Advanced R Programming - Lecture 3

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(slides based on Leif Jonsson's and Måns Magnusson's)

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Today

Scientific Computing: Best Practices

R packages

Git and GitHub

Creating R packages

Documentation with ROxygen

Unit testing with testthat

R-Studio debugger

Questions since last time?

Scientific Computing: Best Practices

Based on the article referred to on course page...

Write code for people

1. Write code for people
   1.1 A program should not require its readers to hold more than a handful of facts in memory at once
   1.2 Make names consistent, distinctive, and meaningful (Hungarian notation)
   1.3 Make code style and formatting consistent
       - camelCase
       - PascalCase
       - snake_case (Python: lower_case_with_underscores)
       - kebab-case
       - *avoid* dot.case

Let the computer do the work

2. Let the computer do the work
   - 2.1 Make the computer repeat tasks
   - 2.2 Save recent commands in a file for re-use (use `.Rhistory` file)
   - 2.3 Use a build tool to automate workflows

Make incremental changes

3. Make incremental changes
    3.1 Work in small steps with frequent feedback and course correction
    3.2 Use a version control system
    3.3 Put everything that has been created manually in version control

Do not repeat yourself (or others)

4. Do not repeat yourself (or others)
   - 4.1 Every piece of data must have a single authoritative representation in the system
   - 4.2 Modularize code rather than copying and pasting
   - 4.3 Re-use code instead of rewriting it

Plan for mistakes

5. Plan for mistakes
   - 5.1 Add assertions to programs to check their operation
   - 5.2 Use an off-the-shelf unit testing library
   - 5.3 Turn bugs into test cases
   - 5.4 Use a symbolic debugger

   - 5.5 **ALWAYS CHECK CORRECTNESS OF INPUT!** (also on exam ...)

Optimize software only after it works correctly

6. Optimize software only after it works correctly
   - 6.1 Use a profiler to identify bottlenecks
   - 6.2 Write code in the highest-level language possible

But prepare code for optimal algorithm . . .

Document design and purpose, not mechanics

7. Document design and purpose, not mechanics
   - 7.1 Document interfaces and reasons, not implementations (but make sure that you are able to understand implementation)
   - 7.2 Refactor code in preference to explaining how it works
   - 7.3 Embed the documentation for a piece of software in that software

Collaborate

8. Collaborate
   - 8.1 Use pre-merge code reviews
   - 8.2 Use pair programming when bringing someone new up to speed and when tackling particularly tricky problems
   - 8.3 Use an issue tracking tool

R packages

An environment with functions and/or data

The way to share code and data

4 000 developers (date?)
$\approx$ 11100 packages (as of 19 July 2017)
nearly 12500 packages (as of 4 May 2018)
18428 packages (as of 15 August 2022) according to CRAN

```
available.packages(available_packages_filters = c("CRAN"))
```

Package basics

Usage

`library()`

`::`

`:::`

Installation

`install.packages()`

`devtools::install_github()`

`devtools::install_local()`

Package namespace

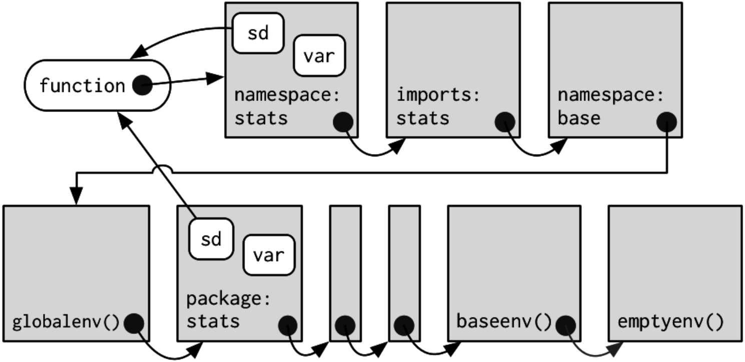

Figure: Package namespace (H. Wickham p.136)

Package namespace

`library()`: **ATTACHES** a package, its functions are available in the search path
`requireNamespace()`: **LOADS** package's code, data, methods, etc., runs `onLoad()`. Package is available in memory but not in search path, package **not** attached, acccess its components by `::`

NEVER use `library()`, `require()` inside your package, CRAN forbids it

H. Wickham, R packages (p. 82–84)

Which are good packages

Examine the package

1. Who?
2. When updated?
3. In development?

Why Version Control?

