Variations on Stochastic Gradient Descent

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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What did we actually do?

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?

Organizing Code

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

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).

R Packages

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

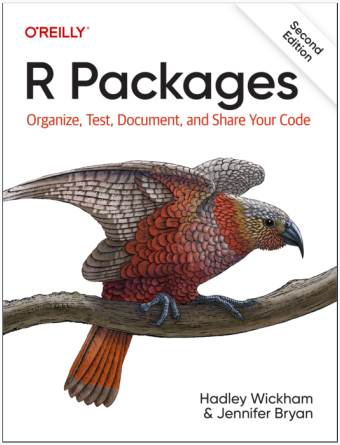


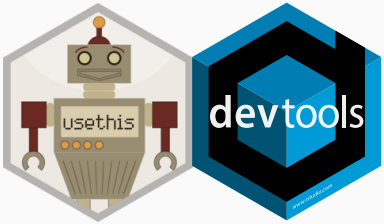
Figure 1: R Packages

Devtools

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

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

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



Rosenbrock Package

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

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

A Toy Example

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- Adding R functions to our package
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- 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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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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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.

Quick but not as robust.

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Try It

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

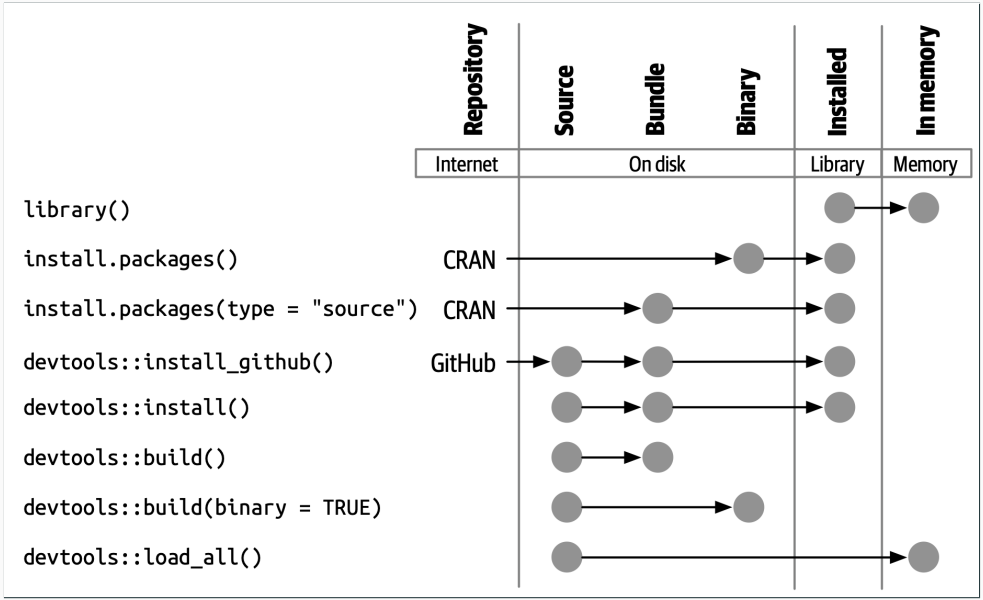

Figure 2: The various states of a package and how to move between them.

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

```
# 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:

```
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```

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

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

roxygen2

roxygen2 is a package that helps with package documentation[1], but it can also be used for handling the namespace.

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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

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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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```

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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NOTE	Typically small issues with your package

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
   to pick a
    license
Encoding: UTF-8
Roxygen: list(markdown = TRUE)
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```

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

Why Do You Need a License?

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

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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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}
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```
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```

In `DESCRIPTION`, you should now see this:

```
Imports:
  numDeriv
```

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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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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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rosenbrock/
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```

Now just need to run `devtools::document()` and `devtools::load_all()` or `devtools::install()` and no your code is available (but not exported).

Exporting Rcpp Code

Wrapping

Call your Rcpp function through an R wrapper:

```
my_fun <- function(x) {
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Exporting Rcpp Code

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Typically easier because checking input and preparing output is easier on the R side.

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Direct Export

You can add roxygen2 comments in Rcpp code too:

```
//' @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.

Why?

Because

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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

```
#' 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
#'
#' @export
my_fun <- function(x) {
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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!

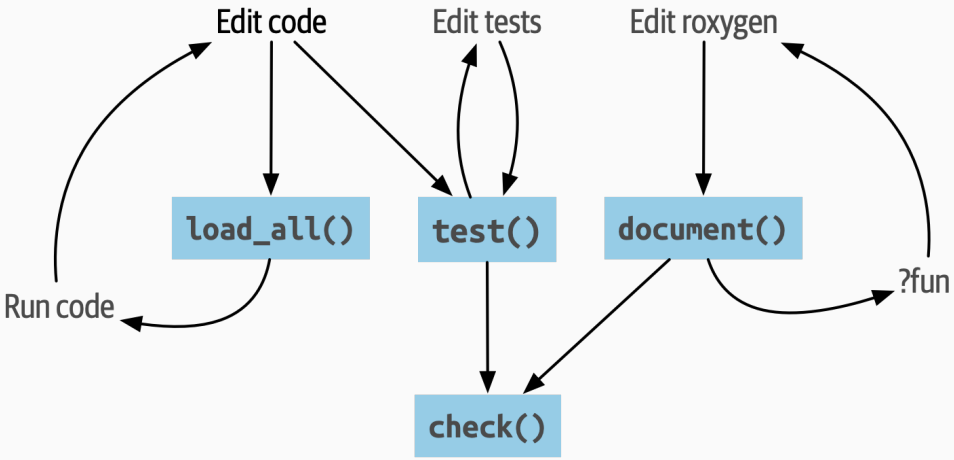

Figure 3: The whole game

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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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

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Continue building the **rosenbrock** package:

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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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- How to properly format metadata (`DESCRIPTION`)

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- Version control through git and github
- How to properly format metadata (`DESCRIPTION`)
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- Publishing to CRAN
- 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 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.

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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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Skills

Ability to implement, test, debug, benchmark, profile and optimize statistical software.

Competence

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

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Statistical Topics

Smoothing Kernel density smoothing and splines (topic 1)

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Computational Topics

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

Thank you (for real this time)!