REPRODUCIBLE RESEARCH IN R

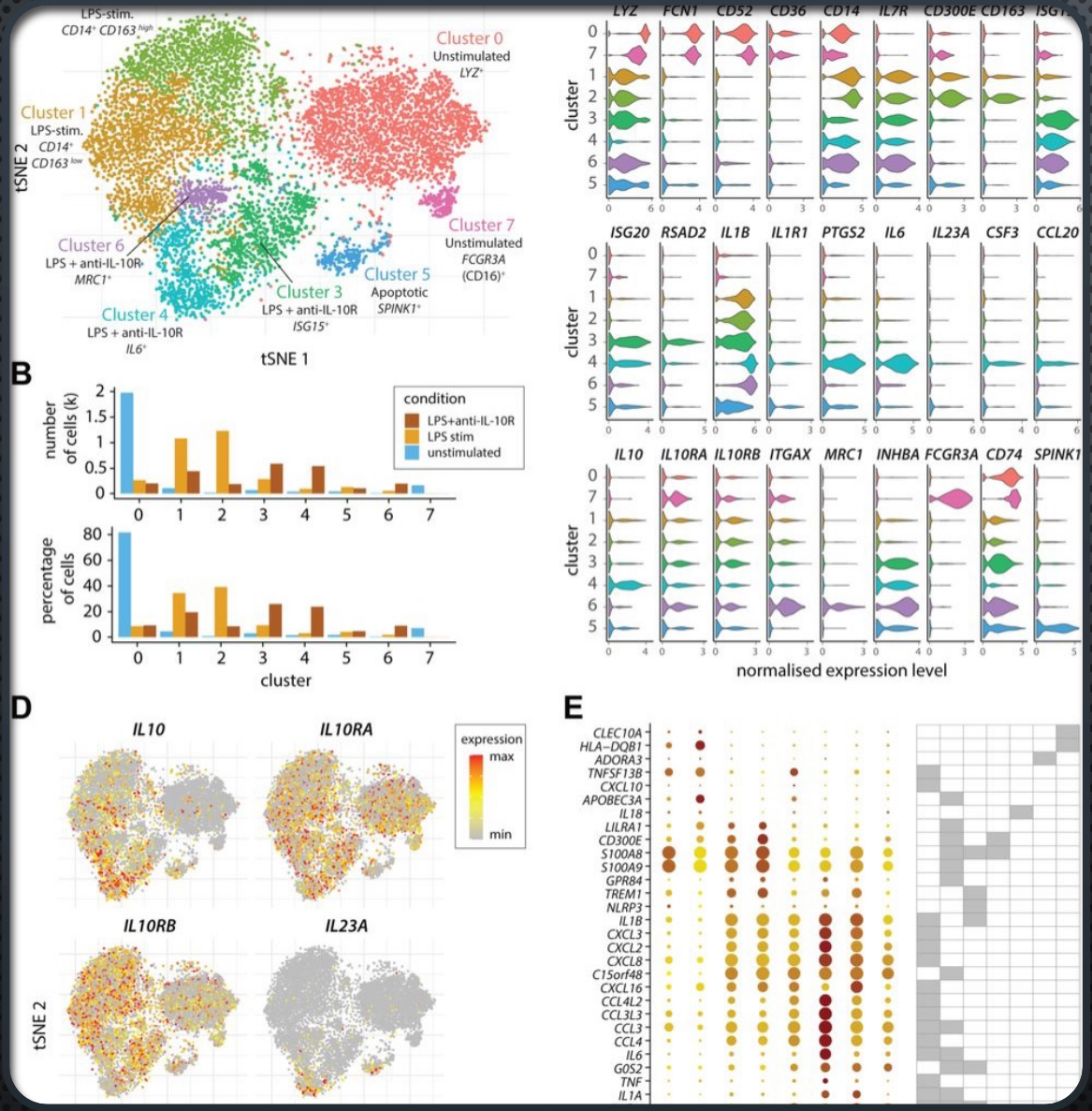
SOUMYA BANERJEE

Rationale

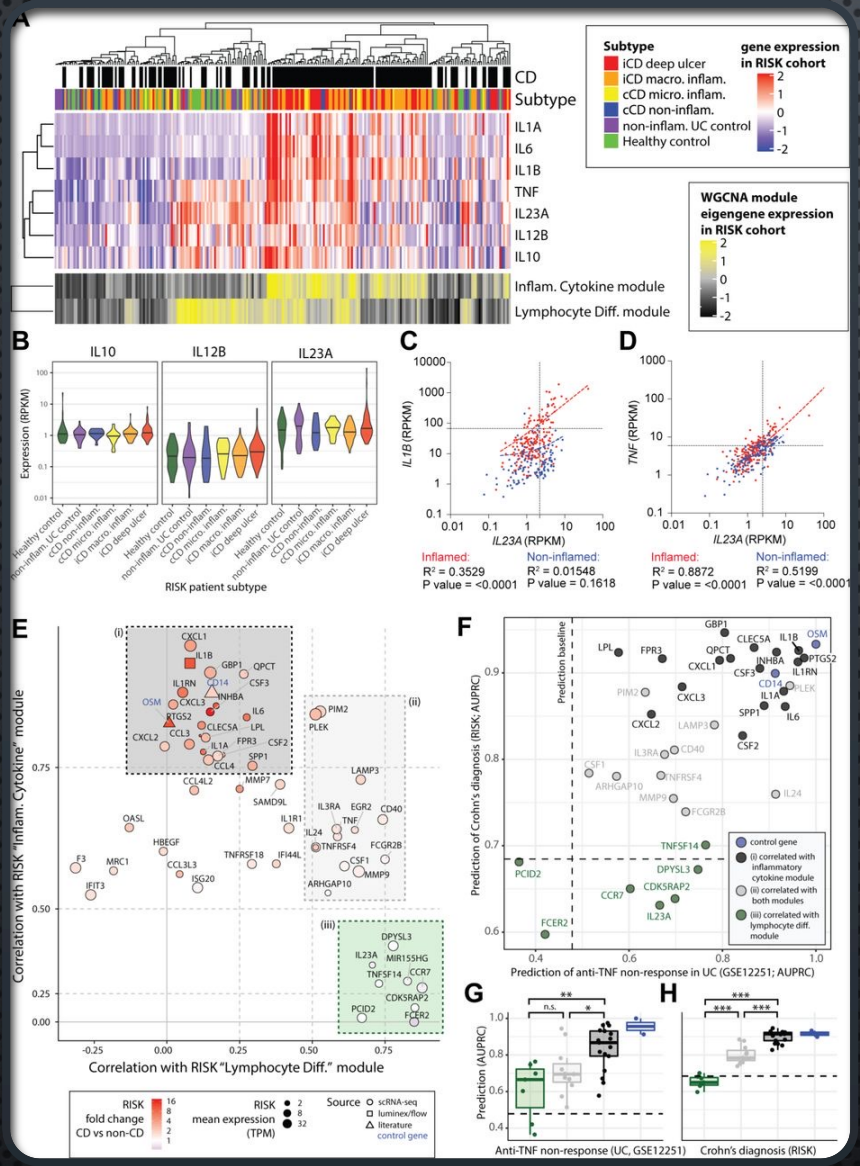
- Your data, your model decisions, parameters and your data filtering decisions will keep on changing. How do you know 6 months later what has changed? Document your code and your output and your design decisions all in one place.
- Reproducible pipeline
- Know exactly what changed and when
- Know how to rerun the analysis and get the (same) results
- This is like your research notebook

