# R 00 Programming and Package Development

Robert Stojnic and Laurent Gatto

Teaching material:

https://github.com/lgatto/TeachingMaterial

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## **Prerequisites**

- good knowledge of R (data types, functions, scripting ...)
- basic knowledge of CLI
- some Latex knowledge helpful but not essential
- object-oriented programming knowledge helpful but not essential

#### Plan

- Introduction
- Revision of basic R
- Object-oriented (OO) Programming
- A few words about R packages
- Package structure
- Writing R documentation
- Other advanced topics
  - Testing your package
  - Debugging
  - Profiling
  - Calling foreign languages
- 8 Distributing packages

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#### **Course introduction**

#### Course agenda

- Object-oriented programming in R: S3 and S4 class systems
- Package development in R: creating and documenting packages
- Other advanced topics: testing, debugging, profiling, C interface
- This is an **intensive** course

# **Objectives**

By the end of the course you should have created a working package written in the S4 class system.

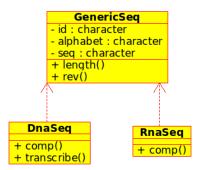
You should be able to use the code as a template for your own work. Our example has been chosen for demonstrative purposes.

# Course working example: "sequences" package

#### Working example

We will make a simple package to handle sequence data.

This package will be able to load a FASTA file and based on sequence type do some operations, like finding the sequence length or reverse sequence. For simplicity we will manipulate single sequences only.



UML class diagram for the "sequences" package

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# Basic R functions (size reflects frequency of usage)

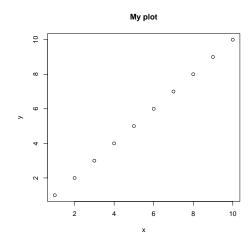


```
Simple function with 4 arguments:
> # Function to calculate area of rectangle
> area <- function(x1, y1, x2, y2) {
    abs(x2-x1) * abs(y2-y1)
> area(0, 0, 5, 5)
[1] 25
Special argument "..." for any:
> # Plot with a message before the plot
> plotMsg <- function(x, y, ...){</pre>
+ cat("Plotting", length(x), "data points!\n")
+ plot(x, y, ...)
+ }
> plotMsg(1:10, 1:10, main="Mv plot")
Plotting 10 data points!
```

# Output of plotMsg()

> plotMsg(1:10, 1:10, main = "My plot")

Plotting 10 data points!



- readLines() reads raw lines of text from a file
- nchar() gives number of characters in a string
   nchar("Some text")

[1] 9

strsplit() - split a string by some separator

```
> strsplit("Some text", " ")
[[1]]
[1] "Some" "text"
> strsplit("Some text", "")
[[1]]
[1] "S" "o" "m" "e" " "t" "e" "x" "t"
```

unique() - unique elements of a vector

```
> unique(c(1, 1, 2, 2, 3))
[1] 1 2 3
> unique(c("a", "b", "a"))
[1] "a" "b"
```

• grep() - find which elements of vector match regular expression
> grep("[AT]+", c("CGC", "TAT", "TATCATA"))
[1] 2 3

• sub() - replace matches to regular expression
> sub("[AT]+", "-", c("CGC", "TAT", "TATCATA"))
[1] "CGC" "-" "-CATA"

- chartr() translate a string by replacing individual characters
   chartr("TA", "AT", "TATCTA")
  - [1] "ATACAT"
- rev() reverse ordering in a vector
  > rev(c("TAT", "ATT", "TTT"))
  [1] "TTT" "ATT" "TAT"
- paste() concatenate variables into a string representation
   paste(c("A", "T", "A"), collapse="")
   [1] "ATA"

#### Lists in R

List is a data structure that can hold a vector of any other variables.

```
> x <- list(a=10, b="text")
> x
$a
[1] 10
$ъ
[1] "text"
> x$a
[1] 10
> x[["b"]]
[1] "text"
> x[[1]]
[1] 10
> names(x)
```

[1] "a" "b"

### **Everything in R has a class**

Everything in R has a type - in object oriented programming called a **class**.

```
> class(10)
[1] "numeric"
> class(c(1, 2, 3))
[1] "numeric"
> class("Some text")
[1] "character"
> class(matrix(0, nrow=10, ncol=10))
[1] "matrix"
> class(plot)
[1] "function"
> class(table(1:4, 1:4))
[1] "table"
```

# Recommended coding standards

### **Coding standards**

- Use <- for assignment rather than =.
- Avoid long lines (80 characters).
- Use spaces for identation (2 or 4).
- No semi-colomns (unless you have several expression in a line).
- Start names with upper case for classes, lower for the rest.
- Use syntax highlighting

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# Object-oriented Programming (OOP)

# Object-oriented vs Procedural programming

- ullet OOP introduced in 1970s in Smalltalk but gained wider popularity in 1990s with programming languages like C++ and Delphi
- Traditional (procedural) programming data and functions decoupled
- Object-oriented programming data and functions tied together in objects

## OOP concepts

- Abstraction related data is stored and handled together
- Inheritance code reuse by hierarchy of more-to-less general object types (classes)
- Polymorphism the most appropriate function is called based on the dataset (e.g various plot functions)

# **Procedural vs Object-oriented Programming**

### Procedural programming

```
> area <- function(x1,y1,x2,y2){
+ abs(x2-x1)*abs(y2-y1)
+ }
> area(0, 0, 5, 5)
[1] 25
```

# Object-oriented programming

```
> setClass("Rectangle",
+ representation = representation(
+ x1 = "numeric".
+ v1 = "numeric".
+ x2 = "numeric",
+ y2 = "numeric")
+ )
> setGeneric("area", function(obj)
     standardGeneric("area"))
[1] "area"
> setMethod("area", "Rectangle", function(obj){
+ abs(obj@x2 - obj@x1) * abs(obj@y2 - obj@y1)
+ })
[1] "area"
> rect = new("Rectangle", x1=0, y1=0, x2=5, y2=5)
> area(rect)
[1] 25
```

#### OOP in R: S3 and S4

R has two object-oriented frameworks:

- S3 older and less formal (i.e. ad-hoc) framework with no explicit class definitions. Many parts of base R use S3, e.g. plotting, linear modelling, ...
  - limited introspection, single inheritance, single dispatch, instance-based
- **S4** full-fledged object-oriented framework, de-facto standard for most modern packages and required for Bioconductor packages.
  - introspection, multiple inheritance, multiple dispatch (introduces a small overhead)

# Course working example

### Working example revisited

Working example for this course will be manipulating DNA/RNA sequence data.

