Advanced Programming in R

Dries Debeer & Benjamin Becker

15. October 2021

Zurich R Courses

Introduction

Introduction

Who are we?

Dries Debeer

Senior Researcher at itec (imec research group at KU Leuven)

scDIFtest, permimp, eatATA, mstDIF

dries.debeer@kuleuven.be

Benjamin Becker

Researcher at IQB (Statistics Department)

eatGADS, eatDB, eatATA, pisaRT

b.becker@iqb.hu-berlin.de

Introduction

Who are you?

1. Occupation, employer?
2. Previous knowledge and experience
    - with R?
    - with other statistical software?
    - with other programming languages?
3. Specific interest/motivation for this workshop?

What do we expect from you?

You ...

- are a frequent R user (e.g. for data wrangling/analyses/plots)
- have a rough understanding of R as a programming language
  $\rightarrow$ e.g. you have already written some R functions yourself
- are interested in learning more about the intricacies of R

Goal of this workshop

A deeper dive into R as a Programming language

- Better understanding of how R works as a programming language
- Better understanding of how larger programming projects can/should be structured
- Practical Git skills
- Practical R package building skills

Agenda

- Scoping & Environments
- Functionals & Split-Apply Paradigm
- Object Orientation (S3)
- Packages & Version Controlling

Environments

Environments

Understanding environments is key to understanding how R behaves, how R finds stuff.

- Scoping
- Closures
- Namespaces

Environments

An environment = "a bag of objects".

It differs from a list with respect to four key points:

1. All elements have names
2. The elements do not have an order
3. Environments are not copied when modified
4. Each environment has an **enclosing environment**

Environments

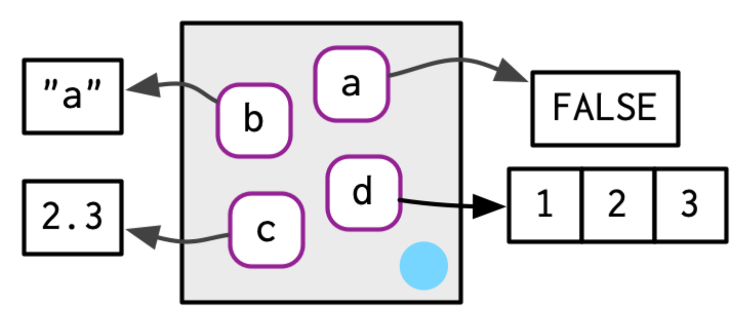
Each environment consists of two parts:

1. a **frame**: a collection of named objects.
    - the objects can be of any type (like in `lists`)
    - the objects have to be named (**unlike** in `lists`)
2. an **enclosing enviroment**: a reference or link to another environment.
    - the link goes in one direction
    - determines the search path

Environments - frame

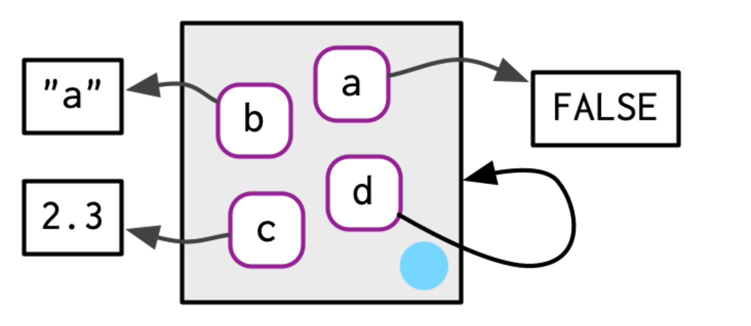
The frame is a “**bag**” of named objects.

- Actually, it is a bag of *bindings* between names and objects
- The combination *environment* + *name* points to a specific object (a location in memory)
- The names in the bag have no order



Environments - frame

An environment can containt itself!