Rationale

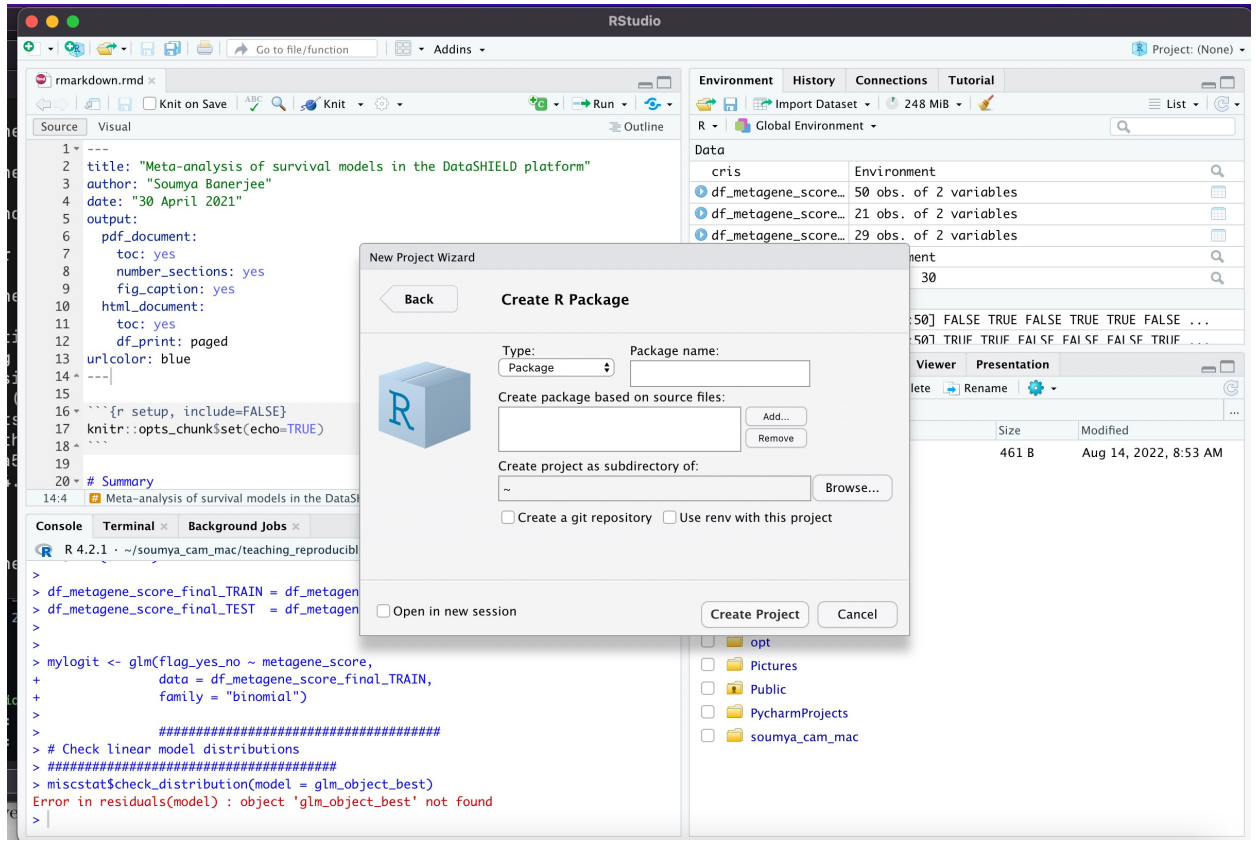
- experiences/case studies of using Rmarkdown notebooks and helping biologists use them to analyze their own data
- When you are deep in your work, it can be difficult to make code pretty, comment it and make it reproducible.
- But you will regret not doing this when you park the work and 6 months later your colloaborators/reviewers ask for additional analysis or changing some assumption, etc.
- Your code should then be ready (you should be able to click a button and reproduce the figures for your paper).


Cluster 0
Unstimulated
LYZ+
Cluster 1
LPS-stim.
CD14+
CD163 low
Cluster 6
LPS + anti-IL-10R
MRC1+
Cluster 4
LPS + anti-IL-10R
IL6+
Cluster 3
LPS + anti-IL-10R
ISG15+
Cluster 5
Apoptotic
SPINK1+
Cluster 7
Unstimulated
FCGR3A
(CD16)+
tSNE 2
tSNE 1
B
number of cells (k)
condition
LPS+anti-IL-10R
LPS stim
unstimulated
percentage of cells
cluster
LYZ FCN1 CD52 CD36 CD14 IL7R CD300E CD163
ISG20 RSAD2 IL1B IL1R1 PTGS2 IL6 IL23A CSF3 CCL20
IL10 IL10RA IL10RB ITGAX MRC1 INHBA FCGR3A CD74 SPINK1
normalised expression level
D
IL10
IL10RA
IL10RB
IL23A
expression
max
min
E
CLEC10A
HLA-DQB1
ADORA3
TNFSF13B
CXCL10
APOBEC3A
IL18
LILRA1
CD300E
S100A8
S100A9
GPR84
TREM1
NLRP3
IL1B
CXCL3
CXCL2
CXCL8
C15orf48
CXCL16
CCL4L2
CCL3L3
CCL3
CCL4
IL6
G052
TNF
IL1A

