From Basics to Brilliance:

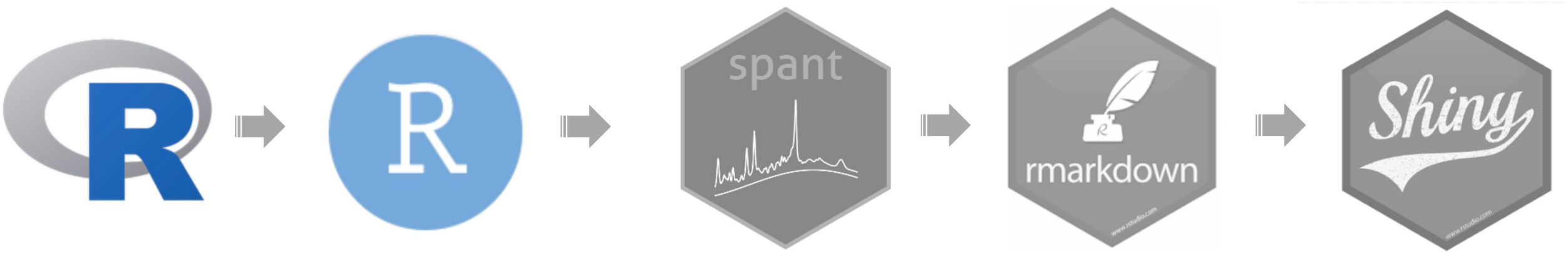
An Introduction to R-Studio for MR Spectroscopy analysis, visualization, and beyond

MRS Hackathon Toronto 2023

Jessica Archibald, PhD.

@ArchibaldJes

Outline



Programming language

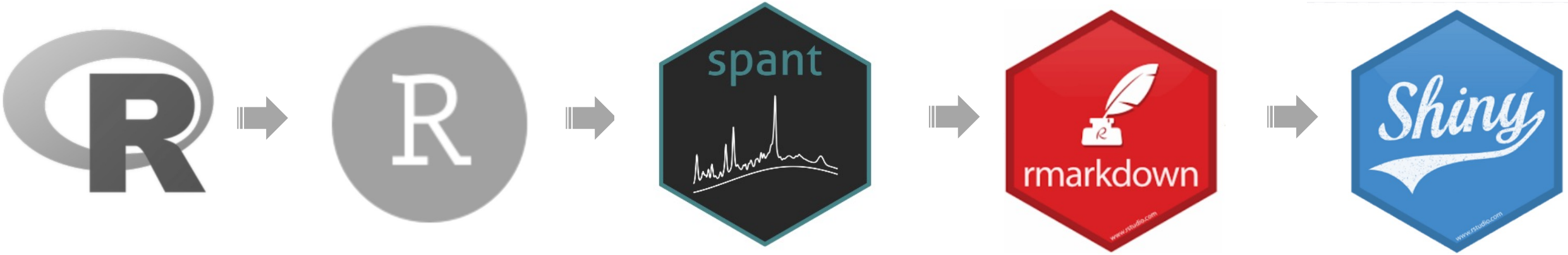
Interface/environment to work with R

Package that integrate text and R code

Package to build interactive web apps

Package to analyze MRS data

Outline



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Why R?

- Signal processing
- Numerical computing
- Simulations and modeling

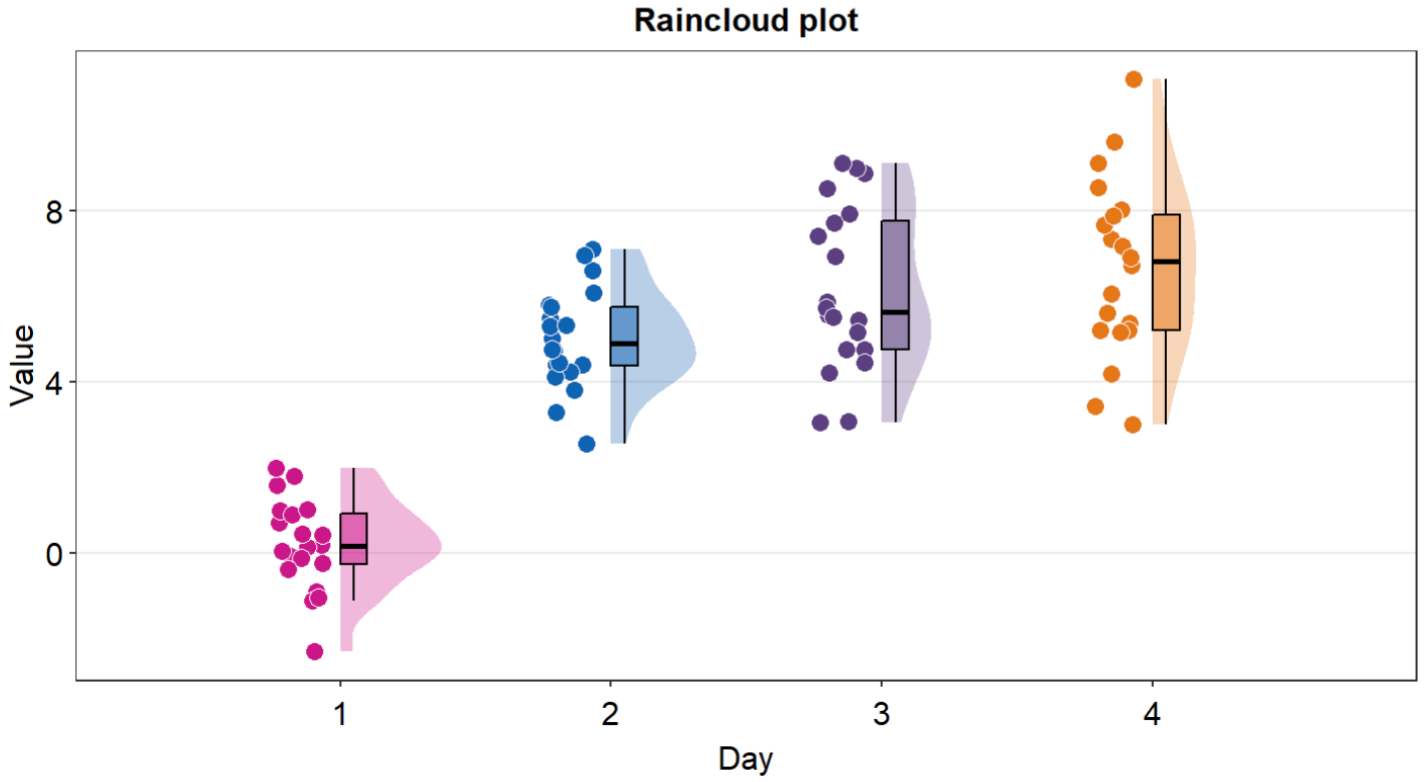
- General–purpose programming
- Data analysis and ML
- Web development

- Statistical Analysis
- Data visualization
- Data science and ML
- Reproducible research

Why R?

- Statistical and data analysis capabilities: collection of packages and libraries
- Data Visualization: high–quality customizable visualizations
- Community–driven approach
- Reproducibility and documentations → RPubs by RStudio
- Free!! & open source

User's creations



Author: Seung Hyun Min

sm_plot

https://www.frontiersin.org/articles/10.3389/fgene.2021.802894/full

How knowing R has improved my research

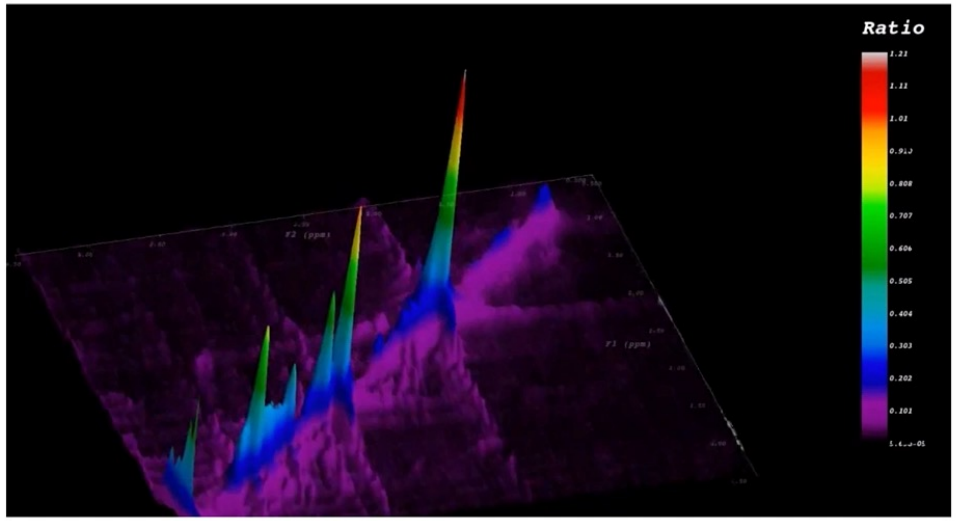
- ⬆ knowledge = ⬇ stress
- Efficacy
    1. Analysis
    2. Presentation
    3. Code access
- Collaboration

Two-Dimensional J-Resolved 1H-MRS using PRESS and Prior Knowledge Fitting (ProFit) in the Posterior Insula

A practical guide for balancing time and quality of metabolic information

JessArchibald

15/12/2021

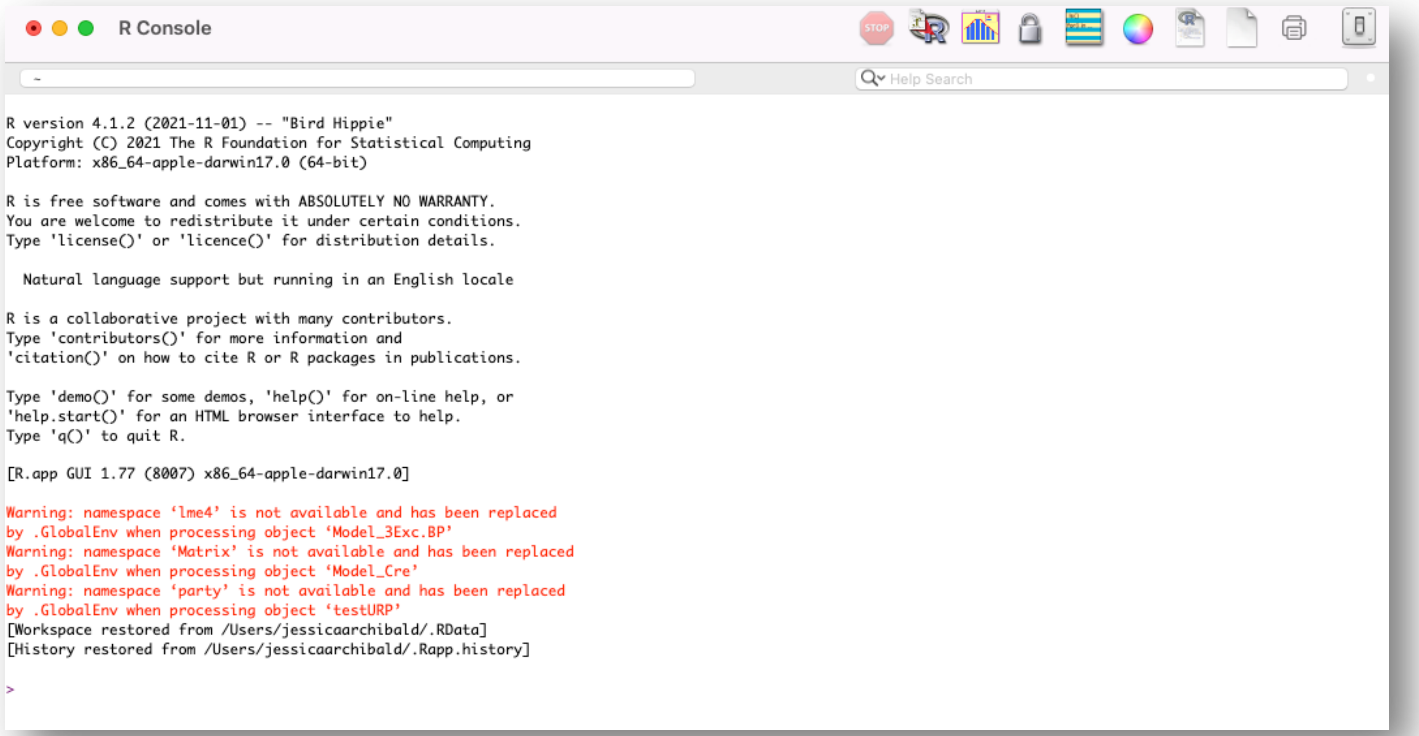


Question 1 - How much is gained when 2 blocks are combined ?