Functions we would like to have:

- readFasta() read in a single sequence from a FASTA file
- id(), seq() return the ID of sequence and the sequence (accessors)
- rev() return reverse DNA/RNA sequence
- length() return DNA/RNA sequence length
- comp() return complementary DNA/RNA sequence
- transcribe() return RNA sequence for DNA sequence

#### Goal

The final product should be an R package using S4 framework. But we need to get there, so lets start with a procedural and S3 implementation...

## readFasta() input file

We will start with the implementation of readFasta(). This function should load the data from a FASTA file and somehow represent it in R.

## A sample FASTA file:

> example dna sequence agcatacgacgactacgacatcagacatcagacatcagactactac gactacagacatcagacatcatatttacatcatcagagattatatta acatcagacatcgacacatcatcatcagcatcat

### Sequence description

Notice that a sequence is described by the:

- name (example dna sequence)
- nucleotide sequence
- sequence alphabet (in case of DNA ATGC, for RNA AUGC)

#### readFasta() implementation

Read in a sequence from FASTA file and return the id, sequence and alphabet in a list:

```
> readFasta <- function(infile){
    lines <- readLines(infile)
    header <- grep("^>", lines)
    if (length(header) > 1) {
      warning("Reading first sequence only.")
      lines <- lines[header[1]:(header[2]-1)]
      header <- header[1]
    id <- sub("^> *","",lines[header],perl=TRUE)
    sequence <- toupper(paste(lines[(header+1):length(lines)],collapse=""))</pre>
    alphabet <- unique(strsplit(sequence, "")[[1]])</pre>
    return.value <- list(id=id, sequence=sequence, alphabet=alphabet)
    class(return.value) <- "GenericSeq"</pre>
    return value
+ }
```

```
> s <- readFasta("aDnaSeg.fasta")
$id
[1] "example dna sequence"
$sequence
[1] "AGCATACGACGACTACGACACTACGACATCAGACACTACAGACTACTACGACTACAGACATCAGACACTACATATTTA
$alphabet
[1] "A" "G" "C" "T"
attr(,"class")
[1] "GenericSeq"
> names(s)
[1] "id"
               "sequence" "alphabet"
```

## S3 object definition

Any variable that has a "class" attribute is an S3 object.

Now we can write class-specific functions - methods.

#### Methods: class-specific functions

Lets write the id() method that will return the sequence id. There are two parts to defining a class-specific function (method):

- Defining a generic function
- Defining the class method

```
> id <- function(x){ UseMethod("id") } # generic</pre>
```

- > id.GenericSeq <- function(x){ x\$id } # method</pre>
- > id(s)
- [1] "example dna sequence"

#### S3 methods mechanism

Generic function has the desired function name and contains only one command UseMethod("functionName") called a dispatch command. This command based on the first parameter's class calls an appropriate function of format functionName.className. If such function doesn't exist functionName.default is called

# The seq() method

Now consider the seq() function. This function already exists (try ?seq). We would like to retain this old function, but also add our seq() that return the DNA/RNA sequence.

The seq() function is already a generic. We don't need to redefine it.

```
> seq
> methods("seq")
> seq.GenericSeq <- function(x) { x$sequence }
> seq(s)
```

[1] "AGCATACGACGACTACGACACTACGACATCAGACACTACAGACTACTACGACTACAGACATCAGACATCACATATTTA

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#### S3 methods exercises

Look at the code we have written so far, understand it, and then solve the following exercise.

#### Exercise 1:

Explore some of the built-in generics and methods. Try the following commands: methods("summary") methods(class="lm")

# Exercise 2: (code:02\_GenericSeq.R, solution:02\_GenericSeq\_solution.R)

Both length() and rev() are already generic functions, but alphabet() is not. Add these methods for class GenericSeq:

- length() should return the length of the DNA/RNA sequence
- alphabet() should return the alphabet of the sequence
- rev() should return the sequence in reverse (Hint: try to use functions strsplit() and the existing base rev() function).

### Reusing class methods

So far we have written methods for GenericSeq that work with any sequence type. Now lets introduce a new class DnaSeq. We want to inherit all methods from GenericSeq - to achieve this simply set the class attribute to all applicable class names.

```
> setSeqSubtype <- function(s){
+    if (all( alphabet(s) %in% c("A","C","G","T") )) {
+      class(s) <- c("DnaSeq", "GenericSeq")
+    } else if (all( alphabet(s) %in% c("A","C","G","U") )) {
+      class(s) <- c("RnaSeq", "GenericSeq")
+    } else {
+      stop("Alphabet ", alphabet(s) ," is unknown.")
+    }
+    return(s)
+ }
> s.dna <- setSeqSubtype(s)
> class(s.dna)
[1] "DnaSeq" "GenericSeq"
```

### DnaSeq methods

> complement(s.dna)

Define a DnaSeq method complement(). All GenericSeq methods still work with DnaSeq objects, but the complement() only works with DnaSeq.

```
> complement <- function(x){ UseMethod("complement") }
> complement.DnaSeq = function(x) chartr("ACGT", "TGCA", seq(x))
> id(s) # works on GenericSeq
[1] "example dna sequence"
> id(s.dna) # works on DnaSeq, GenericSeq
[1] "example dna sequence"
> try({ complement(s) }) # fails with error
```

[1] "TCGTATGCTGATGCTGTGATGCTGTAGTCTGTGATGTCTGATGATGCTGATGTCTGTAGTCTGTGATGTATAAAT

# S3 dispatch and inheritance

The dispatching will look for appropriate methods for all x (sub-)classes (in order in which they are set).

#### S3 inheritance exercise

Look at the inheritance code and understand how it works. Then solve the following exercise.

```
Exercise 3: (code: 03_inherit.R, solution: 03_inherit_solution.R)
```

Write the complement() method for RnaSeq class. Since we don't have a RNA FASTA file you will have to make a new RnaSeq object by hand and assign the right classes to test your code.

