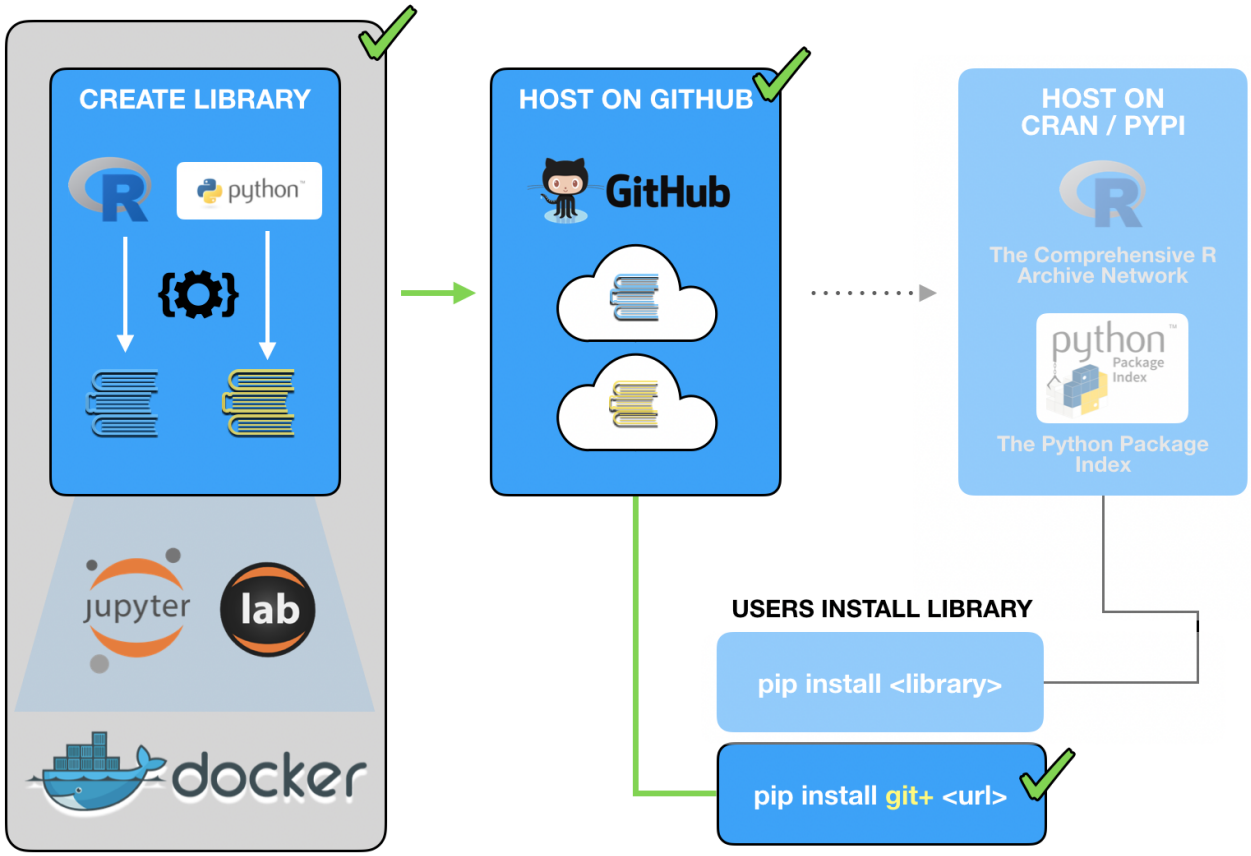
Step-by-Step Guide to Creating R and Python Libraries (in JupyterLab)

Sean McClure Follow
Mar 31 · 32 min read



R and Python are the *bread and butter* of today's machine learning languages. R provides powerful statistics and quick visualizations, while Python offers an intuitive syntax, abundant support, and is the choice interface to today's major AI frameworks.

In this article we'll look at the steps involved in creating libraries in R and Python. This is a skill every machine learning practitioner should have in their toolbox. Libraries help us

organize our code and share it with others, offering packaged functionality to the data community.

> *NOTE: In this article I use the terms "*library*" and "*package*" interchangeably. While some people differentiate these words I don't find this distinction useful, and rarely see it done in practice. We can think of a* ***library*** *(or* ***package****) as a directory of scripts containing functions. Those functions are grouped together to help engineers and scientists solve challenges.*

THE IMPORTANCE OF CREATING LIBRARIES

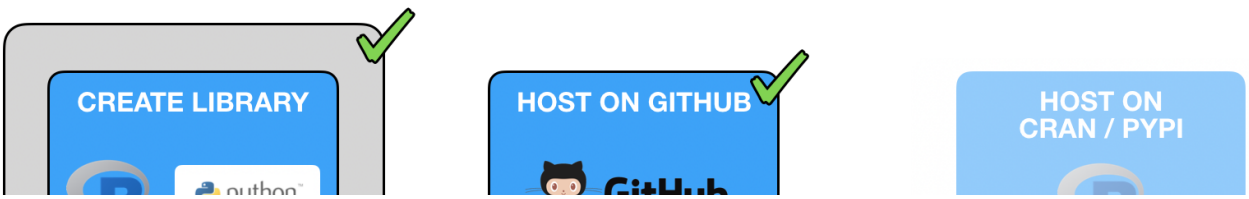
Building today's software doesn't happen without extensive use of libraries. Libraries dramatically cut down the time and effort required for a team to bring work to production. By leveraging the open source community engineers and scientists can move their unique contribution towards a larger audience, and effectively improve the quality of their code. Companies of all sizes use these libraries to sit their work on top of existing functionality, making product development more productive and focused.