Environments - Reference Semantics

How lists work:

```
original <- list(a = 15, b = "original", c = mean)
copy <- original
copy$b <- "new"
c(original$b, copy$b)

> [1] "original" "new"

original$a <- NULL
names(original)

> [1] "b" "c"
```

Environments - Reference Semantics

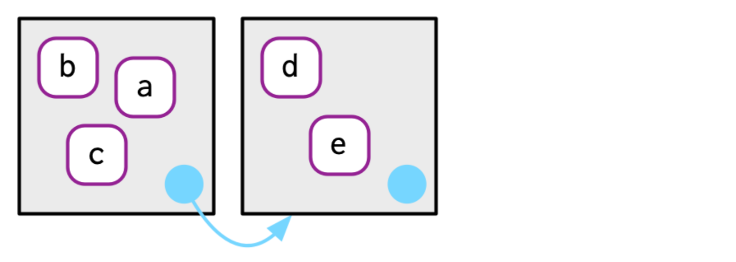
How environments work:

```
original <- rlang::env(a = 15, b = "original", c = mean)
copy <- original
copy$b <- "new"
c(original$b, copy$b)

> [1] "new" "new"

original$a <- NULL
names(original)

> [1] "a" "b" "c"
```

Environments - enclosing environment

The link is used for lexical scoping:

If the reference to an object is not found in the environment, R starts searching in the enclosing environment



- the link goes in **one** direction
- an environment has only one enclosing environment
- an environment can enclose multiple environments (but it is hard to find out if so, and which)

Exercises

Environments - scoping

`?exists` returns a logical if a reference is found in an environment. The search jumps to the enclosing environment until the object is found when `inherits = TRUE` (the default).

`?get` returns an object based on a name and an environment. The search jumps to the enclosing environment until the object is found when `inherits = TRUE` (the default).

`?assign` assigns an object to a name in an environment.

If the reference to an object is not found in the environment, R starts searching in the enclosing environment

Environments

Some important environments:

- the global environment (`.GlobalEnv` or `globalenv()`)
- the empty enviornment (`emptyenv()`)
- the `package`-environment
- the `namespace`-environment
- the `imports`-environment

Environments

The global enviroment

- the user's work space
- first item on the search path
- `.GlobalEnv` or `globalenv()`

The empty enviroment

- An “empty bag”
- last item on the search path
- has no enclosing environment
- `emptyenv()`

Search path

Where does R find objects *during interactive use*?

`?search()`

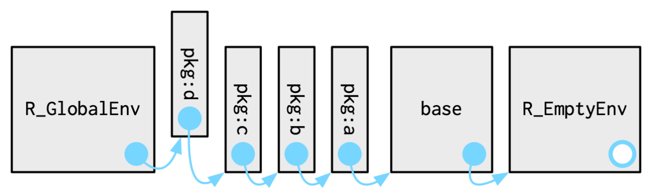
```
search()
```

```
>  [1] ".GlobalEnv"         "package:knitr"     "package:stats"
>  [4] "package:graphics"   "package:grDevices" "package:utils"
>  [7] "package:datasets"   "package:methods"   "Autoloads"
> [10] "package:base"
```

`package:<name>` environments have bindings to the exported objects (functions) of the package.

Search path

Where does R find objects *during interactive use*?



Newly attached packages get a specific place in the search path. They become the enclosing environment of the global environment, and they are enclosed by the previously attached package.

Environments and functions

Four environments are related to functions:

1. the environment that **binds** the function
2. the environment in which the body of the function is **executed**
3. the environment from which the function is **called**
4. the **enclosing** environment

Environments and functions

1. the environment that binds the function

`?find` (can be misleading)

`?pryr::where`

```
add_10 <- function(x) x + 10
find("add_10")

> [1] ".GlobalEnv"

find("sd")

> [1] "package:stats"
```

Environments and functions

1. the environment that binds the function

```
sd <- sd
find("add_10")

> [1] ".GlobalEnv"

find("sd")

> [1] ".GlobalEnv"    "package:stats"
```

One name can be used in different environments (for different objects).