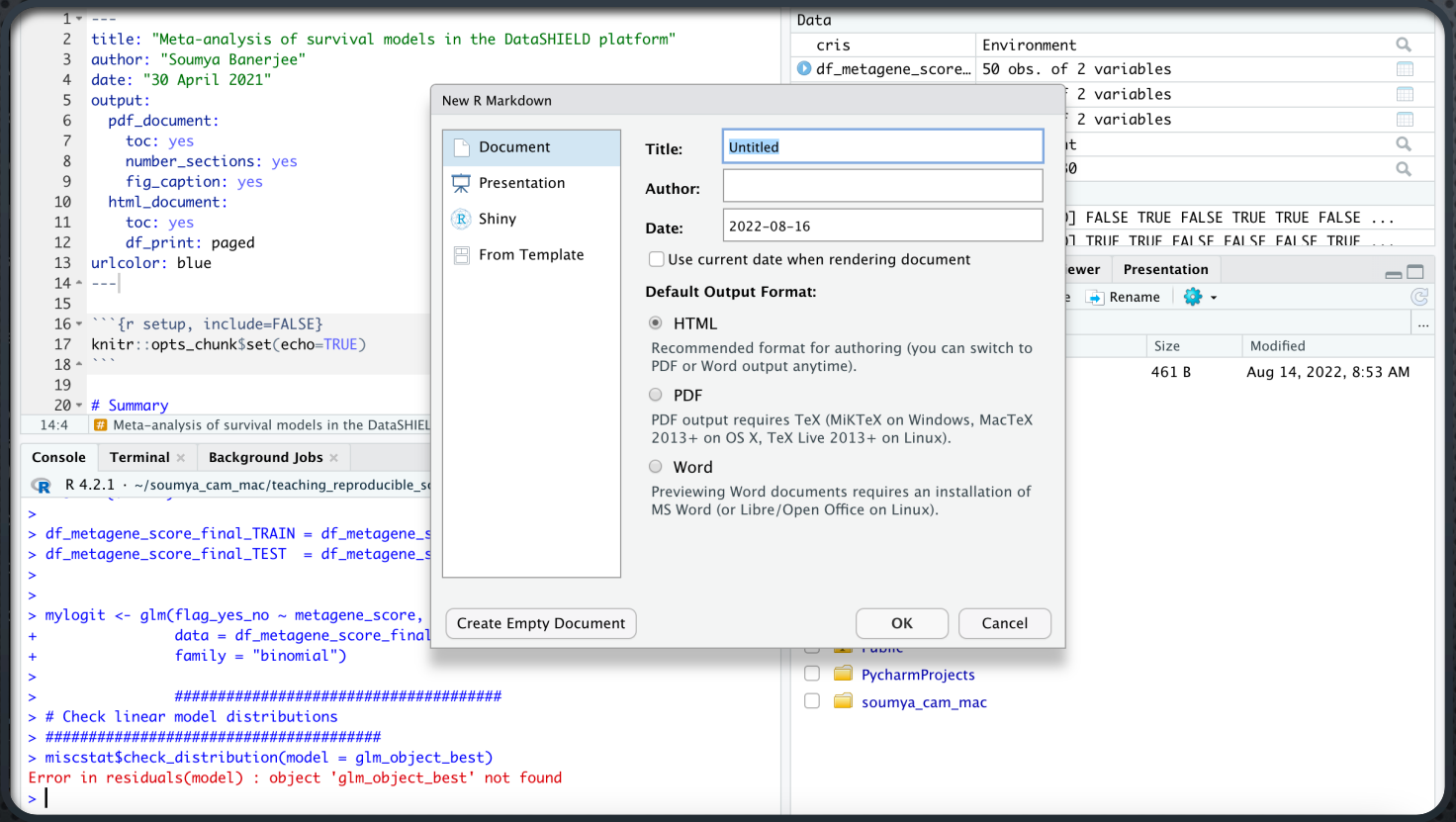
CASE STUDY


A
CD
Subtype
IL1A
IL6
IL1B
TNF
IL23A
IL12B
IL10
Inflam. Cytokine module
Lymphocyte Diff. module
Subtype
iCD deep ulcer
iCD macro. inflam.
cCD micro. inflam.
cCD non-inflam.
non-inflam. UC control
Healthy control
gene expression in RISK cohort
WGCNA module eigengene expression in RISK cohort
B
IL10
IL12B
IL23A
Expression (RPKM)
RISK patient subtype
C
IL1B (RPKM)
IL23A (RPKM)
Inflamed:
R² = 0.3529
P value = <0.0001
Non-inflamed:
R² = 0.01548
P value = 0.1618
D
TNF (RPKM)
IL23A (RPKM)
Inflamed:
R² = 0.8872
P value = <0.0001
Non-inflamed:
R² = 0.5199
P value = <0.0001
E
Correlation with RISK "Inflam. Cytokine" module
Correlation with RISK "Lymphocyte Diff." module
RISK fold change CD vs non-CD
RISK mean expression (TPM)
Source
scRNA-seq
luminex/flow
literature
control gene
F
Prediction baseline
Prediction of Crohn's diagnosis (RISK; AUPRC)
Prediction of anti-TNF non-response in UC (GSE12251; AUPRC)
control gene
(i) correlated with inflammatory cytokine module
(ii) correlated with both modules
(iii) correlated with lymphocyte diff. module
G
Prediction (AUPRC)
Anti-TNF non-response (UC, GSE12251)
H
Crohn's diagnosis (RISK)