When working alone, we just might manage our work the way we each prefer. But things can get hairy when we must collaborate:

1. Imagine you and a colleague writing different modules of a software. You changed something this morning that your colleague was expecting to remain unchanged. 🤯
2. An important stakeholder doesn't link a recent change and wants your team to rollback. Have you stored previous versions? Can you retrieve them easily?
3. Your main server just crashed. Do you have backup?
4. Version Control is ubiquitous. IOW, your **recruiter** probably wants you to have Version Control skills.

Version Control: What is it exactly?

Hear from a professional!

https://vimeo.com/41027679

Why Git?

1. Simple to use
2. Distributed
   - No single copy of the work product (it's distributed!)
   - Each collaborator has all the files and change history
3. Fast
4. Common in practice
5. R packages uses GitHub
6. Integrated with R-Studio

Why Git?

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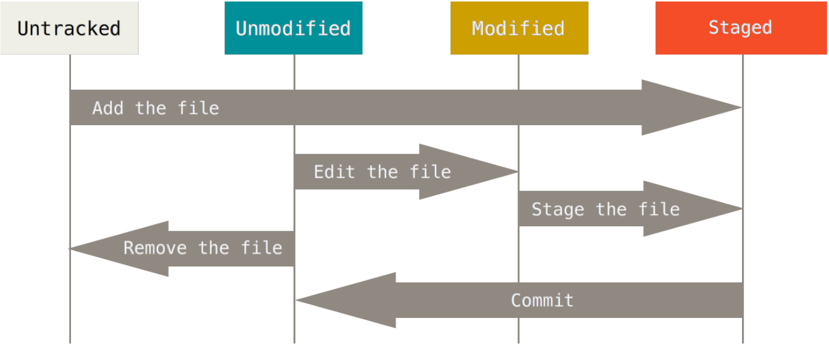
Created by Linus Torvalds! ;)

Git: Getting Started & Basics

The Lifecycle of Files on Git

Source: Pro Git, a book by Chacon and Straub



Chapters 1 & 2 of the book are highly recommended if you are new to Git!

Git: Getting Started & Basics

1. A repository (repo) is basically where the files of your project will reside
2. Any file that have only just been created will, by default, be ‘untracked’
3. To track a file (which you must do if you want to share it, for instance, with your collaborators), ‘add’ it to the repo
4. ‘Commit’ an added file to save it in the repo; when a file is committed, its state will change to ‘unmodified’
5. To edit an ‘unmodified’ file, you (collaborators) can access a copy of the file and perform edits; this will chage the file’s state to ‘modified’
6. To save your edits, stage and commit the file again

GitHub

1. Local (commit)
2. Remote (push/pull)
3. Barebone homepage (using md)
4. Collaborations
5. Issue tracker / Wiki / discussions

Public and private repos

Student accounts

Merge conflicts

1. Competing commits from different contributors.
2. Git cannot resolve this by itself
3. Manually resolve.

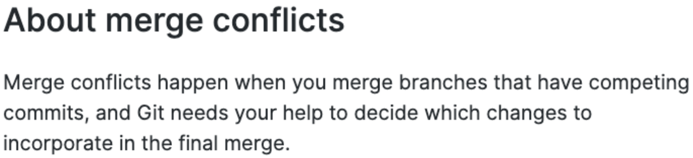
4. Supporting merge tools.
   4.1 `p4merge`
   presentation by Agustín Valencia and Marcos Mourao
   4.2 `sublime merge`
   `https://www.sublimemerge.com/`

Setting p4merge as diff/merge tool for git

Agustín Valencia

Marcos Mourao

The merge issue



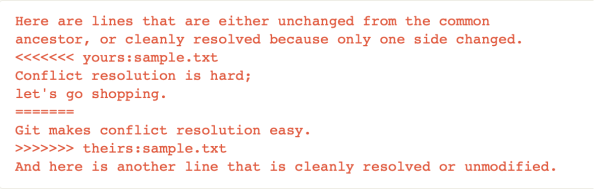
About merge conflicts

Merge conflicts happen when you merge branches that have competing commits, and Git needs your help to decide which changes to incorporate in the final merge.