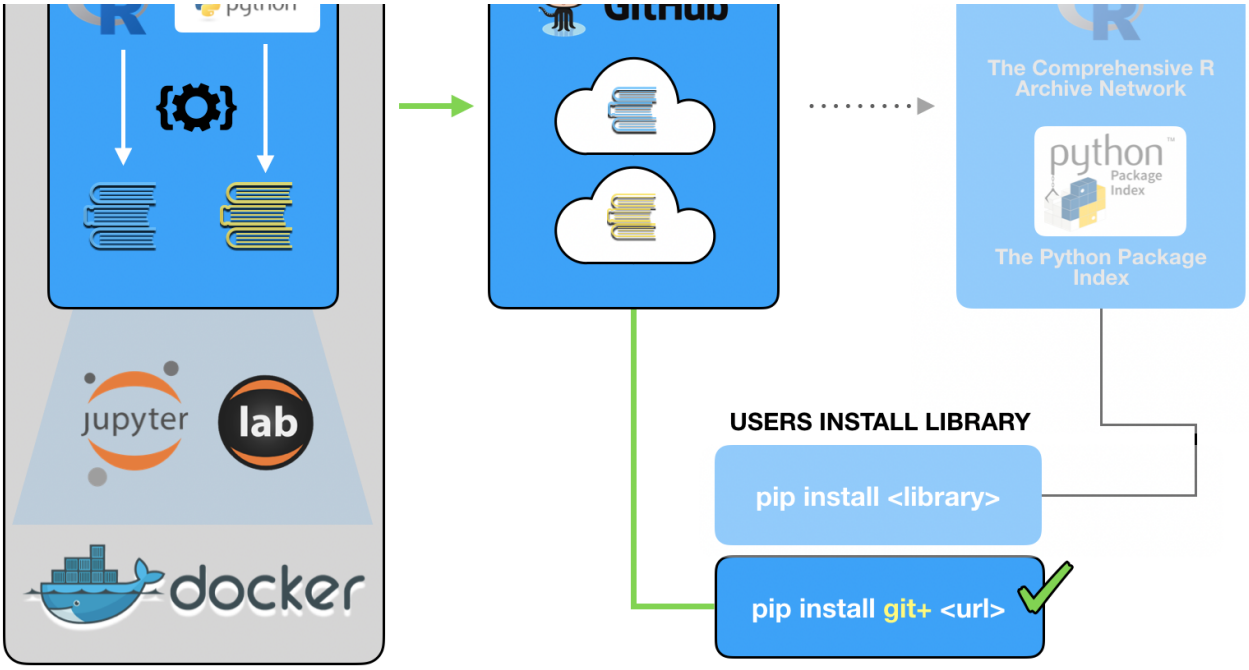
But creating libraries isn't just for production software. Libraries are critical to rapidly prototyping ideas, helping teams validate hypotheses and craft experimental software quickly. While popular libraries enjoy massive community support and a set of best practices, smaller projects can be converted into libraries overnight.

By learning to create lighter-weight libraries we develop an ongoing habit of maintaining code and sharing our work. Our own development is sped up dramatically, and we anchor our coding efforts around a tangible unit of work we can improve over time.

ARTICLE SCOPE

In this article we will focus on creating libraries in R and Python as well as hosting them on, and installing from, GitHub. This means we won't look at popular hosting sites like **CRAN** for R and **PyPI** for Python. These are extra steps that are beyond the scope of this article.





Focusing only on GitHub helps encourage practitioners to develop and share libraries more frequently. CRAN and PyPI have a number of criteria that must be met (and they change frequently), which can slow down the process of releasing our work. Rest assured, it is just as easy for others to install our libraries from GitHub. Also, the steps for CRAN and PyPI can always be added later should you feel your library would benefit from a hosting site.

We will build both R and Python libraries using the same environment (JupyterLab), with the same high-level steps for both languages. This should help you build a working knowledge of the core steps required to package your code as a library.

Let's get started.

SETUP

We will be creating a library called **datapeek** in both R and Python. The datapeek library is a simple package offering a few useful functions for handling raw data. These functions are:

```
encode_and_bind
```

```
remove_features
```

```
apply_function_to_column

get_closest_string
```

We will look at these functions later. For now we need to setup an R and Python environment to create datapeek, along with a few libraries to support packaging our code. We will be using **JupyterLab** inside a **Docker** container, along with a "docker stack" that comes with the pieces we need.

Install and Run Docker

The Docker Stack we will use is called the **jupyter/datascience-notebook**. This image contains both R and Python environments, along with many of the packages typically used in machine learning.