What do you notice about the S3 class system, is it easy to make mistakes? Could you also make your RNA sequence to be of class "1m"?

# S3 class system revision

- Classes are implicit (no formal class definition)
- Making new objects is done by simply setting the class attribute
- Making class methods is done by defining a generic function functionName() and a normal function functionName.className().
   Methods can be retrieved using the methods() function.
- Objects can inherit multiple classes by setting the class attribute to a vector of class names
- Many functions in base R use the S3 system
- Easy to make new ad-hoc classes and objects, but also mistakes and inconsistencies

The S4 class system is designed to address some of these concerns.

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#### Differences of S4 class system to S3

- Classes are explicit they have slots which describe what kind of data is stored
- Improved introspection class, method and slot introspection
- Consistency checking can no longer assign any class name, class hierarchy is explicitly checked and reinforced
- Validity checking custom automatic checks of data consistency
- Multiple inheritance, multiple dispatch, virtual classes

S4 class system is the de-facto standard in Bioconductor.

#### **Defining S4 class**

Each class in S4 needs to be defined before it can be used. At this stage data types and inheritance are specified.

#### S4 class slots

Slots define the **names and types** of variables that are going to be stored in the object. Types can be any of the basic R type or S3/S4 classes. To inspect how basic R types are called use class(), e.g.

```
> class("hello")
[1] "character"
```

### **Creating S4 objects**

[1] "sequence name"

Once we have a class definition, we can make an object by filling out the slots. We can directly access the slots using the @ notation although this is discouraged.

```
> genseq <- new("GenericSeq", id="sequence name",
         alphabet=c("A", "C", "G", "T"), sequence="AGATACCCCGAAACGA")
> genseq
An object of class "GenericSeq"
Slot "id":
[1] "sequence name"
Slot "alphabet":
[1] "A" "C" "G" "T"
Slot "sequence":
[1] "AGATACCCCGAAACGA"
> genseq@id
[1] "sequence name"
> slot(genseq, "id")
```

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x="GenericSeg"

### **Creating S4 methods**

Similar to S3 we define object methods in two steps: by defining a **generic** and the **method**.

```
> setGeneric("rev", function(x) standardGeneric("rev"))
[1] "rev"
> setMethod("rev", "GenericSeq",
            function(x) paste(rev(unlist(strsplit(x@sequence, ""))), collapse=""))
[1] "rev"
> rev(genseq)
[1] "AGCAAAGCCCCATAGA"
> showMethods("rev")
Function: rev (package .GlobalEnv)
x="ANY"
x="character"
    (inherited from: x="ANY")
```

#### S4 accessor methods

It is considered bad practice to use @ in your code to access slots. It breaks the division between the internal class implementation and class usage.

Instead, create getter and setter methods for all slots you want to expose.

```
> setGeneric("id", function(object) standardGeneric("id"))
[1] "id"
> setMethod("id", "GenericSeq", function(object) object@id)
[1] "id"
> setGeneric("id<-", function(object,value) standardGeneric("id<-"))
[1] "id<-"
> setReplaceMethod("id", signature(object="GenericSeq",
                             value="character"),
+
                   function(object, value) {
                     object@id <- value
                     return(object)
                   7)
[1] "id<-"
> id(genseq) <- "new sequence name"
> id(genseq)
```

# S4 introspection and methods exercises

# Exercise 4: (code: 04\_basic\_S4.R)

Try the following introspection functions:

```
showMethods("rev")
getClass("GenericSeq")
slotNames(genseq)
getMethod("rev", "GenericSeq")
findMethods("rev")
isGeneric("rev")
```

What do these function output? In some cases the result is an object. Use the introspection functions to find out more about the results (e.g. class(), getClass(),...).

# Exercise 5: (code as above, solution: 05\_accessors\_solution.R)

Lets complete our GenericSeq implementation with some more methods. Implement getter/setter method seq() and getter only alphabet(). Then implement the method length() to return sequence length. First check if "length" is already a generic though.

### **Special methods** - show()

You might have noticed that many object print a custom description instead of a plain list of slots. We can add this functionality by setting show() and print() methods.

```
> setMethod("show",
            "GenericSea",
            function(object) {
              cat("Object of class",class(object),"\n")
              cat(" Id:",id(object),"\n")
              cat(" Length: ",length(object), "\n")
              cat(" Alphabet:",alphabet(object),"\n")
              cat(" Sequence: ", seq(object), "\n")
            7)
[1] "show"
> genseq
Object of class GenericSeq
 Id: new sequence name
Length: 16
 Alphabet: A C G T
Sequence: AGATACCCCGAAACGA
```

# Special methods - print()

The print() function already exists, but is not an S4 generic.

```
> setGeneric("print", function(x,...) standardGeneric("print"))
[1] "print"
> setMethod("print", "GenericSeq",
            function(x) {
+
              sq \leftarrow strsplit(seq(x),"")[[1]]
              cat(">",id(x),"\n"," 1\t")
              for (i in 1:length(x)) {
                if ((i %% 10)==0) {
                  cat("\n".i."\t")
                cat(sq[i])
              cat("\n")
[1] "print"
> print(genseq)
> new sequence name
  1 AGATACCCC
     GAAACGA
```

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### Special methods - initialize()

Sequence: ATATTA

We might need to do some special processing on object creation. We can do this with a custom initialize() method.

Use named arguments with default values (otherwise class checking might fail).

```
> setMethod("initialize", "GenericSeq",
+ function(.0bject, ..., id="", sequence=""){
+ .0bject@id <- id
+ .0bject@sequence <- toupper(sequence)
+ callNextMethod(.0bject, ...) # call parent class initialize()
+ })
[1] "initialize"
> show(new("GenericSeq", id="new seq.", alphabet=c("A", "T"), sequence="atatta"))
Object of class GenericSeq
Id: new seq.
Length: 6
Alphabet: A T
```

### Inheritance in S4 class system

Implementation of GenericSeq is finished. Now we want to re-use this code and add some extra functionality for DnaSeq and RnaSeq.

We start by defining the new classes that will inherit (contain) our GenericSeq class. It is good practise to provide some default (prototype) values.