CASE STUDY



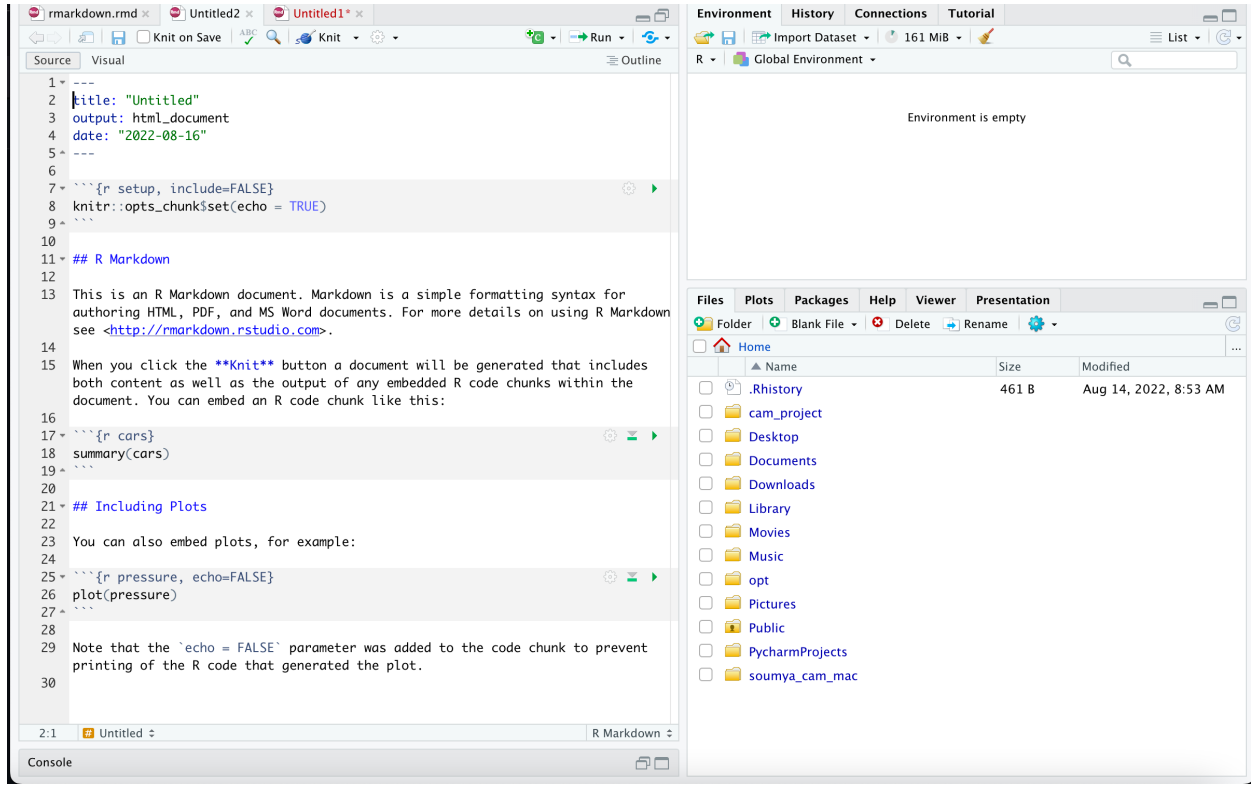
CREATING PACKAGES



CREATING R MARKDOWN

Rationale

- The concepts are the same in any programming language (R/Python)
- Bottomline: we are all busy and we would all rather publish papers, but in the long term these best practices will make us more productive
- This is like protocols (used in experimental biology) for computer scientists. Also like a lab notebook but for computational people.


rmarkdown.rmd
Untitled2
Untitled1*
Knit on Save
Knit
Run
Source
Visual
Outline
---
title: "Untitled"
output: html_document
date: "2022-08-16"

```{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 authoring HTML, PDF, and MS Word documents. For 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 the output of any 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 that generated the plot.
2:1
Untitled
R Markdown
Console
Environment
History
Connections
Tutorial
Import Dataset
161 MiB
List
R
Global Environment
Environment is empty
Files
Plots
Packages
Help
Viewer
Presentation
Folder
Blank File
Delete
Rename
Home
Name
Size
Modified
.Rhistory
461 B
Aug 14, 2022, 8:53 AM
cam_project
Desktop
Documents
Downloads
Library
Movies
Music
opt
Pictures
Public
PycharmProjects
soumya_cam_mac

DEMO

Syntax	Becomes
Make a code chunk with three back ticks followed by an r in braces. End the chunk with three back ticks: ```{r} paste("Hello", "World!") ```	Make a code chunk with three back ticks followed by an r in braces. End the chunk with three back ticks: `paste("Hello", "World!")` `## [1] "Hello World!"`
