

2024 Reproducible work in Data Science (X. de Pedro)

"Data Science. Applications to Biology and Medicine with Python and R", at IL3 - University of Barcelona^[1]. April 10th, 2024 (16-19:15h).

Content at <https://seeds4c.org/reproduciblework2024>^[2]

Slides in PDF

The screenshot shows the Posit Cloud interface in a Mozilla Firefox browser. The address bar displays <https://posit.cloud/content/5488234>. The workspace is named "Your Workspace / datascience2023". The main editor shows R code for data manipulation using dplyr. The environment pane on the right shows the R version 4.2.2 selected. The file pane on the bottom right lists project files like .gitignore, .Rhistory, .Rprofile, project.Rproj, README.md, recipes, renv, renv.lock, and ReproducibleWork_HandsOnExer... The console at the bottom shows the terminal output of the R session.

```
60 select(
61   ACRONIM_VARIABLE,
62   DATA_LECTURA,
63   VALOR_LECTURA) %>%
64   pivot_wider(
65     names_from = "ACRONIM_VARIABLE",
66     values_from = "VALOR_LECTURA")
67
68 data_wide
69 ...
```

DATA_LECTURA	T	Pn
13/05/2013 12:00:00 AM	11.6	973.9
13/05/2013 12:30:00 AM	11.4	973.7
13/05/2013 01:00:00 AM	11.3	973.7

```
/ccloud/project$ uname -r
5.4.0-1088-aws
/ccloud/project$ lsb_release -a
No LSB modules are available.
Distributor ID: Ubuntu
Description: Ubuntu 20.04.5 LTS
Release: 20.04
Codename: focal
/ccloud/project$
```

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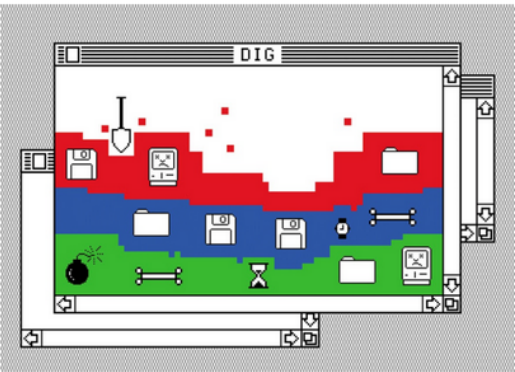
1. Introduction - the problems (i)

TECHNOLOGY FEATURE • 24 AUGUST 2020

Challenge to scientists: does your ten-year-old code still run?


Missing documentation and obsolete environments force participants in the Ten Years Reproducibility Challenge to get creative.

Jeffrey M. Perkel



Perkel, J. (2020). Challenge to scientists: does your ten-year-old code still run? Nature. <https://www.nature.com/articles/d41586-020-02462-7>

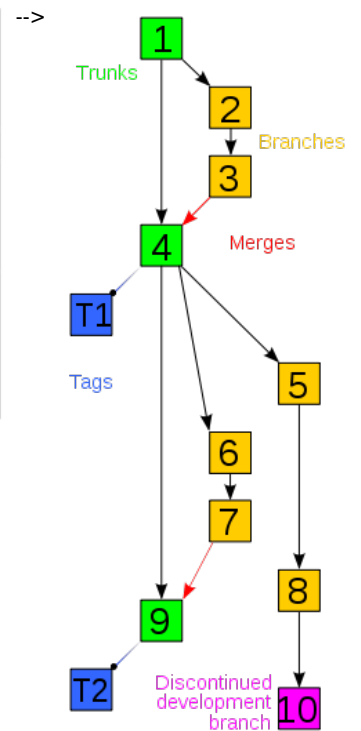
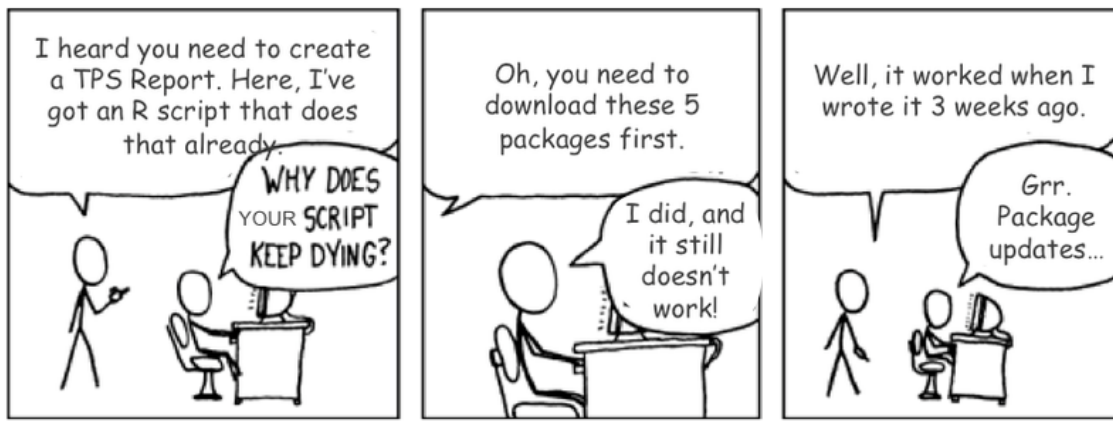
-->



From <https://www.shutterstock.com/image-illustration/3d-illustration-evolution-storage-devices-1420443290>

Obsolete Devices storing code & data --> Ease copying to new devices (legally also: copyleft, ...) + online repositories

1.1. The problems (ii)



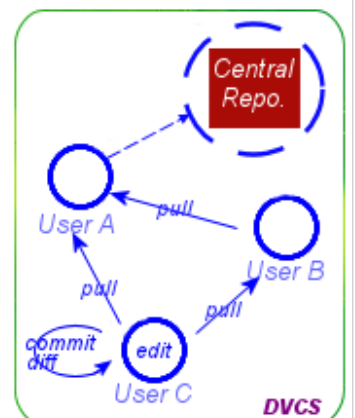
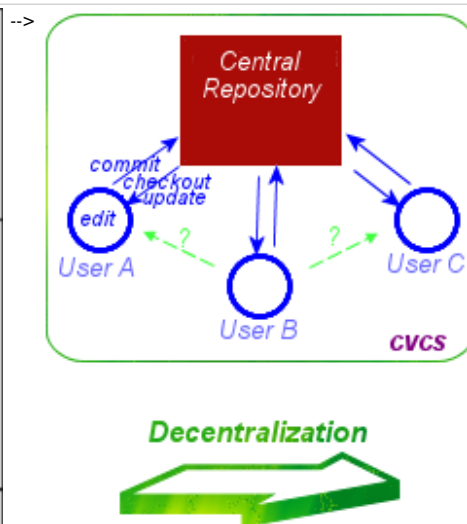
Software obsolescence and incompatible dependency versions

--> Adapt to code evolution:

- Controlling Package Versions (`renv`)
- VCS (**git**, bazaar, svn...)

VCS = Version Control Systems

1.2. The problems (iii)

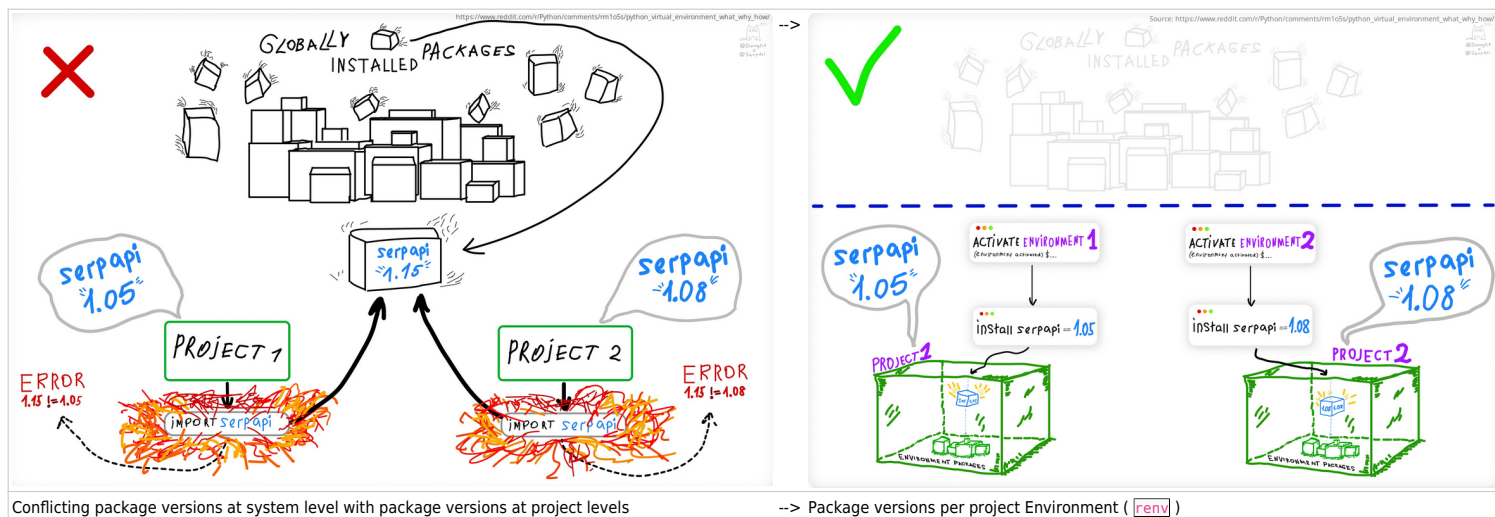


Centralization (such as **Subversion** VCS (**svn**)) may increase efficiency but it also **decreases Resilience** ("shit happens")