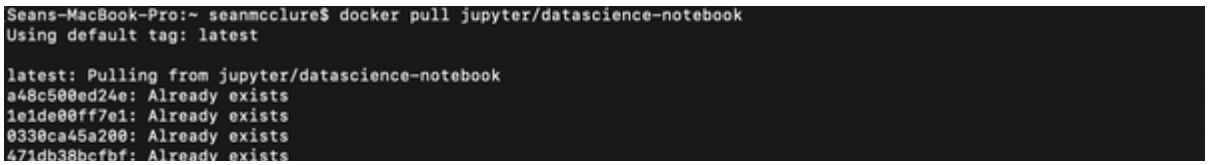
Since these run inside Docker you must have Docker installed on your machine. So **install Docker** if you don't already have it, and once installed, run the following in **terminal** to *pull* the datascience-notebook:

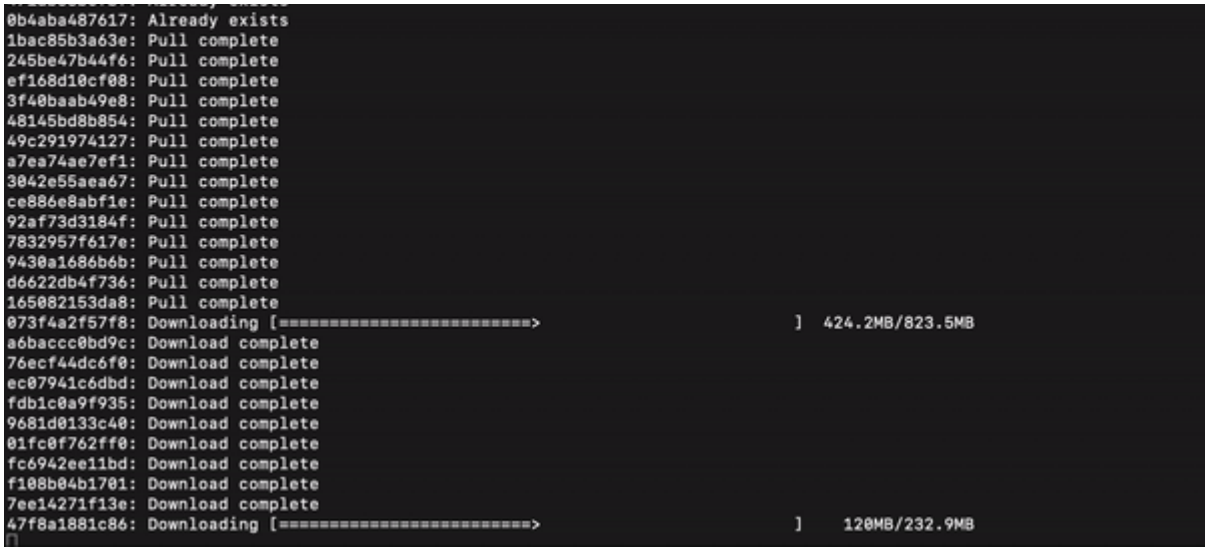
```
docker pull jupyter/datascience-notebook
```

This will pull the most recent image hosted on Docker Hub.

> **NOTE:** *Anytime you pull a project from Docker Hub you get the latest build. If some time passes since your last pull, pull again to update your image.*

Immediately after running the above command you should see the following:





Once everything has been pulled we can **confirm** our new image exists by running the following:

```
docker images
```

… showing something similar to the following:

```
jupyter/datascience-notebook   latest              4bfc95677b8d        16 hours ago        5.61GB
```

Now that we have our Docker stack let's setup JupyterLab.

JupyterLab

We will create our libraries inside a **JupyterLab** environment. JupyterLab is a web-based user interface for programming. With JupyterLab we have a lightweight IDE in the

browser, making it convenient for building quick applications. JupyterLab provides everything we need to create libraries in R and Python, including:

- A **terminal** environment for running shell commands and downloading/installing libraries;
- An R and Python **console** for working interactively with these languages;
- A simple **text editor** for creating files with various extensions;
- Jupyter **Notebooks** for prototyping ML work.

The datascience-notebook we just pulled contains an installation of JupyterLab so we don't need to install this separately. Before running our Docker image we need to **mount a volume** to ensure our work is **saved outside the container**.

First, **create a folder called datapeek** on your desktop (or anywhere you wish) and change into that directory. We need to **run our Docker container with JupyterLab**, so our full command should look as follows:

```
docker run -it -v `pwd`:/home/jovyan/work -p 8888:8888
jupyter/datascience-notebook start.sh jupyter lab
```

You can learn more about Docker commands here. Importantly, the above command exposes our environment on port 8888, meaning we can access our container through the browser.

After running the above command you should see the following output at the end:

```
To access the notebook, open this file in a browser:
    file:///home/jovyan/.local/share/jupyter/runtime/nbserver-8-open.html
Or copy and paste one of these URLs:
    http://(73c37a7b46a8 or 127.0.0.1):8888/?token=11e5027e9f7cacebac465d79c9548978b03aaf53131ce5fd
```

This tells us to **copy and paste** the provided URL into our browser. Open your browser and add the link in the address bar and hit enter (your token will be different):

```
localhost:8888/?
token=11e5027e9f7cacebac465d79c9548978b03aaf53131ce5fd
```

This will automatically open JupyterLab in your browser as a new tab:

We are now ready to start building libraries.

We begin this article with **R**, then look at **Python**.

