R Packages and Wrap-Up

Computational Statistics

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October 24, 2024

Today

Distributing and Organizing Code

Workshop in creating an R package

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Workshop in creating an R package

Course Summary

What did we actually do?

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Workshop in creating an R package

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Oral Examination Prep (Afternoon Session)

What to think of during examination

Organizing Code as an R Package

Organizing Code

Components

- Code for experiments
- Source code for functions (which we should be able to reuse)
- Tests
- Rcpp code
- Data

There are many ways to organize this.
Which one to choose?

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R Package

One way is to make an R package, makes it easy to

- connect to C++ code through Rcpp,
- set up automatic testing,
- document your code, and
- declare dependencies (other packages, R version).

Different approaches, but we will follow **R Packages** (Wickham and Bryan 2023), which is based around the **devtools** package.

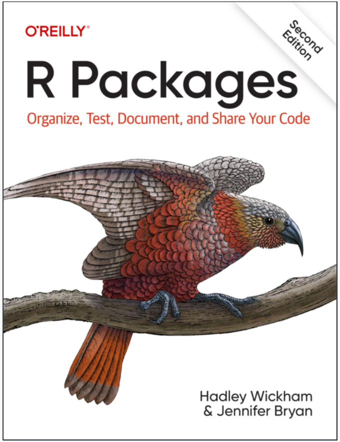

Figure 1: R Packages

Devtools

Meta-package for various helpers that aid in developing R packages (and projects). First off, install and load **devtools**:

```r
install.packages("devtools")
library(devtools)
```

This loads other packages that will be useful for setting up your package, most importantly the **usethis** package.

A Toy Example

Rosenbrock Package

Let's build a simple package that solves the Rosenbrock optimization problem, i.e. find

$$x^* = \arg\min \left((a - x_1)^2 + b(x_2 - x_1^2)^2 \right).$$

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- Testing our code
- Interfacing with Rcpp
- Adding dependencies to other packages
- Licensing our package
- Documenting the code

A First Package

Create It
Call

```
usethis::create_package("rosenbrock")
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or use `File > New Project > New Directory > R Package using devtools` in R Studio.

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 └── NAMESPACE
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You may also have `.Rbuildignore` and `.rosenbrock.Rproj` depending on how you created the package.

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You may also have `.Rbuildignore` and `.rosenbrock.Rproj` depending on how you created the package.

Install It

Open up the package in your editor (R Studio[a]).

```
devtools::install()
```

Voila, you have made an R package!

[a] In which case it should alread be opened.

R Code

`.R/`

- All R code should live in `.R`-files in `R/`.
- These files should (almost) always contain only functions.
- Many ways to organize your files: one function per file, all functions of a certain S3 class in one file etc.

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- These files should (almost) always contain only functions.
- Many ways to organize your files: one function per file, all functions of a certain S3 class in one file etc.

Let's create a first file: `R/objective.R`. Use `usethis::use_r("objective")` and insert this:

```
objective <- function(x, a = 1, b = 100) {
  (a - x[1])^2 + b * (x[2] - x[1]^2)^2
}
```

Workflow

We have created a first R file, but how do we use it? Two major options:

`devtools::install()`
Installs the package, like calling
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Sources all of your code.

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Quick but not as robust.

Try It

Try both options and see if you can call your newly defined function, `objective()`.

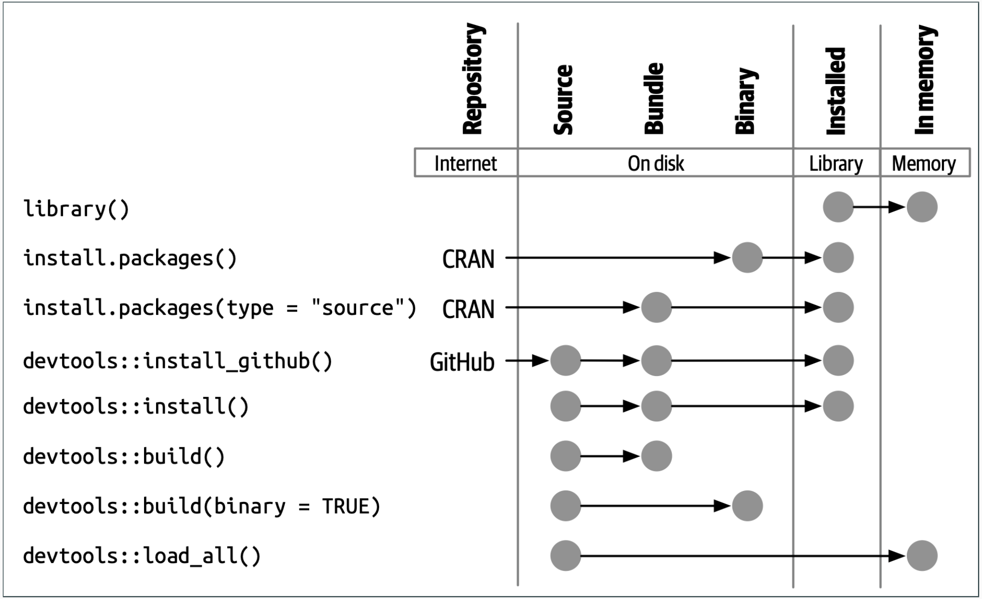

Figure 2: The various states of a package and how to move between them.

Exporting Functions

If you called `devtools::load_all()` then everything is sourced and you can just call `objective()` directly.

But if you use `devtools::install()` and `library(rosenbrock)`, the you would need to use `rosenbrock:::objective()`. The reason is that the function is not yet exported.

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`NAMESPACE`
Decides what functions you want exported. But right now it just contains a comment:

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# Generated by roxygen2: do not edit by hand
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NAMESPACE
Decides what functions you want exported. But right now it just contains a comment:

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

If you want to just export everything, you can remove this file and recreate it with this content:

```
exportPattern("^[[:alpha:]]+")
```

roxygen2

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```r
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Go ahead and place this before your `objective()` definition. Then run `devtools::document()` to roxygenize your package.

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export(objective)
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Reinstall the package and see if you can call `objective()` after loading it.

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testthat

- We have already encountered **testthat** for writing tests in a formalized way.
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```

This creates some new files and directories:

```
rosenbrock/
└── tests/
    ├── testthat/
    │   └── test-<some_fun>.R ........ Your test file for some_fun()
    └── testthat.R
```

A First Simple Test

For the Rosenbrock function, $f^* = f(a, a^2) = f(1, 1) = 0$. Let's make sure this is the case for us too!

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To create a test, we can use `usethis::use_test()`.

Call `use_test("objective")`[2] and insert this:

```
test_that("multiplication works", {
  # add a test using expect_equal()
})
```

[2] It's good practice to name the test file the same as the file where the function you're testing is defined.

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Call `use_test("objective")`[2] and insert this:

```
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  # add a test using expect_equal()
})
```

Check That Everything Works

Run `devtools::test()`, and hopefully see:

```
[ FAIL 0 | WARN 0 | SKIP 0 | PASS 1 ]
```

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Checking

`R CMD check`

R contains functionality for checking that your package is built correctly and you can access this functionality through `devtools::check()`.

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Now run `devtools::check()`. Is there a problem? Yes, let's fix it!

Metadata

The metadata for your package lives in DESCRIPTION. Right now it looks like this:

```
Package: rosenbrock
Title: What the Package Does (One Line, Title Case)
Version: 0.0.0.9000
Authors@R:
    person("First", "Last", , "first.last@example.com", role =
        c("aut", "cre"),
            comment = c(ORCID = "YOUR-ORCID-ID"))
Description: What the package does (one paragraph).
License: `use_mit_license()`, `use_gpl3_license()` or friends
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Encoding: UTF-8
Roxygen: list(markdown = TRUE)
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```

For now we'll leave most of these files alone, but let's fix one thing: the license

Licensing

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So we need to pick a license: for now we’ll pick the MIT license.[3]

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Choosing a License

So we need to pick a license: for now we'll pick the MIT license.[3]

```
usethis::use_mit_license()
```

This will add new files to your package: `LICENSE`, `LICENSE.md`, and modify `DESCRIPTION`, in which you should see:

```
License: MIT + file LICENSE
```

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One way to do so is to use numerical differentiation through the **numDeriv** package:

```
gradient <- function(x, a = 1, b = 100) {
  numDeriv::grad(objective, x, a = a, b = b)
}
```

Now our package depends on **numDeriv**, so we need to add it to `DESCRIPTION`:

```
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In DESCRIPTION, you should now see this:

```
Imports:
  numDeriv
```

Rcpp works best in a package:

- No more manual sourcing (no need to call `Rcpp::sourceCpp()`)
- You don't need to add directives for dependencies to **RcppArmadillo** and other packages.

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We will rely on **roxygen2**. First, call

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usethis::use_package_doc()
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to set up a package doc file in `R/rosenbrock-package.R`.

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```
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to set up a package doc file in `R/rosenbrock-package.R`.

Then use `usethis::use_rcpp()` to put the pieces in place:

```
rosenbrock/
└─ src/
   └─ slop-package.cpp/
```

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Then use `usethis::use_rcpp()` to put the pieces in place:

```
rosenbrock/
└─src/
  └─slop-package.cpp/
```

Now just need to run `devtools::document()` and `devtools::load_all()` or `devtools::install()` and now your code is available (but not exported).

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Exporting Rcpp Code

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Direct Export

You can add roxygen2 comments in Rcpp code too:

```cpp
//' @export
double my_fun_cpp() {...}
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Direct Export

You can add roxygen2 comments in Rcpp code too:

```
//' @export
double my_fun_cpp() {...}
```

Saves you having to write and maintain an R function.