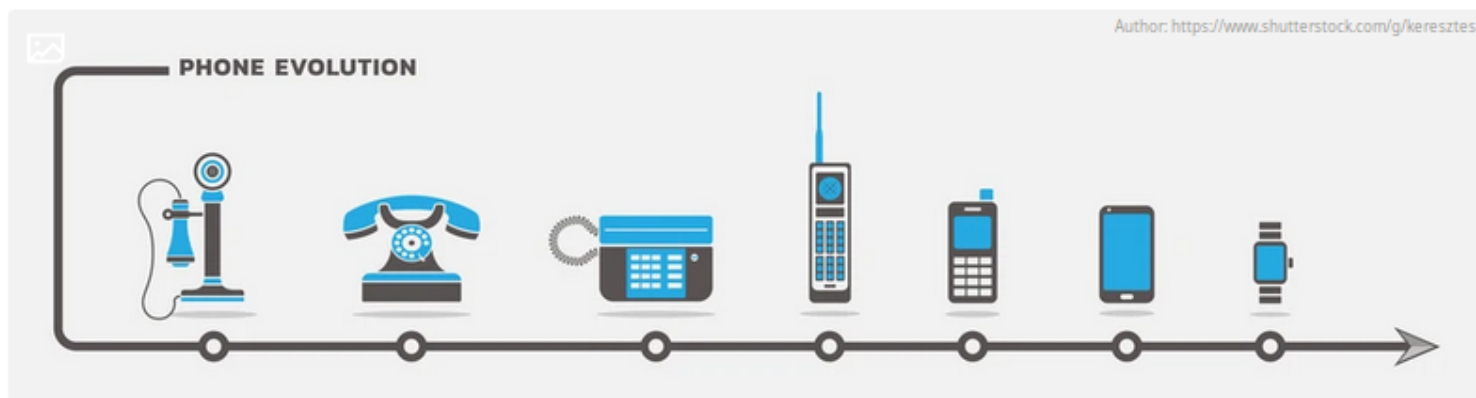
--> From **Centralized** VCS (such as **svn**) to **Decentralized** VCS (such as **git**)

VCS = Version Control Systems

1.3. The problems (iv)



1.4. The problem (v)



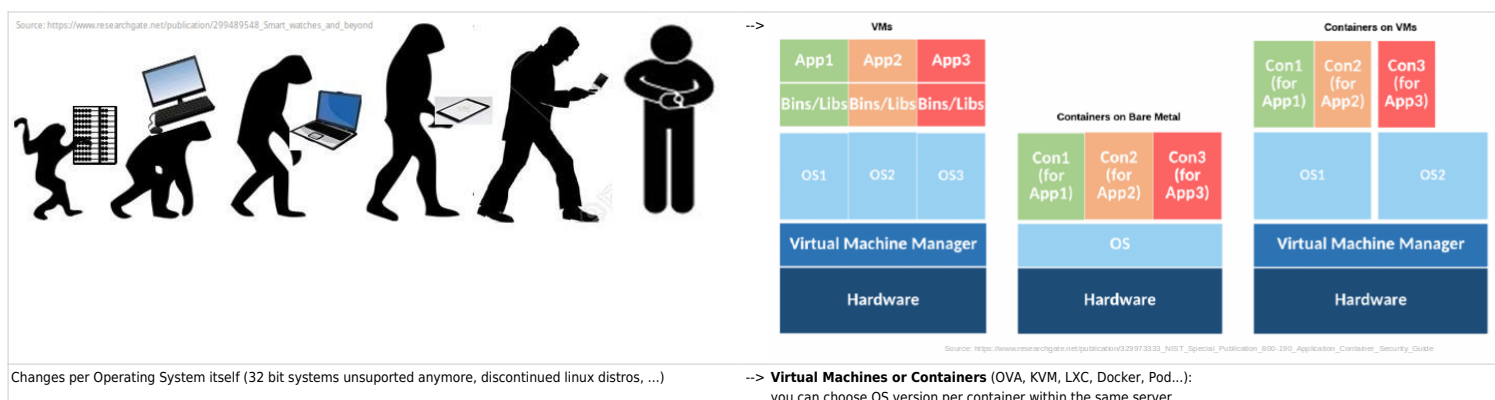
Sometimes a project was developed with a major version of a programming language (R 3.x, Python 2.x), while another project in the same server requires a different major version (R 4.x, Python 3.x)

--> **R case:** from RStudio Server to Posit Workbench (former *RStudio Server Pro*)

You can choose R version per project

Python: Several approaches (`conda`, `PyCharm`, ...): see this as an example^[3].

1.5. The problem (vi)



2. Enemies of reproducibility & adaptability

Enemies of reproducibility and adaptability (in levels): Changes / Evolution / Versions!

1. **Operating system** and its **dependencies** (and their versions)
2. **Programming language** (and its version)
3. **Specific Packages** (and versions) as dependencies for your Work Project
4. **Versions** of your **own code** (algorithm and param variations, etc): lacking versioning system
5. **Readability and tidyness** of your own code / routines / scripts
6. Lack of **documentation/help resources** + steep learning curve to use it or adapt it to your context or infrastructure

3. Reproducibility & Adaptability

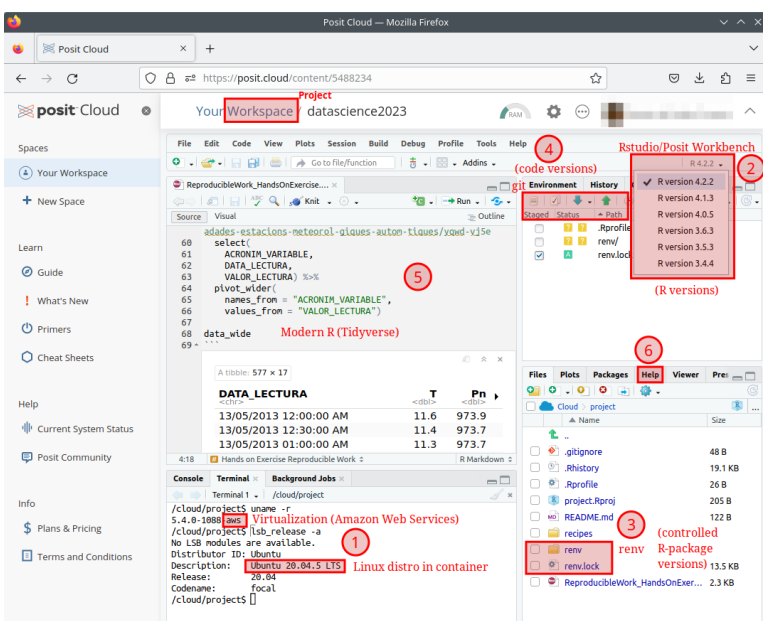
How to avoid reproducibility & adaptability enemies (in R & Python for Data Science):

<u>ISSUES</u>	<u>SOLUTIONS / WORKAROUNDS</u>
(Level 1) Versions in OS repos & critical dependencies: curl, ssl, GDAL, Java, cpp, V8...	<u>Virtual Machines</u> or <u>Containers</u> (VBox, KVM, LXC, Docker, Pod...)
(Level 2) Versions in Programming language: Python 2.x vs 3.x, R 3.x vs 4.x, ...	Python: Conda, Google Colab, ... R: RStudio/Posit Workbench General (in Linux clusters): <i>software modules</i> .
(Level 3) Versions in Specific packages	=== Py: <u>.env</u> , <u>poetry</u> R: Packrat, <u>Renv</u> (by versions), <u>MRAN</u> (by date)
(Level 4) Versions in Your own scripts	Decentralized VCS: <u>Git</u> (Gitlab, Github, ...), <u>Bazaar</u> (Launchpad), ... Centralized VCS: CVS, SVN (Sourceforge, ...), ... <i>VCS = Version Control system</i>
(Level 5) Tidy script content and organization	<u>Literate Coding</u> (Scripting & Coding) / Analysis - R: Rstudio Notebooks with modern R (<i>Tidyverse</i>). VS Notebooks, G-Colab, ... - Python: Jupyter Notebooks , Rstudio Notebooks, VS Notebooks, G-Colab, ... (<u>Quarto</u> Markdown and rendering for both and more)
(Level 6) Help to lower the learning curve	Documentation, Code Vignettes, Examples, Tutorials, Learning material (<u>Learnr</u>), Books (<u>bookdown</u>)...

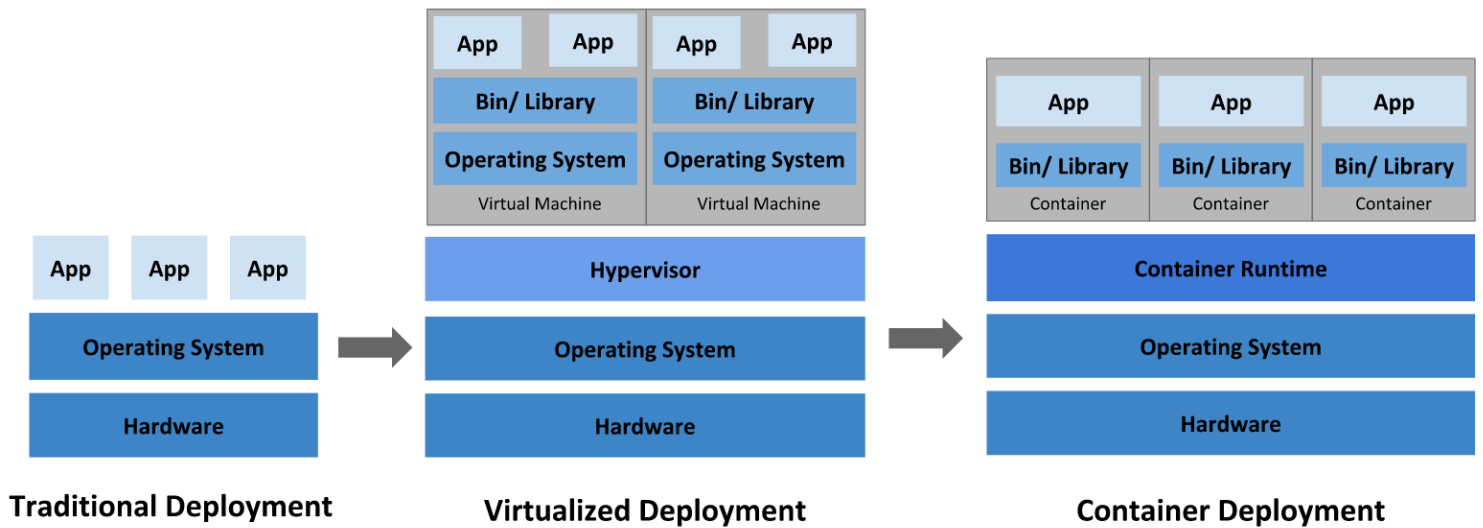
4. Reproducibility & Adaptability - Example in Posit Cloud

Example in <https://posit.cloud>^[4] (former *RStudio Server Pro*) :

- **Level 1:** A **Container** with a specific linux distro (e.g. Ubuntu Linux 20.04 Focal LTS) per project.
- **Level 2:** RStudio/**Posit Workbench** (which allows choosing R version per project)
- **Level 3:** **renv** for your R package collection (and specific versions) in your project
- **Level 4:** **git** or svn for your scripts in your project
- **Level 5:** YOU (*Tidyverse* is your friend)
- **Level 6:** YOU (+ helpers: **roxygen2**, **blogdown**, **learnr**, **bookdown**, ...)