Subjects: 24.

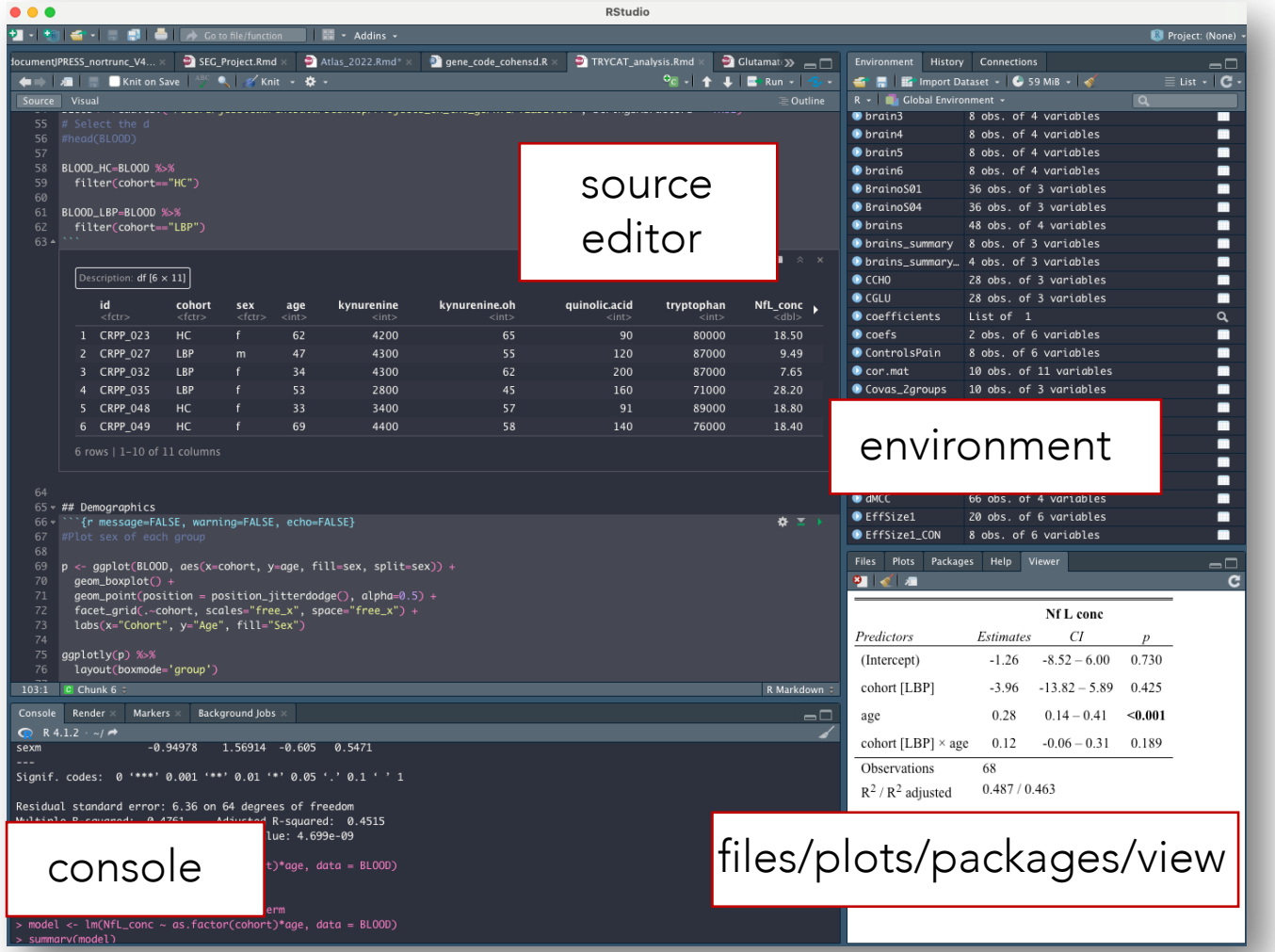
R

- Programming language for statistical computing.
- Comprehensive toolset for exploring, visualizing, and modeling data.

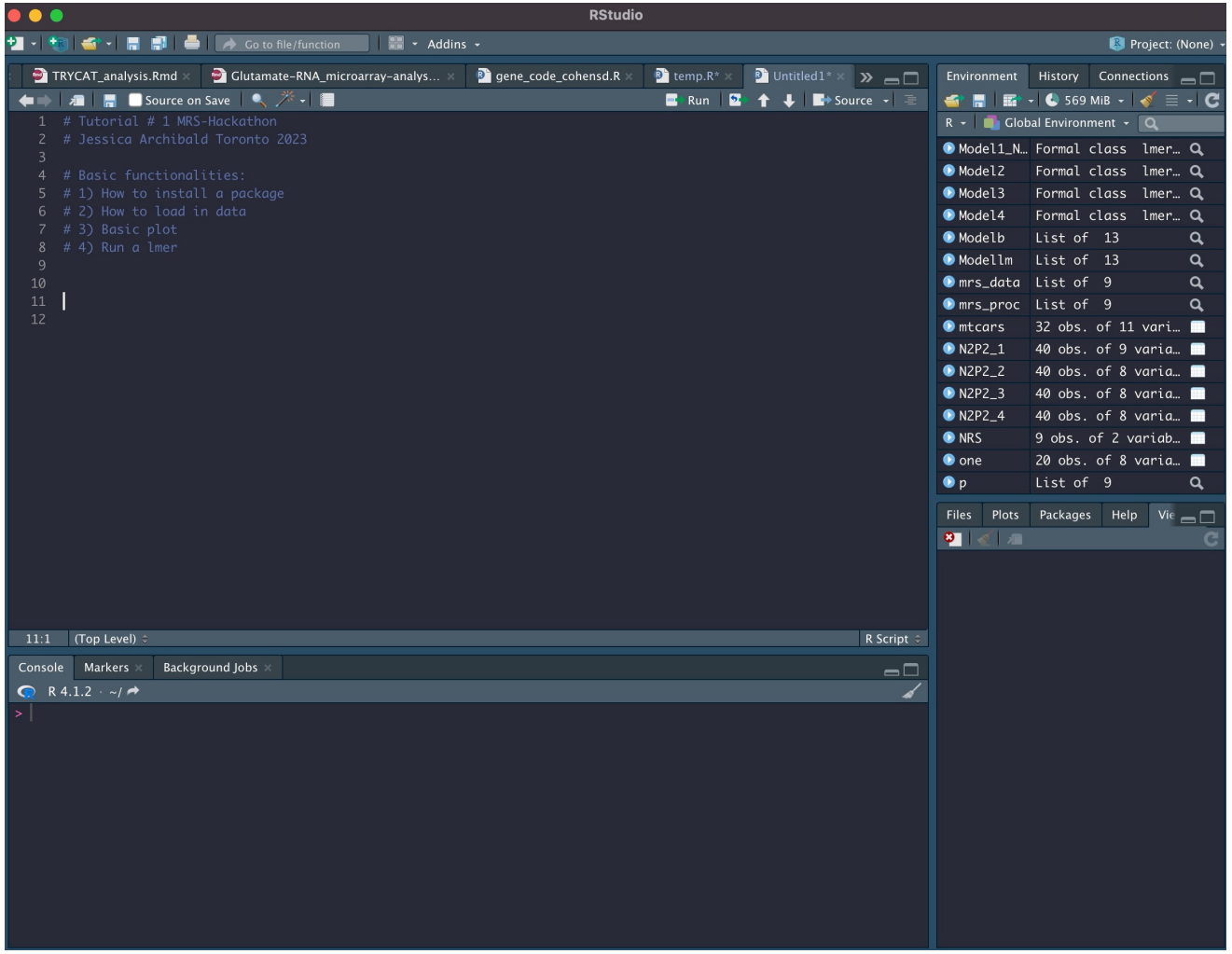


R Studio

- Integrated development environment
- User–friendly
- Enhance programming experience



Tutorial 1


RStudio
Go to file/function
Addins
Project: (None)
TRYCAT_analysis.Rmd
Glutamate-RNA_microarray-analys...
gene_code_cohensd.R
temp.R*
Untitled1*
Source on Save
Run
Source
1 # Tutorial # 1 MRS-Hackathon
2 # Jessica Archibald Toronto 2023
4 # Basic functionalities:
5 # 1) How to install a package
6 # 2) How to load in data
7 # 3) Basic plot
8 # 4) Run a lmer
11:1
(Top Level)
R Script
Console
Markers
Background Jobs
R 4.1.2 · ~/
Environment
History
Connections
569 MiB
R
Global Environment
Model1_N... Formal class lmer...
Model2 Formal class lmer...
Model3 Formal class lmer...
Model4 Formal class lmer...
Modelb List of 13
Modellm List of 13
mrs_data List of 9
mrs_proc List of 9
mtcars 32 obs. of 11 vari...
N2P2_1 40 obs. of 9 varia...
N2P2_2 40 obs. of 8 varia...
N2P2_3 40 obs. of 8 varia...
N2P2_4 40 obs. of 8 varia...
NRS 9 obs. of 2 variab...
one 20 obs. of 8 varia...
p List of 9
Files
Plots
Packages
Help

Data types & functions

- Character
- Factor
- Integer
- Numeric

```
> str(BLOOD)
'data.frame':   68 obs. of  11 variables:
 $ id            : Factor w/ 68 levels "CRPP_023","CRPP_0
 $ cohort        : Factor w/ 2 levels "HC","LBP": 1 2 2 2
 $ sex           : Factor w/ 2 levels "f","m": 1 2 1 1 1
 $ age           : int  62 47 34 53 33 69 26 34 71 78 ...
 $ kynurenine    : int  4200 4300 4300 2800 3400 4400 270
 $ kynurenine.oh: int  65 55 62 45 57 58 44 52 38 41 ...
 $ quinolic.acid: int  90 120 200 160 91 140 120 120 130
 $ tryptophan    : int  80000 87000 87000 71000 89000 760
 $ NfL_conc      : num  18.5 9.49 7.65 28.2 18.8 18.4 6.2
 $ NfL_CV        : num  6.89 5.45 5.77 3.56 3.21 ...
```

