

Machine Learning in R: Workshop Series

Structuring Data Projects

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1 Learning Objectives



This workshop should support you in optimizing your overall data science and machine learning workflow by setting up an RStudio project, conducting your analyses in an interactive notebook environment and maintaining local project libraries (so-called *virtual environments*).

More specifically, after this workshop you will

- › be familiar with the main features of RStudio projects (`.Rproj`) as well as the differences between absolute and relative directory paths,
- › know your way around R Markdown documents (`.Rmd`) and embrace R Notebooks as your primary tool for doing interactive data science and machine learning in R,
- › see the value in using local project environments to prevent dependency errors, promote collaboration, and ensure reproducibility.

2 Introduction to RStudio Projects



2 Introduction to RStudio Projects (.Rproj)

What is an RStudio project?

RStudio projects offer you a way to structure your data science projects and improve your workflow:

- › Keep all the files related to your data science project in a single place.
- › Stop working on one or multiple R scripts and return later to continue where you left.
- › Structure your project or analysis in a modular manner.
- › Easily share your whole project with collaborators.

R Studio Project

```
| README.md  
| main_script.R  
+ figures  
|   fig_01.PNG  
|   fig_02.PNG  
|   ...  
+ data  
|   raw_data.csv  
|   clean_data.rds  
+ scripts  
|   01_pkg_mgmt.R  
|   02_functions.R  
|   03_params.R  
|   04_analysis.R
```



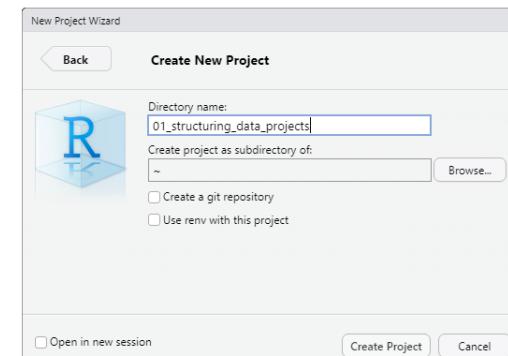
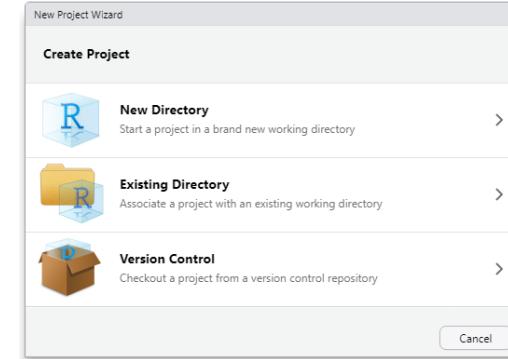
2 Introduction to RStudio Projects (.Rproj)

How do I create an RStudio project?

RStudio provides three ways of creating an **.Rproj** (*File -> New Project...*):

1. As a new file directory
2. As part of an existing file directory
3. By cloning a version control repository (e.g., from GitHub)

Here, I create a brand new directory, called **01_structuring_data_projects** in which I organize this presentation:





2 Introduction to RStudio Projects (.Rproj)

What happens when a new project is created?

- › RStudio creates a `.Rproj` file within the specified directory. This file contains certain project options and enables to open the RStudio project from your machine's filesystem (e.g., desktop).
- › RStudio creates a hidden directory (`.Rproj.user`) where project-related temporary files (e.g. auto-saved documents) are stored.
- › RStudio loads the `.Rproj` file and displays the project name on the far right side of the main toolbar.



2 Introduction to RStudio Projects (.Rproj)

What happens when a new project is created?

- › RStudio creates a `.Rproj` file within the specified directory. This file contains certain project options and enables to open the RStudio project from your machine's filesystem (e.g., desktop).
- › RStudio creates a hidden directory (`.Rproj.user`) where project-related temporary files (e.g. auto-saved documents) are stored.
- › RStudio loads the `.Rproj` file and displays the project name on the far right side of the main toolbar.

What happens when a new RStudio Project is opened?

- › A fresh R session is started.
- › The `.RData` file in the project directory is loaded (depending on the project options).
- › The `.Rhistory` file in the project directory is loaded into the *RStudio history pane*.
- › Previously edited scripts are restored.
- › The current *working directory* is set to the project directory (as specified upon creation, see [slide 6](#)).