CREATING LIBRARIES IN R

R is one of the “big 2” languages of machine learning. At the time of this writing it has well-over 10,000 libraries. Going to *Available CRAN Packages By Date of Publication* and running…

```
document.getElementsByTagName('tr').length
```

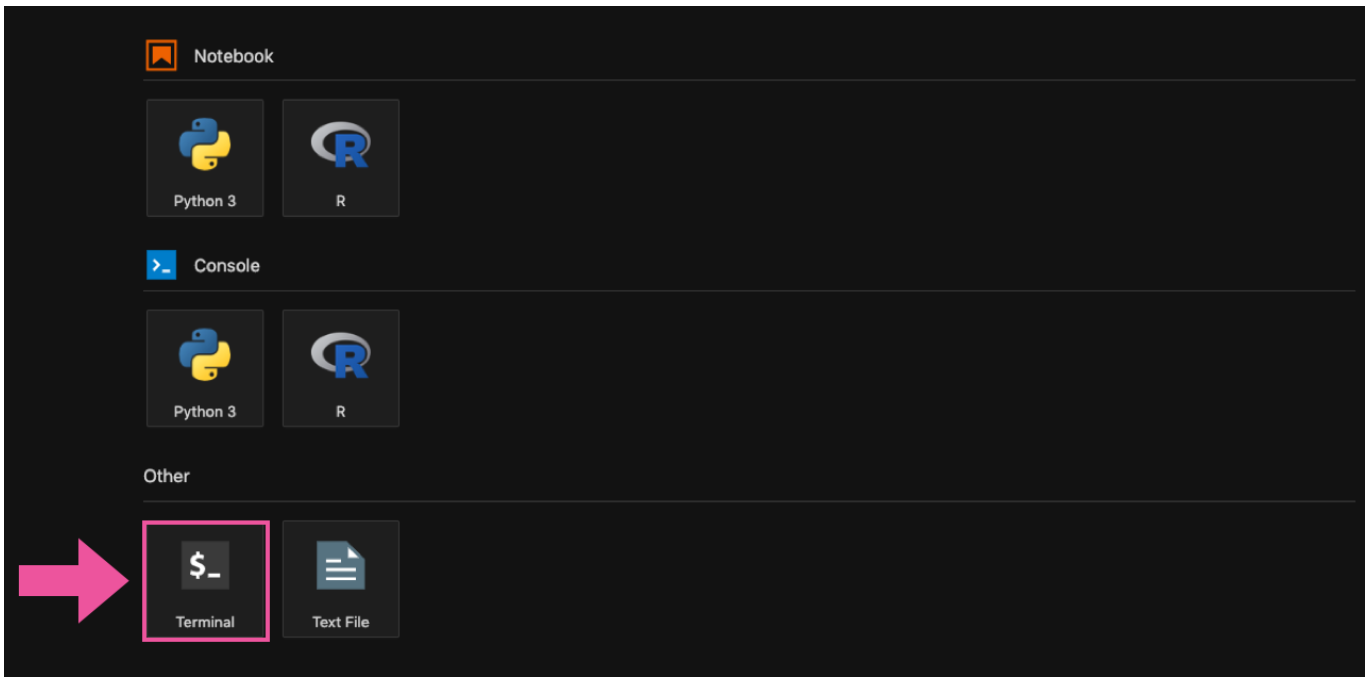
…in the browser console gives me 13858. Minus the header and final row this gives **13856** packages. Needless to say R is not in need of variety. With strong community support and a concise (if not intuitive) language, R sits comfortably at the top of statistical languages worth learning.

The most well-known treatise on creating R packages is **Hadley Wickam**'s book R Packages. Its contents are available for free online. For a deeper dive on topic I recommend looking there.

We will use Hadley's **devtools** package to abstract away the tedious tasks involved in creating packages. devtools is *already installed* in our Docker Stacks environment. We also require the **roxygen2** package, which helps us document our functions. Since this doesn't come pre-installed with our image let's install that now.

> ***NOTE:*** *From now on we'll* ***use the terminal in JupyterLab*** *in order to conveniently keep our work within the browser.*

Open terminal inside JupyterLab's Launcher:



> ***NOTE**: If you'd like to change your JupyterLab to **dark theme**, click on* Settings *at the top,* JupyterLab Theme*, then* JupyterLab Dark*:*

Inside the console type R, then….

```
install.packages("roxygen2")
library(roxygen2)
```

With the necessary packages installed we're ready to tackle each step.

STEP 1: Create Package Framework

We need to create a directory for our package. We can do this in one line of code, using the devtools **create** function. In terminal run:

```
devtools::create("datapeek")
```

This automatically creates the bare bone files and directories needed to define our R package. In JupyterLab you will see a set of new folders and files created on the left side.