`as.factor()` `as.character()` `as.integer()` `as.numeric()`

Manipulate the data

rows

- `Filter()`
- `Slice()`
- `Arrange()`

columns

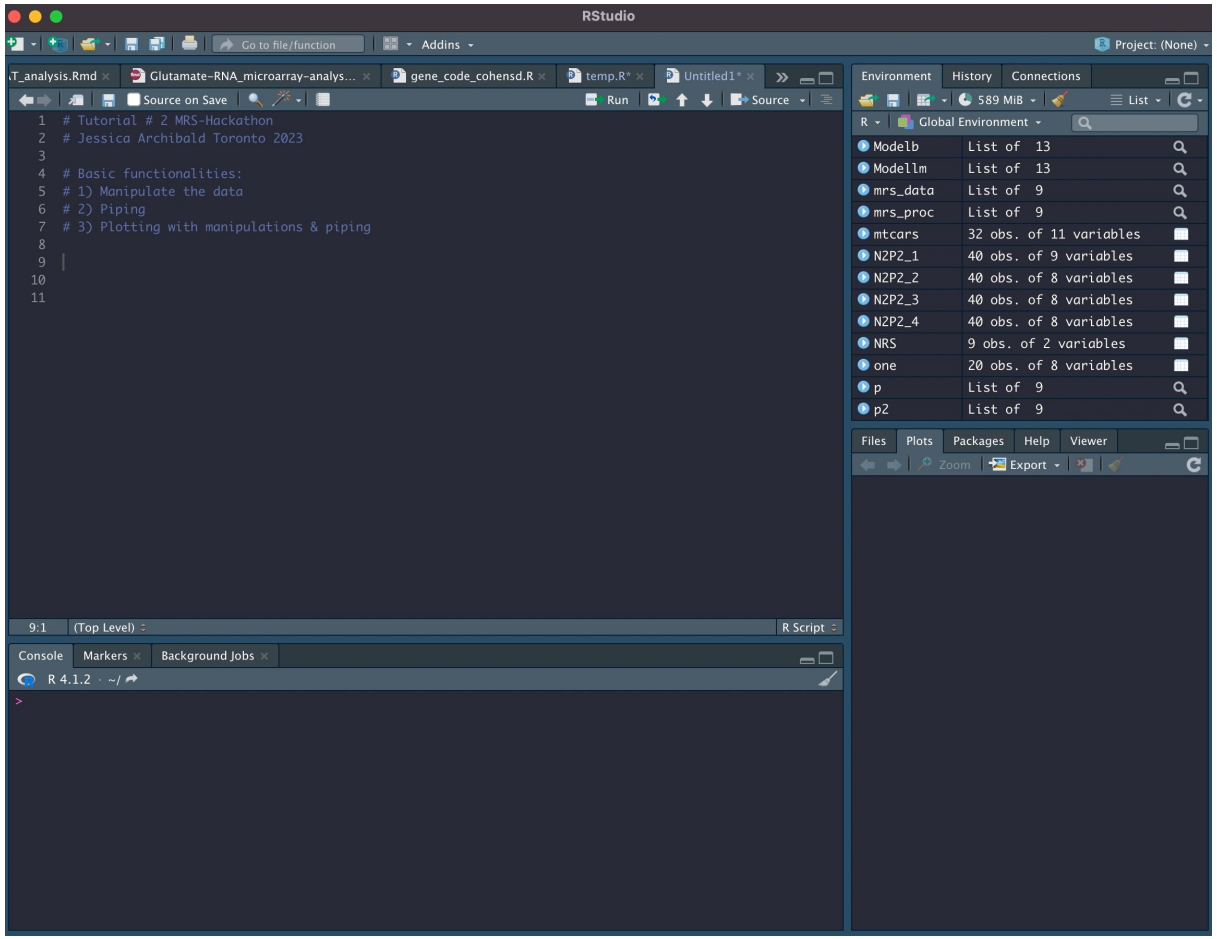
- `Select()`
- `Rename()`
- `Mutate()`
- `Relocate()`

pivoting

- `Pivot_longer`
- `Pivot_wider`

https://github.com/rstudio/cheatsheets/blob/main/data-transformation.pdf

Tutorial 2


RStudio
Go to file/function
Addins
Project: (None)
Glutamate-RNA_microarray-analys...
gene_code_cohensd.R
temp.R*
Untitled1*
Source on Save
Run
Source
1 # Tutorial # 2 MRS-Hackathon
2 # Jessica Archibald Toronto 2023
4 # Basic functionalities:
5 # 1) Manipulate the data
6 # 2) Piping
7 # 3) Plotting with manipulations & piping
9:1
(Top Level)
R Script
Console
Markers
Background Jobs
R 4.1.2 · ~/
Environment
History
Connections
589 MiB
List
Global Environment
Modelb List of 13
Modellm List of 13
mrs_data List of 9
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mtcars 32 obs. of 11 variables
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N2P2_3 40 obs. of 8 variables
N2P2_4 40 obs. of 8 variables
NRS 9 obs. of 2 variables
one 20 obs. of 8 variables
p List of 9
p2 List of 9
Files
Plots
Packages
Help
Viewer
Zoom
Export

Short–cuts

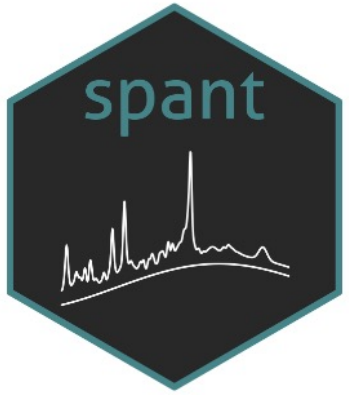
- Control + L Clear the console
- ⌘ command + enter Run code
- ⌘ command + left/right Cursor to the start or end of code

Short–cuts

- shift + ⌘ command + c → Comment/uncomment code
- shift + ⌘ command + p → Re–run last chunk of code
- ⌘ command + d → Deletes a line of code

Programming language

Interface/environment to work with R

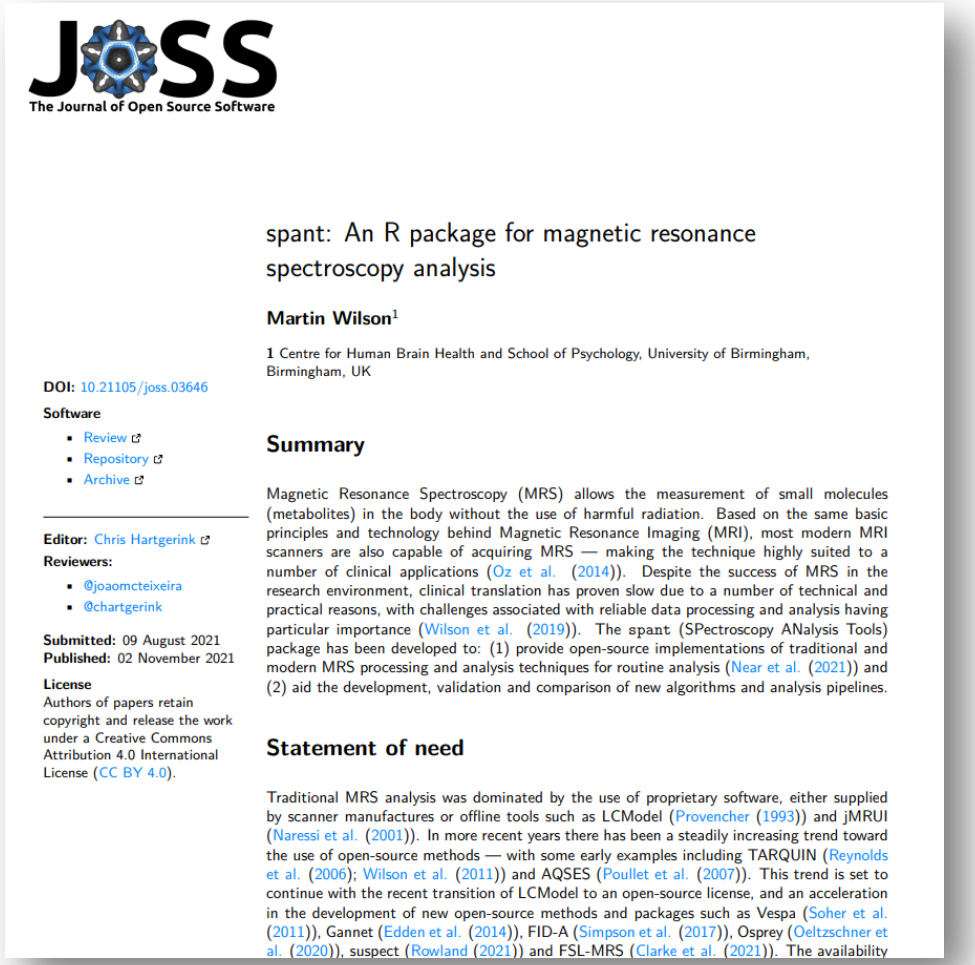


Package to analyze MRS data

Package that integrate text and R code

Package to build interactive web apps

Spant– (SPectroscopy ANalysis Tools)



JOSS
The Journal of Open Source Software

spant: An R package for magnetic resonance spectroscopy analysis

Martin Wilson[1]

1 Centre for Human Brain Health and School of Psychology, University of Birmingham, Birmingham, UK

DOI: 10.21105/joss.03646

Software

- Review
- Repository
- Archive

Editor: Chris Hartgerink

Reviewers:

- @joaomcteixeira
- @chartgerink

Submitted: 09 August 2021
Published: 02 November 2021

Summary

Magnetic Resonance Spectroscopy (MRS) allows the measurement of small molecules (metabolites) in the body without the use of harmful radiation. Based on the same basic principles and technology behind Magnetic Resonance Imaging (MRI), most modern MRI scanners are also capable of acquiring MRS — making the technique highly suited to a number of clinical applications (Oz et al. (2014)). Despite the success of MRS in the research environment, clinical translation has proven slow due to a number of technical and practical reasons, with challenges associated with reliable data processing and analysis having particular importance (Wilson et al. (2019)). The spant (SPectroscopy ANalysis Tools) package has been developed to: (1) provide open-source implementations of traditional and modern MRS processing and analysis techniques for routine analysis (Near et al. (2021)) and (2) aid the development, validation and comparison of new algorithms and analysis pipelines.