Place code inline with a single back ticks. The first back tick must be followed by an R, like this `r paste("Hello", "World!")`.	Place code inline with a single back ticks. The first back tick must be followed by an R, like this Hello World!.
Add chunk options within braces. For example, `echo=FALSE` will prevent source code from being displayed: ```{r eval=TRUE, echo=FALSE} paste("Hello", "World!") ```	Add chunk options within braces. For example, `echo=FALSE` will prevent source code from being displayed: `## [1] "Hello World!"`

DEMO

DEMO

- See the link below for more details
- https://www.rstudio.com/wp-content/uploads/2015/03/rmarkdown-reference.pdf
- Now head over to the file named rmarkdown.rmd
- https://github.com/neelsoumya/teaching_reproducible_science_R/blob/main/rmarkdown.rmd
- Running this will create a report like the following:
- https://github.com/neelsoumya/teaching_reproducible_science_R/blob/main/rmarkdown.pdf

Simple demo of rmarkdown

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30 August 2022

Contents

1 Summary

This is a document that outlines a demo of an R markdown.

2 Visualize data

todo histogram

3 Perform logistic regression

```
## [1] 0.3666667
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
```

DEMO

CONCEPTS ARE LANGUAGE AGNOSTIC

```
# This is a test

Testing pandoc

``` code
import GPy
```


``` code
print("Cat")
```
```

CONCEPTS ARE LANGUAGE AGNOSTIC

- HTTPS://GITHUB.COM/NEELSOUMYA/TEACHING_REPRODUCIBLE_SCIENCE_R/BLOB/MAIN/TST.MD

- *PANDOC TST.MD -O TEST.IPYNB*

Resources

- https://github.com/neelsoumya/teaching_reproducible_science_R/
- Code, resources and templates
- EXERCISES with sample data
- Installation instructions