> ***NOTE**: You will also see your new directory structure created on your desktop (or wherever you chose to create it) since we **mounted a volume** to our container during setup.*

If we inspect our package in JupyterLab we now see:

```
datapeek
├── R
├── datapeek.Rproj
├── DESCRIPTION
├── NAMESPACE
```

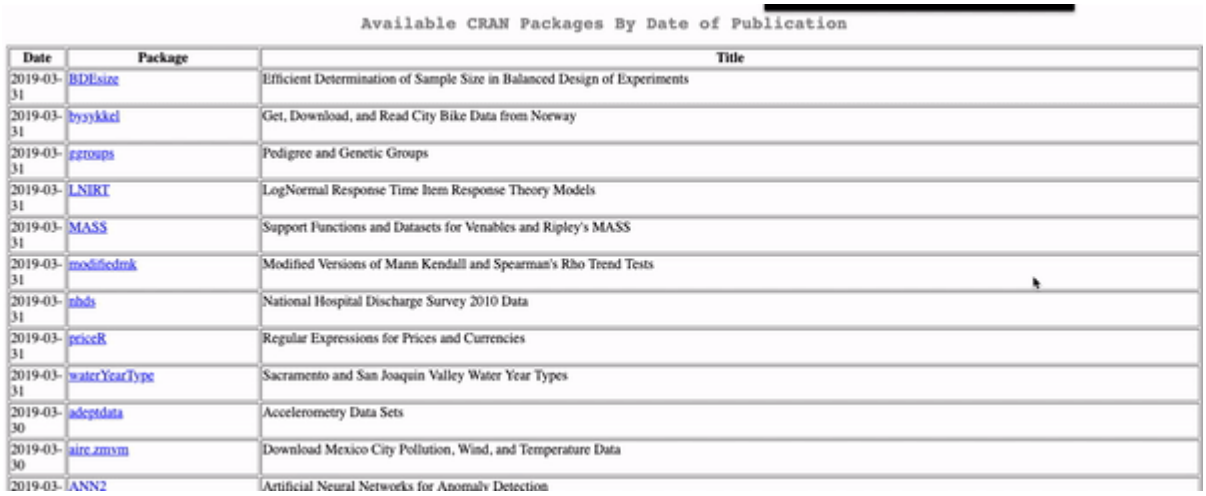
The **R** folder will eventually contain our *R code*. The **my_package.Rproj** file is specific to the *RStudio* IDE so we can ignore that. The **DESCRIPTION** folder holds our package's *metadata* (a detailed discussion can be found here). Finally, **NAMSPACE** is a file that ensures our library plays nicely with others, and is more of a CRAN requirement.

Naming Conventions

We must follow these **rules** when naming an R package:

- must be unique on **CRAN** (you can check all current R libraries here);
- can *only consist* of **letters**, **numbers** and **periods**;
- *cannot contain* an **underscore** or **hyphen**;
- must *start* with a **letter**;
- cannot *end* in a **period**;

You can read more about naming packages here. Our package name "datapeek" passes the above criteria. Let's head over to CRAN and do a *Command+F* search for "datapeek" to ensure it's not already taken:



Available CRAN Packages By Date of Publication

Date	Package	Title
2019-03-31	BDEsize	Efficient Determination of Sample Size in Balanced Design of Experiments
2019-03-31	bysykkel	Get, Download, and Read City Bike Data from Norway
2019-03-31	pgroups	Pedigree and Genetic Groups
2019-03-31	LNIRT	LogNormal Response Time Item Response Theory Models
2019-03-31	MASS	Support Functions and Datasets for Venables and Ripley's MASS
2019-03-31	modifiedmk	Modified Versions of Mann Kendall and Spearman's Rho Trend Tests
2019-03-31	nhds	National Hospital Discharge Survey 2010 Data
2019-03-31	priceR	Regular Expressions for Prices and Currencies
2019-03-31	waterYearType	Sacramento and San Joaquin Valley Water Year Types
2019-03-30	adeptdata	Accelerometry Data Sets
2019-03-30	aire.zmvm	Download Mexico City Pollution, Wind, and Temperature Data
2019-03-	ANN2	Artificial Neural Networks for Anomaly Detection

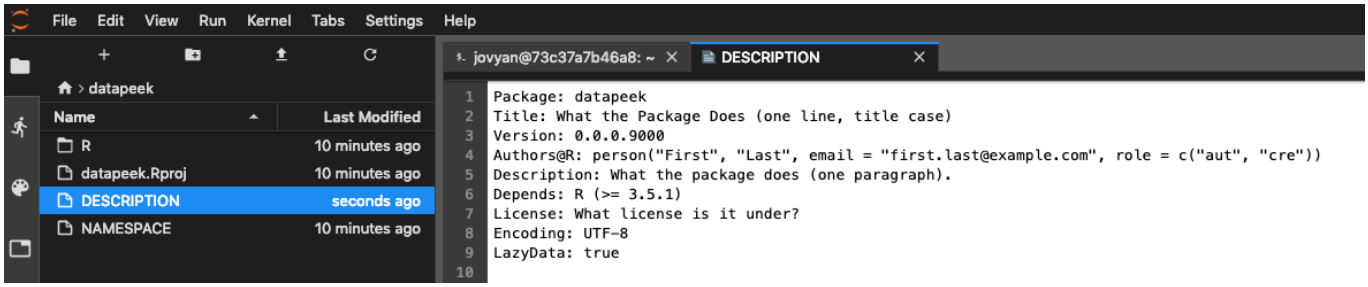
Command + F search on CRAN to check for **package name uniqueness.**

…looks like we're good.

STEP 2: Fill Out Description Details

The job of the `DESCRIPTION` file is to store important *metadata* about our package. These data include **others packages** required to run our library, our **license**, and our **contact** information. Technically, the definition of a package in R is any directory containing a `DESCRIPTION` file, so always ensure this is present.