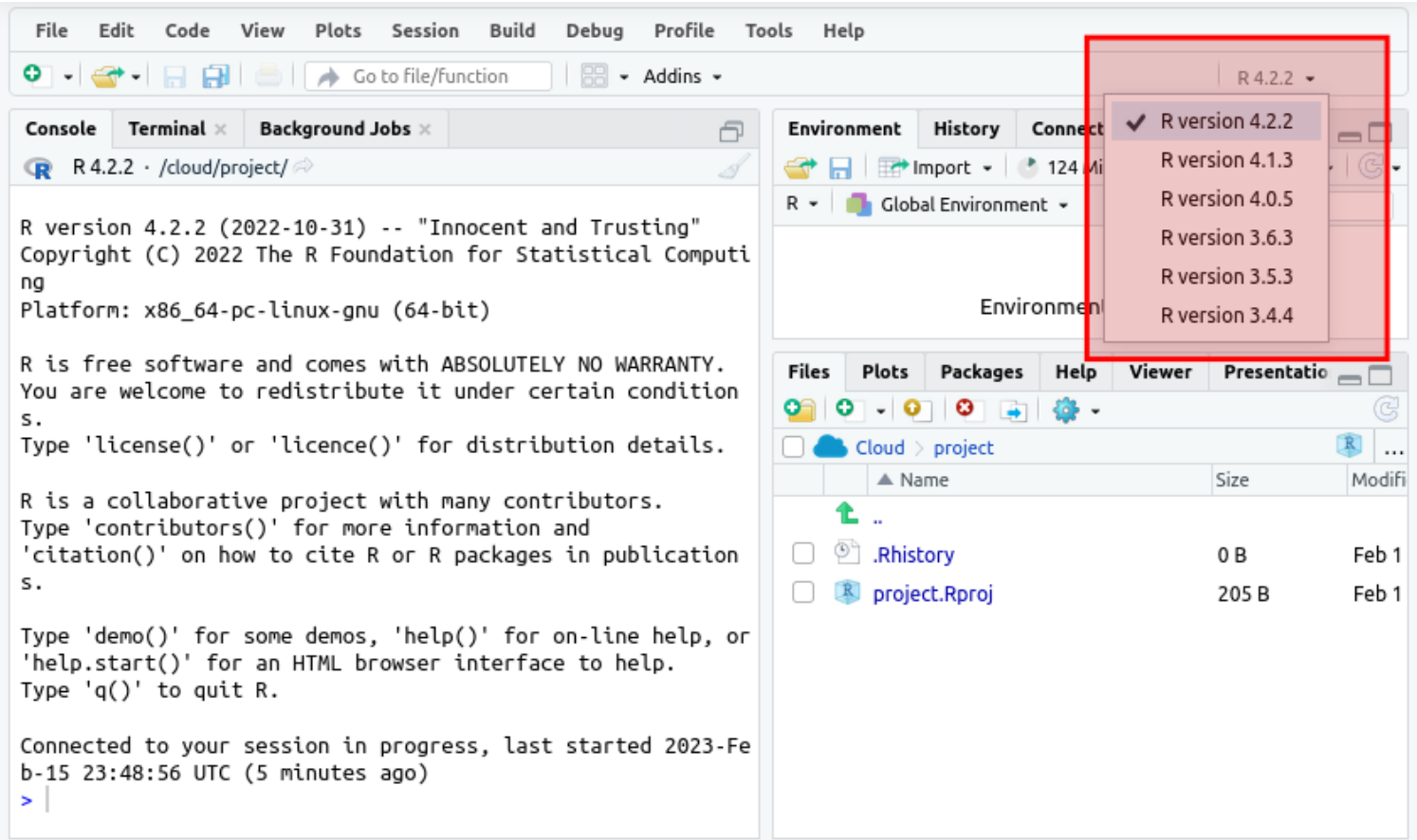


4.1. Level 1: Virtual Machines or Containers



From:
<https://kubernetes.io/docs/concepts/overview/>^[5]

4.2. Level 2: RStudio-Posit Workbench



4.3. Level 3: renv - for packages

Version control in work "environments"


```
utils::sessionInfo()> sessionInfo() R version 4.1.2
(2021-11-01) Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Ubuntu 22.04.1 LTS Matrix products:
default BLAS: /usr/lib/x86_64-linux-
gnu/blas/libblas.so.3.10.0 LAPACK: /usr/lib/x86_64-linux-
gnu/lapack/liblapack.so.3.10.0 locale: [1]
LC_CTYPE=ca_ES.UTF-8 LC_NUMERIC=C
LC_TIME=ca_ES.UTF-8 [4] LC_COLLATE=ca_ES.UTF-8
LC_MONETARY=ca_ES.UTF-8
LC_MESSAGES=ca_ES.UTF-8 [7] LC_PAPER=ca_ES.UTF-8
LC_NAME=C LC_ADDRESS=C [10] LC_TELEPHONE=C
LC_MEASUREMENT=ca_ES.UTF-8 LC_IDENTIFICATION=C
attached base packages: [1] stats graphics grDevices
datasets utils methods base other attached packages:
[1] kableExtra_1.3.4 fs_1.5.2 tictoc_1.1 lubridate_1.9.0
timechange_0.1.1 [6] janitor_2.1.0 knitr_1.40
markdown_1.3 RODBC_1.3-19 fst_0.9.8 [11]
forcats_0.5.2 stringr_1.4.1 dplyr_1. (cont.)
```

renv::snapshot() i ./renv.lock

```
{
  "R": {
    "Version": "4.1.2",
    "Repositories": [
      {
        "Name": "CRAN",
        "URL": "https://cloud.r-project.org"
      }
    ]
  },
  "Packages": {
    "DBI": {
      "Package": "DBI",
      "Version": "1.1.3",
      "Source": "Repository",
      "Repository": "CRAN",
      "Hash":
        "b2866e62bab9378c3cc9476a1954226b",
      "Requirements": []
    },
    "tinytex": {
      "Package": "tinytex",
      "Version": "0.42",
      "Source": "Repository",
      "Repository": "CRAN",
      "Hash":
        "7629c6c1540835d5248e6e7df265fa74",
      "Requirements": [
        "xfun"
      ]
    },
    "tzdb": {
      "Package": "tzdb",
      "Version": "0.3.0",
      "Source": "Repository",
      "Repository": "CRAN",
      "Hash":
        "b2e1cbce7c903eaf23ec05c58e59fb5e",
      "Requirements": [
        "cpp11"
      ]
    },
    "zip": {
      "Package": "zip",
      "Version": "2.2.2",
      "Source": "Repository",
      "Repository": "CRAN",
      "Hash":
        "c42bfcec3fa6a0cce17ce1f8bc684f88",
      "Requirements": []
    }
  }
}
```

(cont'd)0.10 purrr_0.3.5 readr_2.1.3 [16] tidyr_1.2.1
tibble_3.1.8 ggplot2_3.4.0 tidyverse_1.3.1 loaded via a
namespace (and not attached): [1] httr_1.4.4
jsonlite_1.8.3 viridisLite_0.4.1 modelr_0.1.10
assertthat_0.2.1 [6] renv_0.16.0 cellranger_1.1.0
yaml_2.3.6 pillar_1.8.1 backports_1.4.1 [11] glue_1.6.2
digest_0.6.30 rvest_1.0.3 snakecase_0.11.0
colorspace_2.0-3 [16] htmltools_0.5.3 pkgconfig_2.0.3
broom_1.0.1 haven_2.5.1 scales_1.2.1 [21]
webshot_0.5.4 svglite_2.1.0 openxlsx_4.2.5.1 rio_0.5.29
tzdb_0.3.0 [26] generics_0.1.3 ellipsis_0.3.2 withr_2.5.0
cli_3.4.1 magrittr_2.0.3 [31] crayon_1.5.2 readxl_1.4.1
evaluate_0.18 fansi_1.0.3 xml2_1.3.3 [36]
foreign_0.8-82 tools_4.1.2 data.table_1.14.4 hms_1.1.2
lifecycle_1.0.3 [41] munsell_0.5.0 reprex_2.0.2 zip_2.2.2
compiler_4.

