have to create a account (lowest tier is free)
 - https://posit.cloud/



R as a calculator

Our first R code

- When you open RStudio, you'll see the console. This is where R waits for commands.
- Arithmetic operators: + * / ^ (exponentiation) %% (modulus) %/% (integer division)
- As in algebra, an R function accepts arguments and returns a value.
- Common mathematical functions: sum(), mean(), median(), mode(), min(), max(), sd(), sqrt(), abs()
- Logarithms: log(x) for natural and log10(x) for base 10 (or log(x, base) for any base you want)
- (Euler's number) is represented with exp(1), where 1 is the desired exponent of .
- Rounding: round() for decimal places, signif() for specifiying significant digits
 - See also: floor(), ceiling()
- NOTE: To operate on more than one value, such as calculating a mean, your values need to be inside a *vector*.

Vectors in R

- An ordered collection of values, all having the same type (e.g., numeric or text)
- Created with the c() function ("combine")
- R loves vectors—so much, that any single value you give to R, is returned as a 1-length vector!
- Very many operations are *vectorized*, meaning that they apply to every value in a vector by default.

Exercise 1.1: console calculations

RStudio orientation

RStudio layout (panes)



Write *scripts* and *R notebooks* in tabs



Objects in your workspace (session); Import Dataset

BL: Console

Run commands

↑ for command history

≒ tab key for suggestions

■ BR: Help, Files, Packages ? <a> □

All extremely useful!

What kinds of files will you use in RStudio? (1)

- R Notebook (.Rmd) or Quarto document (.qmd): mix formatted text and code and code outputs
- R script (.R): plain-text file that can be executed by R directly
 - ⚠ The only permitted "natural language" is in code comments.
- R Project (.Rproj): lives in the directory for a given project, and holds information like command history and settings. Optional but recommended.
- .RData: a workspace (session) snapshot
- .rds: an R data structure, i.e., an R object which has been saved to the filesystem

What kinds of files will you use in RStudio? (2)

Of course, you will also be loading files in whatever format your data take (spreadsheets, shapefiles, etc.).

Protip: make sure your operating system is set to display *all* file extensions!

- Windows instructions
- macOS instructions

Ways to run your session

- Console: quick calculations, one-line pieces of code
- Scripts: multiple console commands saved in one file
 - You can send to console line-by-line, or entire file at once
- Notebooks: a document with "code chunks" (mini scripts)
 - You can run the chunk one line at a time, or entire chunk at once

Keyboard shortcuts	
Windows:	Mac:
 Ctrl-Enter runs one line of code Ctrl-Shift-Enter runs the whole chunk 	 ₩-Enter runs one line of code ₩-Shift-Enter runs the whole chunk

Working Directory (1)

- Suppose your project folder has a subfolder called data, and a file called patients.csv.
 - Absolute path:

```
/users/djb190/Documents/projects/R/study-
x/data/patients.csv
```

- Relative path: data/patients.csv
- We would rather use the relative path, but R needs to know, "relative to where?"

Working Directory (2)

- Use getwd() to check your current working directory
- To set your working directory:
 - In the **Files** tab (bottom right), click the three dots ... at right, find the folder you would like to use as Working Directory, and click Open
 - Now click the

 More

 button and choose Set As Working Directory
- When you run a <u>script</u>, you should set the working directory
- When you open a <u>notebook</u>, RStudio will automatically treat the notebook's location as the working directory

Packages

Packages

- Packages are additional functionality created by individuals and collaborations in the R user community
- So far, we have only used base R
- Packages greatly extend R! You'll use them all the time.
- The authoritative place for packages is CRAN, the Comprehensive R Archive Network (https://cran.rproject.org/)
 - A convenient directory and repository
 - QA/QC process; trusted as reliable and safe



Install a package

- 1. Google "Rstats" where is whatever you want to do (or maybe "R package for"). Read about available packages for your job and choose one.
- 2. Go to Packages tab (bottom right pane) and click Install.
- 3. Type the name of the package you want and click install.