Click on the DESCRIPTION file in JupyterLab's directory listing. You will see the basic details created automatically when we ran `devtools::create("datapeek")` :



Let's add our specific details so our package contains the necessary metadata. Simply edit this file inside JupyterLab. Here are the details I am adding:

- **Package**: `datapeek`
- **Title**: `Provides useful functions for working with raw data.`
- **Version**: `0.0.0.1`
- **Authors@R**: `person("Sean", "McClure", email="sean.mcclure@example.com", role=c('aut','cre'))`
- **Description**: The datapeek package helps users transform raw data for machine learning development.
- **Depends**: `R (≥ 3.5.1)`
- **License**: `MIT`
- **Encoding**: `UTF-8`
- **LazyData**: `true`

Of course you should fill out these parts with your own details. You can read more about the definitions of each of these in Hadley's chapter on metadata. As a brief overview…

the `package`, `title`, and `version` parts are self-explanatory, just be sure to *keep* `title` *to one line*. `Authors@R` must adhere to the format you see above, since it contains executable R code. Note the **role** argument, which allows us to list the main contributors of our library. The usual ones are:

`aut` : *author*

`cre` : *creator or maintainer*

`ctb` : *contributors*

`cph` : *copyright holder*

There are many more options, with the full list found here.

You can add **multiple authors** by listing them as a vector:

```
Authors@R: as.person(c(
    "Sean McClure <sean.mcclure@example.com> [aut, cre]",
    "Rick Deckard <rick.deckard@example.com> [aut]",
    "Rachael Tyrell <rachel.tyrell@example.com> [ctb]"
))
```

> ***NOTE**: If you do plan on hosting your library on CRAN be sure your email address is correct, as CRAN will use this to contact you.*

The `description` can be multiple lines, limited to 1 paragraph. We use `depends` to specify the minimum version of R our package depends on. You should use an R version equal or greater than the one you used to build your library. Most people today set their `License` to MIT, which permits anyone to "use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software" as long as your copyright is included. You can learn more about the MIT license here. `Encoding` ensures our library can be opened, read and saved using modern parsers, and `LazyData` refers to how data in our package are loaded. Since we set ours to true it means our data won't occupy memory until they are used.

STEP 3: Add Functions

3A: Add Functions to R Folder

Our library wouldn't do much without functions. Let's add the 4 functions mentioned in the beginning of this article. The following GIST shows our datapeek functions in R:

```r
library(data.table)
library(mltools)

encode_and_bind <- function(frame, feature_to_encode) {
    res <- cbind(iris, one_hot(as.data.table(frame[[feature_to_encode]])))
    return(res)
}

remove_features <- function(frame, features) {
  rem_vec <- unlist(strsplit(features, ', '))
  res <- frame[,!(names(frame) %in% rem_vec)]
  return(res)
}

apply_function_to_column <- function(frame, list_of_columns, new_col, funct) {
    use_cols <- unlist(strsplit(list_of_columns, ', '))
    new_cols <- unlist(strsplit(new_col, ', '))
    frame[new_cols] <- apply(frame[use_cols], 2, function(x) {eval(parse(text=funct))})
    return(frame)
}

get_closest_string <- function(vector_of_strings, search_string) {
    all_dists <- adist(vector_of_strings, search_string)
    closest <- min(all_dists)
    res <- vector_of_strings[which(all_dists == closest)]
    return(res)
}
```

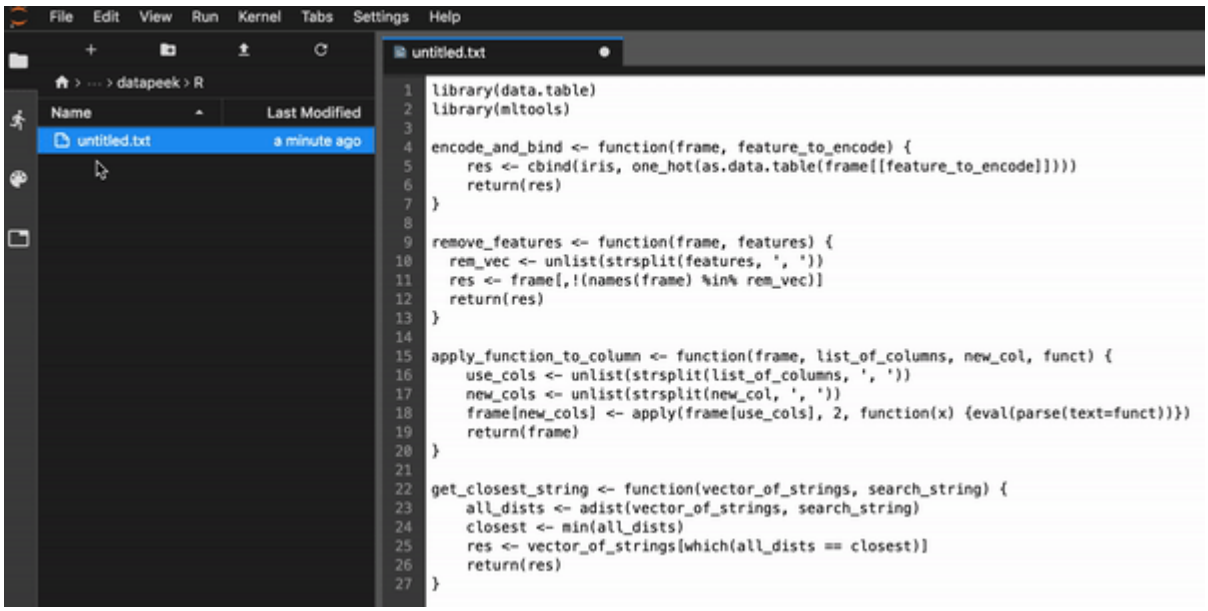
utilities.R hosted with ♡ by GitHub view raw