(cont'd)

(cont'd)1.2 systemfonts_1.0.4 [46] rlang_1.0.6
grid_4.1.2 fstcore_0.9.12 rstudioapi_0.14
rmarkdown_2.18 [51] gtable_0.3.1 DBI_1.1.3 curl_4.3.3
R6_2.5.1 fastmap_1.1.0 [56] utf8_1.2.2 stringi_1.7.8
parallel_4.1.2 Rcpp_1.0.9 vctrs_0.5.0 [61] dbplyr_2.2.1
tidyselect_1.2.0 xfun_0.34 >

4.3.3. "Happy path"

For a reproducible environment

Commands in terminal - Computer 1



```
cd project_folder
git init
R
[obrir projecte de RStudio]
renv::init() # to initialize renv in
your code project
renv::snapshot() # to make a
snapshot "picture" of the list of R
packages used within the whole R
project and their respective package
versions
q()
git commit ...
git push
```

Commands in terminal - Computer 2



```
cd project_folder
```

```
git clone/git pull ...
R
[open same RStudio project]
renv::status() # for a report on
which steps are suggested for you to
follow
renv::restore() # to restore the
package library (with the required
package versions) for this project
[continue working in/developing your
code]
renv::snapshot() # to make a new
snapshot "picture" (in case there
are new packages and/or versions or
R packages newer or older in use in
your project ;- )
q()
git commit ...
git push
```

4.3.4. Infraestructure

Projects with `renv` write and use these files in order to work:

File	Use
.Rprofile	Used to activate renv for new R sessions launched in the project.
renv.lock	The lockfile, describing the state of your project's library at some point in time.
renv/activate.R	The activation script run by the project .Rprofile .
renv/library	The private project library.
renv/settings.dcf	Project settings - see <code>?settings</code> for more details.

By default, `renv` uses a package memory-cache here:

Platform	Location
Linux	<code>~/.local/share/renv</code>
macOS	<code>~/Library/Application Support/renv</code>
Windows	<code>%LOCALAPPDATA%/renv</code>

4.3.5. Advanced use



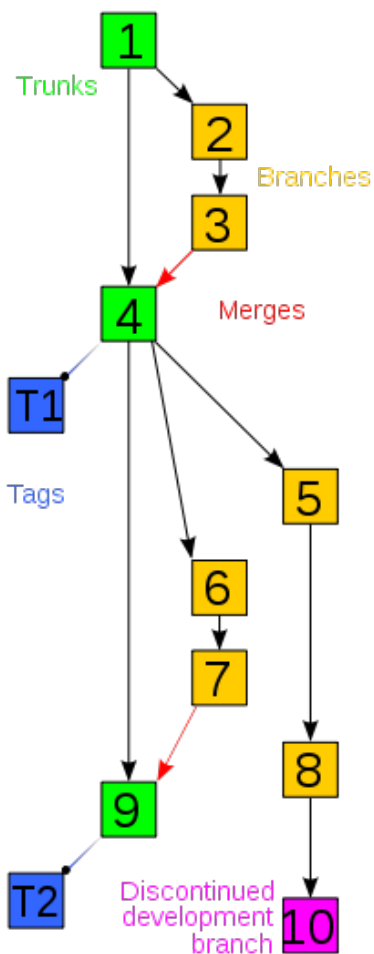
```
renv::install("packagename", version="0.1") # to install old versions from a
```

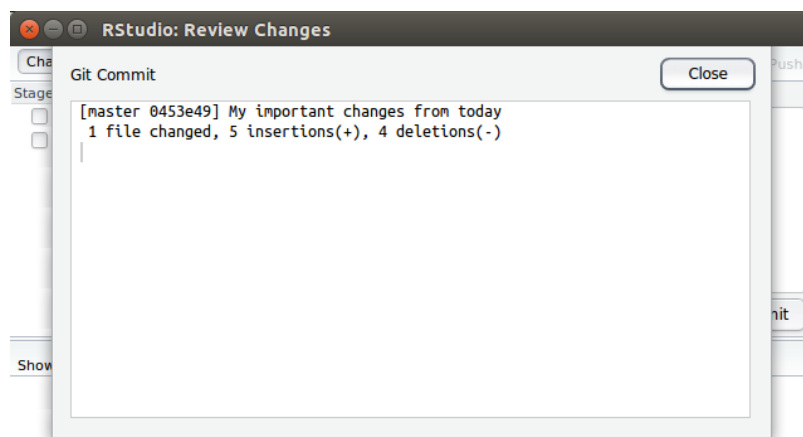
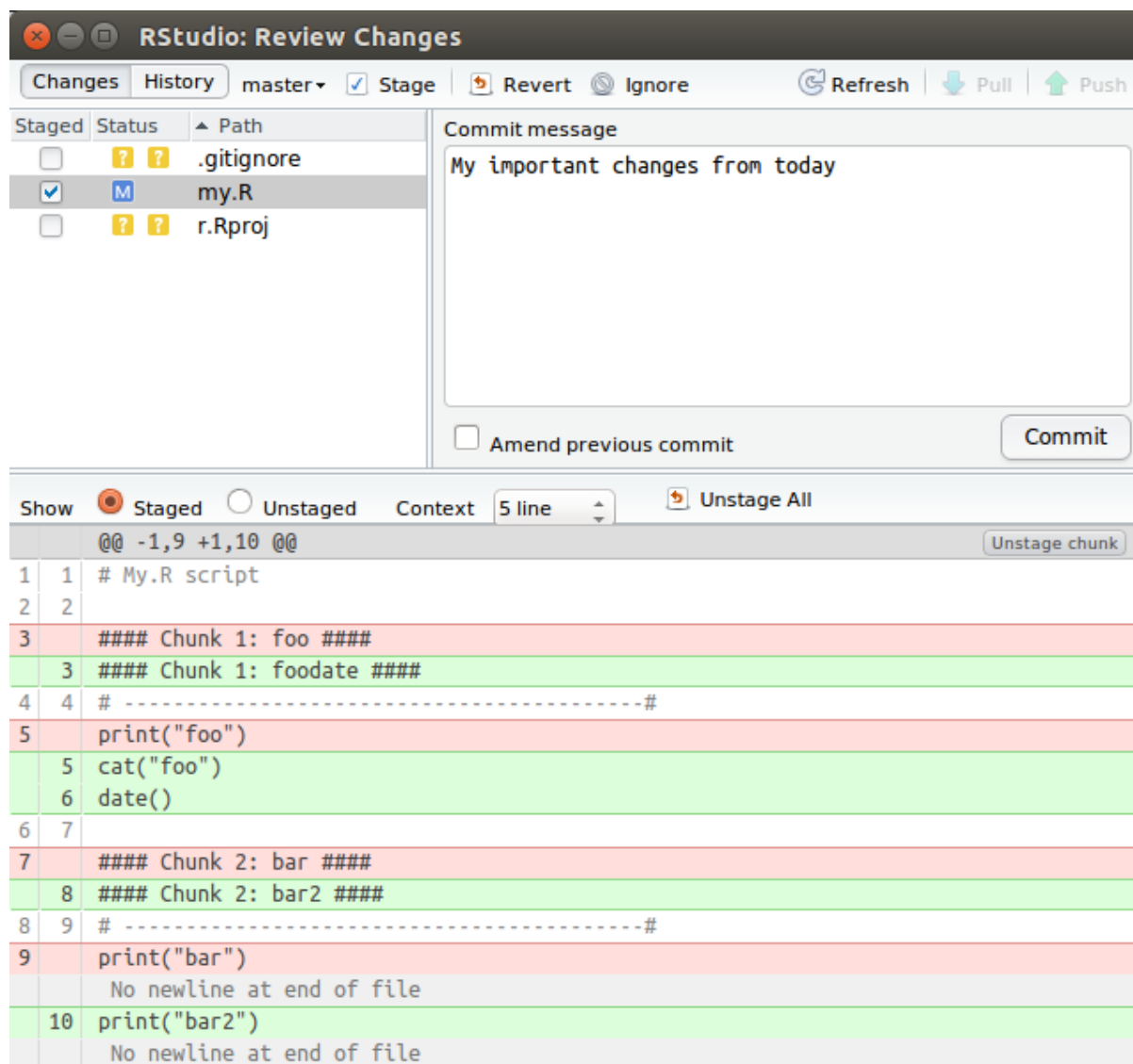
```
package (useful also for discontinued packages in CRAN!). See possible package-  
version numbers at https://cran.r-project.org/src/contrib/Archive/yourpackage/  
renv::record("packagename", version="0.1") # to save at renv.lock the specific  
version you need for this package  
renv::deactivate() # to temporarily deactivate renv in your project  
renv::activate() # to reactivate renv in your project  
renv::equip() # for special installations in MS Windows  
vignette("docker", package = "renv") # for a combined use with Docker  
vignette("collaborating", package = "renv") # to improve collaborative use in work  
teams
```

And much more. See:

- <https://rstudio.github.io/renv/articles/renv.html>^[6]
- <https://solutions.posit.co/envs-pkgs/environments/>^[7]

4.4. Level 4: git - for code





See: <https://gitlab.com/radup/curs-r-introduccio/>^[8] > Folder "codi"^[9] > **10.compartir.via.git.Rmd** (or .pdf^[10])

See also my own git recipes over some years, github cheatsheet, ...: <https://seeds4c.org/git>^[11]

5. More information

Work Environments in R

- <https://solutions.posit.co/envs-pkgs/environments/>^[12]

Videos

- An Introduction to Reproducible Research Practices. 29 d'abr. 2022. John Little. Duke University. Video^[13]
- Designing a Reproducible Workflow with R and GitHub. John Little. 22 de nov. 2021 Video^[14] | Tutorial^[15]
- The workflowr R package: a framework for reproducible and collaborative data science. 13 de jul. 2018. R Consortium. Video^[16]
- Kevin Ushey | renv: Project Environments for R | RStudio (2020). Posit PBC.. 20 de des. 2020. Video^[17]

R Packages

[renv](#)^[18] | [workflowr](#)^[19] | [learnr](#)^[20] | [roxygen2](#)^[21] | [Tidyverse](#)^[22]

Free Work environments for Collaborative Data Science with R & Python

- <https://posit.cloud/plans/free>^[23]

Additional tutorial with big data to follow on site (R Cloud)

- Danielle Navarro. 2022. "Using Amazon S3 with R"^[24] March 17, 2022.