Source : https://help.github.com/en/articles/about-merge-conflicts

Git way to solve merge conflicts

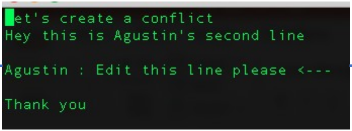
- Open the conflicting file in a text editor.
- Conflict markers:



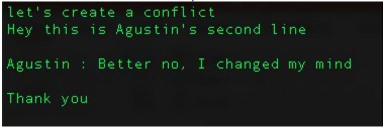
```
Here are lines that are either unchanged from the common
ancestor, or cleanly resolved because only one side changed.
<<<<<<< yours:sample.txt
Conflict resolution is hard;
let's go shopping.
=======
Git makes conflict resolution easy.
>>>>>>> theirs:sample.txt
And here is another line that is cleanly resolved or unmodified.
```

- Manually delete the conflict markers and choose which version (or both) to maintain in your file.

Source: https://git-scm.com/docs/git-merge

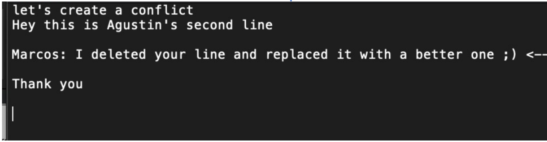


```
let's create a conflict
Hey this is Agustin's second line

Agustin : Edit this line please <---

Thank you
```



```
let's create a conflict
Hey this is Agustin's second line

Agustin : Better no, I changed my mind

Thank you
```

Agustín: commit

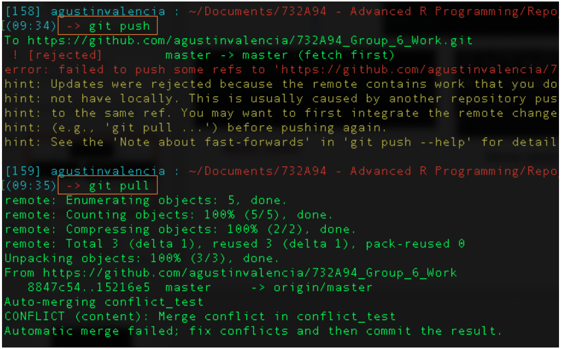


```
let's create a conflict
Hey this is Agustin's second line

Marcos: I deleted your line and replaced it with a better one ;) <--

Thank you

|
```