2 Introduction to RStudio Projects (.Rproj)

Let's have a look at the project directory for this presentation (maintained as an `.Rproj`):

```
abs_path <- getwd()  
abs_path  
  
> [1] "C:/Users/.../workshops/01_structuring_data_projects"
```

This path is referred to as an **absolute path**. What files do we find under this path?

```
dir(abs_path)  
  
> [1] "01_rstudio_projects.Rmd"          "02_r_notebooks.Rmd"           "03_project_environments.Rmd"  
> [4] "custom"                           "demo"                      "img"  
> [7] "index.html"                      "index.Rmd"                 "libs"  
> [10] "README.md"                     "renv"                      "renv.lock"  
> [13] "slides"                          "structuring_data_projects.Rproj"
```

This is basically all the stuff required for rendering this presentation. Put differently: With an `.Rproj`, I organize all the files related to the project in one folder (e.g., script files, data sets, figures, manuscripts, etc.).



2 Introduction to RStudio Projects (.Rproj)

Instead of using `dir("C:/Users/.../workshops/01_structuring_data_projects")`, you should rather use `dir(".").` When specifying a path on your computer, the single dot (`.`) reflects a **relative path**, i.e. a path relative to your current working directory. Hence, `"."` again refers to:

```
> [1] "C:/Users/.../workshops/01_structuring_data_projects"
```



2 Introduction to RStudio Projects (.Rproj)

Instead of using `dir("C:/Users/.../workshops/01_structuring_data_projects")`, you should rather use `dir(".").` When specifying a path on your computer, the single dot (`.`) reflects a **relative path**, i.e. a path relative to your current working directory. Hence, `"."` again refers to:

```
> [1] "C:/Users/.../workshops/01_structuring_data_projects"
```

Now, let's assume you want to access `raw_data.txt` in the subfolder `data`, i.e. you search for this file under:

```
> [1] "C:/Users/.../workshops/01_structuring_data_projects/data"
```

What is the corresponding relative path when reading in the data?



2 Introduction to RStudio Projects (.Rproj)

Instead of using `dir("C:/Users/.../workshops/01_structuring_data_projects")`, you should rather use `dir(".").` When specifying a path on your computer, the single dot (`.`) reflects a **relative path**, i.e. a path relative to your current working directory. Hence, `."` again refers to:

```
> [1] "C:/Users/.../workshops/01_structuring_data_projects"
```

Now, let's assume you want to access `raw_data.txt` in the subfolder `data`, i.e. you search for this file under:

```
> [1] "C:/Users/.../workshops/01_structuring_data_projects/data"
```

What is the corresponding relative path when reading in the data?

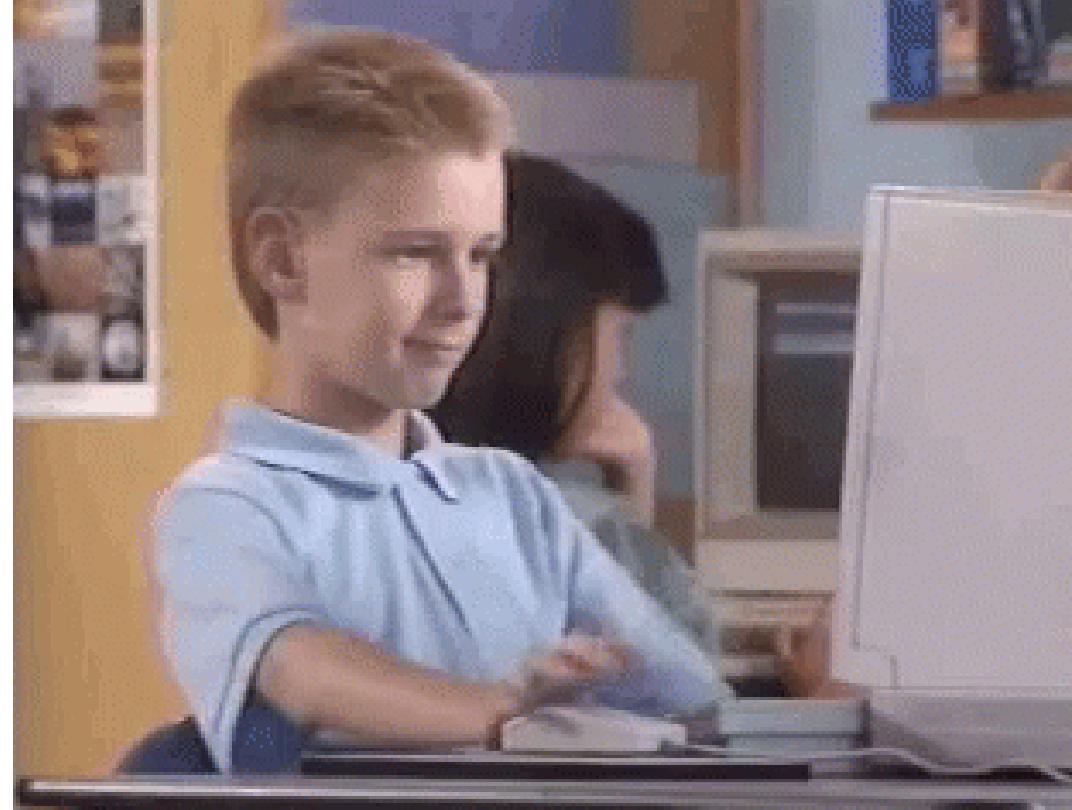
```
read.delim("./data/raw_data.txt", header = T, sep = ",")
```