Papers

- Wallach JD, Boyack KW, Ioannidis JPA. (2018) Reproducible research practices, transparency, and open access data in the biomedical literature, 2015–2017. PLoS Biol 16 (11): e2006930. <https://doi.org/10.1371/journal.pbio.2006930>^[25]
- Leek JT, Peng RD. Opinion: Reproducible research can still be wrong: adopting a prevention approach. Proc Natl Acad Sci U S A. 2015 Feb 10;112(6):1645-6. doi: 10.1073/pnas.1421412111. PMID: 25670866; PMCID: PMC4330755

6. Hands-on practical exercise

The screenshot displays the Posit Cloud web application interface. The browser window shows the URL `https://posit.cloud/content/5488234`. The interface includes a sidebar with navigation options like 'Spaces', 'Learn', 'Help', and 'Info'. The main workspace area is titled 'Your Workspace / datascience2023' and features a menu bar, a toolbar, and a code editor. The code editor contains R code for data manipulation. Below the code, a tibble preview is shown with columns `DATA_LECTURA`, `T`, and `Pn`. The console at the bottom displays system information. On the right side, there is an 'Environment' panel with a dropdown menu for selecting R versions, and a 'Files' panel showing the file structure of the current project.

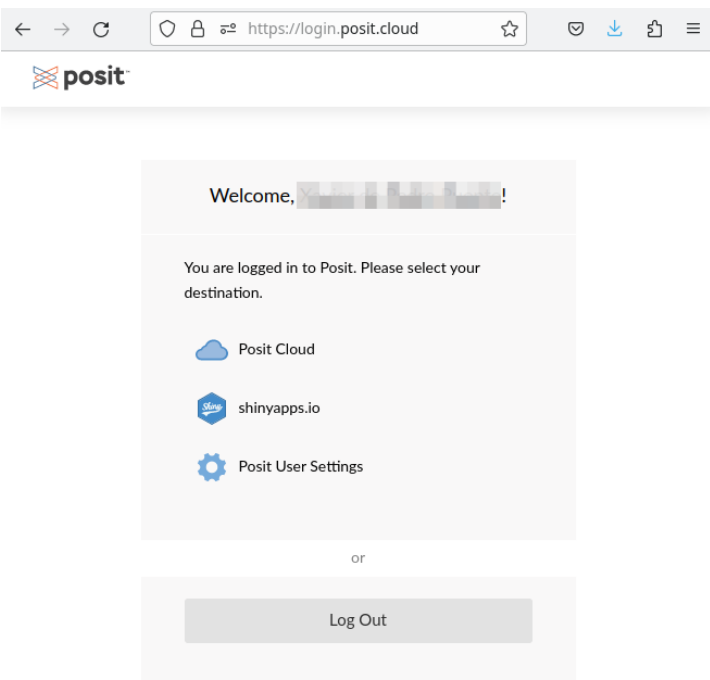
6.1. Register a free account at Posit Cloud

You can do so at:

- <https://posit.cloud/plans/free>^[26]

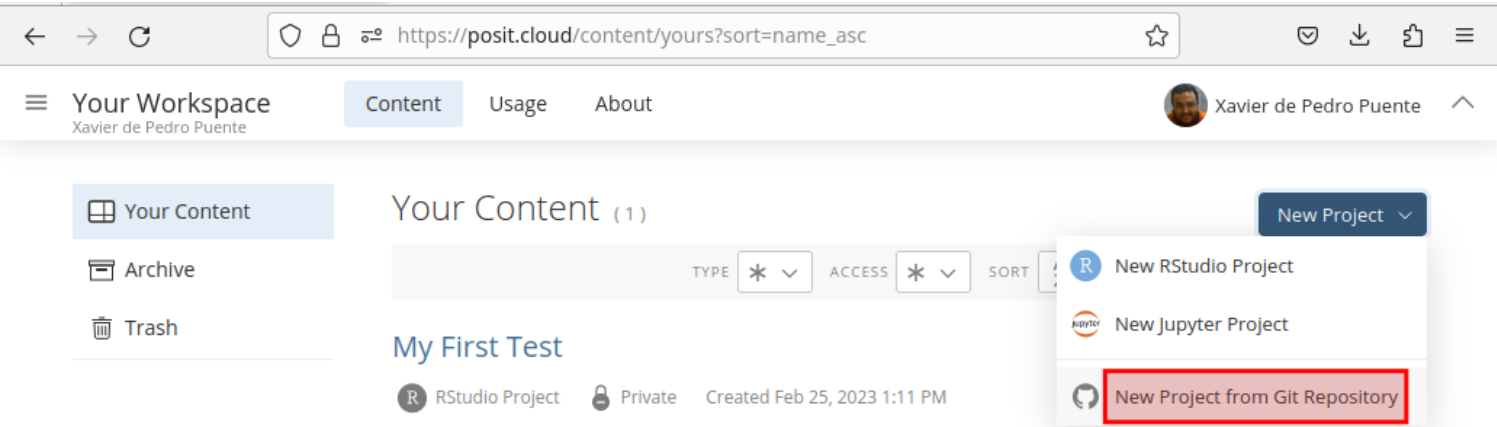
You will need to click on a link sent to your email inbox to validate your account.

Once done, you'll see something like:



6.2. Create a Project from git repository

Enter Posit cloud and click at **New Project > New Project from Git Repository**



6.2.1. Visit gitlab to get clone url

Visit this code project in gitlab to get the project clone url:
<https://gitlab.com/xavidp/datascience2023>^[27]

The screenshot shows the GitLab web interface for a repository named 'DataScience2023' by user 'Xavier de Pedro'. The URL in the browser is `https://gitlab.com/xavidp/datascience2023`. The repository has 5 commits, 1 branch, 0 tags, and 236 KB of project storage. A recent commit titled 'Base Rmd file' is shown. The 'Clone' button is highlighted with a red box. A dropdown menu is open, showing options to clone with SSH or HTTPS. The HTTPS URL is `https://gitlab.com/xavidp/datascience2023.git`, which is also highlighted with a red box. Below the clone options, there are links to open the project in Visual Studio Code or IntelliJ IDEA using either SSH or HTTPS.

6.2.2. Create project from git repo

Paste it in the Posit cloud popup window and click at OK:

The screenshot shows the Posit Cloud web interface. A dialog box titled 'New Project from Git Repository' is open in the center. It contains a text input field with the URL `https://gitlab.com/xavidp/datascience2023.git` and an 'OK' button. The background shows the 'Your Workspace' section with tabs for 'Content', 'Usage', and 'About'. The 'Content' tab is active, showing a list of items: 'Your Content', 'Archive', and 'Trash'. The user's name 'Xavier de Pedro Puente' is visible in the top right corner.

6.3. Choose R 3.6.x & Run Rmd

The screenshot shows the Posit Cloud interface in a Mozilla Firefox browser. The URL is <https://posit.cloud/content/5488234>. The workspace is named "Your Workspace / datascience2023". The R version is set to "R 3.6.3" (indicated by a red circle 1). The source editor shows an R Markdown file named "ReproducibleWork_HandsOnExercise.Rmd" with the following content:

```
1 ---
2 title: "Hands on Exercise Reproducible Work"
3 author: "Xavier"
4 date: "2023-02-25"
5 output: html_document
6 ---
7
8 {r setup, include=FALSE}
9 knitr::opts_chunk$set(echo = TRUE)
10
11 # Session Reproducible Work
12
13 Monday Feb 27, 2023. IL3-UB.
```

The "Run" button in the toolbar is highlighted with a red circle 3, and the "Run All" option in the dropdown menu is highlighted with a red circle 4. The "Environment" panel on the right shows "Environment is empty". The "Files" panel at the bottom right shows a list of files, with "ReproducibleWork_HandsOnExercise.Rmd" highlighted by a red circle 2.

6.3.1. Install dependencies also

The screenshot shows the Posit Cloud interface with a warning message: "Packages markdown and knitr required but are not installed". The "Install" button is highlighted with a red box. The source editor shows the same R Markdown file as in the previous screenshot. The "Environment" panel on the right shows "Environment is empty". The "Files" panel at the bottom right shows a list of files, with "ReproducibleWork_HandsOnExercise.Rmd" highlighted by a red circle 2.

```
11
12 # Session Reproducible Work
13
14 Monday Feb 27, 2023. IL3-UB.
15
16 Related to:
17 https://seeds4c.org/reproduciblework2023
18
4:5 # Hands on Exercise Reproducible Work R Markdown
```

Console Terminal Background Jobs

Install R packages 0:05

```
* DONE (base64enc)
* installing *binary* package 'mime' ...
* DONE (mime)
* installing *binary* package 'ellipsis' ...
* DONE (ellipsis)
* installing *binary* package 'cachem' ...
* DONE (cachem)
```

6.3.2. Running Rmd will perform GNU/Linux system commands also

**GNU/Linux system
commands will usually be
much more efficient in
memory & cpu**

It helps to prevent RAM
bottlenecks with just 1Gb
RAM on Posit Cloud Free
plan

(while csv file from reduced
meteorological dataset is
already 0.5 Gb).

RAM

Your Workspace / datascience2023

File Edit Code View Plots Session Build Debug Profile Tools Help

Go to file/function

Addins

R 4.2.2

ReproducibleWork_HandsOnExercise....

Source Visual Outline

```
15 Monday, Feb 27, 2023 12:00
16 Related to:
17 https://seeds4c.org/reproduciblework2023
18
19 ## Hands on Exercise
20
21 ```{r}
22 if (!require(readr)) {install.packages("readr")}
23
24 Loading required package: readr
25
26 ```{r}
27 if (!file.exists("data_subset.csv")) {
28   system("wget http://cloud.seeds4c.org/data_smc.csv.bz2")
29   system("bunzip2 data_smc.csv.bz2 -k")
30   system("cat data_smc.csv | head -n1000001 >
31     data_subset.csv")
32 }
33 data <- read_csv("data_subset.csv")
34
```

Environment History Connections Git

R Global Environment

Data

data 1000000 obs. of 8 varia...