Marcos: commit & push

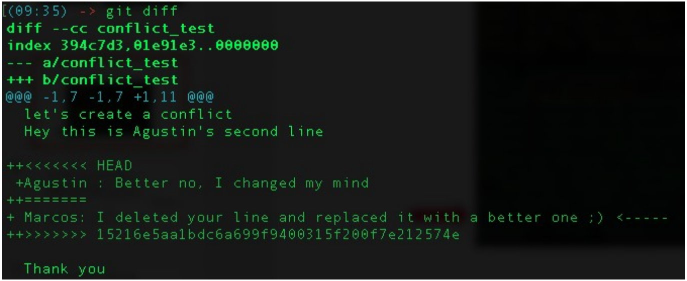
Try to push → **CONFLICT !**

Trying to push an outdated file



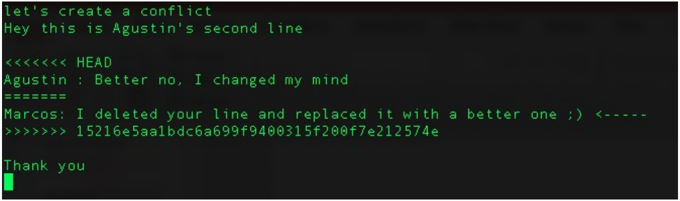
```
[158] agustinvalencia : ~/Documents/732A94 - Advanced R Programming/Repo
[(09:34) -> git push
To https://github.com/agustinvalencia/732A94_Group_6_Work.git
 ! [rejected]        master -> master (fetch first)
error: failed to push some refs to 'https://github.com/agustinvalencia/7
hint: Updates were rejected because the remote contains work that you do
hint: not have locally. This is usually caused by another repository pus
hint: to the same ref. You may want to first integrate the remote change
hint: (e.g., 'git pull ...') before pushing again.
hint: See the 'Note about fast-forwards' in 'git push --help' for detail

[159] agustinvalencia : ~/Documents/732A94 - Advanced R Programming/Repo
[(09:35) -> git pull
remote: Enumerating objects: 5, done.
remote: Counting objects: 100% (5/5), done.
remote: Compressing objects: 100% (2/2), done.
remote: Total 3 (delta 1), reused 3 (delta 1), pack-reused 0
Unpacking objects: 100% (3/3), done.
From https://github.com/agustinvalencia/732A94_Group_6_Work
   8847c54..15216e5  master     -> origin/master
Auto-merging conflict_test
CONFLICT (content): Merge conflict in conflict_test
Automatic merge failed; fix conflicts and then commit the result.
```

Git diff



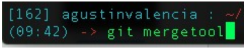
```
[(09:35) -> git diff
diff --cc conflict_test
index 394c7d3,01e91e3..0000000
--- a/conflict_test
+++ b/conflict_test
@@@ -1,7 -1,7 +1,11 @@@
  let's create a conflict
  Hey this is Agustin's second line

++<<<<<<< HEAD
 +Agustin : Better no, I changed my mind
++=======
+ Marcos: I deleted your line and replaced it with a better one ;) <-----
++>>>>>>> 15216e5aa1bdc6a699f9400315f200f7e212574e

  Thank you
```

How the file looks now

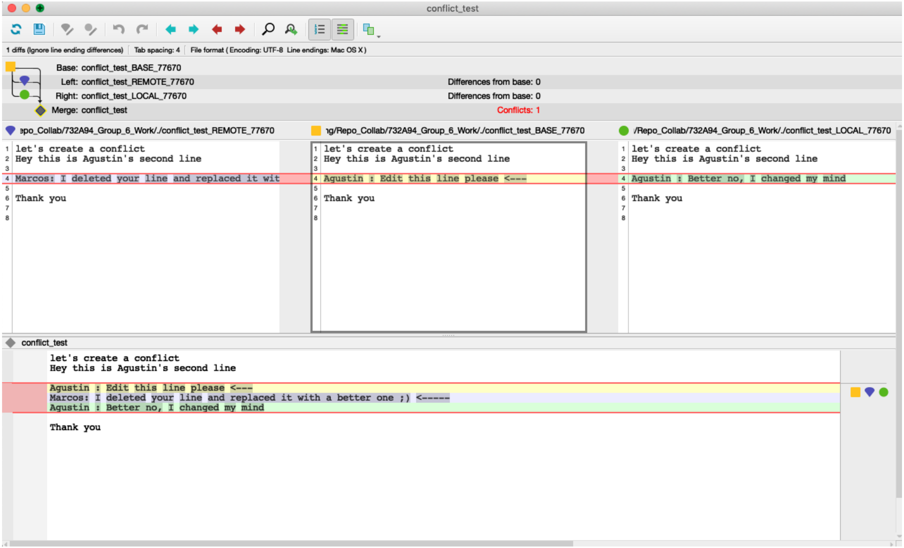


```
let's create a conflict
Hey this is Agustin's second line

<<<<<<< HEAD
Agustin : Better no, I changed my mind
=======
Marcos: I deleted your line and replaced it with a better one ;) <-----
>>>>>>> 15216e5aa1bdc6a699f9400315f200f7e212574e

Thank you
```