Statement of need

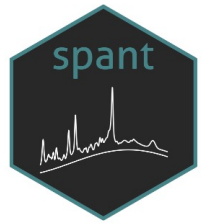
Traditional MRS analysis was dominated by the use of proprietary software, either supplied by scanner manufactures or offline tools such as LCModel (Provencher (1993)) and jMRUI (Naressi et al. (2001)). In more recent years there has been a steadily increasing trend toward the use of open-source methods — with some early examples including TARQUIN (Reynolds et al. (2006); Wilson et al. (2011)) and AQSES (Poullet et al. (2007)). This trend is set to continue with the recent transition of LCModel to an open-source license, and an acceleration in the development of new open-source methods and packages such as Vespa (Soher et al. (2011)), Gannet (Edden et al. (2014)), FID-A (Simpson et al. (2017)), Osprey (Oeltzschner et al. (2020)), suspect (Rowland (2021)) and FSL-MRS (Clarke et al. (2021)). The availability

- Provide open–source implementations of traditional and modern MRS processing and analysis.

spant

https://cran.r–project.org/web/packages/spant/spant.pdf

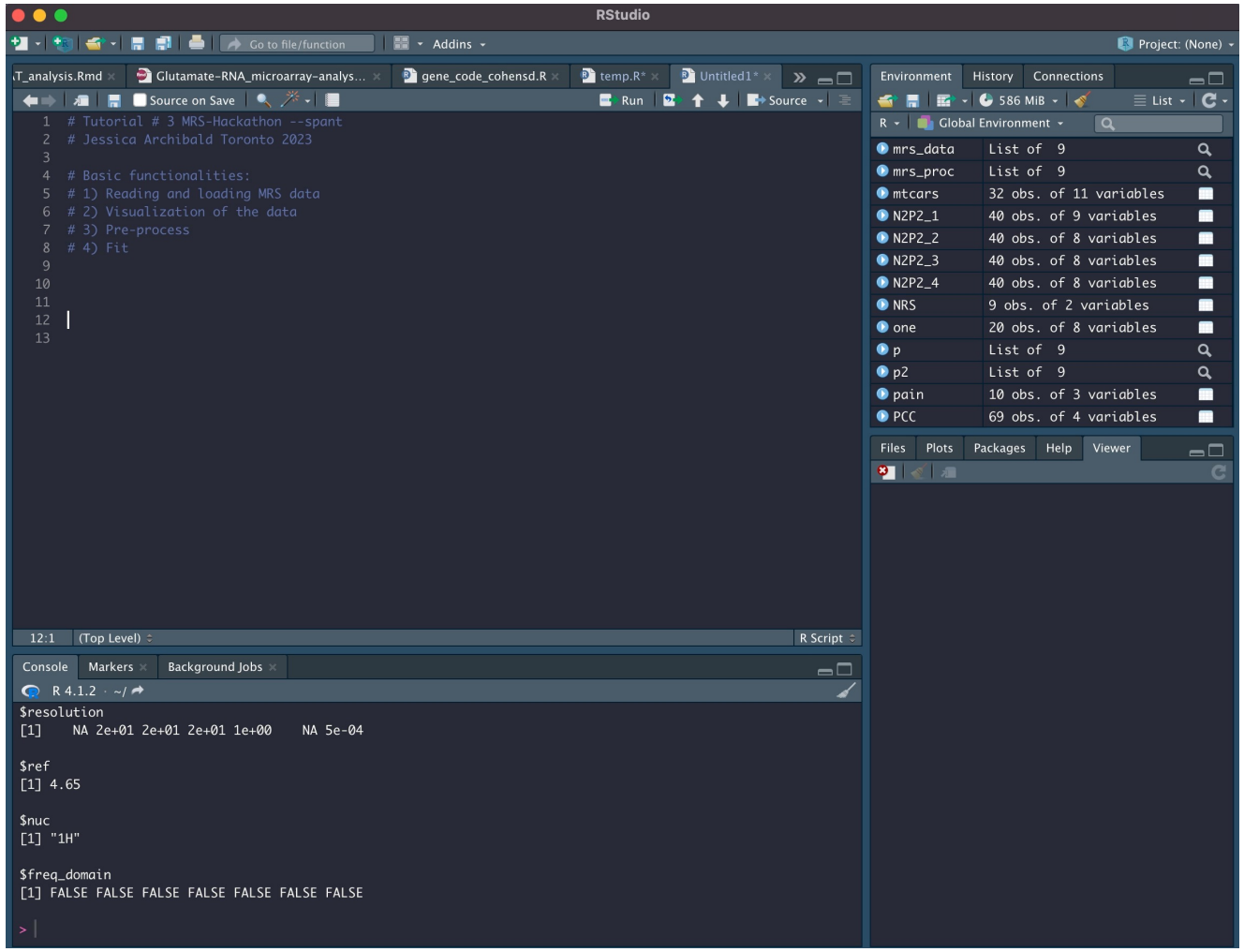
Spant– (SPectroscopy ANalysis Tools)



- Aid the development, validation and comparison of new algorithms and analysis pipelines.

- Particularly suited to the interactive exploration and batch processing of large and complex datasets.

Tutorial 3


RStudio
Go to file/function
Addins
Project: (None)
T_analysis.Rmd
Glutamate-RNA_microarray-analys...
gene_code_cohensd.R
temp.R*
Untitled1*
Source on Save
Run
Source
1 # Tutorial # 3 MRS-Hackathon --spant
2 # Jessica Archibald Toronto 2023
4 # Basic functionalities:
5 # 1) Reading and loading MRS data
6 # 2) Visualization of the data
7 # 3) Pre-process
8 # 4) Fit
12:1
(Top Level)
R Script
Console
Markers
Background Jobs
R 4.1.2 · ~/
$resolution
[1] NA 2e+01 2e+01 2e+01 1e+00 NA 5e-04
$ref
[1] 4.65
$nuc
[1] "1H"
$freq_domain
[1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
Environment
History
Connections
586 MiB
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R
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mrs_data List of 9
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pain 10 obs. of 3 variables
PCC 69 obs. of 4 variables
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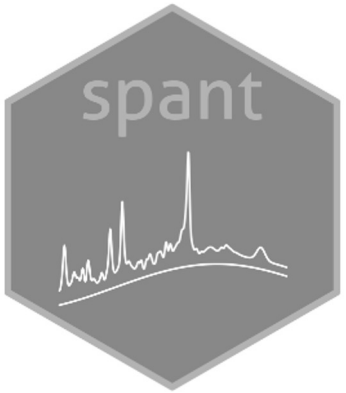
Viewer

Programming language

Interface/environment to work with R



Package to analyze MRS data

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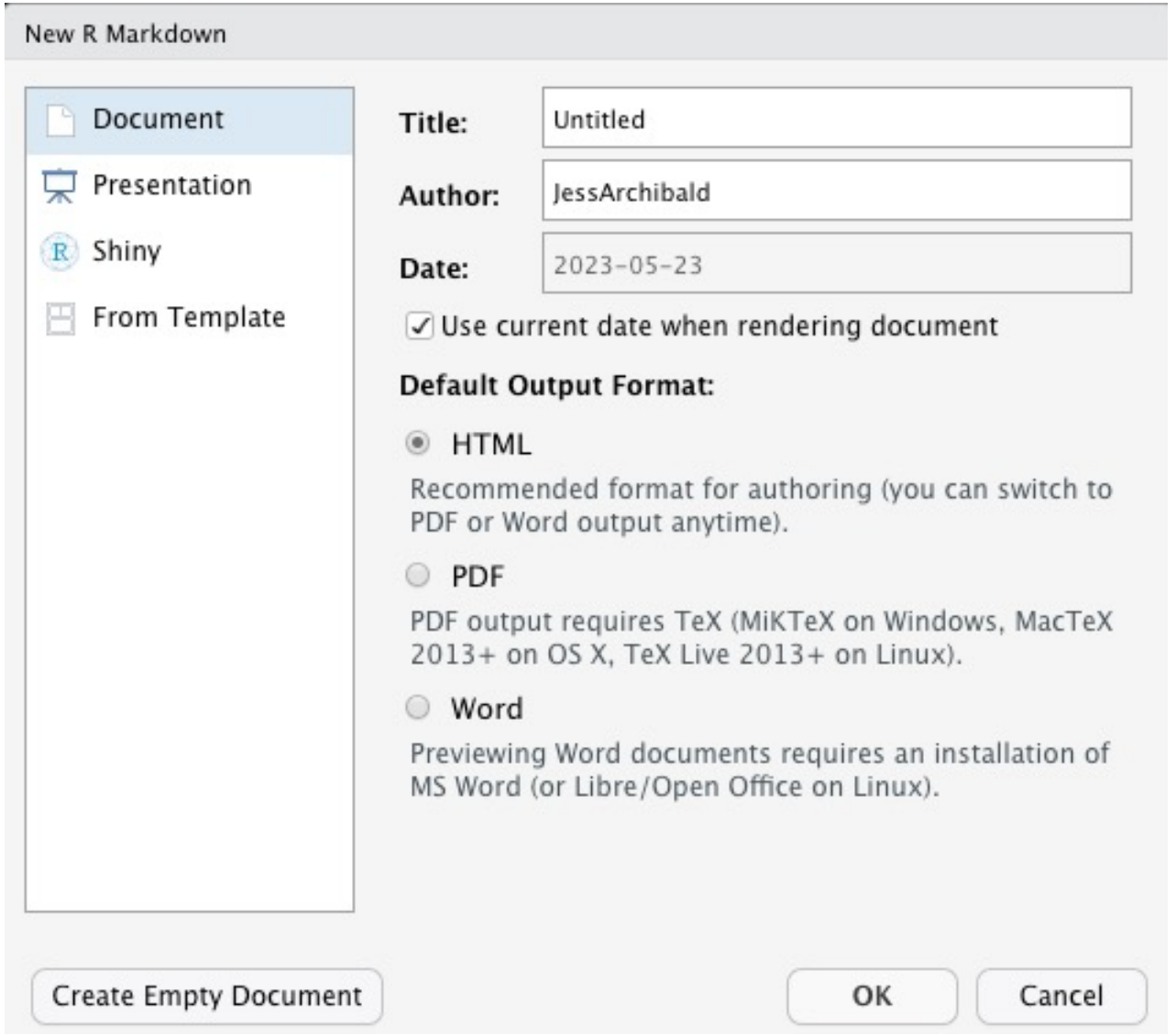
Package to build interactive web apps

R Markdown

- .Rmd file
- Output formats



https://www.rstudio.com/wp-content/uploads/2015/02/rmarkdown-cheatsheet.pdf

R Markdown

```
---
title: "Untitled"
author: "JessArchibald"
date: "`r Sys.Date()`"
output: html_document
---

```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
```

R Markdown

This is an R Markdown document. Markdown is a simple formatting syntax for author
more details on using R Markdown see <http://rmarkdown.rstudio.com>.

When you click the **Knit** button a document will be generated that includes both content as well as th
embedded R code chunks within the document. You can embed an R code chunk like this:

```{r cars}
summary(cars)
```

Including Plots

You can also embed plots, for example:

```{r pressure, echo=FALSE}
plot(pressure)
```

Note that the `echo = FALSE` parameter was added to the code chunk to prevent printing of the R code tha
```