The use of relative paths makes it very easy to navigate your project or share it with collaborators without having to adjust every path manually!

Note: If you want to step one folder up in the folder hierarchy, you may use two dots (`..`). When writing paths on Windows, use `/` instead of `\`, otherwise R interprets it as an escape character.



2 Introduction to RStudio Projects (.Rproj)





2 Introduction to RStudio Projects (.Rproj)

Project options: For each RStudio project you can specify a set of project-specific options (these override the set of global options). Access project options within RStudio by navigating to *Tools -> Project Options...*.

- › **Save workspace to .RData on exit:** Stores your current *global environment* (workspace resp. *RStudio environment pane*) in an `.RData`-file in your project directory when closing your RStudio project.

Note: Not recommended! You should always be able to recreate your global environment from your scripts. Hence, I would set this behavior of Rstudio to "never" (Tools -> Global Options...).

- › **Restore .RData into workspace at startup:** Loads your previously saved workspace from the `.RData` file into the *global environment*.
- › **Always save history:** Writes your code history (*RStudio history pane*) into an `.Rhistory` file located in your project directory.

3 R Markdown Documents

3 The Story So Far: R Scripts (.R)

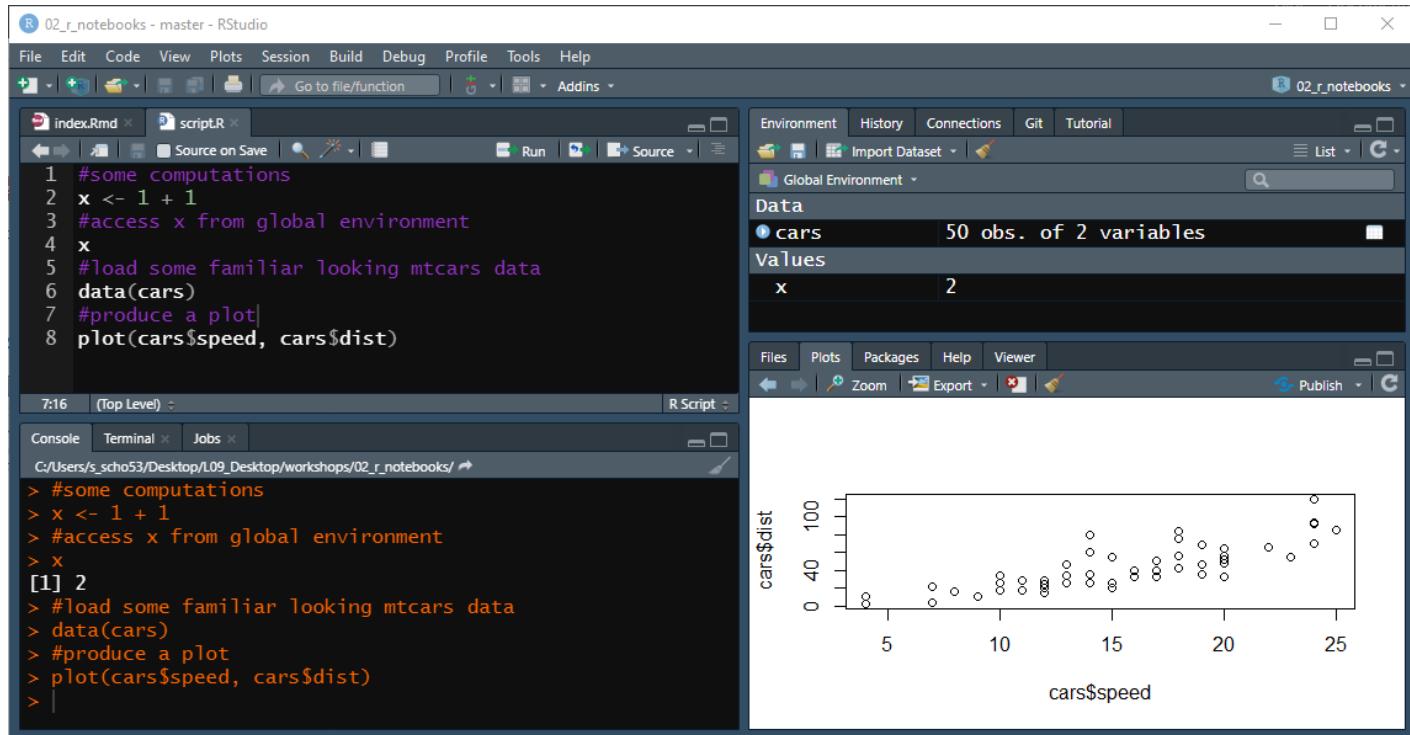
The screenshot shows the RStudio interface with the following components:

- File Bar:** File, Edit, Code, View, Plots, Session, Build, Debug, Profile, Tools, Help.
- Toolbar:** Source on Save, Run, Source.
- Project Bar:** 02_r_notebooks - master - RStudio.
- Script Editor:** Shows the content of `script.R` with the following code:

```
1 #some computations
2 x <- 1 + 1
3 #access x from global environment
4 x
5 #load some familiar looking mtcars data
6 data(cars)
7 #produce a plot
8 plot(cars$speed, cars$dist)
```
- Console:** Shows the output of running the script:

```
> #some computations
> x <- 1 + 1
> #access x from global environment
> x
[1] 2
> #load some familiar looking mtcars data
> data(cars)
> #produce a plot
> plot(cars$speed, cars$dist)
> |
```
- Data View:** Shows the `cars` dataset with 50 observations of 2 variables. The variable `x` has a value of 2.
- Plots View:** Displays a scatter plot of `cars$dist` versus `cars$speed`. The x-axis ranges from 5 to 25, and the y-axis ranges from 0 to 100. The plot shows a positive correlation between speed and distance.

3 The Story So Far: R Scripts (.R)



With R scripts (.R), a report of your analysis must be drawn separately from your code (e.g., in MS Word) while collecting all plots and results you have previously written to file (e.g., .PNG or .csv). More importantly, each change of the code requires a whole review of the report! 😞



3 R Markdown Documents (.Rmd)

The `rmarkdown` package:

- › Markdown-based authoring framework for data science
- › Intertwine R code and plain text in one document
- › Generate high-quality reports from .Rmd-files

Document elements:

- › Header
- › Text body
- › Code & output

Note: The different document elements apply to R Markdown Documents (.Rmd-files) and do not appear in common R Scripts (.R-files).



[What is R Markdown?](#) from [RStudio, Inc.](#) on Vimeo.



3 R Markdown Documents (.Rmd)

3.1 The Header

The **YAML header** appears at the top of each `.Rmd` document. It contains a bunch of metadata as well as formatting options for your final report. The syntax for the header is based on [YAML](#).

```
---
```

```
title: "Rmarkdown Demo"      #Title/headline of your markdown report
author: John Doe              #Name of the author
date: 2020-11-02              #Date of the report
output:
  html_document:
    toc: true                 #Output format
    toc_float: true           #Table of contents (toc)
    toc_depth: 2              #Floating toc on the left side of the document
    #Depth of headers to generate toc
---
```



3 R Markdown Documents (.Rmd)

3.2 The Text Body

You can write plain text,

in *italics* or in **bold**,

and use S^{uperscript} or S_{ubscript}.

You can format text as `fancy R code` ,

and even embed LaTeX equations:

```
$$
x_{1/2} = -\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 - q}
$$
```

You can write plain text,

in *italics* or in **bold**,

and use Superscript or Subscript.