Functions (objects) can have references in more than one environment!

Environments and functions

2. the environment in which the body is executed
`environment(NULL)`

```
get_executing_env <- function() environment()
get_executing_env()

> <environment: 0x0000000016f12640>

get_executing_env()  # always new

> <environment: 0x0000000017095f88>
```

The execution environment disappears when the body is executed.
Unless it becomes the enclosing environment of another function.

Environments and functions

3. the environment from which the function is called
`?parent.frame`

```
print_calling_env <- function() parent.frame()
print_calling_env()

> <environment: R_GlobalEnv>

other_fun <- function() print_calling_env()
other_fun()

> <environment: 0x000000001654d868>
```

3. the environment from which the function is called

This environment is often a execution environment of another function.

- To get the calling function use `?sys.call`.
- To get the complete call stack use `?sys.calls`.

Environments and functions

3. the environment from which the function is called

`?sys.calls`

```
print_calling_funs <- function() sys.calls()
print_calling_funs()
other_fun <- function() print_calling_funs()
other_fun()
```

Environments and functions

4. the enclosing environment

`environment(function)`

```
get_enclosing_env <- function() parent.env(environment())
get_enclosing_env()

> <environment: R_GlobalEnv>
```

Environments and functions

4. the enclosing environment `environment(function)`

```
make_adder <- function(add = 0) {
  print(environment())
  return(function(x) x + add)}
add_5 <- make_adder(5)

> <environment: 0x0000000016376c20>

environment(add_5)

> <environment: 0x0000000016376c20>
```

The execution environment disappears when the body is executed.
Unless it becomes the enclosing environment of another function

Environments and functions

4. the enclosing environment

When a function is created, the binding environment and the enclosing environment are typically equal. But the enclosing environment can be changed (using `environment <-`)

```
strange_mean <- function(x, ...) mean(x, ...)
strange_mean(1:3)

> [1] 2

env1 <- rlang::env(mean = function(x, ...) "Strange!")
environment(strange_mean) <- env1
strange_mean(1:3)

> [1] "Strange!"
```

Environments and functions

Four environments are related to functions:

1. the environment that **binds** the function
2. the environment in which the body of the function is **executed**
3. the environment from which the function is **called**
4. the **enclosing** environment

Where does R find stuff?

From *inside functions*?

1. the execution environment
2. the enclosing environment
3. the enclosing environment of that environment
4. ...
5. the empty environment

Where does R find stuff?

From inside functions *defined in the global environment*?

1. the executing environment
2. the global environment (i.e., the enclosing environment)
3. the `package:<name>` environment of the last attached package
4. ...
5. the empty environment

Where does R find stuff?

From inside functions *defined in packages*?

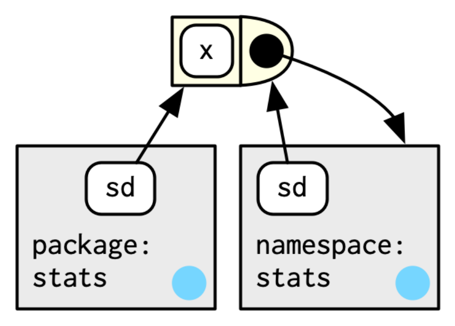
1. the executing environment
2. the `namespace:<name>` environment
3. the `imports:<name>` environment
4. the `namespace:base` environment
5. the global environment (i.e., the enclosing environment)
6. the `package:<name>` environment of the last attached package
7. ...
8. the empty environment

Where does R find stuff?

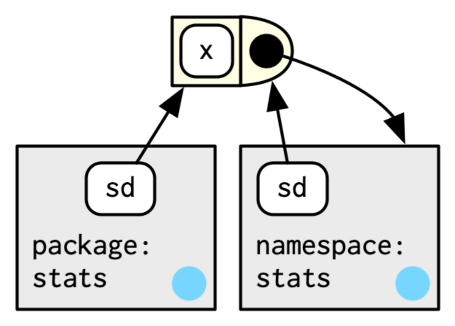
Exported functions from packages have two binding environments!