~/Desktop/Projects_on_the_go/NfL/TRYCAT_analysis.html

TRYCAT_analysis.html | Open in Browser | Find | Publish

Zurich Project - GM and NfL

JessArchibald

2022-11-05

– add normality of the data : age, nfl, etc

JANUARY 2023 - NfL DATA & TRYCAT DATA

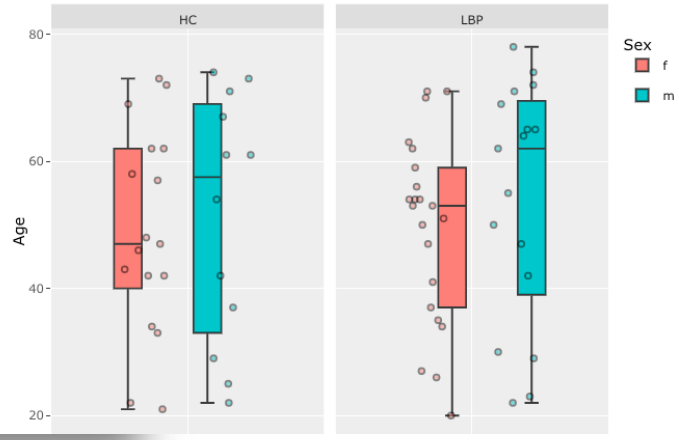
> n= 68 (39 LBP 29 HC)

> 7 of these are semi-quantitative (4 HC and 3 LBP)

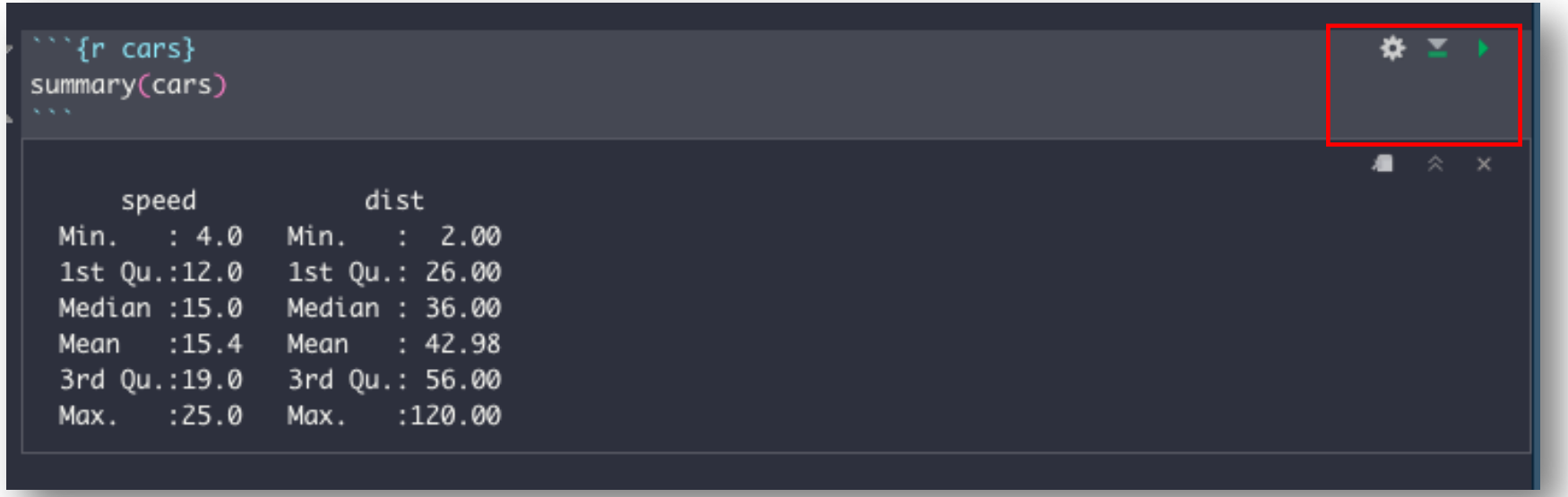
> mean age = 50.77 SD= 16.70 range= 20-78

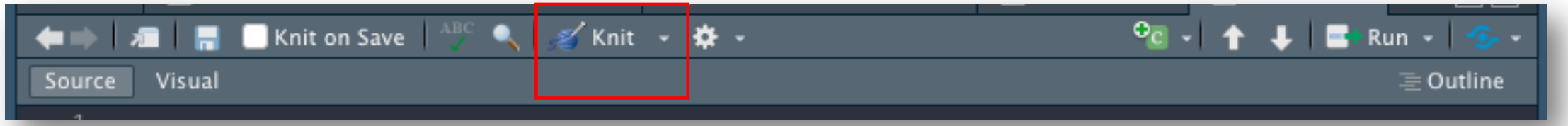
> 29 Male

Demographics

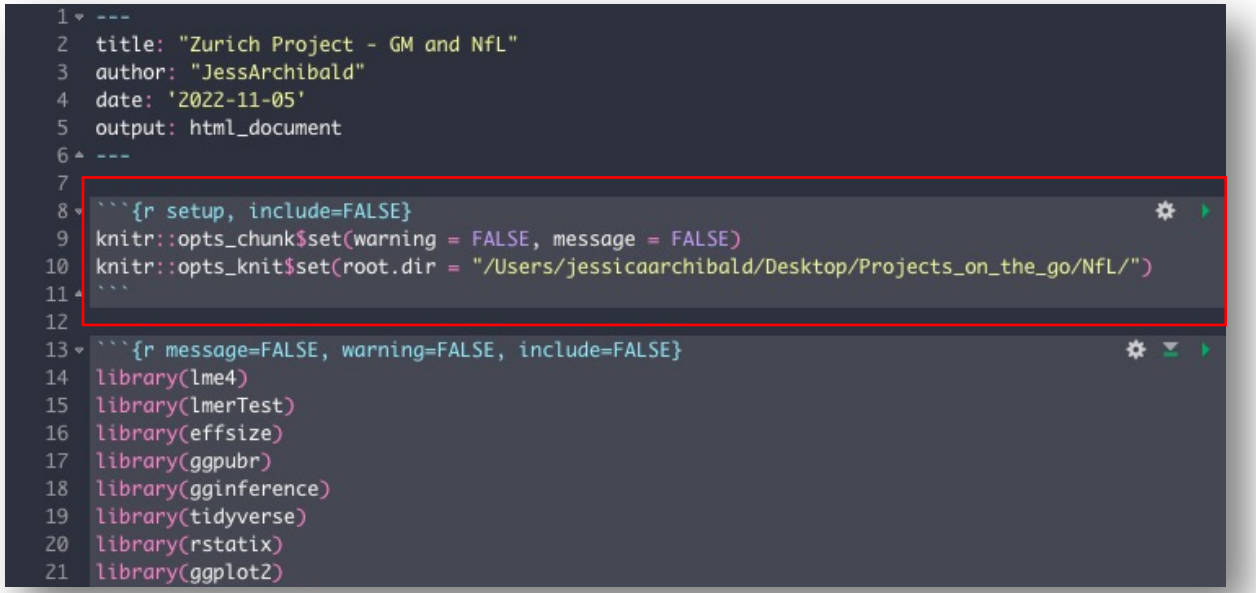


R Markdown


```{r cars}
summary(cars)
```
speed dist
Min. : 4.0 Min. : 2.00
1st Qu.:12.0 1st Qu.: 26.00
Median :15.0 Median : 36.00
Mean :15.4 Mean : 42.98
3rd Qu.:19.0 3rd Qu.: 56.00
Max. :25.0 Max. :120.00


Knit on Save
Knit
Run
Source
Visual
Outline

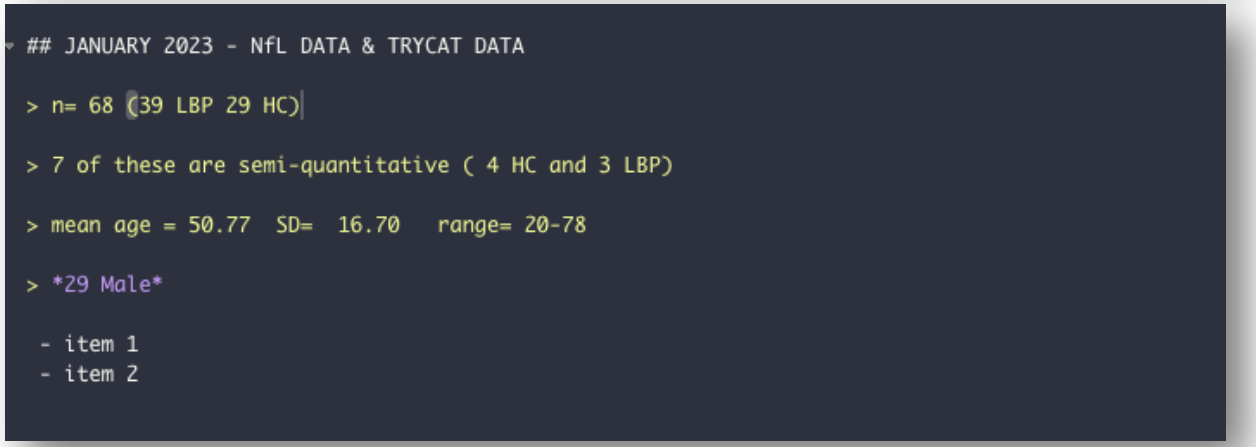
R Markdown



```
---
title: "Zurich Project - GM and NfL"
author: "JessArchibald"
date: '2022-11-05'
output: html_document
---

```{r setup, include=FALSE}
knitr::opts_chunk$set(warning = FALSE, message = FALSE)
knitr::opts_knit$set(root.dir = "/Users/jessicaarchibald/Desktop/Projects_on_the_go/NfL/")
```

```{r message=FALSE, warning=FALSE, include=FALSE}
library(lme4)
library(lmerTest)
library(effsize)
library(ggpubr)
library(gginference)
library(tidyverse)
library(rstatix)
library(ggplot2)
```
```



```
## JANUARY 2023 - NfL DATA & TRYCAT DATA

> n= 68 (39 LBP 29 HC)

> 7 of these are semi-quantitative ( 4 HC and 3 LBP)

> mean age = 50.77  SD=  16.70   range= 20-78

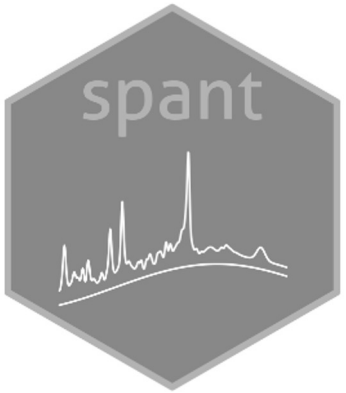
> *29 Male*

 - item 1
 - item 2
```