### Custom comp() methods in two subclasses

Now we can write the comp() method which is going to work differently for DNA and RNA sequences.

```
> setGeneric("comp",function(object) standardGeneric("comp"))
[1] "comp"
> setMethod("comp", "DnaSeq",
            function(object) {
              chartr("ACGT", "TGCA", seq(object))
            7)
   "comp"
> setMethod("comp", "RnaSeq",
            function(object) {
              chartr("ACGU", "UGCA", seq(object))
            7)
   "comp"
[1]
```

### Creating objects of appropriate class

We could use new() to create new object instances, but it is tedious and error prone. Instead, we should provide a function that reads in some data and sets the right class for the data.

```
> readFasta <- function(infile){
   lines <- readLines(infile)
   header <- grep("^>", lines)
   if (length(header)>1) {
     warning("Reading first sequence only.")
     lines <- lines[header[1]:(header[2]-1)]
     header <- header[1]
   .id <- sub("^> *", "", lines[header], perl=TRUE)
   .sequence <- toupper(paste(lines[(header+1):length(lines)],collapse=""))</pre>
    .alphabet <- toupper(unique(strsplit(.sequence, "")[[1]]))
   if (all(.alphabet %in% c("A", "C", "G", "T"))) {
     newseg <- new("DnaSeg",
                    id= id
                    sequence=.sequence)
   } else if (all(.alphabet %in% c("A", "C", "G", "U"))) {
     newsea <- new("RnaSea".
                    id=.id.
                    sequence=.sequence)
   } else {
     stop("Alphabet "..alphabet," is unknown.")
   return(newseq)
```

### Object validity tests

The user can still use new in an inconsistent way or change a consistent object in the way that will render it inconsistent (e.g. assign an RNA sequence to an object of class DnaSeq).

First lets make sure each new object is consistent, e.g. that alphabet matches sequence.

```
> setClass("GenericSeg",
           representation = representation(
             id = "character".
             alphabet = "character".
             sequence = "character",
             "VIRTUAL").
           validity = function(object) {
             isValid <- TRUE
             if (nchar(object@sequence)>0) {
               chars <- casefold(unique(unlist(strsplit(object@sequence,""))))</pre>
               isValid <- all(chars %in% casefold(object@alphabet))</pre>
             if (!isValid)
               cat("Some characters are not defined in the alphabet.\n")
             return(isValid)
           7)
```

### Validity tests - setters

Now lets make sure the user cannot render the objects inconsistent by modifying the object.

```
setReplaceMethod("id",
                   signature(object="GenericSeq",
                              value="character").
                   function(object, value) {
                     object@id <- value
                     if (validObject(object))
                       return(object)
                   })
[1] "id<-"
> setReplaceMethod("seg",
                   signature(object="GenericSeq",
                              value="character").
                   function(object, value) {
                     object@sequence <- value
                     if (validObject(object))
                       return(object)
                   })
    "sea<-"
```

Look at the code we wrote so far and understand it. Then solve the following exercise.

### Exercise 6: (code: 06\_S4\_complete.R)

Try again reading the supplied fasta file using

Inspect the resulting object using object introspection tools. Try to break the resulting object by assigning invalid values to sequence. What happens if you do:

$$seq(x) <- "!"$$

and what if:

x@sequence <- "!"

# Exercise 7: (code as above, solution: 07\_transcribe\_solution.R)

Implement a new method transcribe() of DnaSeq. This method should take a DnaSeq, replace the T's with U's and return a RnaSeq object.

### More \$4 features and considerations

#### Virtual classes

A class can be marked to be **virtual** so that no objects can be made, but it can only be inherited. In our case, we might want to mark GenericSeq as virtual, to do so just add parameter "VIRTUAL" into class representation.

#### Class unions

In some cases we might want a slot to contain an object from one of multiple unrelated classes. In that case we would create a "dummy" class to serve as a place holder. For this we can use **class union**, for example setClassUnion("AOrB", c("A", "B")) would create a new virtual class AOrB that is a parent class to both A and B.

### **Overriding operators**

**Operators** in R can also be over-ridden. For instance setMethod("[", MyClass, ....) will override the subsetting operator [] for MyClass to give it custom functionality.

## **Mutability**

[1] "ACGTAA"

R objects are not **mutable**; R has a **copy on modify** semantics: whenever you pass an a object to a function, a copy is passed as argument. This is how things work for both S3 and S4 class systems.

```
> a <- new("DnaSeq", sequence="ACGTaa")
> seq(a)
[1] "ACGTAA"
> comp(a)
[1] "TGCATT"
> seq(a)
```

#### Reference classes

A recent OO system, based on S4 classes, that implements a **pass by reference** semantic. See ?ReferenceClasses for details.

### **Example**

```
## here, you would have
```

- > a\$seq ## equivalent of seq(a)
- [1] "AGCATG"
- > a\$comp()
- > a\$seq
- [1] "TCGTAC"

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#### References

- R Installation and Administration [R-admin], R Core team
- Writing R Extensions [R-ext], R Core team

Use help.start() to access them from your local installation, or http://cran.r-project.org/manuals.html from the web.

## **Terminology**

A **package** is loaded from a **library** by the function library(). Thus a library is a directory containing installed packages.

Calling library("foo", lib.loc = "/path/to/bar") loads the package (book) foo from the library bar located at /path/to/bar.

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# **Packages**

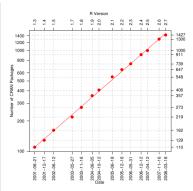
One of the aspects that make R appealing:

**CRAN** package repository features 2868 available packages.

R-forge 986 packages.

**Bioconductor** 517 reviewed packages in latest release (version 2.9).

Numbers checked on 2<sup>nd</sup> March 2011



# Why packages

Packages provide a mechanism for loading optional code and attached documentation as needed.

There is more to it – packages are a means to

- logically group your own functions
- keep code and documentation together and consistent
- keep code and data together
- keep track of changes in code
- summarise all packages used for a analysis (see sessionInfo())
- make a reproducible research compendium (container for code, text, data as a means for distributing, managing and updating)
- optionally test your code
- ... project managment

even if you do not plan to distribute them.