How we did it



```
[162] agustinvalencia : ~/
(09:42) -> git mergetool
```



conflict_test

1 diffs (Ignore line ending differences) | Tab spacing: 4 | File format (Encoding: UTF-8 Line endings: Mac OS X)

Base: conflict_test_BASE_77670
Left: conflict_test_REMOTE_77670 — Differences from base: 0
Right: conflict_test_LOCAL_77670 — Differences from base: 0
Merge: conflict_test — Conflicts: 1

epo_Collab/732A94_Group_6_Work/./conflict_test_REMOTE_77670

```
let's create a conflict
Hey this is Agustin's second line

Marcos: I deleted your line and replaced it wit

Thank you
```

ng/Repo_Collab/732A94_Group_6_Work/./conflict_test_BASE_77670

```
let's create a conflict
Hey this is Agustin's second line

Agustin : Edit this line please <---

Thank you
```

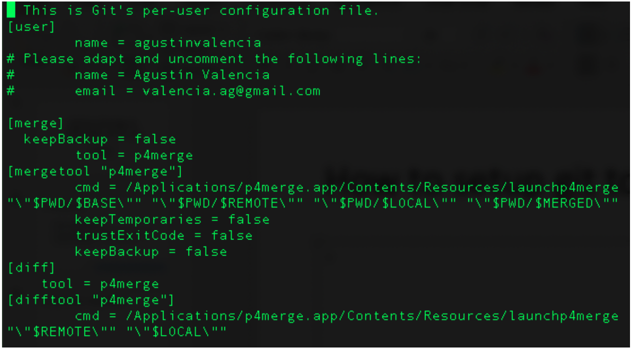
/Repo_Collab/732A94_Group_6_Work/./conflict_test_LOCAL_77670

```
let's create a conflict
Hey this is Agustin's second line

Agustin : Better no, I changed my mind

Thank you
```

conflict_test

```
let's create a conflict
Hey this is Agustin's second line

Agustin : Edit this line please <---
Marcos: I deleted your line and replaced it with a better one ;) <-----
Agustin : Better no, I changed my mind

Thank you
```

How to setup git to use p4merge



```
█ This is Git's per-user configuration file.
[user]
        name = agustinvalencia
# Please adapt and uncomment the following lines:
#       name = Agustín Valencia
#       email = valencia.ag@gmail.com

[merge]
  keepBackup = false
        tool = p4merge
[mergetool "p4merge"]
        cmd = /Applications/p4merge.app/Contents/Resources/launchp4merge
"\"$PWD/$BASE\"" "\"$PWD/$REMOTE\"" "\"$PWD/$LOCAL\"" "\"$PWD/$MERGED\""
        keepTemporaries = false
        trustExitCode = false
        keepBackup = false
[diff]
    tool = p4merge
[difftool "p4merge"]
        cmd = /Applications/p4merge.app/Contents/Resources/launchp4merge
"\"$REMOTE\"" "\"$LOCAL\""
```

.gitconfig file

Source : https://gist.github.com/SeanSSDing/d56d8b8aa4c79a05939b9ad3a6a63c8f

Why part of the course?

Writing performant code (best practice)
The way to collaborate (R ecosystem)
Combine code, data and analysis
Easy to distribute and reuse (public api)

Learn how to reuse code from other packages

Package structure

Package structure

```
DESCRIPTION
```

DESCRIPTION: Imports, Suggests, Depends **(LABS!!)**

Your package will nearly always use functions from other packages!

Imports: These packages have to be present (or installed) when your package is installed. However, attaching your package `library(your package)` will **load** them (not attach). To use functions from them it is recommended to call them in your package as `packagename::function()`.

Suggests: Your package can use these functions, but does not require them, e.g. datasets, for tests, vignettes. Before using functions from them you need to check if they are available, `requireNamespace()`

Depends: Packages here will be **attached**. **NOT** recommended, heavy on the environment, CRAN has a limit on the number of packages in `Depends`. Can be used to specify version of `R`.