1. Set working directory
2. Load my libraries
3. Lightweight markup language

Programming language

Interface/environment to work with R



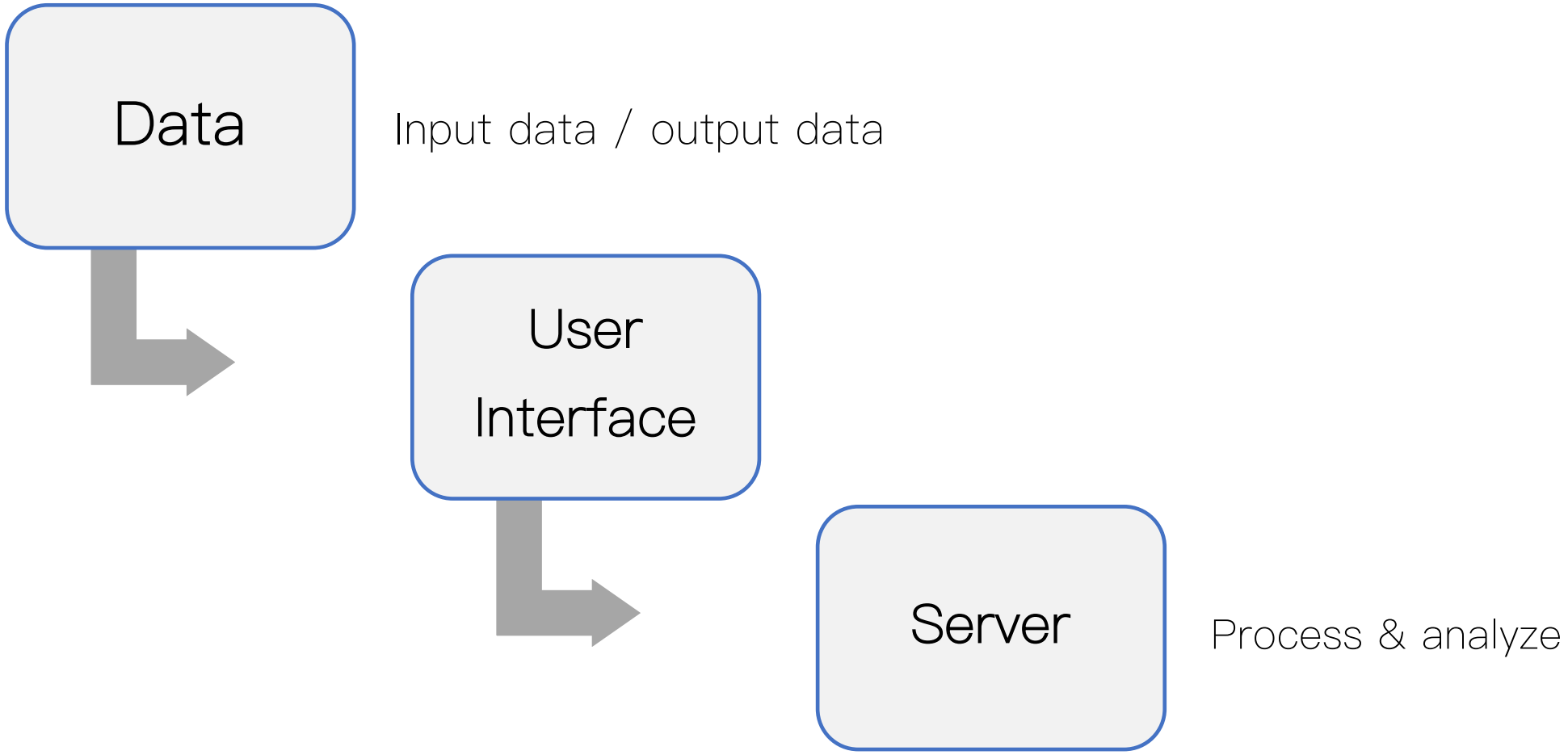
Package to analyze MRS data

Package that integrate text and R code

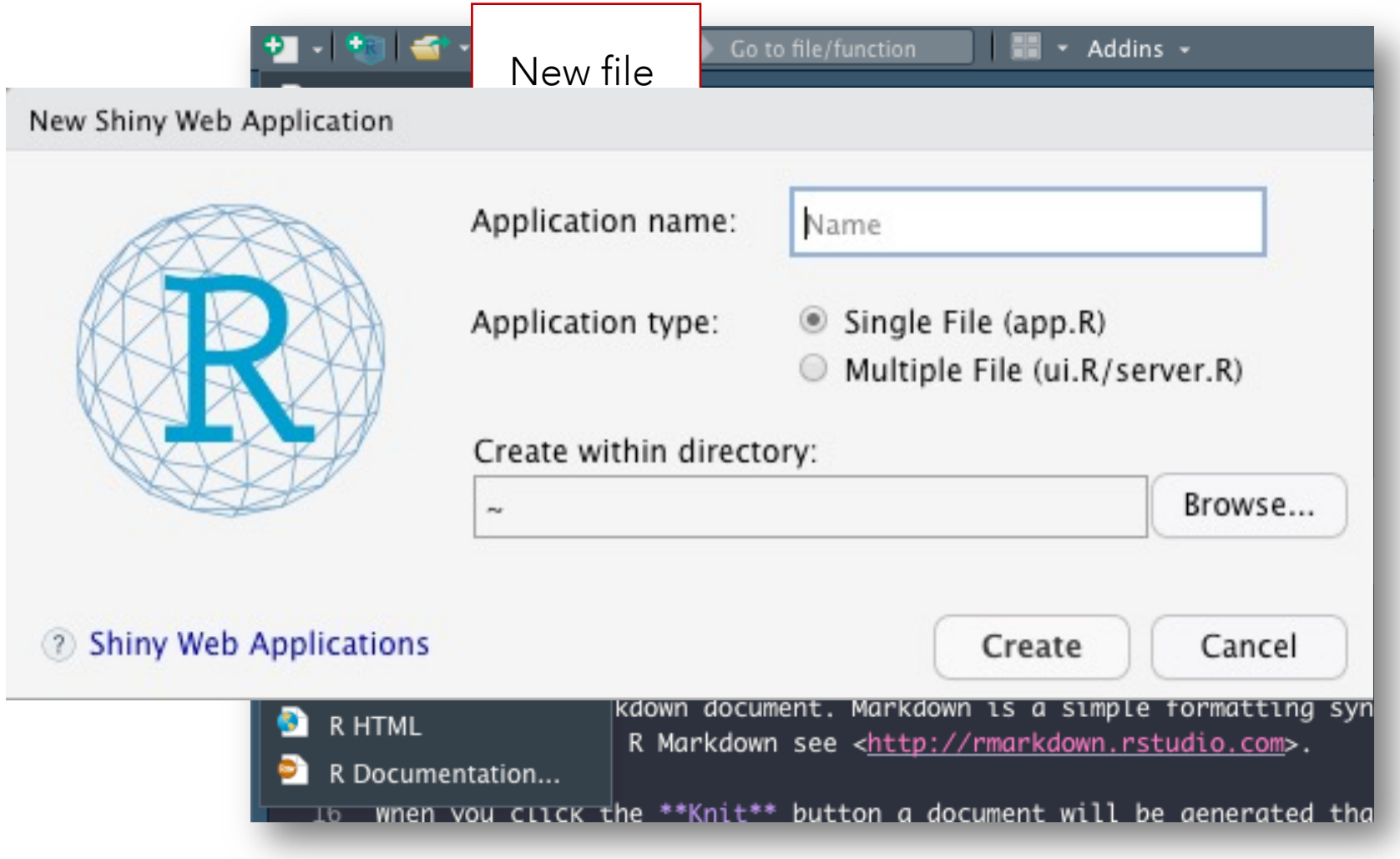
Package to build interactive web apps

Shiny– package for web apps

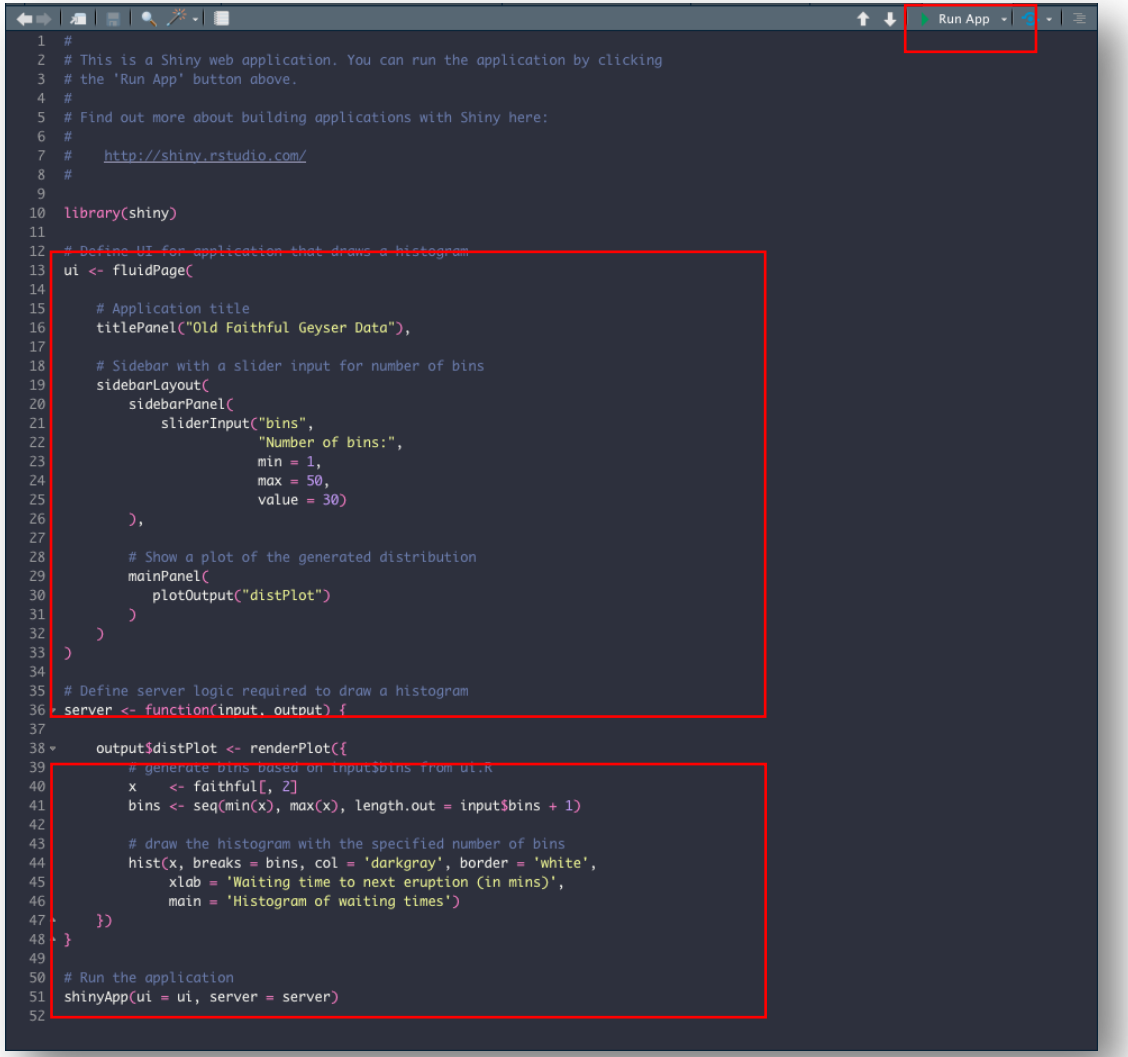
Workflow



Shiny– building the app



Shiny– building the app



1. Run the app
2. User Interface
3. Server

Shiny– building the app

```
#
# This is a Shiny web application. You can run the application by clicking
# the 'Run App' button above.
#
# Find out more about building applications with Shiny here:
#
#    http://shiny.rstudio.com/
#

library(shiny)

# Define UI for application that draws a histogram
ui <- fluidPage(

    # Application title
    titlePanel("Old Faithful Geyser Data"),

    # Sidebar with a slider input for number of bins
    sidebarLayout(
        sidebarPanel(
            sliderInput("bins",
                        "Number of bins:",
                        min = 1,
                        max = 50,
                        value = 30)
        ),

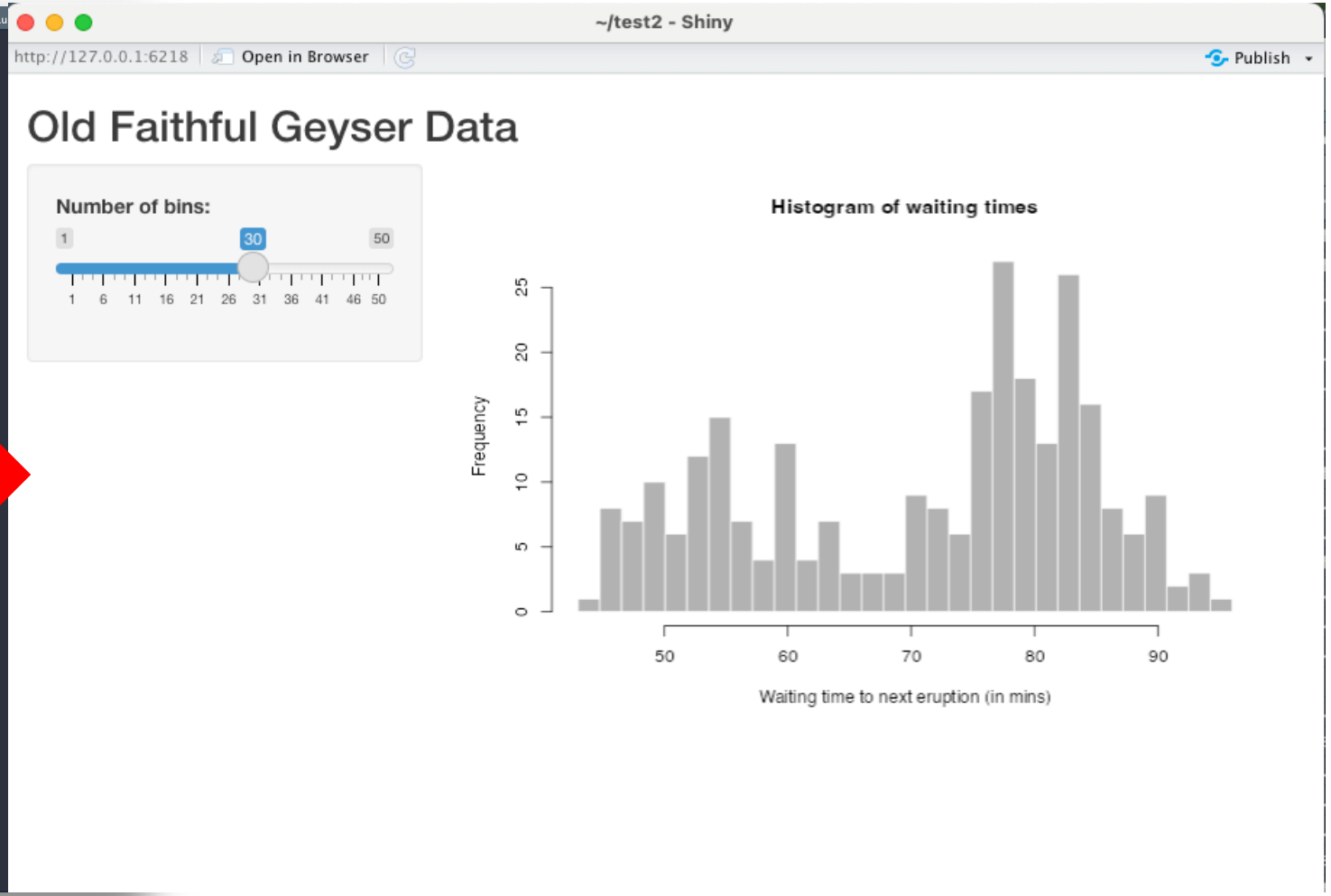
        # Show a plot of the generated distribution