Documentation

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Types

- Comments in code
- Manual (help files)
- Long-form articles (vignettes)

roxygen2

Primary purpose of the package. You write code is a special syntax and it converts it into manual files that R understands.

roxygen2 Syntax

```r
#' Function Title
#'
#' Here you describe what the function does, possibly
#' using several lines.
#'
#' @param x Explanation of argument x
#'
#' @return Explanation of what the function returns
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Your Turn

Document `objective()` with roxygen2 syntax. No need for sensible documentation. Just make sure you have the bare minimum.

Documentation in This Course

- Not making a package for CRAN, so lower standards.
- You don't need to document to benefit from building a package.
- But it's not a bad idea to do so anyway!

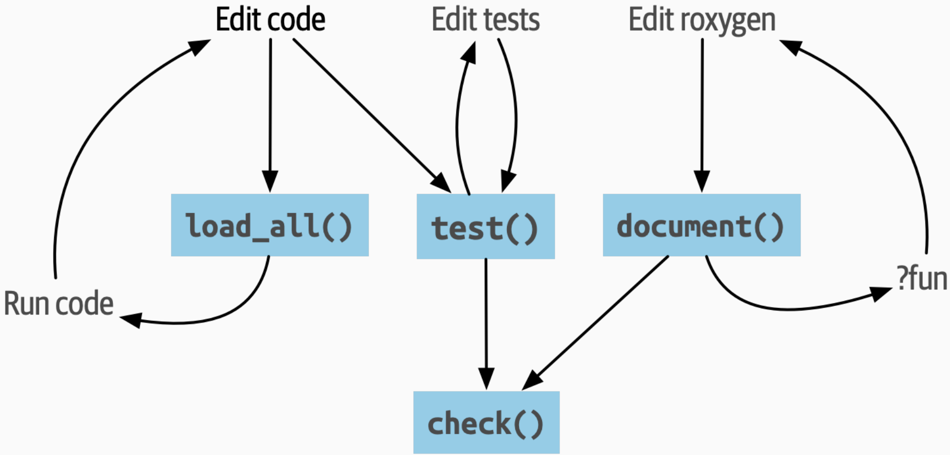

Figure 3: The whole game

Projects

When you have a project, you typically need more things:

- scripts with simulations, etc, which produce output
- datasets stored in different formats
- notebooks (or latex sources)

These things do not naturally fit into a package framework.

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1. Just store these things directly into the package folder. Optionally, you can use `.Rbuildignore` to ignore these files when building the package.

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These things do not naturally fit into a package framework.

Two Choies of Structure

1. Just store these things directly into the package folder. Optionally, you can use `.Rbuildignore` to ignore these files when building the package.
2. Put your **package** into a subdirectory of your project. This cleanly separates the part of your project that contains reusable code (the package) and the part that is experiments and reports. But a little trickier to setup.

Exercise: Two Options

Rosenbrock

Continue building the **rosenbrock** package:

- Write a gradient descent (or stochastic gradient descent) implementation that minimizes the rosenbrock function.

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- Write a gradient descent (or stochastic gradient descent) implementation that minimizes the rosenbrock function.
- Write the code in Rcpp. If you want, you can first write it in R to see that everything is working, and then port it.
- Feel free to use generative AI to write the code.

Exercise: Two Options

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An Assignment

Start trying to convert your work for one assignment into a package

What We Didn't Cover

- Version control through git and github

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- Principled approaches to reproducibility (renv, containers)

Oral Examination Prep

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Examiners
Me and Jonas Gyde Hermansen

It's possible that Niels will show up during one or two of the examinations.

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The Five Points

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- Can you implement alternative solutions?
- Can the code be restructured e.g. by modularization, abstraction or object oriented programming to improve generality, extendability and readability?
- How does the implementation perform (benchmarking)?
- Where are the bottlenecks (profiling), and what can you do about them?

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- Use plots as much as possible
- Good to include math and code, but avoid overwhelming us.

Evaluation Criteria

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Knowledge of fundamental algorithms for statistical computations and R packages that implement some of these algorithms or are useful for developing novel implementations.

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Competence

Ability to select appropriate numerical algorithms for statistical computations and evaluate implementations in terms of correctness, robustness, accuracy and memory and speed efficiency.

Course Summary

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Statistical Topics

Smoothing Kernel density smoothing and splines (topic 1)

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Simulation MC methods: rejection and importance sampling (topic 2)

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Computational Topics

- Debugging
- Profiling
- Benchmarking
- Debugging
- Writing performant code

Thank you (for real this time)!