#### **Administration**

### **Building packages**

R CMD build myPackage — the R package builder builds R package (and vignettes if available).

# **Checking packages**

R CMD check myPackage\_0.1.1.tar.gz or R CMD check myPackage — the R package checker tests whether the package or source work correctly.

- The package is installed (checks missing cross-references and duplicate aliases in help files).
- File names validity, permissions.
- Package DESCRIPTION file is checked for completeness, and some of its entries for correctness.
- R and .Rd files are checked for syntax errors.
- A check is made for missing documentation entries.
- Codoc checking
- Examples provided by the package's documentation are run.
- If available, package tests are run and vignettes are executed and compiled.

### **Administration**

### **Installing packages**

R CMD INSTALL myPackage\_0.1.1.tar.gz or install.packages("myPackage\_0.1.1.tar.gz") — installs the package in the default library. Other libraries can be specified with the -1 option or lib argument.

# Loading

Use library() or require().

#### On Windows

R is very much Unix centric. To build from source on Windows, you will need Rtools<sup>a</sup> See the *The Windows toolset* in R-Admin for more details.

ahttps://cran.r-project.org/bin/windows/Rtools/

### Plan

- Introduction
- Revision of basic R
- Object-oriented (OO) Programming
- A few words about R packages
- Package structure
- Writing R documentation
- **Other advanced topics** 
  - Testing your package
  - Debugging
  - Profiling
  - Calling foreign languages
- B Distributing packages

### A minimal package

Function package.skeleton() automates some of the setup for a new source package. Calling it with minimal arguments produces the following hierarchy:

```
> foo <- function(x) x
> package.skeleton(name="myRpackage",list="foo")
```

### produces

```
myRpackage/

|-- DESCRIPTION

|-- man

| |-- foo.Rd

| +-- myRpackage-package.Rd

|-- R

| +-- foo.R

+-- Read-and-delete-me
```

#### **DESCRIPTION**

Package: myRpackage

Type: Package

Title: What the package does (short line)

Version: 1.0

Date: 2016-09-21

Author: Who wrote it

Maintainer: Who to complain to <yourfault@somewhere.net>

Description: More about what it does (maybe more than one line)

License: What license is it under?

### **Lazy loading**

A mechanism used to defer initialization of an object until the point at which it is needed. The individual objects in the package's environment are indirect references to the actual objects until, for example a function is called or an object loaded.

The LazyLoad and LazyData fields control whether the R objects and the datasets (respectively) use lazy-loading. LazyLoad must be set if the *methods* package is used.

LazyLoad is now on by default.

### **Example**

R uses Lazy evaluation, which delays the evaluation of an expression (here the argument) until its value is actually required [a]:

<sup>&</sup>lt;sup>a</sup>example from Hadley Wickham's devtools

### **Example**

```
> suppressWarnings(dump("dnaseq","",evaluate=FALSE))
dnaseq <-
<pre>cpromise: lazyLoadDBfetch(c(OL, 195L), datafile, compressed,
```

#### **DESCRIPTION**

### Other important fields

- **Depends** A comma-separated list of package names (optionally with versions) which this package depends on.
- **Suggests** Packages that are not necessarily needed: used only in examples, tests or vignettes, packages loaded in the body of functions (see require()).
  - Imports Packages whose name spaces are imported from (as specified in the NAMESPACE file) but which do not need to be attached to the search path.
    - **Collate** Controls the collation order for the R code files in a package. If filed is present, all source files must be listed.
      - **URL** A list of URLs separated by commas or whitespace.

. . .

#### The NAMESPACE file

Stored in the package directory. Restrict the symbols that are exported and imports functionality from other packages. Only the exported symbols will have to be documented.

Note: NAMESPACE is now required (since R 2.14).

```
export(f, g) ## exports f and g
exportPattern("^[^\\.]")
import(foo) ## imports all symbols from package foo
importFrom(foo, f, g) ## imports f and g from foo
```

It is possible to explicitly use symbol s from package *foo* with foo::s or foo:::s if s is not exported.

### Attach and load

Packages are attached to the search path with library or require.

- Attach When a package is attached, then all of its dependencies (see Depends field in its DESCRIPTION file) are also attached.

  Such packages are part of the evaluation environment and will be searched.
  - Load One can also use the Imports field in the NAMESPACE file. Imported packages are loaded but are not attached: they do not appear on the search path and are available only to the package that imported them.

### R

Contains source()able R source code to be installed. Files must start with an ASCII (lower or upper case) letter or digit and have one of the extensions .R (recommended), .S, .q, .r, or .s. File order is important if code relies on *earlier* code — order use Collate filed in DESCRIPTION file.

### **Example**

```
## works fine without Collate field AllGenerics.R DataClasses.R methods-ClassA.R methods-ClassB.R functions-ClassA.R ...
```

zzz.R is generally used to define special functions used to initialize (called after a package is loaded and attached) and clean up (just before the package is detached). See help(".onLoad")), ?.First.Lib and ?.Last.Lib for more details.

#### man

Manuals for the objects (package, functions, generics, methods, classes and data sets) in the package in R documentation (Rd) format. The filenames must start with an ASCII (lower or upper case) letter or digit and have the extension .Rd or .rd and should be URL compatible. If you use a NAMESPACE, only exported symbols need to be documented. Without NAMESPACE, internal use only objects should be documented in pkg-internal.Rd.

#### data

Contains data files, made available via *lazy-loading* or for loading using data(). Data types that are allowed are

R code self-sufficient plain R code (.R or .r),

Tables possibly compressed tables (.tab, .txt, or .csv, see ?data for the file formats)

Objects created using save() (.RData or .rda).

### **Example**

There is a DnaSeq object in sequences/data.

#### inst

Content is copied recursively to the installation directory, for example **CITATION** file (see citation() function),

doc directory for additional documents (see vignettes, later).
 extdata directory for other data files, not belonging in data.
 tests code for unit tests (see later).

## **Example**

In our sequences package, there is a fasta sequence in sequences/inst/extdata used to illustrate the readFasta function.

#### tests

Contains additional package-specific test code. We will talk about unit tests later.

#### src

Contains sources and headers for the compiled code, plus optionally a file Makevars or Makefile.