You can format text as fancy R code,

and even embed LaTeX equations:

$$x_{1/2} = -\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 - q}$$



3 R Markdown Documents (.Rmd)

3.2 The Text Body

```
# You can use headers (H1)
```

You can use headers (H1)

```
## You can use headers (H2)
```

You can use headers (H2)

```
### You can use headers (H3)
```

You can use headers (H3)



3 R Markdown Documents (.Rmd)

3.2 The Text Body

> You can highlight quotes,

| You can highlight quotes,

embed [Hyperlinks](url),

embed [Hyperlinks](#),

or include images: ,

or include images:



,



3 R Markdown Documents (.Rmd)

3.2 The Text Body

- You can
 - create
 - an unordered
 - list
 - of items
1. Or even
 2. better
 3. you create an ordered list
 1. which should
 2. also look
 1. familiar!

And finally, since we are in an academic context you might also want to use some footnotes.^[^1]

[^1]: *Note: Find more information about the `rmarkdown` syntax by consulting the official [cheat sheet](url).*

And finally, since we are in an academic context you might also want to use some footnotes.¹

[1] Note: Find more information about the `rmarkdown` syntax by consulting the official [cheat sheet](#).



3 R Markdown Documents (.Rmd)

3.3 Code Chunks & Output

Code Chunks: Self-contained part of your R code for which, upon code evaluation, the output of your code is shown directly below the chunk instead of in your console or the *RStudio viewer* or the *plots pane*.

```
14 ````{r fibonacci, warning=F}
15 fib <- function(n) {
16   x <- numeric(n)
17   x[1:2] <- c(1,1)
18   for(i in 3:n) {
19     x[i] = x[i-1] + x[i-2]
20   }
21   return(x)
22 }
23
24 Sys.sleep(5)
25
26 fib(10)
27 ````
```

[1] 1 1 2 3 5 8 13 21 34 55

Creating code chunks:

Using the *insert* button in the RStudio interface  **Insert**, or via the keyboard shortcut: *Ctrl + Alt + I*.

Note: In fact, code chunks even allow you to write and evaluate code in other languages, such as Python, SQL or C++.

3 R Markdown Documents (.Rmd)



3.3 Live Demo

02 : 00



3 R Markdown Documents (.Rmd)

3.3 Code Chunks & Output

Chunk Options: Can be set as boolean (`True`/`False`) arguments in the chunk header `{r ...}`.

Argument	Description
<code>include=F</code>	Code and Output does not appear in the final report (yet, code is still evaluated).
<code>eval=F</code>	Output does not appear in the final report as the code is not evaluated.
<code>result=F</code>	Output does not appear in the final report but the code is evaluated.
<code>echo=F</code>	Code does not appear in the final report.
<code>message=F</code>	Messages generated by the code do not appear in the final report.
<code>warning=F</code>	Warnings generated by the code do not appear in the final report.



3 R Markdown Documents (.Rmd)

3.4 Generating High-Quality Reports

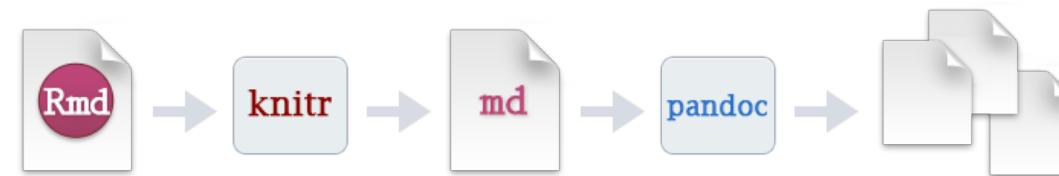
Render the `.Rmd` document into your desired output format by using `knitr:::render()` command from the `knitr` package or hit the *Knit* button in your RStudio toolbar.



3 R Markdown Documents (.Rmd)

3.4 Generating High-Quality Reports

Render the `.Rmd` document into your desired output format by using `knitr:::render()` command from the `knitr` package or hit the *Knit* button in your RStudio toolbar.



Workflow in the background:

1. `knitr` takes your `.Rmd`-file and converts it into a plain markdown file (`.md`).
2. The `.md`-file is processed by `pandoc` and converted into the final output format (e.g., PDF, HTML, Word).