We have to add our functions to the **R folder**, since this is where R looks for any functions inside a library.

```
datapeek
├── R
├── datapeek.Rproj
├── DESCRIPTION
├── NAMESPACE
```

Since our library only contains 4 functions we will place all of them into a single file called **utilities.R**, with this file residing inside the R folder.

Go into the **directory** in JupyterLab and open the R folder. **Click on *Text File*** in the Launcher and paste in our 4 R functions. Right-click the file and **rename** it to utilities.R.



3B: Export our Functions

It isn't enough to simply place R functions in our file. Each function must be *exported* to expose them to users of our library. This is accomplished by adding the **@export tag** above each function.

The export syntax comes from *Roxygen*, and ensures our function gets added to the NAMESPACE. Let's **add the @export tag** to our first function:

```r
#' @export
encode_and_bind <- function(frame, feature_to_encode) {
    res <- cbind(iris, one_hot(as.data.table(frame[[feature_to_encode]])))
    return(res)
}
```

encode_and_bind.R hosted with ♡ by GitHub view raw

Do this for the remaining functions as well.

> **NOTE**: *In larger libraries we would only export functions that need to be usable outside our package. This helps reduce the chances of a conflict with another library.*

3C: Document our Functions

It is important to document our functions. Documenting functions provides information for users, such that when they type `?datapeek` they get details about our package. Documenting also supports working with vignettes, which are a long-form type of documentation. You can read more about documenting functions here.

There are **2 sub-steps** we will take:

- **add** the document annotations
- **run** `devtools::document()`

— Add the Document Annotations

Documentation is added **above our function**, directly above our `#' @export` line. Here's the example with our first function:

```
#' One-hot encode categorical variables.
#'
#' This function one-hot encodes categorical variables and binds the entire frame.
#'
#' @param data frame
#' @param feature to encode
#' @return hot-encoded data frame
#'
#' @export
encode_and_bind <- function(frame, feature_to_encode) {
    res <- cbind(iris, one_hot(as.data.table(frame[[feature_to_encode]])))
    return(res)
}
```

encode_and_bind.R hosted with ♡ by GitHub view raw

We space out the lines for readability, adding a title, description, and any parameters used by the function. Let's do this for our remaining functions:

```
library(data.table)
```

```
library(mltools)

#' One-hot encode categorical variables.
#'
#' This function one-hot encodes categorical variables and binds the entire frame.
#'
#' @param data frame
#' @param feature to encode
#' @return hot-encoded data frame
#'
#' @export
encode_and_bind <- function(frame, feature_to_encode) {
    res <- cbind(iris, one_hot(as.data.table(frame[[feature_to_encode]])))
    return(res)
}

#' Remove specified features from data frame.
#'
#' This function removes specified features from data frame.
#'
#' @param data frame
#' @param features to remove
#' @return original data frame less removed features
#'
#' @export
remove_features <- function(frame, features) {
  rem_vec <- unlist(strsplit(features, ', '))
  res <- frame[,!(names(frame) %in% rem_vec)]
  return(res)
}

#' Apply function to multiple columns.
#'
#' This function enables the application of a function to multiple columns.
#'
#' @param data frame
#' @param list of columns to apply function to
#' @param name of new column
#' @param function to apply
#' @return original data frame with new column attached
#'
#' @export
apply_function_to_column <- function(frame, list_of_columns, new_col, funct) {
    use_cols <- unlist(strsplit(list_of_columns, ', '))
    new_cols <- unlist(strsplit(new_col, ', '))
```

```
    new_cols <- unlist(strsplit(new_col, ","))
    frame[new_cols] <- apply(frame[use_cols], 2, function(x) {eval(parse(text=funct))})
    return(frame)
}

#' Discover closest matching string from set.
#'
#' This function discovers the closest matching string from vector of strings.
#'
#' @param vector of strings
#' @param search string
#' @return closest matching string
#'
#' @export
get_closest_string <- function(vector_of_strings, search_string) {
    all_dists <- adist(vector_of_strings, search_string)
    closest <- min(all_dists)
    res <- vector_of_strings[which(all_dists == closest)]
    return(res)
}
```

all_functions.R hosted with ♡ by GitHub view raw

— Run `devtools::document()`

With documentation added to our functions we then **run the following in terminal**, just outside the root directory:

```
devtools::document()
```

> ***NOTE:*** *Make sure you're one level outside the datapeek directory.*

You may get the **error**:

```
Error: 'roxygen2' >= 5.0.0 must be installed for this functionality.
```

In this case **open terminal in JupyterLab** and **install roxygen2**. You should also install data.table and mltools, since our first function uses these:

```
install.packages('roxygen2')
install.packages('data.table')
install.packages('mltools')
```

Run the `devtools::document()` again. You should see the following:

```
[7]: devtools::document()

     Updating datapeek documentation
     Loading datapeek
     Updating roxygen version in /home/jovyan/work/datapeek/DESCRIPTION
     Writing NAMESPACE
     Writing NAMESPACE
     Writing encode_and_bind.Rd
     Writing remove_features.Rd
     Writing apply_function_to_column.Rd
     Writing get_closest_string.Rd
```

This will generate **.Rd files** inside a new **man folder**. You'll notice an .Rd file is created for *each* function in our package.