H. Wickham, R packages (p. 34–36, 84)

Package structure

```
DESCRIPTION
NAMESPACE
```

NAMESPACE **(LABS!!)**

What is used from other packages and provided to others!

`importFrom(package, function)`: package has to be listed in `DESCRIPTION`, do not `import(package)` (i.e. all) but only what you need. No need to call function as `package::function` now but **RECOMMENDED**

`export(function)`: what you make available for your users

`exportPattern(regular expression)`: make available functions with name matching a pattern, e.g. does not start with .

`S3method(method, class)`: export S3 methods

S4 classes, methods import and export **see book**

`useDynLib`: Import a function from C

H. Wickham, R packages (p. 84–90)

Imported functions (tips)

Do not call imported functions directly but through your own wrapper function.

1. Better control over what you pass: wrapper's interface.
2. Foreign package or function gets deprecated: change only in one place.

Use syntax `package::function()` for imported functions, as it makes code more clear and easier to update.

Package structure

```
DESCRIPTION
NAMESPACE
R/
```

Package structure

```
DESCRIPTION
NAMESPACE
R/
man/
```

Package structure

```
DESCRIPTION
NAMESPACE
R/
man/
vignette/
```

Package structure

```
DESCRIPTION
NAMESPACE
R/
man/
vignette/
tests/
```

Package structure

```
DESCRIPTION
NAMESPACE
R/
man/
vignette/
tests/
data/
```

Package structure

```
DESCRIPTION
NAMESPACE
R/
man/
vignette/
tests/
data/
scr/
```

Package structure

```
DESCRIPTION
NAMESPACE
R/
man/
vignette/
tests/
data/
scr/
inst/
```

Why roxygen2?

R requires that package documentation be stored in **.Rd** files in the `man/` folder. These files must conform to a number of specs, which may be tedious to accomplish manually.

Enter **roxygen2**: package elements can be documented in **.R** files (in the `R/` folder), and roxygen2 will generate the `man/` files.

Remember:

1. **roxygen2** is no free-lunch, but it does simplify documentation; importantly, it help manage the package NAMESPACE
2. Having docs near code can help with writing performant code
3. **roxygen2** is similar to JavaDoc & DOxygen, which are widely adopted standards for documenting Java & C++ packages

roxygen2: Workflow and Syntax

Standard Workflow:

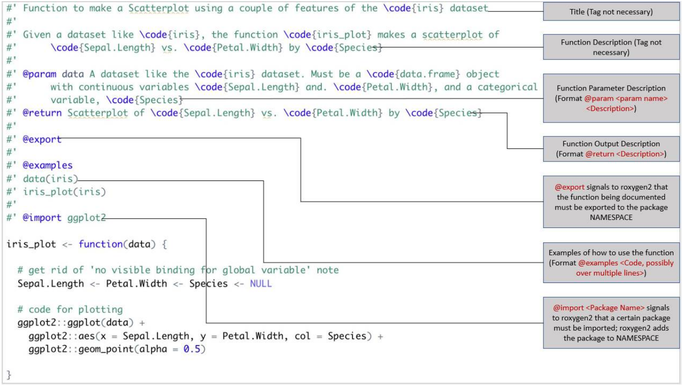
1. Add comments to .R files (see Syntax below)
2. Run the command `devtools::document()`
3. Preview documents and repeat above steps if/as needed

Generic Syntax:

1. All roxygen2 comments must begin with the token `#!`
2. These must be placed **before** the function code
3. Most (if not all) such comments must be written out as tags; each tag must be in the `@tagnames details` format.
4. roxygen2 requires that specific elements of a function/dataset/class be documented by means of specific tags; see link below for details.