Or if you like to write code: install.packages("name-of-package")

Let's install the **tidyverse**, a collection of packages that we'll use for the rest of the course: **install.packages("tidyverse")**

Attach a package

- To use a package, we need to attach it:
 - In Packages tab, click the checkbox next to the package name
 - or run library(package-name)
- Once a package is attached, its functions and/or datasets are available in the workspace. (But all packages are detached when the session ends.)
- Some packages will display a message or warning when they attach; some will not;
 depending on the package and your setup

Now let's attach tidyverse: library(tidyverse)

Loading data

Tabular data

You are likely to encounter tabular data in the following storage formats:

- Comma-separated values (CSV) or tab-separated values (TSV): .csv, .tsv, .dat,
 .txt
- Excel spreadsheets: .xlsx, .xls
- OpenDocument spreadsheet from OpenOffice/LibreOffice: .ods
- Parquet, a columnar format which is very efficient: .parquet
- Relational databases: usually via remote connection
 - Requires writing structured query language (SQL) or using a SQL-based package.

We are going to focus on CSV, since it is a non-proprietary and extremely common format.

Loading a CSV

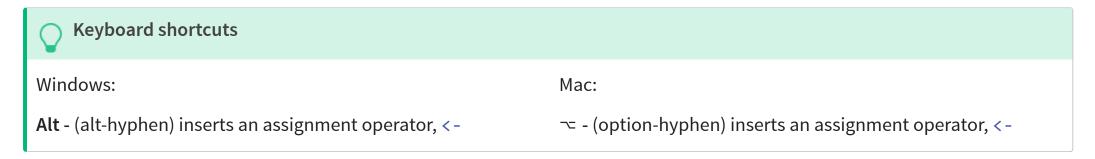
- readr is a package for reading CSVs and other characterdelimited formats
 - (also possible with base R, but readr is recommended)
- library(readr) will attach readr, but it is included in tidyverse (which we already have attached)
- This means we can call readr's read_csv() function!
- You can also call a function from an installed package, without attaching it, by prepending the package name and two colons: readr::read_csv().



Object assignment

In order to do something with our data, besides look at them once, we need to tell R to assign the result of our expression—i.e., the output of read_csv()—to an object. We also sometimes call this storing or saving an object

We use a left-pointing arrow, < − (type less-than and hyphen) for assignment:



You may also use = (equals) for object assignment, although it is not recommended.

Viewing the data

Use the **View()** function on our loaded data to launch the Data Viewer, for example: **View(my_values)**. This is the same as clicking the object's name in the Environment pane.

You can also type the object's name to see a brief textual representation of it, in the console or notebook.

A few more useful functions:

- dplyr::glimpse() or str() shows all columns listed top-to-bottom
- head() and tail() shows the top or bottom of the data frame
- **Q** summary() summarizes a vector (or each vector in a data frame) according to its data type

R data types and structures

Data types

Every value in R has one of these types:

- numeric: real, decimal numbers
- integer: whole numbers
- character: text; should always be in quotation marks " " in code
- logical: TRUE and FALSE, also called Boolean
- complex: for imaginary values i.e. complex numbers (rare)
- raw: values are stored as bytes and not human-readable (rare)

Data structures

Regardless of type, every value is organized into a structure (usually with other values). These are the most common structures:

- **Vector**: we have already used this ordered collection of single type; R's default structure; 1D
- List: ordered collection of varying types; 1D
- Data frame: a tabular structure; 2D
 - "table" and "data.table" are two alternatives to data frames with different use cases
- Matrix (2D), Array (D): Used for linear algebra, and some machine learning algorithms operate on matrices
- A special vector is the factor, which allows only certain values (defined in the structure);
 used for categorical variables
- Model object: produced by a modeling function such as linear regression
- Many other specialized structures are offered by packages, built upon these components

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The data frame

- A table in which each column ("variable") is a vector of equal length
- Row (or "case" or "observation") is read by retrieving the th value of each variable
- To reference a variable/column, use the format data_frame\$var_name
- We'll be spending the rest of our time in this course with data frames and vectors.
- (Under the hood, a data frame is a list with some added features.)

Saving data

Writing a CSV

- readr can also write: write_csv()
- Remember Working Directory and relative paths.
- The file name must be in quotation marks, e.g.,
 write_csv("patients.csv")

The data frame is the "R-native" representation of the data. We read and write to an interchange format (CSV) to save and/or share our work.

Exercise 1.2: loading and addressing data

Wrap up

Conclusion

We learned about:

- Orienting to R and RStudio
- Performing basic calculations and function calls
- Opening, viewing, and saving data
- Writing our first R code

Next time: exploring data frames!