- the `namespace:<name>` environment
- the `package:<name>` environment

Both `::` and `:::` work.



Where does R find stuff?



But, only one enclosing environment: the `namespace:<name>` environment!

Thus, form inside a (package-) function, R first looks for imported and exported functions of that package!

Where does R find stuff?

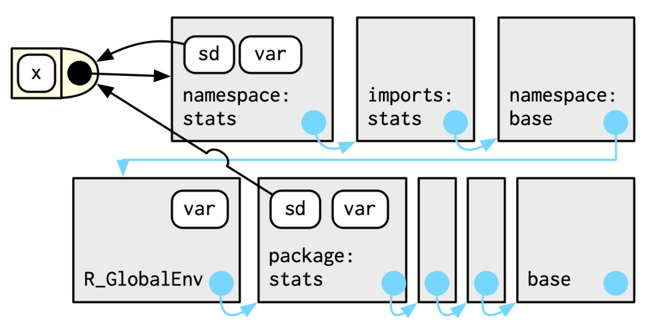
Unexported functions from packages have one binding environment: the `namespace:<name>` environment

Which is also the enclosing environment

Only `:::` works.

Where does R find stuff?

Where does R find functions from packages?



Enviroments

You can do crazy things with environments.

If you want to make use of reference semantic (i.e., modify objects in place), use R6

Programming advice

Keep it simple, avoid chaos!

Exercises

Functionals

Higher Order Functions

Higher order functions are functions that either **take functions as input** or **return functions as output**.

Functionals

As defined by Hadley Wickham: A **functional** is a function that takes another function as an input. Common argument names are `FUN` or `f`.

Examples

- `apply`-family
- `Reduce`, `Filter`
- `nlm`
- `optimize`
- ...

`apply`-family

The `apply`-family *applies* a function repeatedly. This can be seen as an abstraction of a for loop, with the following advantages:

- requires less code to write
- can be easier to read / understand
- does not store intermediate results
- no need to replace / grow

`apply`-family

The members of the `apply`-family in Base R are:

- `lapply` vector / list $\rightarrow$ list
- `sapply` vector / list $\rightarrow$ vector (matrix)
- `apply` matrix / array / data.frame $\rightarrow$ vector (matrix)
- `tapply`, `by`
- `mapply`, `Map`
- `rapply`, `eapply`, `vapply`

A popular alternative from the tidyverse: `purrr`

- `map` vector / list $\rightarrow$ list
- `map2` multiple vectors / lists $\rightarrow$ list
- ...

`apply`-family

Our focus: `lapply` and `Map`

Why?

- Consistent output
- Fast
- No dependencies
- We want to understand R basics

lapply

`lapply` takes mainly two arguments

`X` the input list/vector

`FUN` the function that should be repeatedly applied

```
example_list <- list(vec1 = c(1, 3, 4),
                     vec2 = c(4, 2, 10),
                     vec3 = c(2, NA, 1))
lapply(example_list, FUN = mean)


> $vec1
> [1] 2.666667
>
> $vec2
> [1] 5.333333
>
> $vec3
> [1] NA
```

lapply

Other arguments can be passed through `lapply` via '...'.

```
example_list <- list(vec1 = c(1, 3, 4),
                     vec2 = c(4, 2, 10),
                     vec3 = c(2, NA, 1))
lapply(example_list, FUN = mean, na.rm = TRUE)


> $vec1
> [1] 2.666667
>
> $vec2
> [1] 5.333333
>
> $vec3
> [1] 1.5
```