Files Plots Packages Help Viewer

Cloud > project

Name	Size
..	
.gitignore	48 B
.Rhistory	0 B
data_smc.csv.bz2	50.2 MB
project.Rproj	205 B
README.md	122 B
ReproducibleWork_HandsOnExer...	629 B
data_smc.csv	613.3 MB
data_subset.csv	61.3 MB

Console Terminal Background Jobs

R 4.2.2 /cloud/project/

```
> data <- read_csv("data_subset.csv")
Rows: 1000000 Columns: 8— Column specification
```

6.3.3. Display raw data

Variables are in numeric codes (not easily readable by humans in a semantic way). We lack some variable names (or acronyms at least) for readability.

ReproducibleWork_HandsOnExercise.... data

Filter

	ID	CODI_ESTACIO	CODI_VARIABLE	DATA_LECTURA	DATA_EXTREM
1	XK721205132330	XK	72	12/05/2013 11:30:00 PM	12/05/2013 11:30:00 PM
2	XK361205132330	XK	36	12/05/2013 11:30:00 PM	NA
3	XK381205132330	XK	38	12/05/2013 11:30:00 PM	NA
4	XK321205132330	XK	32	12/05/2013 11:30:00 PM	NA
5	XK401205132330	XK	40	12/05/2013 11:30:00 PM	12/05/2013 11:30:00 PM
6	XK421205132330	XK	42	12/05/2013 11:30:00 PM	12/05/2013 11:51:00 PM
7	XK331205132330	XK	33	12/05/2013 11:30:00 PM	NA
8	XK441205132330	XK	44	12/05/2013 11:30:00 PM	12/05/2013 11:32:00 PM
9	XK031205132330	XK	3	12/05/2013 11:30:00 PM	12/05/2013 11:51:00 PM
10	XK301205132330	XK	30	12/05/2013 11:30:00 PM	NA
11	XK311205132330	XK	31	12/05/2013 11:30:00 PM	NA
12	XL031205132330	XL	3	12/05/2013 11:30:00 PM	12/05/2013 11:51:00 PM
13	XL301205132330	XL	30	12/05/2013 11:30:00 PM	NA

Environment History

R Global Environment

Data

data 1000000 ...

Files Plots Packages

Cloud > project

Name

..

.gitignore

.Rhistory

6.3.4. Transform in tidy way (i)


```

34
35 {r}
36 # Get the description of the variable codes
37 # From here: https://analisi.transparenciacatalunya.cat/Medi-Ambient/Metadades-variables-meteorol-giques/4fb2-n3yi/data
38 variables <- read_csv("https://analisi.transparenciacatalunya.cat/api/views/4fb2-n3yi/rows.csv?accessType=DOWNLOAD&sorting=true")
39

```

Rows: 26 Columns: 6 — Column specification

Delimiter: ","

chr (4): NOM_VARIABLE, UNITAT, ACRONIM, CODI_TIPUS_VAR

dbl (2): CODI_VARIABLE, DECIMALS

i Use 'spec()' to retrieve the full column specification for this data.

i Specify the column types or set 'show_col_types = FALSE' to quiet this message.

```

40
41 {r}
42 # We prepare a small dataframe from the variable definition to join on the smc data frame
43 variables.to.join <- variables %>%
44   select(CODI_VARIABLE, ACRONIM) %>%
45   arrange(CODI_VARIABLE)
46
47 variables.to.join
48

```

A tibble: 26 x 2

	CODI_VARIABLE <dbl>	ACRONIM <chr>
1	Px	
2	Pn	
3	HRx	
30	VV10	

6.3.5. Transform in tidy way (ii) - result

```

49
50 {r}
51 # Let's join variable df on to the data df
52 data <- left_join(data, variables.to.join) %>%
53   rename(ACRONIM_VARIABLE = ACRONIM)
54

```

Joining, by = "CODI_VARIABLE"

```

55
56 {r}
57 # Let's convert the source data frame (which is long shape, as database) into a wide shape (table like, with meteorological variables as
58 # columns) while selecting just one meteorological station as an example
59 data_wide <- data %>%
60   filter(CODI_ESTACIO == "D5") %>% # D5 corresponds to "Barcelona Observatori Fabra" Meteorological Observatory (at Collserola Mountain)
61   https://analisi.transparenciacatalunya.cat/Medi-Ambient/Metadades-estacions-meteorol-giques-auton-tiques/vawd-vj5e
62   select(
63     ACRONIM_VARIABLE,
64     DATA_LECTURA,
65     VALOR_LECTURA) %>%
66   pivot_wider(
67     names_from = "ACRONIM_VARIABLE",
68     values_from = "VALOR_LECTURA")
69 data_wide
70

```

A tibble: 577 x 17

DATA_LECTURA <chr>	T <dbl>	Pn <dbl>	Tn <dbl>	HR <dbl>	HRn <dbl>	HRx <dbl>	VV10 <dbl>	DV10 <dbl>	VVx10 <dbl>
13/05/2013 12:00:00 AM	11.6	973.9	11.4	91	91	92	2.0	238	2.7
13/05/2013 12:30:00 AM	11.4	973.7	11.4	90	90	91	1.5	238	2.4
13/05/2013 01:00:00 AM	11.3	973.7	11.3	89	87	91	1.1	174	2.3
13/05/2013 01:30:00 AM	11.3	973.6	11.3	89	88	91	1.5	209	2.4

6.3.6. Last code chunks

```

70
71 ```{r}
72 # Save resulting dataset to disk
73 write_csv(data_wide, "data_subset_d5_wide.csv")
74 ```
75
76
77 ```{r}
78 # Produce a simple R version of this R Markdown document
79 knitr::purl("ReproducibleWork_HandsOnExercise.Rmd", documentation=2)
80 ```

```

```
[1] "ReproducibleWork_HandsOnExercise.R"
```

```
81
82
```

4:18 # Hands on Exercise Reproducible Work

6.4. Choose R 4.2.x & Run Rmd again

Repeat the previous steps but in a R 4.2.x environment: install dependent R packages again... (new environment, but still installing from CRAN repos). renv not needed in this case still (lucky you!).

So far, so good.

The screenshot shows the Posit Cloud workspace interface. The browser address bar displays `https://posit.cloud/content/5488234`. The workspace name is "Your Workspace / datascience2023". The R version is set to "R 4.2.2", which is highlighted with a red box. The interface includes a menu bar (File, Edit, Code, View, Plots, Session, Build, Debug, Profile, Tools, Help) and a toolbar with icons for file operations and running code. The main editor shows the R Markdown file "ReproducibleWork_HandsOnExercise.Rmd" with the following content:

```

1 ---
2 title: "Hands on Exercise Reproducible Work"
3 author: "Xavier"
4 date: "2023-02-25"
5 output: html_document
6 ---
7

```

A yellow warning banner at the bottom of the editor states: "Packages rmarkdown, dplyr, and knitr others required but are not installed. Install Don't Show Again". The right sidebar shows the "Environment" tab with a list of files: `data_smc.csv`, `data_smc.csv.bz2`, `data_subset_all.csv`, and `data_subset_d5_wide.csv`. The status bar indicates "Your branch is ahead of 'origin/master' by 1 commit."

6.5. Choose R 3.4.x & Run Rmd

Now let's touch some issues with R package versions in a R 3.4.x environment

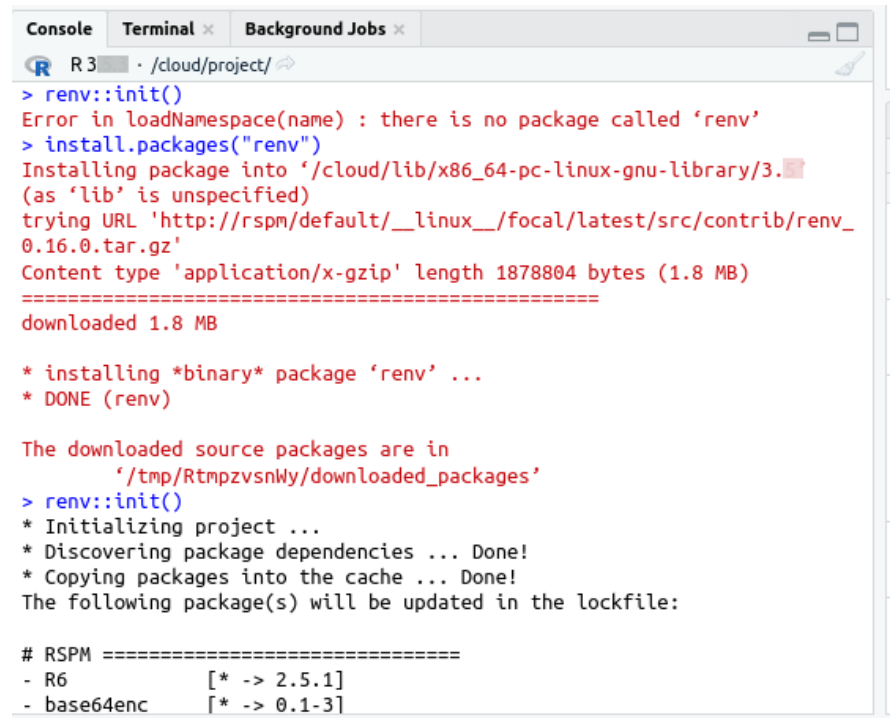
Running Rmd will fail at some package installations

- `dplyr` installation fails
- `readr` is reported as unavailable in R 3.4.4
- `tidyr` installation also fails (as well as `purrr`)

Solution

In this case, the solution involves finding some valid previous package version for each conflicting R package, and using this type of commands:

- `renv::init()`
- `renv::install("packagename@x.y.z")` # being x.y.z a valid package version number, as taken from <https://cran.r-project.org/src/contrib/Archive/packagename/>^[28]
- `renv::record("packagename@x.y.z")`
- `renv::snapshot()` # after all packages installed without any more issues



```
Console Terminal Background Jobs
R 3.4.4 - /cloud/project/
> renv::init()
Error in loadNamespace(name) : there is no package called 'renv'
> install.packages("renv")
Installing package into '/cloud/lib/x86_64-pc-linux-gnu-library/3.4.4'
(as 'lib' is unspecified)
trying URL 'http://rspm/default/__linux__/focal/latest/src/contrib/renv_0.16.0.tar.gz'
Content type 'application/x-gzip' length 1878804 bytes (1.8 MB)
=====
downloaded 1.8 MB

* installing *binary* package 'renv' ...
* DONE (renv)

The downloaded source packages are in
'/tmp/RtmpzvsnWY/downloaded_packages'
> renv::init()
* Initializing project ...
* Discovering package dependencies ... Done!
* Copying packages into the cache ... Done!
The following package(s) will be updated in the lockfile:

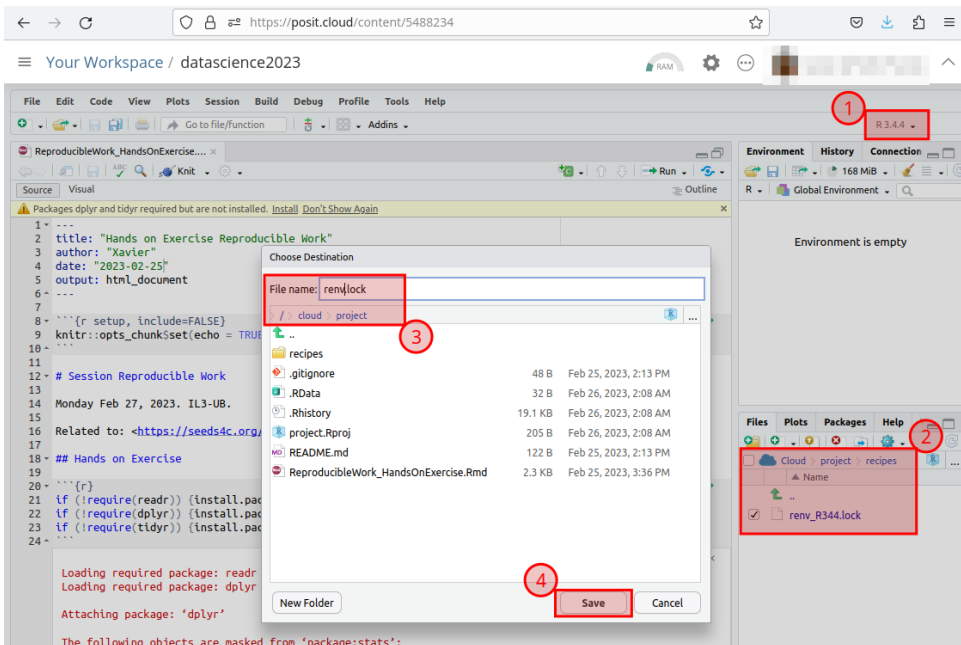
# RSPM =====
- R6 [* -> 2.5.1]
- base64enc [* -> 0.1-3]
```

6.5.1. Use renv.lock recipe (i)

Let's get `renv` to the rescue. Once somebody solved these issues, and found a valid recipe of package versions for this environment, a file `./renv.lock` will have been produced in the project root folder after running the command `renv::snapshot()`

I did this already, and I uploaded the produced `renv.lock` file to the manually created `./recipes/` folder in this project as a backup for you (as `renv_R344.lock`).

You can then copy now the `./recipes/renv_R344.lock` file provided in the project as `./renv.lock` in the project root folder, for `renv` to be able use it.

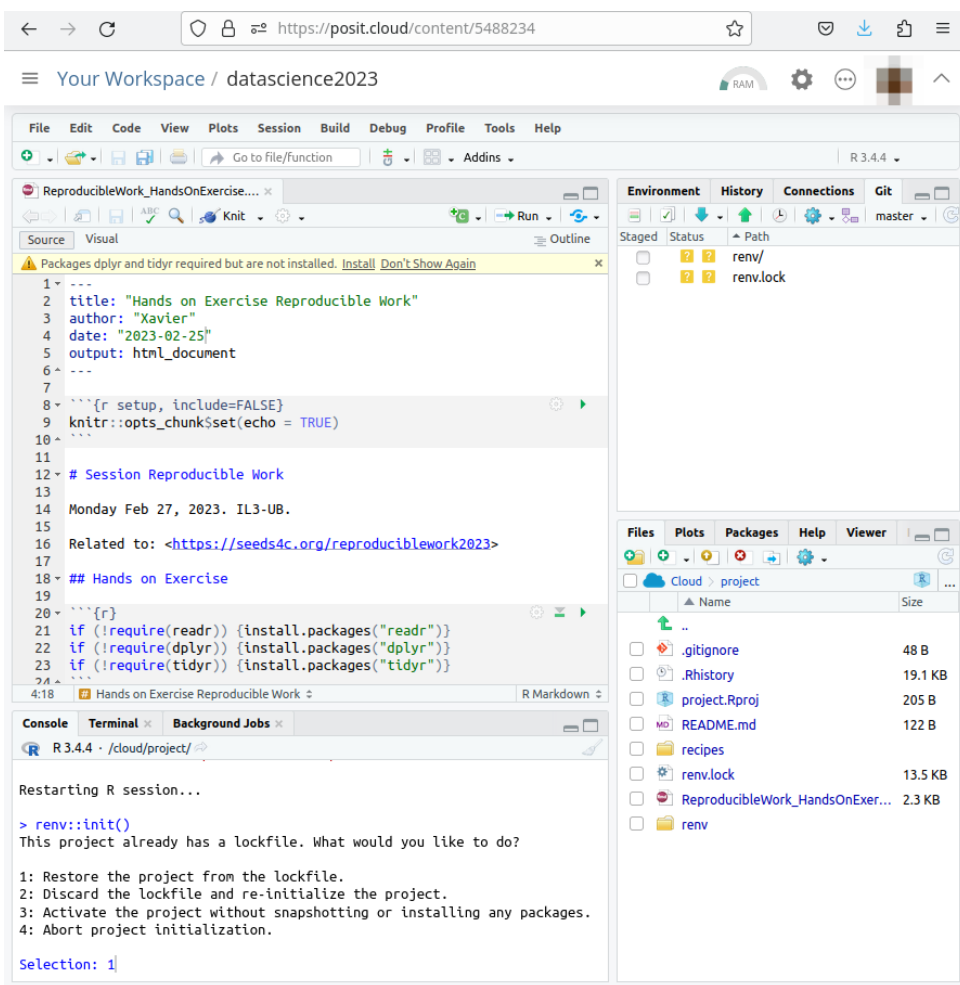


6.5.2. Use renv.lock recipe (ii)

Run `renv::init()` in the R console.

Choose restore the renv.lock package versions:

"1. Restore the project from the lockfile"



6.5.3. Use renv.lock recipe (iii)

You will be ready to go with minimum human intervention.

All R packages will be installed in the background to their required package versions, following the recipe that someone created for R 3.4.4. already.

The key file is the **renv.lock** file.

The screenshot displays the RStudio environment with the following components:

- Source Editor:** Contains an R Markdown document titled "Hands on Exercise Reproducible Work" by "Xavier" dated "2023-02-25". The document includes a YAML header, a session setup block, and a code chunk for installing packages. The code is as follows:

```
1 ---
2 title: "Hands on Exercise Reproducible Work"
3 author: "Xavier"
4 date: "2023-02-25"
5 output: html_document
6 ---
7 
8 {r setup, include=FALSE}
9 knitr::opts_chunk$set(echo = TRUE)
10 
11 
12 # Session Reproducible Work
13 
14 Monday Feb 27, 2023. IL3-UB.
15 
16 Related to: <https://seeds4c.org/reproduciblework2023>
17 
18 ## Hands on Exercise
19 
20 {r}
```
- Environment:** Shows the loaded environment with files: .Rprofile, renv/, and renv.lock.
- Files:** Lists the project files and their sizes:

Name	Size
..	
.gitignore	48 B
.Rhistory	19.1 KB
project.Rproj	205 B
README.md	122 B
recipes	
renv.lock	13.5 KB
ReproducibleWork_HandsOnExer...	2.3 KB
renv	
.Rprofile	26 B
- Console:** Shows the output of the R session, including the installation of packages (tinytex, rmarkdown, tidyverse) and the message "Restarting R session...".

6.5.4. Use renv.lock recipe (iv) - finished

File Edit Code View Plots Session Build Debug Profile Tools Help

Go to file/function

Addins

R 3.4.4

ReproducibleWork_HandsOnExercise...