Source: `https://r-pkgs.org/man.html`

roxygen2: Example I



```
#' Function to make a Scatterplot using a couple of features of the \code{iris} dataset
#'
#' Given a dataset like \code{iris}, the function \code{iris_plot} makes a scatterplot of
#'     \code{Sepal.Length} vs. \code{Petal.Width} by \code{Species}
#'
#' @param data A dataset like the \code{iris} dataset. Must be a \code{data.frame} object
#'     with continuous variables \code{Sepal.Length} and. \code{Petal.Width}, and a categorical
#'     variable, \code{Species}
#' @return Scatterplot of \code{Sepal.Length} vs. \code{Petal.Width} by \code{Species}
#'
#' @export
#'
#' @examples
#' data(iris)
#' iris_plot(iris)
#'
#' @import ggplot2

iris_plot <- function(data) {

  # get rid of 'no visible binding for global variable' note
  Sepal.Length <- Petal.Width <- Species <- NULL

  # code for plotting
  ggplot2::ggplot(data) +
    ggplot2::aes(x = Sepal.Length, y = Petal.Width, col = Species) +
    ggplot2::geom_point(alpha = 0.5)

}
```

Title (Tag not necessary)

Function Description (Tag not necessary)

Function Parameter Description (Format @param <param name> <Description>)

Function Output Description (Format @return <Description>)

@export signals to roxygen2 that the function being documented must be exported to the package NAMESPACE

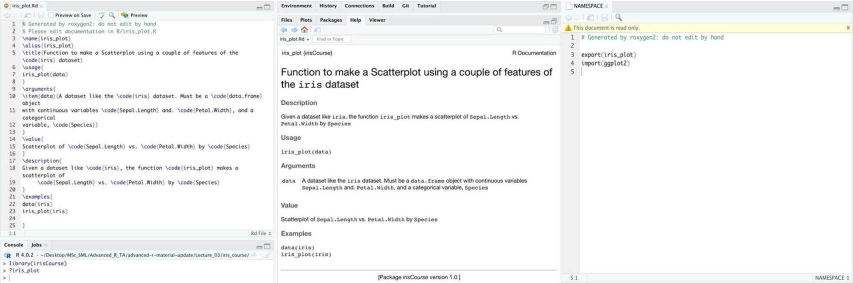
Examples of how to use the function (Format @examples <Code, possibly over multiple lines>)

@import <Package Name> signals to roxygen2 that a certain package must be imported; roxygen2 adds the package to NAMESPACE

Figure: Including roxygen2 compatible documentation

Source Code: ./iris_course/R/iris_plot.R

roxygen2: Example II



```
% Generated by roxygen2: do not edit by hand
% Please edit documentation in R/iris_plot.R
\name{iris_plot}
\alias{iris_plot}
\title{Function to make a Scatterplot using a couple of features of the
\code{iris} dataset}
\usage{
iris_plot(data)
}
\arguments{
\item{data}{A dataset like the \code{iris} dataset. Must be a \code{data.frame}
object
with continuous variables \code{Sepal.Length} and. \code{Petal.Width}, and a
categorical
variable, \code{Species}}
}
\value{
Scatterplot of \code{Sepal.Length} vs. \code{Petal.Width} by \code{Species}
}
\description{
Given a dataset like \code{iris}, the function \code{iris_plot} makes a
scatterplot of
    \code{Sepal.Length} vs. \code{Petal.Width} by \code{Species}
}
\examples{
data(iris)
iris_plot(iris)

}
```

```
R 4.0.2 · ~/Desktop/MSc_SML/Advanced_R_TA/advanced-r-material-update/Lecture_03/iris_course/
> library(irisCourse)
> ?iris_plot
> 
```

iris_plot {irisCourse} R Documentation

Function to make a Scatterplot using a couple of features of the `iris` dataset

Description

Given a dataset like `iris`, the function `iris_plot` makes a scatterplot of `Sepal.Length` vs. `Petal.Width` by `Species`

Usage

`iris_plot(data)`

Arguments

`data` A dataset like the `iris` dataset. Must be a `data.frame` object with continuous variables `Sepal.Length` and. `Petal.Width`, and a categorical variable, `Species`

Value

Scatterplot of `Sepal.Length` vs. `Petal.Width` by `Species`

Examples

```
data(iris)
iris_plot(iris)
```

[Package *irisCourse* version 1.0]

```
# Generated by roxygen2: do not edit by hand

export(iris_plot)
import(ggplot2)

```

Figure: `man` and `NAMESPACE` files automatically updated by roxygen2!