### demo

R scripts runned via demo() that demonstrate some of the functionality of the package. Execution of these scripts is not checked.

### Exercise 8: Let's create a package

So far, you have defined a set of classes, methods and functions ... Create the required directory structure and files using package.skeleton(name="sequences") or manually. For the former, you can use different arguments:

**list** to specify the R objects by their names.

code\_files to specify R code files.

**environment** to specify an environment where objects are looked for.

See ?package.skeleton for more details.

### Exercise 9: Let's build/check it

Do you expect the package to build/check/INSTALL:

R CMD build sequences

R CMD check sequences\_1.0.tar.gz

R CMD INSTALL sequences\_1.0.tar.gz

Why? Have a look at R CMD build | check --help.

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### Rd format

### R documentation format

R objects are documented in files written in *R documentation* (Rd) format, a simple markup language much of which closely resembles LATEX, which can be processed into a variety of formats, including LATEX, HTML, pdf and plain text.

#### Rd format

#### An Rd file constists of

**Header** provides basic information about the name of the file, the topics documented, a title, a short textual description and R usage information – mandatory.

**Body** gives further information defined within *sections* (for example, on the function's arguments and return value, as in the example)

Footer with keyword information – optional.

Every (exported) object must be documented. Package documentation is optional.

% File src/library/base/man/load.Rd

```
\name{load}
\alias{load}
\title{Reload Saved Datasets}
\description{
 Reload the datasets written to a file with the function
 \code{save}.
\usage{
load(file, envir = parent.frame())
\arguments{
 \item{file}{a connection or a character string giving the
   name of the file to load.}
 \item{envir}{the environment where the data should be
   loaded.}
\seealsof
 \code{\link{save}}.
\examples{
## save all data
save(list = ls(), file= "all.RData")
## restore the saved values to the current environment
load("all.RData")
## restore the saved values to the workspace
load("all.RData", .GlobalEnv)
}
\kevword{file}
```

#### **Documentation**

#### **General comments**

- Different objects are documented with different types of Rd files, as defined by the \docType{} tag.
- Different object documentation require or are advised to contain different sections.
- One .Rd file can document several objects by defining multiple \alias{}'es.

#### **Documentation**

#### **Guidelines for Rd files**

These are suggested guidelines for the system help files (in .Rd format) that are intended for core developers but may also be useful for package writers. (see http://developer.r-project.org/Rds.html)

There are many different sections and marking text (for mathematical notation, tables, cross-references, ...), that will look very familiar to LATEX users. All are described in *Writing R documentation files* (section 2) of the R-ext manual.

Fortunately, the prompt(object) et. al. functions will inspect the object to be documented and create a specific documentation skeleton for us to be completed.

## Package documentation

Provides an short and optional overview of a package.

# **Example**

promptPackage("sequences")

## Exercise 10:

Create a sequences-package. Rd and document your package.

# **Example**

```
\name{rivers}
\docType(data\)
\alias[rivers]
\title{Lengths of Major North American Rivers}
\description{
   This data set gives the lengths (in miles) of 141 \dQuote{major} rivers in North America, as compiled by the US Geological Survey.
}
\usage{rivers}
\format{A vector containing 141 observations.}
\source{World Almanac and Book of Facts, 1975, page 406.}
\references{
   McNeil, D. R. (1977) \emph{Interactive Data Analysis}.
   New York: Wiley.
}
\keyword{datasets}
```

# **Example**

prompt(myDataFrame) or promptData(myDataObject)

## Exercise 11:

Document the dnaseq object.

#### **Function documentation**

```
Many markup command, including \usage{fun(arg1, arg2, ...)}, \arguments{...}, \section{Warning}{...} and \examples{...}, which are executed!
```

# **Example**

```
prompt(object=myFunction) or prompt(name="myFunction")
```

## Exercise 12:

Choose one of the functions and document it.

# **Documenting S4 classes and methods**

Documentation is 'similar' than for functions. Note that aliases are of the form MyClass-class or MyGeneric, signature\_list-method.

Additionnal aliases should be added to refer to MyGeneric,

 $\label{thm:mygeneric-method} \begin{tabular}{ll} MyGeneric-method, ... and the manuals are accessed with class?topic and method?topic. Overall documentation for methods should be aliased with MyGeneric-methods \end{tabular}$ 

See help("Documentation", package = "methods") for more details.

# **Example**

promptClass("MyClass") and promptMethods("myMethod")

## Exercise 13:

Document one class and one method of the package.

NB: we have used aliases for the methods to refer to the class documentation.

#### What is it?

Roxygen is a Doxygen-like documentation system for R; allowing **in-source** specification of Rd files, collation and namespace directives.

See https://github.com/klutometis/roxygen.

Install with install.packages("roxygen2").

Use R CMD roxygen myPackage to generate manuals and NAMESPACE.

```
Example
```

```
## Reads sequences data in fasta and create \code{DnaSeq}
##' and \code{RnaSeq} instances.
##
## This funtion reads DNA and RNA fasta files and generates
##' valid \code{"DnaSeq"} and \code{"RnaSeq"} instances.
##
##' Otitle Read fasta files.
## Cparam infile the name of the fasta file which the data are to be read from.
## Oreturn an instance of \code{DnaSeq} or \code{RnaSeq}.
##' @seealso \code{\linkS4class{GenericSeq}}, \code{\linkS4class{DnaSeq}} and \code
## @examples
##' f <- dir(system.file("extdata",package="sequences"),pattern="fasta",full.names="
##' f
##' aa <- readFasta(f[1])
##' aa
##' @author Laurent Gatto \email{lg390@cam.ac.uk}
##' @keywords IO, file
readFasta <- function(infile) {
}
```

# Roxygen2

## **Good points**

Makes (1) to get from code to full package straightforward and also (2) maintenance much easier.

## Since roxygen2

S4 support (classes, generics, methods).

#### See also

Rd2roxygen - Convert Rd to roxygen documentation and utilities to improve documentation

http://cran.r-project.org/web/packages/Rd2roxygen/index.html

# **Vignettes**

## Package vignette

These executable documents are in Sweave (.Rnw extension) or Rmarkdown (Rmd) which is an extended LATEX document (markdown) that includes code chunks. These are executed and the output (variable, but also tables and graphs) are displayed in the document. These dynamic reports, are updated automatically if data or analysis change.