lapply

We can use our own functions as input.

```
dropNAs <- function(x) {
  x[!is.na(x)]
}
lapply(example_list, FUN = dropNAs)
```

```
> $vec1
> [1] 1 3 4
>
> $vec2
> [1]  4  2 10
>
> $vec3
> [1] 2 1
```

lapply

Anonymous functions can be used as input.

```
lapply(example_list, FUN = function(x) x[!is.na(x)])


> $vec1
> [1] 1 3 4
>
> $vec2
> [1]  4  2 10
>
> $vec3
> [1] 2 1
```

lapply

Data.frames are lists, too.

```
lapply(iris, FUN = class)


> $Sepal.Length
> [1] "numeric"
>
> $Sepal.Width
> [1] "numeric"
>
> $Petal.Length
> [1] "numeric"
>
> $Petal.Width
> [1] "numeric"
>
> $Species
> [1] "factor"
```

lapply

Atomic vectors can be used as input, but often vectorization could be used instead.

```
lapply(c(1, 2, 3), FUN = function(x) {
  paste0("ID", x)
})


> [[1]]
> [1] "ID1"
>
> [[2]]
> [1] "ID2"
>
> [[3]]
> [1] "ID3"
```

lapply

Limitation of `lapply`:
Only a single list/vector can be supplied as input. `Map` is a generalization of `lapply`! It is usually needed less often but a very powerful tool.

Map

Works very similar to `lapply`, with a few differences:

- Multiple input lists/vectors
- The list input should be named explicitly
- The order of the function and the list-input is switched

```
list1 <- list(mtcars[1:2, 1:3], iris[1:2, c(1, 2, 5)])
list2 <- list(mtcars[3:4, 1:3], iris[3:4, c(1, 2, 5)])

Map(rbind, x = list1, y = list2)
```

Map

```
> [[1]]
>                 mpg cyl disp
> Mazda RX4      21.0   6  160
> Mazda RX4 Wag  21.0   6  160
> Datsun 710     22.8   4  108
> Hornet 4 Drive 21.4   6  258
>
> [[2]]
>   Sepal.Length Sepal.Width Species
> 1          5.1         3.5  setosa
> 2          4.9         3.0  setosa
> 3          4.7         3.2  setosa
> 4          4.6         3.1  setosa
```

Map

Again, anonymous functions can be supplied as input:

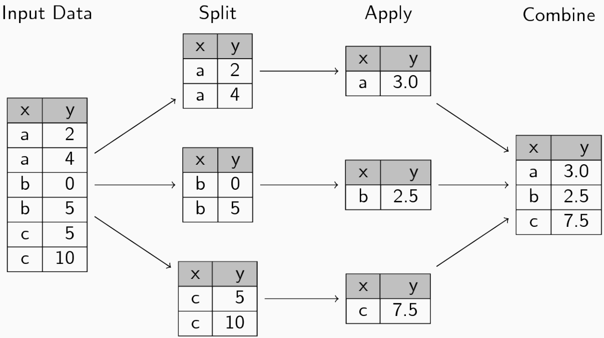
```
list1 <- list(mtcars[1:2, 1:3], iris[1:2, c(1, 2, 5)])
list2 <- list(mtcars[3:4, 1:3], iris[3:4, c(1, 2, 5)])

Map(function(x, y) {
  rbind(x, y)
  },
  x = list1, y = list2)
```

Split & Apply & Combine

A common use case for the `apply`-family is the **Split & Apply & Combine** paradigm. Here, we want to perform the same analyses for various subgroups in our data set:

- **split** a data.frame or vector (`?split`)
- **apply** computations on each split (`?lapply`)
- **combine** the results (`?do.call`)

Split & Apply & Combine



Split & Apply & Combine

```
head(iris)
```

```
>   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
> 1          5.1         3.5          1.4         0.2  setosa
> 2          4.9         3.0          1.4         0.2  setosa
> 3          4.7         3.2          1.3         0.2  setosa
> 4          4.6         3.1          1.5         0.2  setosa
> 5          5.0         3.6          1.4         0.2  setosa
> 6          5.4         3.9          1.7         0.4  setosa
```

```
table(iris$Species)
```

```
> 
>     setosa versicolor  virginica 
>         50         50         50
```