Source Visual

Outline

```

1 ---
2 title: "Hands on Exercise Reproducible Work"
3 author: "Xavier"
4 date: "2023-02-25"
5 output: html_document
6 ---
7
8 ```{r setup, include=FALSE}
9 knitr::opts_chunk$set(echo = TRUE)
10 ```
11
12 # Session Reproducible Work
13
14 Monday Feb 27, 2023. IL3-UB.
15
16 Related to: <https://seeds4c.org/reproduciblework2023>
17
18 ## Hands on Exercise
19
20 ```{r}
21 if (!require(readr)) {install.packages("readr")}
22 if (!require(dplyr)) {install.packages("dplyr")}
23
24 Hands on Exercise Reproducible Work

```

Environment History Connections Git

Staged Status Path

<input type="checkbox"/>	?	?	.Rprofile
<input type="checkbox"/>	?	?	ReproducibleWork_HandsOnExercise.R
<input type="checkbox"/>	?	?	data_smc.csv
<input type="checkbox"/>	?	?	data_smc.csv.bz2
<input type="checkbox"/>	?	?	data_subset_all.csv
<input type="checkbox"/>	?	?	data_subset_d5_wide.csv
<input type="checkbox"/>	?	?	renv/
<input type="checkbox"/>	?	?	renv.lock

Files Plots Packages Help Viewer

Cloud > project

	Name	Size
	..	
<input type="checkbox"/>	.gitignore	48 B
<input type="checkbox"/>	.Rhistory	19.1 KB
<input type="checkbox"/>	project.Rproj	205 B
<input type="checkbox"/>	README.md	122 B
<input type="checkbox"/>	recipes	
<input type="checkbox"/>	renv.lock	13.5 KB
<input type="checkbox"/>	ReproducibleWork_HandsOnExer...	2.3 KB
<input type="checkbox"/>	renv	
<input type="checkbox"/>	.Rprofile	26 B
<input type="checkbox"/>	data_smc.csv.bz2	50.2 MB
<input type="checkbox"/>	data_smc.csv	613.3 MB
<input type="checkbox"/>	data_subset_all.csv	61.3 MB
<input type="checkbox"/>	data_subset_d5_wide.csv	48.6 KB
<input type="checkbox"/>	ReproducibleWork_HandsOnExer...	2.8 KB

Console Terminal Background Jobs

R 3.4.4 · /cloud/project/

```

+ values_from = "VALOR_LECTURA")
>
> data_wide
> # Save resulting dataset to disk
> write_csv(data_wide, "data_subset_d5_wide.csv")
> # Produce a simple R version of this R Markdown document
> knitr::purl("ReproducibleWork_HandsOnExercise.Rmd", documentation=2)

processing file: ReproducibleWork_HandsOnExercise.Rmd

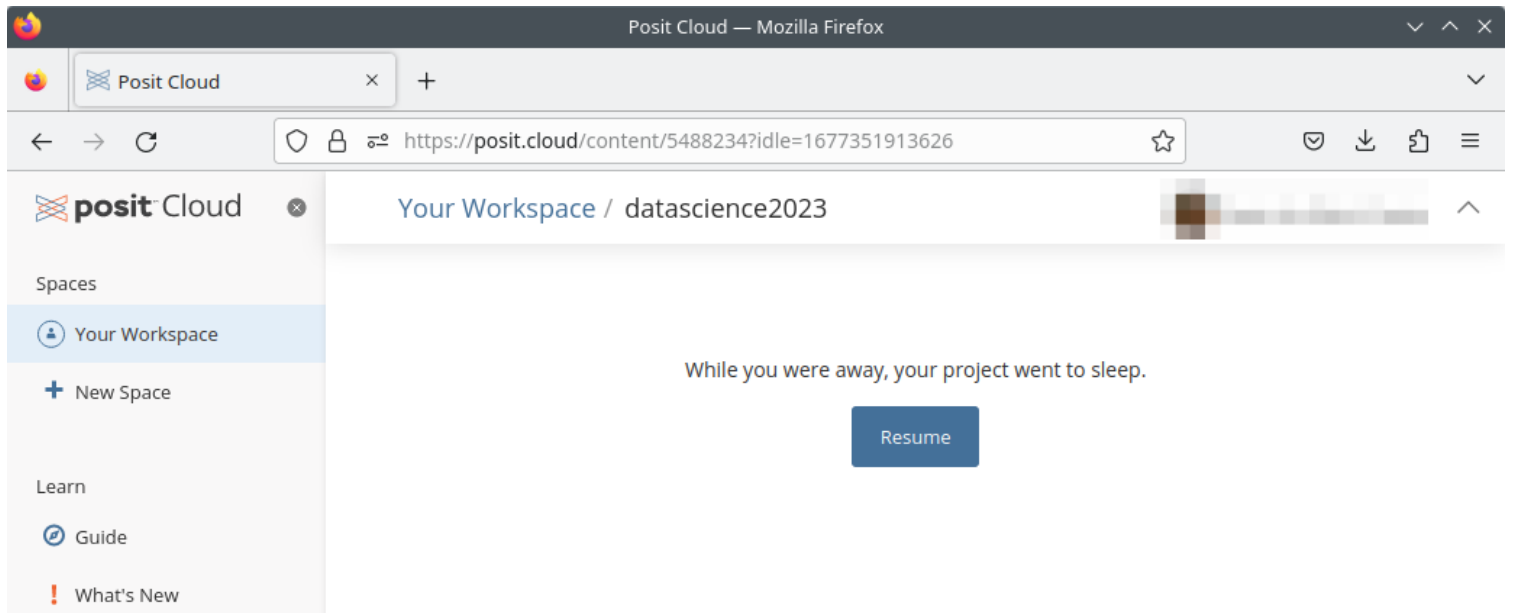
output file: ReproducibleWork_HandsOnExercise.R

[1] "ReproducibleWork_HandsOnExercise.R"
>

```

6.6. Additional info

Project (Container) goes to sleep on inactivity



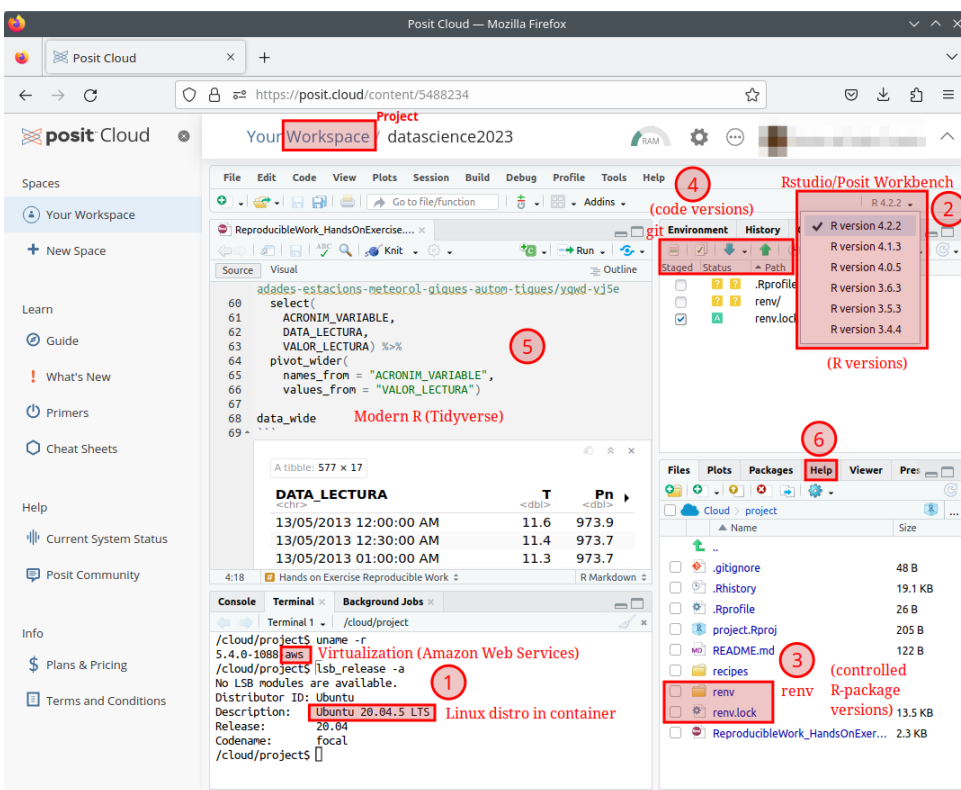
Thanks

Xavier de Pedro Puente,
Ph.D. -
xavier.depedro@seeds4c.org

Slides available at:
<https://seeds4c.org/reproduciblework2024>^[29]

^[30]

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- [1] <https://www.il3.ub.edu>
- [2] <https://seeds4c.org/reproduciblework2024>
- [3] <https://stackoverflow.com/questions/30492623/using-both-python-2-x-and-python-3-x-in-ipynotebook>
- [4] <https://posit.cloud>
- [5] <https://kubernetes.io/docs/concepts/overview/>
- [6] <https://rstudio.github.io/renv/articles/renv.html>
- [7] <https://solutions.posit.co/envs-pkgs/environments/>
- [8] <https://gitlab.com/radup/curs-r-introduccio/>
- [9] <https://gitlab.com/radup/curs-r-introduccio/-/tree/master/codi>
- [10] <https://gitlab.com/radup/curs-r-introduccio/-/raw/master/codi/10.compartir.via.git.pdf>
- [11] <https://seeds4c.org/git>
- [12] <https://solutions.posit.co/envs-pkgs/environments/>
- [13] <https://www.youtube.com/watch?v=VjDM-XsoHUQ>
- [14] <https://www.youtube.com/watch?v=Cn-72tbRNFc&t=79s>
- [15] <https://github.com/data-and-visualization/git-tutorial>
- [16] <https://www.youtube.com/watch?v=GrqM2VqlQ20>
- [17] <https://www.youtube.com/watch?v=yjIEblDevOs>
- [18] <https://rstudio.github.io/renv/>
- [19] <https://github.com/workflowr/workflowr>
- [20] <https://rstudio.github.io/learnr/>
- [21] <https://roxygen2.r-lib.org/>
- [22] <https://www.tidyverse.org/>
- [23] <https://posit.cloud/plans/free>
- [24] <https://blog.djnavarro.net/using-aws-s3-in-r>
- [25] <https://doi.org/10.1371/journal.pbio.2006930>

^[26] <https://posit.cloud/plans/free>

^[27] <https://gitlab.com/xavidp/datascience2023>

^[28] <https://cran.r-project.org/src/contrib/Archive/packageName/>

^[29] <https://seeds4c.org/reproduciblework2024>

^[30] <http://creativecommons.org/licenses/by-sa/3.0/>

^[31] <http://creativecommons.org/licenses/by-sa/3.0/>