The package vignettes are compiled at build time and are the prefered place for more extensive package documentation and use-cases.

#### References:

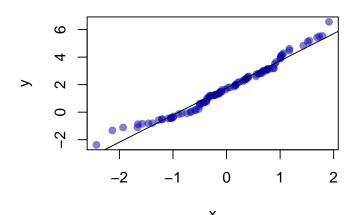
http://www.stat.uni-muenchen.de/~leisch/Sweave/ and

http://yihui.name/knitr/

```
... LaTeX document ...
<<label=myCode,echo=TRUE,fig=TRUE>>=
x <- sort(rnorm(100))
y <- sort(rnorm(100,2,2))
plot(x,y,pch=19,col="#0000BB80")
abline(lm(y~x))
@
... LaTeX document ...</pre>
```

# **Vignettes**

```
> x <- sort(rnorm(100)); y <- sort(rnorm(100,2,2))
> plot(x,y,pch=19,col="#0000BB80"); abline(lm(y~x))
```



# **Vignettes**

## **Example**

Have a look at the *sequences* package vignette in sequences/inst/doc.

#### Exercise 14:

The vignette is very basic. Try to add some code chunks to improve it. You can also embed code in-line with \Sexpr{}.

Prints version information about R and attached or loaded packages.

```
Example
> sessionInfo()
R version 3.3.1 Patched (2016-08-02 r71022)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Ubuntu 14.04.5 LTS
locale:
 [1] LC CTYPE=en GB.UTF-8
                         LC NUMERIC=C
 [3] LC TIME=en GB.UTF-8
                          LC COLLATE=en GB.UTF-8
 [5] LC_MONETARY=en_GB.UTF-8 LC_MESSAGES=en_GB.UTF-8
 [7] LC PAPER=en GB.UTF-8
                            LC NAME=C
 [9] LC ADDRESS=C
                             LC TELEPHONE=C
[11] LC_MEASUREMENT=en_GB.UTF-8 LC_IDENTIFICATION=C
attached base packages:
[1] stats
             graphics grDevices utils datasets methods base
loaded via a namespace (and not attached):
[1] tools 3.3.1 msdata 0.12.1
```

#### **Example**

- > toLatex(sessionInfo())
  - R version 3.3.1 Patched (2016-08-02 r71022), x86\_64-pc-linux-gnu
  - Locale: LC\_CTYPE=en\_GB.UTF-8, LC\_NUMERIC=C, LC\_TIME=en\_GB.UTF-8, LC\_COLLATE=en\_GB.UTF-8, LC\_MONETARY=en\_GB.UTF-8, LC\_MESSAGES=en\_GB.UTF-8, LC\_PAPER=en\_GB.UTF-8, LC\_NAME=C, LC\_ADDRESS=C, LC\_TELEPHONE=C, LC\_MEASUREMENT=en\_GB.UTF-8, LC\_IDENTIFICATION=C
  - Base packages: base, datasets, graphics, grDevices, methods, stats, utils
  - Loaded via a namespace (and not attached): msdata 0.12.1, tools 3.3.1

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# Plan

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# How to test the code in your package?

Or how to make sure that changes in your code do not break existing functionality?

- Implicitely, documentation examples and a vignette do some tests.
- Using R's build-in testing, that runs some code and compares the output to a saved template.
- Specific packages for unit testing: RUnit<sup>a</sup> or testthat<sup>b</sup>.

ahttp://cran.r-project.org/web/packages/RUnit/index.html

bhttp://cran.r-project.org/web/packages/testthat/index.html

# In package/tests/

#### Create

- mytest.R with code to be tested
- mytest.Rout.save with the reference output

When checking your package R will

- 1 execute the code in mytest.R
- 2 save the output to mytest.Rout
- Ocompare mytest.Rout to mytest.Rout.save
- report any differences

```
Test individual expression
expect_that(object_or_expression, condition) with conditions
    equals expect_that(1+2,equals(3)) or expect_equal(1+2,3)
gives_warning expect_that(warning("a"), gives_warning())
       is_a expect_that(1, is_a("numeric")) or
           expect_is(1,"numeric")
    is_true expect_that(2 == 2, is_true()) or
           expect_true(2==2)
  matches expect_that("Testing is fun", matches("fun")) or
           expect_match("Testing is fun", "f.n")
takes_less_than expect_that(Sys.sleep(1),takes_less_than(3))
```

## **Example**

```
> library(testthat)
> test_that("ok test", {
+ expect_equal(length(a), 6)
+ expect_true(seq(a) == "ACGTAA")
+ expect_is(a, "DnaSeq")
+ })
> try(expect_true(seq(a) == "ACGTaa")) ## fails with
> ## Error: seq(aa) == "ACGTaa" isn't true
```

## Exercise 15:

Update sequences/tests/sequences-test.R and sequences-test.Rout.save accordingly.

Hint: check the updated package and look in sequences.Rcheck/tests/

# Debugging

## Using R's tools

- Call traceback() after error to print the sequence of calls that lead to the error.
- Use debug(faultyFunction) to register faultyFunction for debugging, so that browser() will be called on entry. In browser mode, the execution of an expression is interrupted and it is possible to inspect the environment (with ls()). Use undebug(faultyFunction) to revert to normal usage.
- Use trace() to insert code into functions, start the browser or recover() from error.
- Set options(error=recover) to get the call stack and browse in any of the function calls.

Good reference: An Introduction to the Interactive Debugging Tools in Ra

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ahttp://www.biostat.jhsph.edu/~rpeng/docs/R-debug-tools.pdf

#### Exercise 16:

Lets debug sequences' readFasta function:

- Prepare for debugging: debug(readFasta)
- 2 Let get a fasta file from the package:

```
fasta <-
```

dir(system.file(dir="extdata",package="sequences"),full.names=TRUE)

- Oall the function to be debugged: readFasta(fasta)
- Oblug!

Hint: when debugging, use n (or an empty line) to advance to the next step, c to continue to the end of the current context (to the end of a loop for instance), where to print the stack trace of all active function calls and Q to exit the browser.

Other hint: use ls(all.names=TRUE) to see all objects, also those that start with a '.'.