Split & Apply & Combine

Splitting the data set via a single (or multiple) grouping variables

```
data_list <- split(iris, f = iris$Species)
class(data_list)

> [1] "list"

length(data_list)

> [1] 3
```

Split & Apply & Combine

Apply the same computation to all data sets

```
out_list <- lapply(data_list, function(subdat) {
  mod <- lm(Sepal.Length ~ Sepal.Width, data = subdat)
  sum_mod <- summary(mod)
  out <- c(Intercept = coef(mod)[[1]],
    Slope = coef(mod)[[2]],
    r2 = sum_mod$r.squared)
  round(out, 3)
})
```

Split & Apply & Combine

```
out_list[["virginica"]]


> Intercept     Slope        r2
>     3.907     0.902     0.209
```

Combine the results

```
do.call(rbind, out_list)
```

```
>            Intercept Slope    r2
> setosa         2.639 0.690 0.551
> versicolor     3.540 0.865 0.277
> virginica      3.907 0.902 0.209
```

Exercises

Object Oriented Programming (S3)

Object Oriented Programming

Why?

- User-friendly: same function for different objects (`summary()`)
- Coder-friendly: implementation can depend on object
- Coder-friendly: easier to maintain & extend

Object Oriented Programming

Basics

- a **class** is a definition
- an object is an **instance** of a class.
- a **method** is specific implementation of procedure, and is associated with classes.
- **inheritance**: classes are organized in hierarchy. "is-a-type-of"-relation.
- **method-dispatch**: the process of finding the correct method to apply for a specific object.

Encapsulated OOP

- methods belong to objects or classes
- method calls look like `object.method(arg1, arg2)`
- most popular
- python, R6

Object Oriented Programming

Functional OOP

- methods belong to **generics** (or generic functions)
- method calls look like `generic(object, arg1, arg2)`
- looks like a normal function
- internally build on functions
- S3

Object Oriented Programming in R

- **S3**
- S4
- RC
- R6
- ...

S3

Compromise between interactive use, functional programming and object-oriented programming.

- "naming conventions"
- used in base R
- flexible: new classes, new methods, new generics

S3

- `class`-attribute
- generics and methods
- inheritance and dispatch

S3 - class

A new class is made by adding an arbitrary `class` attribute to an object.

```
object <- 1:10
class(object) <- "myClass"
attributes(object)


> $class
> [1] "myClass"
```

Very flexible! Use it wisely!

S3 - class

```r
class(iris)
```

```
> [1] "data.frame"
```

```r
iris[1:4, 1:3]
```

```
>   Sepal.Length Sepal.Width Petal.Length
> 1          5.1         3.5          1.4
> 2          4.9         3.0          1.4
> 3          4.7         3.2          1.3
> 4          4.6         3.1          1.5
```

S3 - class

Changing the class changes the behavior!

```
class(iris) <- "no data.frame"
class(iris)

> [1] "no data.frame"

iris[1:4, 1:3]

> Error in iris[1:4, 1:3]:  falsche Anzahl von Dimensionen
```

S3 - class

Good practice: ***constructor function***

- defines the structure of the class
- should be used to create objects of that class

```
myClass <- function(element1, element2){
  # validation of the elements
  structure(list(element1),
            attribute1 = element2,
            class = "myClass")
}
```

Write a separate validation-function for computationally intensive validation.