        mainPanel(
           plotOutput("distPlot")
        )
    )
)

# Define server logic required to draw a histogram
server <- function(input, output) {

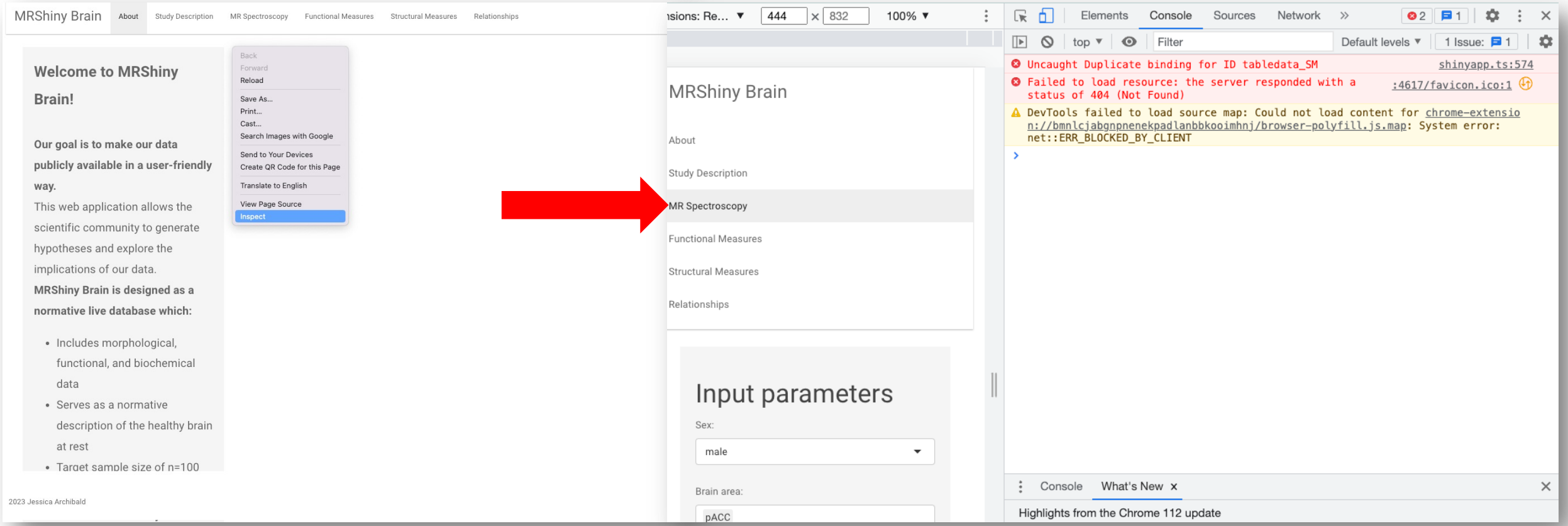
    output$distPlot <- renderPlot({
        # generate bins based on input$bins from ui.R
        x    <- faithful[, 2]
        bins <- seq(min(x), max(x), length.out = input$bins + 1)

        # draw the histogram with the specified number of bins
        hist(x, breaks = bins, col = 'darkgray', border = 'white',
             xlab = 'Waiting time to next eruption (in mins)',
             main = 'Histogram of waiting times')
    })
}

# Run the application
shinyApp(ui = ui, server = server)
```



Shiny– debugging tip



Shiny– deploy

SHINY SERVER

Get your Shiny apps online

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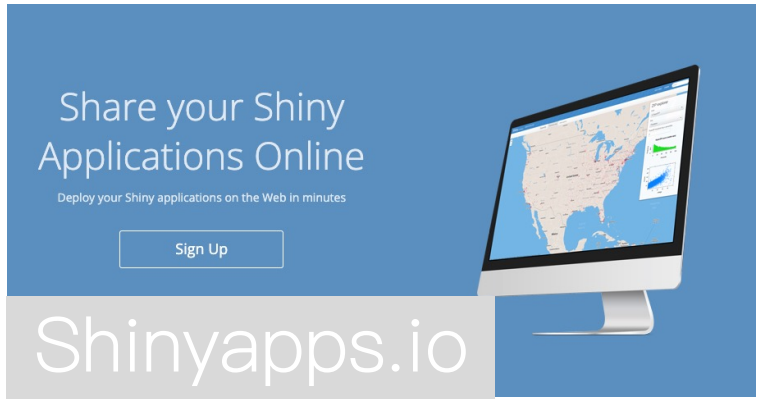
Shiny Server

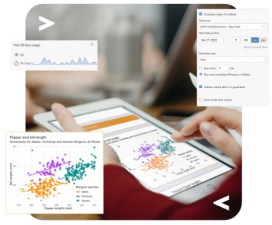


POSIT CONNECT

For data products worth sharing

Deploy everything you create in R & Python, including interactive applications (Shiny, Streamlit, Dash), documents, notebooks, and dashboards. Automate code execution so your data products are always up to date. Give stakeholders and collaborators the right access to the content they need.