Note: `knitr` can only convert your final `.Rmd`-file if your code is free of errors as `knitr` tries to run your entire code (so-called batch execution) as part of the conversion workflow!

3 R Markdown Documents (.Rmd)



4 Interactive Data Science



4 Interactive Data Science

4.1 Introduction to Computational Notebooks

Computational notebooks are virtual interfaces used for [Literate Programming](#). They combine features of word processors (e.g., MS Word) and the programming language kernel (e.g., the R shell which you find in the *RStudio console pane*).



4 Interactive Data Science

4.1 Introduction to Computational Notebooks

Computational notebooks are virtual interfaces used for [Literate Programming](#). They combine features of word processors (e.g., MS Word) and the programming language kernel (e.g., the R shell which you find in the *RStudio console pane*).

Features:

- › Interactivity
- › Iteration
- › Sharing & Communication
- › Transparency
- › Reproducibility



4 Interactive Data Science

4.1 Introduction to Computational Notebooks

This sounds pretty familiar after learning about R Markdown documents right?
So what is the R Notebook all about?



4 Interactive Data Science



4.2 R Markdown Documents vs. R Notebooks

Primarily, both formats are based on `.Rmd`-files:

- › An R Markdown document can be used as a computational notebook,
- › and an R Notebook can be rendered to other R Markdown document types (e.g., PDF, HTML, Word).

A notebook (in the `R` universe) can be viewed as a special version of a Markdown document (it is a special way of executing an R Markdown document).

4 Interactive Data Science



4.2 R Markdown Documents vs. R Notebooks

Primarily, both formats are based on `.Rmd`-files:

- › An R Markdown document can be used as a computational notebook,
- › and an R Notebook can be rendered to other R Markdown document types (e.g., PDF, HTML, Word).

A notebook (in the R universe) can be viewed as a special version of a Markdown document (it is a special way of executing an R Markdown document).

The use case is determined by your goal: generating high-quality reports with R Markdown documents vs. doing data science / machine learning using R Notebooks.

R Markdown documents:

- › Execution of the whole code before rendering (batch execution)
- › Requires code to be free of errors

R Notebooks:

- › Preview is simply a snapshot of your notebook (see `.nb.html`-file)
- › No R code is executed

4 Interactive Data Science



4.2 Live Demo

02 : 00

5 Project Environments

5 renv: Project Environments

5.1 Library Paths

Question: Where does R generally store my installed packages respectively loads them from?

5 renv: Project Environments

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Answer: Your user-specific *active library path*, i.e. from disk.

5 renv: Project Environments

5.1 Library Paths

Question: Where does R generally store my installed packages respectively loads them from?

Answer: Your user-specific *active library path*, i.e. from disk.

```
.libPaths()
```

```
> [1] "C:/Users/.../Documents/R/R-4.0.2/library"
```

5 renv: Project Environments

5.1 Library Paths

Question: Where does R generally store my installed packages respectively loads them from?

Answer: Your user-specific *active library path*, i.e. from disk.

```
.libPaths()
```

```
> [1] "C:/Users/.../Documents/R/R-4.0.2/library"
```

Packages are stored and loaded from the root installation folder (here for Windows operating systems). R crawls this path when loading (`library()`) or downloading (`install.packages()`) packages.

```
find.package("splines")
```

```
> [1] "C:/Users/.../Documents/R/R-4.0.2/library/splines"
```

5 `renv`: Project Environments

5.1 Library Paths

By default, this path is accessed each time you run a new `R` session or create a new `.Rproj`. Yet, the required version of a given package may vary across projects (e.g., depending on the project's start date):

- › Project A requires `dplyr 1.0.0`,
- › Project B requires `dplyr 0.8.1`, and
- › Project C requires the dev version of `dplyr`.

According to what you have learned, the three projects share the same mutual library path:

```
C:/Users/.../Documents/R/R-4.0.2/library
```

An upgrade or downgrade of the package version increases the chance that one of the projects does not work seamlessly any longer.



5 `renv`: Project Environments

5.2 Features of `renv`

R package for initializing and managing local project environments, i.e. collections of R packages utilized only within a certain `.Rproj`.