S3 - Generics and Methods

- **methods** for a class belong to **generics**
- when a generic is called for a specific class, the corresponing method for that class will be used.
- common generics are: `print()`, `plot()`, `summary()`, `anova()`
- same function, but different computation depending on object-class

```
body(print)


> UseMethod("print")
```

S3 - Generics and Methods

Creating a new method (for an existing generic):

```
print.myClass <- function(x, ...){
  cat("This is a myClass-print:\n")
  cat(round(c(nValues = length(x),
              mean = mean(x),
              SD = sd(x)), 3), ...)
}
my_object <- 1:5
class(my_object) <- "myClass"
print(my_object)

> This is a myClass-print:
> 5 3 1.581
```

S3 - Generics and Methods

Good practices (enforced for packages on CRAN):

- A method must have all the arguments of the generic, including `...` if the generic does.
- A method must have arguments in exactly the same order as the generic.
- If the generic specifies defaults, all methods should use the same defaults.

S3 - Generics and Methods

Inspect the generic!

```
formalArgs(print)

> [1] "x"   "..."

formalArgs(summary)

> [1] "object" "..."
```

S3 - Generics and Methods

Creating a new generic:

```
center <- function(x, ...)
  UseMethod("center")

center.myClass <- function(x, ...){
  print("centering myClass:\n")
  return(x - mean(x))
}

center(my_object)

> [1] "centering myClass:\n"
> This is a myClass-print:
> 5 0 1.581
```

S3 - Inheritance and Dispatch

Objects can have more than one class

```
my_model <- glm(as.factor(books) ~ pared, data = pisa,
                family = "binomial")
class(my_model)

> [1] "glm" "lm"

class(my_model) == "lm"

> [1] FALSE  TRUE

inherits(my_model, "lm")

> [1] TRUE
```

Good practice: hierachical inheritance (subclass and superclass)

S3 - Inheritance and Dispatch

When a method is not available for a (sub)class, the next available method (i.e., for the supperclass) will be used.

```
"variable.names.glm" %in% methods(class = "glm")

> [1] FALSE

"variable.names.lm" %in% methods(class = "lm")

> [1] TRUE

variable.names(my_model)

> [1] "(Intercept)" "pared"
```

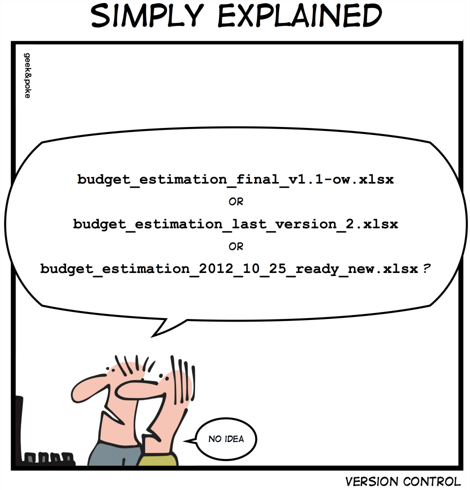
Exercises

Version Controlling (Git + Github)

Version Controlling

- Motivation
- Setup
- Work flow
- Recommendations
- Resources

Motivation


SIMPLY EXPLAINED
geek&poke
budget_estimation_final_v1.1-ow.xlsx
OR
budget_estimation_last_version_2.xlsx
OR
budget_estimation_2012_10_25_ready_new.xlsx ?
NO IDEA
VERSION CONTROL

Motivation

- Implementation of long term change history
  - No ridiculous file names
  - No archive subfolder
  - Always perfect overview of file history and changes
- Collaborations
  - What has changed?
  - Who has changed it?
  - Documentation of changes
  - Parallel working possible (merging)

But...


THIS IS GIT. IT TRACKS COLLABORATIVE WORK ON PROJECTS THROUGH A BEAUTIFUL DISTRIBUTED GRAPH THEORY TREE MODEL.
COOL. HOW DO WE USE IT?
NO IDEA. JUST MEMORIZE THESE SHELL COMMANDS AND TYPE THEM TO SYNC UP. IF YOU GET ERRORS, SAVE YOUR WORK ELSEWHERE, DELETE THE PROJECT, AND DOWNLOAD A FRESH COPY.