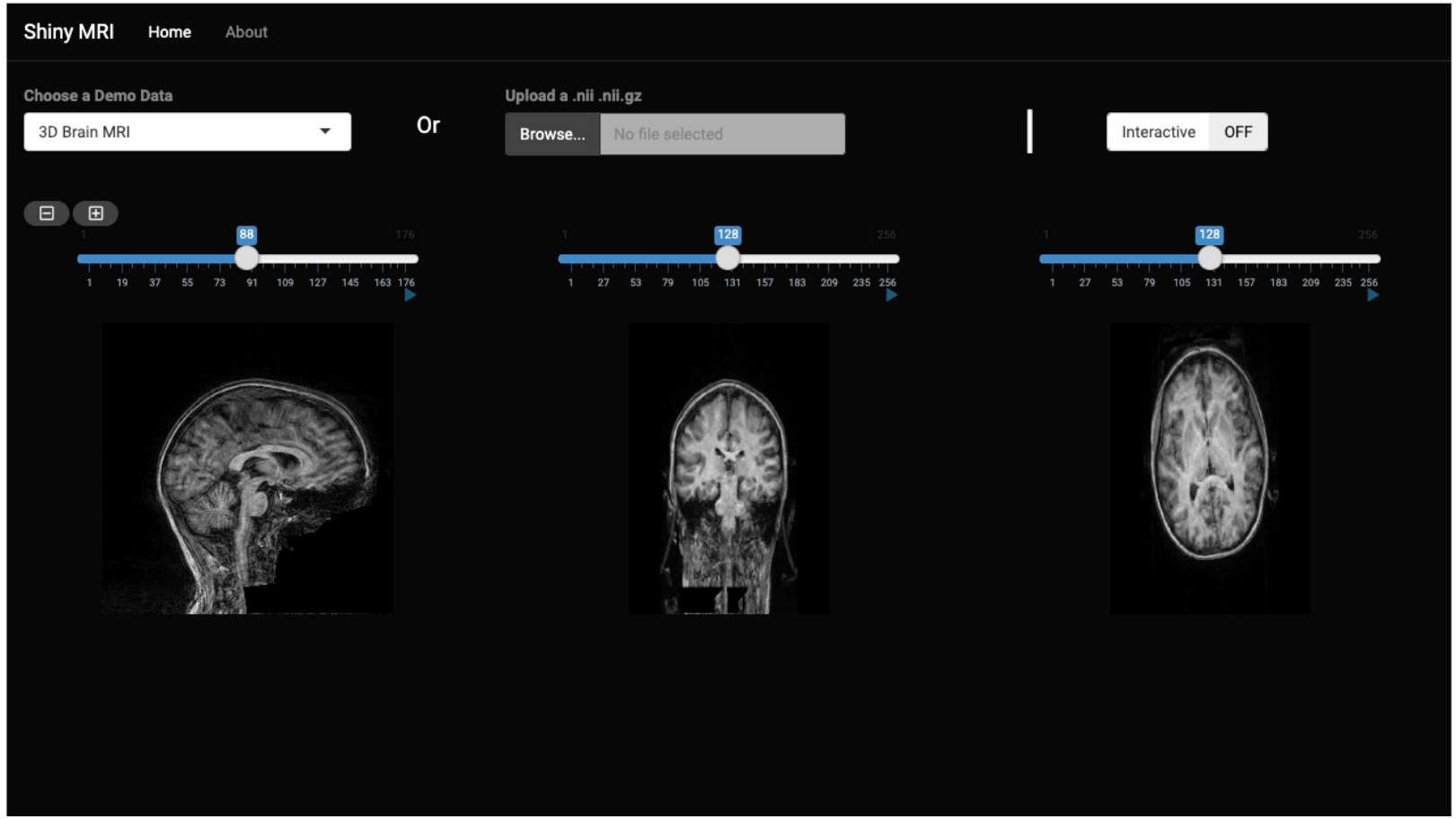
SCHEDULE A DEMO | WATCH THE VIDEO



Posit Connect

https://shiny.posit.co/r/deploy

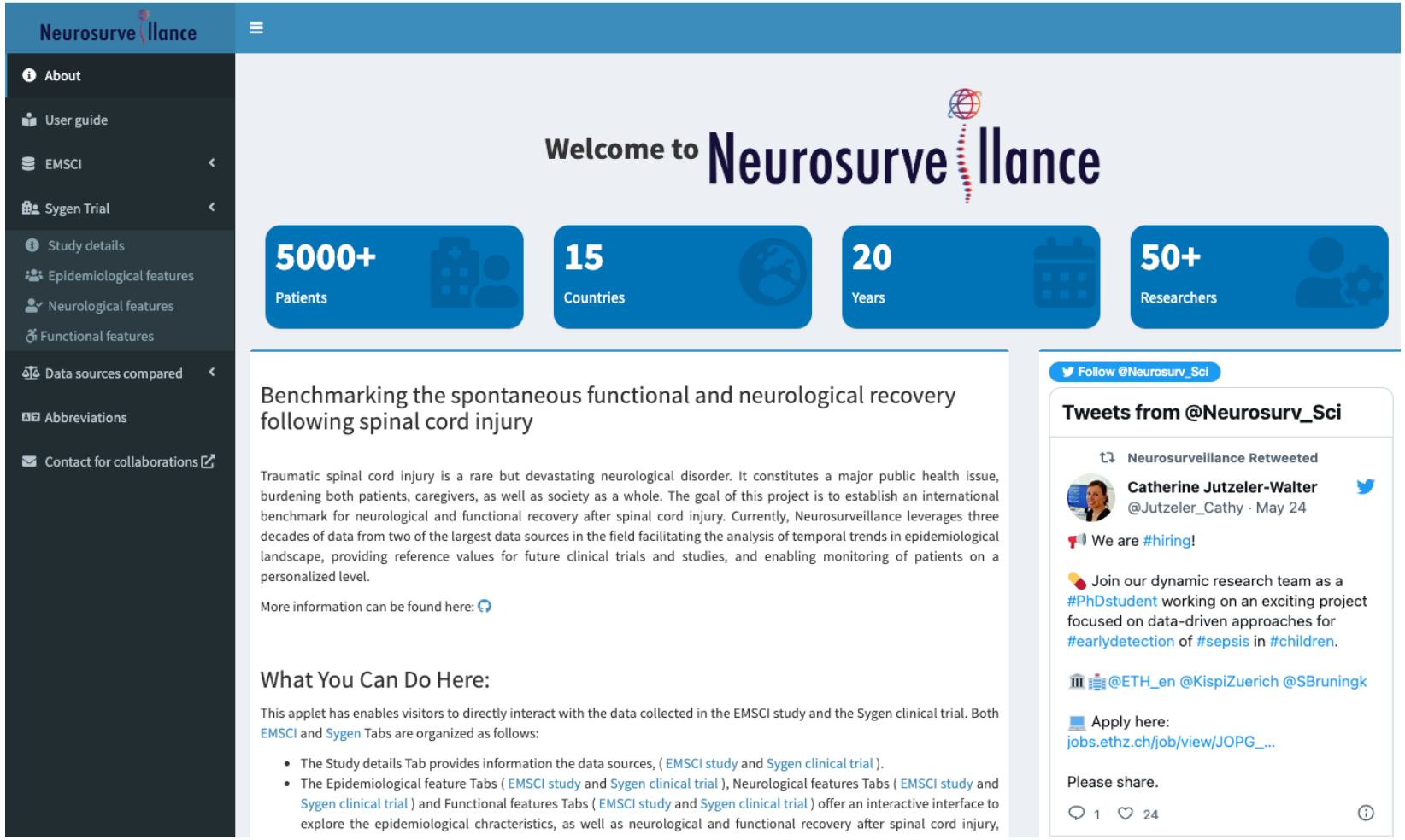
Illustrative examples



Author: Hao Zhuname

[Shiny-contest]

Illustrative examples



Author: Lucie Bourguignon

Neurosurvellance

Illustrative examples

Author: Jessica Archibald

[MRShiny Brain]

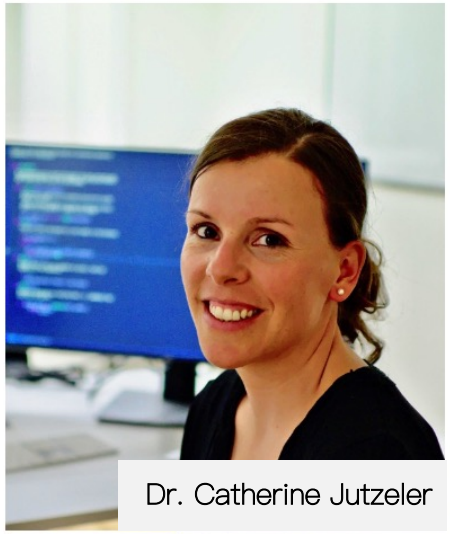
Pros & Cons

Take home message

Why you should use R studio, R Markdown, Spant, and Shiny

- Enhance the efficiency, reproducibility, and interactivity of your data analysis and presentation workflow.
- Enhance quality, transparency, and accessibility.
- By using spant, you can seamlessly integrate MRS analysis into your broader R analysis pipeline.

Acknowledgements



Dr. Catherine Jutzeler

Dr. Niklaus Zölch

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1st MR Spectroscopy Hackathon

MRS Hackathon 2023 team

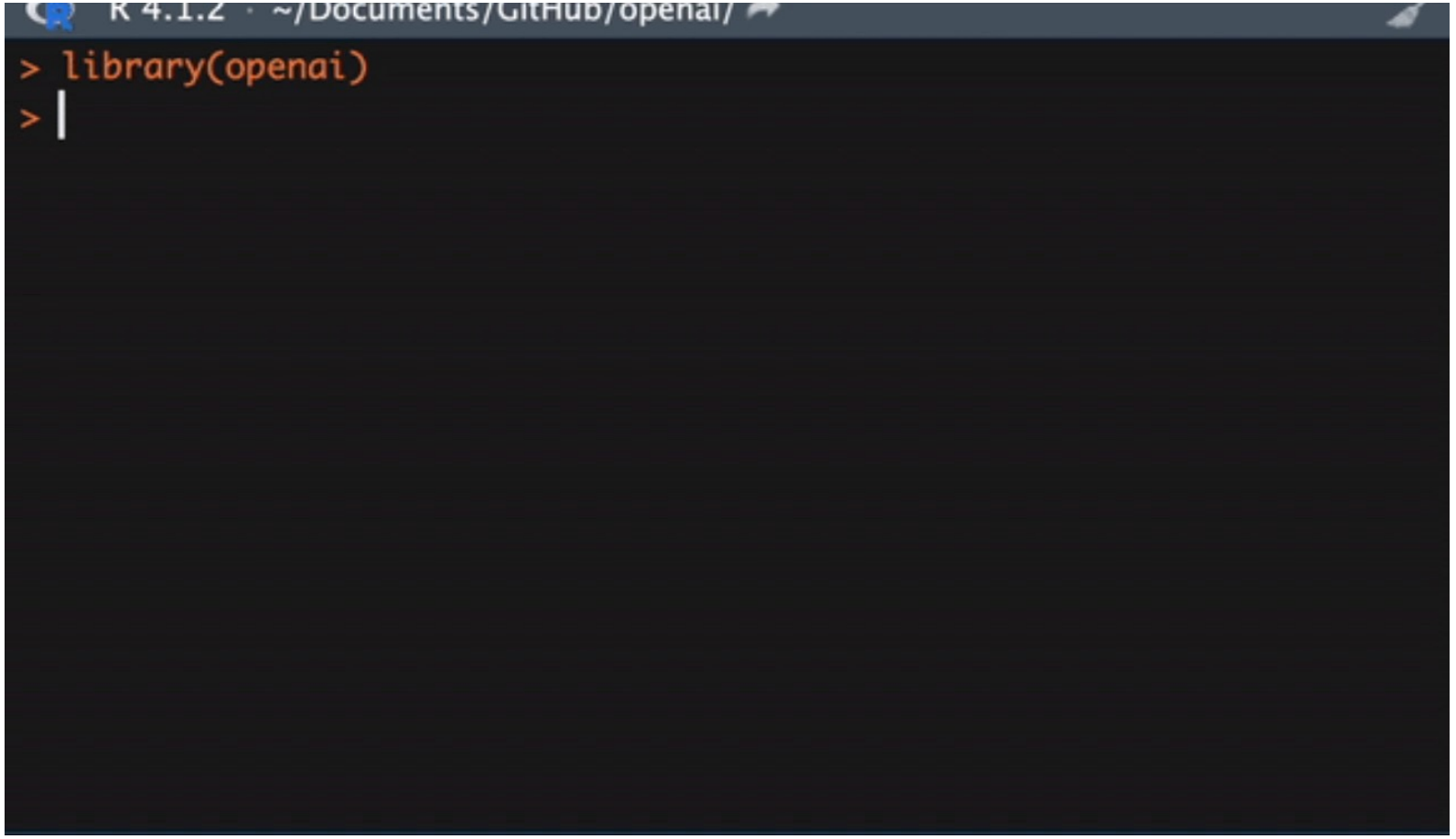
Antonia Kaiser

Georg Oeltzschner

Candace Fleischer

Jaime Near

R via AI



Author: Sam Terfa

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