# Measuring time

```
> m <- matrix(runif(1e4), nrow=1000)
```

```
> system.time(apply(m, 1, sum))
```

```
user system elapsed 0.002 0.000 0.001
```

## **Replicate**

```
> replicate(5, system.time(apply(m, 1, sum))[[1]])
```

```
[1] 0.001 0.001 0.002 0.002 0.001
```

# **Profiling time**

## **Execution time**

[1] 0.06

```
> Rprof("rprof")
> res <- apply(m,1,mean,trim=.3)</pre>
> Rprof(NULL); summaryRprof("rprof")
$by.self
                       self.time self.pct total.time total.pct
"mean.default"
                              0.02
                                         33.33
                                                         0.06 100.00
"anv"
                                         33 33 0 02 33 33
                             0.02
"unique.default"
                             0.02
                                         33.33 0.02 33.33
$bv.total
                       total.time total.pct self.time self.pct
"mean.default"
                               0.06
                                          100.00
                                                           0.02
                                                                     33.33
"apply"
                               0.06
                                         100.00
                                                           0.00
                                                                       0.00

        0.06
        100.00
        0.00
        0.00

        0.02
        33.33
        0.02
        33.33

        0.02
        33.33
        0.02
        33.33

        0.02
        33.33
        0.00
        0.00

"FIIN"
"anv"
"unique.default"
"sort int"
                               0.02 33.33
"unique"
                                                           0.00
                                                                       0.00
$sample.interval
[1] 0.02
$sampling.time
```

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```
Memory usage using tracemem*
> a
Object of class DnaSeq
 Id:
 Length: 6
 Alphabet: A C G T
 Sequence: GCATCA
> tracemem(a)
[1] "<0x20f0978>"
> seq(a) <- "GTGT"
tracemem[0x20f0978 \rightarrow 0x242a700]:
tracemem[0x242a700 \rightarrow 0x2223df0]: seq<- seq<-
```

 $^st$  tracemem requires to build R with --enable-memory-profiling

# Calling foreign languages

## The difficult route

- When R is getting too slow or is not doing well in terms of memory management.
- Implement the heavy stuff in C, C++a, Fortran or Javab.

```
ahttp://dirk.eddelbuettel.com/code/rcpp.html
bhttp://www.rforge.net/rJava/
```

# Other scripting languages

- R/Perl<sup>a</sup> and R/Python<sup>b</sup> bidirectional interfaces.
- There is also the system() function for direct access to OS functions.

```
ahttp://www.omegahat.org/RSPerl/
```

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bhttp://www.omegahat.org/RSPython/

## R's build-in C interfaces

- Better know how to program in C.
- Documentation is not always easy to follow: R-Ext, R Internals as well as R and other package's code.

#### .C

- Easy way
- Arguments and return values must be primitive (vectors of doubles or integers)

#### .Call

- Accepts R data structures as arguments and return values (SEXP and friends) (no type checking is done though).
- Memory management: memory allocated for R objects is garbage collected. Thus R objects in C code, you must be explicitly PROTECTed to avoid being gc()ed, and subsequently UNPROTECTed.

# **Example**

```
#include <R.h>
#include <Rdefines.h>
SEXP gccount(SEXP inseq) {
 int i. 1:
 SEXP ans, dnaseq;
 PROTECT(dnaseg = STRING_ELT(inseq, 0));
 1 = LENGTH(dnaseg):
 printf("length %d\n",1);
 PROTECT(ans = NEW_NUMERIC(4));
 for (i = 0: i < 4: i++)
   REAL(ans)[i] = 0;
 for (i = 0; i < 1; i++) {
    char p = CHAR(dnaseq)[i];
   if (p=='A')
      REAL(ans)[0]++:
   else if (p=='C')
      REAL(ans)[1]++;
   else if (p=='G')
      REAL(ans)[2]++;
   else if (p=='T')
      REAL(ans)[3]++:
    else
      error("Wrong alphabet");
 UNPROTECT(2):
 return(ans);
```

# Using your C code

## **Directly**

- Oreate a shared library: R CMD SHLIB gccount.c
- 2 Load the shared object: dyn.load("gccount.so")
- ① Create an R function that uses it: gccount <- function(inseq)
  .Call("gccount",inseq)</pre>
- Use you C code: gccount("GACAGCATCA")

## In a package

- Document you function.
- Overwrite .First.lib to dyn.load you shared object.
- If you have a NAMESPACE, export the shared objects with useDynLib.

## **Example**

In sequences, we have

- The gccount.c code in src.
- Defined a R function in R/functions.R gccount <- function(inseq) {</li>

```
.Call("gccount",
inseq,
PACKAGE="sequences")
```

- }
- Written the man/gccount.Rd man page.
- Exported the function in NAMESPACE using export(gccount) and the shared library with useDynLib(sequences)

```
Example
> s <- "GACTACGA"
> gccount
function (inseq)
{
    .Call("gccount", inseq, PACKAGE = "sequences")
}
<environment: namespace:sequences>
> gccount(s)
[1] 3 2 2 1
> table(strsplit(s,""))
ACGT
3 2 2 1
```

## Plan

- Object-oriented (OO) Programming
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- - Testing your package
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  - Profiling
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- **Distributing packages**

- CRAN Upload your checked myPackage\_x.y.z.tar.gz to
   ftp://cran.R-project.org/incoming and optionally
   send a message to CRAN@R-project.org. Your package will
   be installable with install.packages("myRpackage").
- R-forge Log in, regitser a project and wait for acceptance. Then commit you code to the svn repository. Your package will be installable with install.packages using repos="http://R-Forge.R-project.org".
- Bioconductor Make sure to satisfy submission criteria (pass check, have a vignette, use S4, have a NAMESPACE, make use of appropriate existing infrastructure, include a NEWS file, must **not** already be on CRAN, ...) and submit by email. Your package will then be reviewed before acceptance. A svn account will then be created. Package will be installable with biocLite("myPackage").

#### References

## **Further reading**

- Writing R Extensions, R Core
- R Programming for Bioinformatics, Robert Gentleman
- Advanced R and R Packages by Hadley Wickham
- https://github.com/lgatto/TeachingMaterial