Source Code: `./iris_course/R/iris_plot.R`

Why unit testing?

Fewer bugs
Better code structure
Faster restarts
Robust code - correct a bug only once

A must in complicated projects!

One unit testing framework for R integrated with R-Studio is `testthat`

Types of testing

1. White box testing
2. Black box testing
3. Probabilistic testing

testthat: Workflow and Test File Structure

Workflow

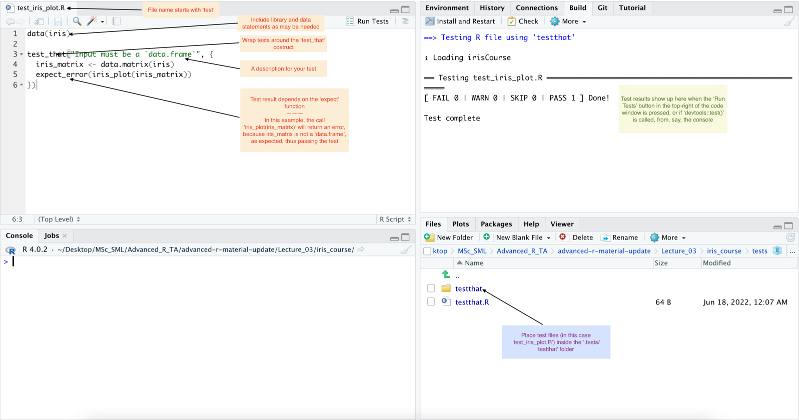
1. Setup the test framework with `usethis::use_testthat()`
2. Write out tests in .R files (viz. test files) and save them in the `tests/testthat/` folder (created through step 1 above) with filename starting with ‘test’ (for e.g. `test_myfun.R`)
3. Run tests with Ctrl/Cmd + Shift + T or `devtools::test()`

Test File Structure

1. As with usual .R scripts, test files must have `library`, `data` or similar statements if needed for the tests
2. Test files typically have ‘test groups’, which in turn have ‘expectations’, the atomic units of the `testthat` framework
3. For those familiar, note that the `context` statement is now deprecated

Source: `https://r-pkgs.org/tests-basics.html`; review this link for syntax details

Test File Example



```
data(iris)

test_that("Input must be a `data.frame`", {
  iris_matrix <- data.matrix(iris)
  expect_error(iris_plot(iris_matrix))
})
```

File name starts with 'test'

Include library and data statements as may be needed

Wrap tests around the 'test_that' costruct

A description for your test

Test result depends on the 'expect' function
— — —
In this example, the call 'iris_plot(iris_matrix)' will return an error, because iris_matrix is not a 'data.frame', as expected, thus passing the test

```
==> Testing R file using 'testthat'

ℹ Loading irisCourse

══ Testing test_iris_plot.R ════════════════════════════════════════════════
═════
[ FAIL 0 | WARN 0 | SKIP 0 | PASS 1 ] Done!

Test complete
```

Test results show up here when the 'Run Tests' button in the top-right of the code window is pressed, or if 'devtools::test()' is called, from, say, the console

```
R 4.0.2 · ~/Desktop/MSc_SML/Advanced_R_TA/advanced-r-material-update/Lecture_03/iris_course/
>
```

	Name	Size	Modified
	..		
□	testthat		
□	testthat.R	64 B	Jun 18, 2022, 12:07 AM

Place test files (in this case 'test_iris_plot.R') inside the '.tests/testthat' folder

Source Code: ./iris_course/tests/test_that/test_iris_plot.R

Introduction to Debugging in R

Another Video!!
Debugging in R
`https://vimeo.com/99375765`

REMEMBER
ALWAYS
CHECK INPUT!

The End... for today.

Questions?

See you next time!