Isolated projects:

- › One local library of R packages per `.Rproj`
- › Upgrade/downgrade packages without breaking other projects

Portable projects:

- › Save the state of your project library in a `lockfile`
- › Share the `lockfile` with others and ensure compatibility

Reproducible projects:

- › Use `renv::snapshot()` to save the state of your project library
- › Use `renv::restore()` to restore the state of your project library as specified in the lockfile



5 `renv`: Project Environments

5.3 The `renv` Workflow

Step 1:

Set up `renv` by running `renv::init()` to initialize your local environment with a private library of R packages specific to your project.

Step 2:

Write some code, install, uninstall and update some packages.

Step 3:

Use `renv::snapshot()` to write the current state of your project library to the so-called *lockfile*.

Step 4:

Write some code, install, uninstall and update some packages.

Step 5:

Use `renv::restore()` to revert to the library state encoded in your *lockfile* in case you run into problems while working with updated packages.



5 renv: Project Environments

5.3 The renv Workflow: `renv::init()`

```
> install.packages("renv")
> renv::init()
```

Under the hood, `renv::init()` establishes the infrastructure to run your project-specific library. More specifically, the following files are written to and used by your `renv`-enabled projects:

File	Usage
.Rprofile	Used to activate renv whenever a new R session is launched within the project
renv.lock	The lockfile, defining the state of your project library
renv/activate.R	The activation script run by the project .Rprofile
renv/library	Your local project library



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv.lock`

The **lockfile** stores all information necessary to re-install the required packages, e.g., when sharing the project with a collaborator, archiving a project or putting code into productive use (*deployment*).

Packages can be downloaded from: [CRAN](#), [Bioconductor](#), [GitHub](#), [Gitlab](#), [Bitbucket](#).



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv.lock`

The **lockfile** stores all information necessary to re-install the required packages, e.g., when sharing the project with a collaborator, archiving a project or putting code into productive use (*deployment*).

Packages can be downloaded from: [CRAN](#), [Bioconductor](#), [GitHub](#), [Gitlab](#), [Bitbucket](#).

Exemplary lockfile entry in JSON format:

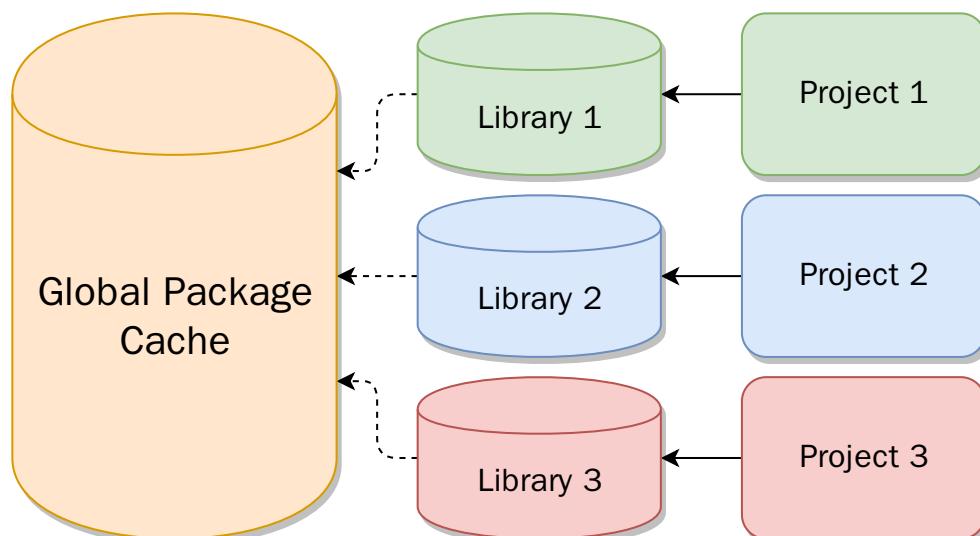
```
"renv": {  
  "Package": "renv",  
  "Version": "0.11.0",  
  "Source": "Repository",  
  "Repository": "CRAN",  
  "Hash": "1c3ef87cbb81c23ac96797781ec7aecc"  
}
```



5 renv: Project Environments

5.3 The renv Workflow: renv/library

renv links your project to a **global package cache** where all your downloaded packages are stored by renv. You can think of it as a repository that contains all package versions ever installed on your machine.



This approach avoids redundancies, if the same package version is used by multiple projects.

In this case, the installation of the respective package is stored in the global cache with renv simply creating a link to this cache within your project. This is what your local **project library** under the path `renv/library` is all about.

Picture by [Kevin Ushey](#).