Setup

See the workshop preparation materials

Work flow 1

Creating a repository

- Create an **online repository** (e.g. on Github)
  - Use an R specific `.gitignore`
  - Initialize with a short readme (`.md`)
- Clone the repository to your local machine via RStudio
- An R-Project is added automatically to the existing repository

Excursion: gitignore

- Plain text file
- Which files should not be tracked by git?
  $\rightarrow$ These then only exist locally in their current version!
- Options
  - Single files
  - Folder
  - Specific data types
  - Combinations of the above
- Use cases
  - Large files (Data, images, ...)
  - Auxiliary files (e.g. created during latex compilation)

Work flow 2

Working with an existing repository

- Before working: Synch your local repo (**Pull** or **clone**)
- Perform changes in your local repository
  $\rightarrow$ Create/modify/delete files
- **Stage** your changes
- **Commit** your changes (aka new version)
- **Push** your changes (online repository is updated)

Excursion: mergen

Conflicts between different updated versions

- Common when working collaborativley
- Discrepancies between your own different local repos $\rightarrow$ Git communicates these and indicates conflicts
- Select the desired changes
- Stage selection, commit and push

Excursion: Branches

Multiple parallel versions of a project within one repository

- e.g. one stable and one development branch
- Only certrain modifications should be made in the stable branch
- **Note**: RStudio GUI has limited support for this

Recommendations

- Keep it simple!
  - If not necessary, no branches/forks/pull requests
- Have meaningful commits
- Keep it lean (no big files)

Resources

Git (+ R) Resources

- Small Intro (https://r-bio.github.io/intro-git-rstudio/)
- Happy Git with R (https://happygitwithr.com/)
- R Packages and Git (https://r-pkgs.org/git.html)
- Git Book (http://git-scm.com/book/en/v2)

R Packages

Motivation

- It is incredibly easy!
- It makes your code easier accessible (for others and yourself)
- It provides a great framework for documenting your code
- It provides great tools for testing your code
- It is a form of scientific output (packages can be cited)

Setup

Use `usethis` and/or `RStudio` to set up everything.

- Create a regular Github Repository
- Clone the repository regularly
- Use `usethis::use_package(getwd())` to create the minimal package structure
- Use `usethis` if you want to add more specific architecture

R functions

Your actual code lives in the `R` folder.

- Write small functions which do one specific thing
- Organize your functions logically
- Avoid very long scripts

Using other packages

If you want to use another package in your source code, add it to the Imports-Field in your description file and use its functions using `package::function`.

Documentation

Use `roxygen2` to document your code and to manage your namespace.

Testing

Use `testthat` for automated testing. This has multiple advantages:

- Good test coverage serves as a quality attribute of a good and stable package
- Modifying existing code becomes much easier
- Your code becomes more robust
- It helps you sleep at night

Resources

Writing R packages

- Writing R Extensions (`https://cloud.r-project.org/doc/manuals/r-release/R-exts.html`)
- R Packages (`https://r-pkgs.org/`)

Wrap Up

General Advice

- Try to always learn new things about R and / or programming
- Try to automate as much as possible
- If you are re-using code regularly, write a package!
- Learn from masters
- Rewrite important code - the first attempt is usually not the best approach

Literature Recommendations

R Resources

- Advanced R Ed. 1 (http://adv-r.had.co.nz/)
- Advanced R Ed. 2 (https://adv-r.hadley.nz/)
- Notes on Functionals (https://www.stat.umn.edu/geyer/8054/notes/functional.html)
- R language definition (https://cloud.r-project.org/doc/manuals/r-release/R-lang.html)
- R Inferno (https://www.burns-stat.com/pages/Tutor/R_inferno.pdf)
- R Packages (https://r-pkgs.org/)
- Clean Code (https://enos.itcollege.ee/~jpoial/oop/naited/Clean%20Code.pdf)

Thank you for your attention!

Thank you for your attention!

Questions? Remarks?