Project documentation

Best Practices for Writing Reproducible Code // part 3

Project documentation

Why do you need documentation?

- You want yourself to understand how code written some time ago works
- You want others to understand how to (re-)use your code

For this you need to

- Explain parts of your code with comments
- Explain what to install and how to get started in your **readme**
- Explain in-depth use of your code in a notebook

Comments

Comments are annotations you write directly in the code source.

They:

- are written for users who deal with your source code
- explain parts that are not intuitive from the code itself
- do not replace readable or structured code
- (in a specific structure) can be used to directly generate documentation for users.

Comic source: Geek & Poke

When not to use comments

• ...to repeat in natural language what is written in your code

```
# Now we check if the age of a patient is greater than 18
if(agePatient > 18)
```

• ...to turn old code into zombie code (fine for troubleshooting, but do not leave it in!)

```
# Do not run this!!
# itDoesNotWork ← optimizeMulticoreDeepLearning(myProteins)
# if(itDoesNotWork = 1444){
# connection ← connectToHPC(currentUser, password)
#}
```

• ...to replace version control, like git

```
# removed on August 5
# if() ...
#Now, it connects to the API with o-auth2, updated 05/05/2016
•••
```

Comment lines: WHY over HOW

Comment lines are used to explain the **purpose** of some piece of code.

```
# Bug fix GH 20601
# If the data frame is too big, the number of unique index combination
# will cause int32 overflow on windows environments.
# We want to check and raise an error before this happens
num_rows = np.max([index_level.size for index_level in self.new_index_levels])
num_columns = self.removed_level.
```

From Pandas reshape.py documentation

Docstrings

- Structured comments, associated to *segments* (rather than lines) of code, can be used to generate documentation for users* of your project.
- These comments are called *docstrings*.
- Docstrings are parsed as the first statement of a module (e.g. a function or class).
- Docstrings allow you to provide documentation to a function, that is relevant to the user of that function.
- Writing docstrings makes you generate your documentation as you are generating the code: efficiently, comprehensively!

^{*)} Remember? That's probably you!

Generating docstrings

In R you will need a separate package to deal with docstrings:

```
library(docstring)

multiply ← function(x,y){
  #' @title Multiply two numbers
  #' @description This function takes two
  #' input numbers and multiplies
  #' them. It returns the multiplied result.
  #' @param x The first value
  #' @param y The second value
  #' @return The two arguments multiplied.
  return(x*y)
}

?multiply
```

multiply {TempPackage}

Multiply two numbers

Description

This function takes two input numbers and multiplies them. It returns the multiplied result.

Usage

multiply(x, y)

Arguments

- x The first value
- The second value

Value

The two arguments multiplied.

Much more information in the vignette for docstring.

Generating docstrings

In Python, docstrings are string literal comments following a function declaration:

```
def multiply(x,y):
    """

Multiply two numbers

This function takes two input numbers and multiplies them.
It returns the multiplied result.
Keyword arguments:
    x -- the first value
    y -- the second value
    """
    return x*y
```

NB: a triple single quote (''') works, but PEP style prefers double quotes for docstrings.

A glimpse into code generation

Docstrings are formatted so that they can easily be turned into documentation of your package.

You will need additional tools:

- http://www.doxygen.nl/ : C++ (and many more languages)
- http://www.sphinx-doc.org/ : Python
- https://roxygen2.r-lib.org/: R

We will not do this today, but it is worth checking out if you want to release your code!

A glimpse into code generation

In the console, in RStudio, run the following command:

roxygen2::roxygenise()

The command above will create documentation files that can be visualized by calling help(your package)



NB This works for R packages, with the proper file structure. See here: http://r-pkgs.had.co.nz/intro.html

Your turn (choose one!)

1. Comment lines

- a. Do you have superfluous comments? Remove them!
 - Remove your zombie code and version control-like comments
 - See if you can replace a 'how' comment for a 'why' comment (what is the purpose of this code? rather than this is how this code works)
- b. Are there elements without comments that need them? Add them!
 - Have you found yourself staring at a piece of code for too long without understanding it? Perhaps it needs more information!
 - Try to comment on the thought behind the code rather than phrasing it in English.

2. Docstrings

- Add a docstring to a function, preferably the last function you worked on (so it's fresh in your memory).
- Keep in mind: what does my user need to know when they are working with this function?

README

The README page is the first thing your user will see!

The contents typically include one or more of the following:

- Configuration instructions
- Installation instructions
- Operating instructions
- A file manifest (list of files included)
- Copyright and licensing information
- Contact information for the distributor or programmer
- Known bugs
- Troubleshooting
- Credits and acknowledgments

From wikipedia's Readme page

An example



build passing op build passing

coverage 88 % pypi v2.0.1 DOI 10.5281/zenodo.596127 launch binder

The goal of mcfly is to ease the use of deep learning technology for time series classification. The advantage of deep learning is that it can handle raw data directly, without the need to compute signal features. Deep learning does not require expert domain knowledge about the data, and has been shown to be competitive with conventional machine learning techniques. As an example, you can apply mcfly on accelerometer data for activity classification, as shown in the tutorial.

Installation

Prerequisites:

- Python 2.7, 3.5 or 3.6
- pip

Installing all dependencies in sparate conda environment:

```
conda env create -f environment.yml
# activate this new environment
source activate mcfly
```

README examples and templates

Some examples from projects with high quality documentation:

Bigger community software projects:

- Python's Pandas
- Scikit-learn
- Tidyverse's Dplyr

Research software:

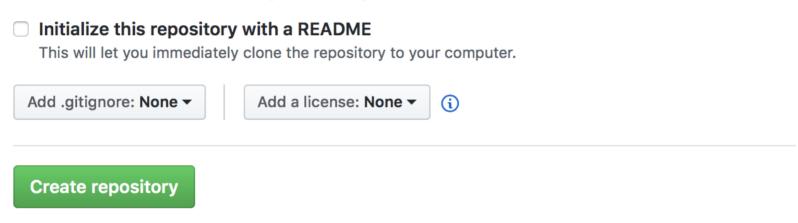
- e-science center's 'McFly' tool
- Utrecht University's: Automatic Systematic Review
- Utrecht University's MICE

Templates and ideas:

- https://gist.github.com/PurpleBooth/109311bb0361f32d87a2
- https://github.com/matiassingers/awesome-readme

README how?

When you create a repository on Github, there is an option to include a README file
 Skip this step if you're importing an existing repository.



- READMEs are files that can be written as text, and commonly use Markdown for formatting.
- Github will show the content of your README file at the root of the repository.
- Your cookiecutter template included a README, so you are all set!

Your turn!

Edit your README file.

Make sure to include the following information:

- What does your project do?
- How do you start running your project?
 - How does the user download your project? (consider git clone!)
 - How does the user call the main script(s) that should be executed?

And perhaps any other elements you are inspired to add (check out the examples!)