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv/library`

Finally, if you now check your *active library path*, you can observe a new project-specific path (as well as an additional system library path which you need not consider further at this point).

```
.libPaths()
```

```
> [1] "C:/Users/.../01_structuring_data_projects/renv/library/R-4.0/x86_64-w64-mingw32"  
> [2] "C:/Users/.../AppData/Local/Temp/Rtmp0aVyVr/renv-system-library"
```



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv::snapshot()`

After having successfully set up our project-specific library, let's consider the two other main features of the `renv` package: `renv::snapshot()` and `renv::restore()`.

`renv::snapshot()` updates the lockfile by writing the current state of the project library to the lockfile.

```
renv::snapshot()
```



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv::snapshot()`

After having successfully set up our project-specific library, let's consider the two other main features of the `renv` package: `renv::snapshot()` and `renv::restore()`.

`renv::snapshot()` updates the lockfile by writing the current state of the project library to the lockfile.

```
renv::snapshot()
```

```
> The following package(s) will be updated in the lockfile:  
>  
> # CRAN =====  
> - glue      [1.4.0 -> 1.4.1]  
> - jsonlite   [1.6.0 -> 1.7.0]  
> - rmarkdown   [* -> 2.3]  
>  
> Do you want to proceed? [y/N]: y  
> * Lockfile written to 'C:/Users/.../01_structuring_data_projects/renv.lock'.
```



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv::restore()`

After having successfully set up our project-specific library, let's consider the two other main features of the `renv` package: `renv::snapshot()` and `renv::restore()`.

`renv::restore()` updates the project library by restoring the state of the project library as specified in the lockfile.

```
renv::restore()
```



5 `renv`: Project Environments

5.3 The `renv` Workflow: `renv::restore()`

After having successfully set up our project-specific library, let's consider the two other main features of the `renv` package: `renv::snapshot()` and `renv::restore()`.

`renv::restore()` updates the project library by restoring the state of the project library as specified in the lockfile.

```
renv::restore()
```

```
> The following package(s) will be updated:  
>  
> # CRAN =====  
> - rmarkdown    [* -> 2.3]  
> - stringr     [* -> 1.4.0]  
>  
> Do you want to proceed? [y/N]: y  
> Installing stringr [1.4.0] ... OK (copied cache)  
> Installing rmarkdown [2.3] ... OK (copied cache)
```



5 `renv`: Project Environments

5.4 Additional Remarks

A project is always bound to a particular version of `renv`. Updating the current version of the `renv` package should be done using the `renv::upgrade()` command.

When setting up `renv` for an existing project, it crawls all project scripts and searches for packages that are mentioned in your code via `renv::dependencies()`. For this presentation, I relied, among others, on the following packages (note that packages are only identified if mentioned in the code by namespace):

```
head(renv::dependencies(), 5)
```

```
> Finding R package dependencies ... Done!  
>  
> 1 C:/Users/s_scho53/.../01_rstudio_projects.Rmd  
> 2 C:/Users/s_scho53/.../01_rstudio_projects.Rmd  
> 3 C:/Users/s_scho53/.../01_rstudio_projects.Rmd  
> 4 C:/Users/s_scho53/.../01_rstudio_projects.Rmd  
> 5 C:/Users/s_scho53/.../02_r_notebooks.Rmd
```

Source	Package
rmarkdown	knitr
knitr	knitr
knitr	rmarkdown

Additional Resources

RStudio Support (2020): Using Projects. URL: <https://support.rstudio.com/hc/en-us/articles/200526207-Using-Projects>.

Wickham, H./Grolemund, G. (2017): R for Data Science: Visualize, Model, Transform, Tidy, and Import Data. URL: <https://r4ds.had.co.nz/workflow-projects.html>, chapter 8 (Workflow: projects).

RStudio (2020): Introduction to Rmarkdown. URL: <https://rmarkdown.rstudio.com/lesson-1.html>.

Xie, Y./Allaire, J.J./Grolemund, G. (2020): R Markdown: The Definitive Guide. URL: <https://bookdown.org/yihui/rmarkdown/>, chapter 2 (Basics) and 3 (Documents).

Ushey, K. (2020): renv: Project Environments for R. URL: <https://kevinushey-2020-rstudio-conf.netlify.app/slides.html#1>.

Ushey, K. (2020): Introduction to renv. URL: <https://rstudio.github.io/renv/articles/renv.html>.