If you look at your DESCRIPTION file it will now show a new line at the bottom:

```
Package: datapeek
Title: Provides useful functions for working with raw data.
Version: 0.0.0.1
Authors@R: person("Sean", "McClure", email="sean.mcclure@example.com", role = c('aut','cre'))
Description: The datapeek package helps users transform raw data for machine learning development.
Depends: R (>= 3.5.1)
License: MIT
Encoding: UTF-8
LazyData: true
RoxygenNote: 6.1.1
```

This will also generate a NAMESPACE file:

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

export(apply_function_to_column)
export(encode_and_bind)
export(get_closest_string)
export(remove_features)
```

We can see our 4 functions have been exposed. Let's now move onto ensuring dependencies are specified inside our library.

STEP 4: List External Dependencies

It is common for our functions to require functions found in other libraries. There are 2 things we must do to ensure external functionality is made available to our library's functions:

1. **Use double colons** inside our functions to specify which library we are relying on;
2. **Add imports** to our DESCRIPTION file.

You'll notice in the above GIST we simply listed our libraries at the top. While this works well in stand-alone R scripts it isn't the way to use dependencies in an R package. When creating R packages we must use the "***double-colon approach***" to ensure the correct function is read. This is related to how "top-level code" (code that isn't an object like a function) in an R package is *only executed when the package is built*, not when it's loaded.

For example:

```
library(mltools)

do_something_cool_with_mltools <- function() {
    auc_roc(preds, actuals)
}
```

…won't work because `auc_roc` will not be available (running library(datapeek) doesn't re-execute library(mltools)). This *will* work:

```
do_something_cool_with_mltools <- function() {
    mltools::auc_roc(preds, actuals)
}
```

The only function in our datapeek package requiring additional packages is our first one:

```
#' One-hot encode categorical variables.
#'
#' This function one-hot encodes categorical variables and binds the entire frame.
#'
#' @param data frame
```

```r
#' @param feature to encode
#' @return hot-encoded data frame
#'
#' @export
encode_and_bind <- function(frame, feature_to_encode) {
    res <- cbind(iris, mltools::one_hot(data.table::as.data.table(frame[[feature_to_encode]])))
    return(res)
}
```

encode_and_bind.R hosted with ♡ by GitHub view raw

Using the double-colon approach to specify dependent packages in R.

Notice **each time** we call an external function we preface it with the external library and double colons.

We must also list external dependencies in our `DESCRIPTION` file, so they are handled correctly. Let's **add our imports to the DESCRIPTION file**:

```
Package: datapeek
Title: Provides useful functions for working with raw data.
Version: 0.0.0.1
Authors@R: person("Sean", "McClure", email="sean.mcclure@example.com", role = c('aut','cre'))
Description: The datapeek package helps users transform raw data for machine learning development.
Depends: R (>= 3.5.1)
License: MIT
Encoding: UTF-8
LazyData: true
RoxygenNote: 6.1.1
Imports:
    data.table,
    mltools
```

Be sure to have the imported libraries comma-separated. Notice we didn't specify any **versions** for our external dependencies. If we need to specify versions we can use parentheses after the package name:

```
Imports:
    data.table (>= 1.12.0)
```

Since our `encode_and_bind` function isn't taking advantage of any bleeding-edge updates we will leave it without any version specified.

STEP 5: Add Data

Sometimes it makes sense to include data inside our library. Package data can allow our user's to practice with our library's functions, and also helps with *testing*, since machine learning packages will always contain functions that ingest and transform data. The 4 options for adding *external data* to an R package are:

1. **binary** data
2. **parsed** data
3. **raw** data
4. **serialized** data

You can learn more about these different approaches here. For this article we will stick with the most common approach, which is to **add external data to an R folder**.

Let's add the Iris dataset to our library in order to provide users a quick way to test our functions. The data must be in the **.rda format**, created using R's `save()` function, and have the **same name** as the file. We can ensure these criteria are satisfied by using devtools' `use_data` function:

```
x <- read.csv("http://bit.ly/2HuTS0Z")
devtools::use_data(x, iris)
```

Above, I read in the Iris dataset from its URL and pass the data frame to `devtools::use_data()`.

In JupyterLab we see a new data folder has been created, along with our iris.rda dataset:

```
datapeek
├── data
│   └── iris.rda
├── man
├── R
├── datapeek.Rproj
├── DESCRIPTION
├── NAMESPACE
```

We will use our added dataset to run tests in the following section.

STEP 6: Add Tests

Testing is an important part of software development. Testing helps ensure our code works as expected, and makes debugging our code a much faster and more effective process. Learn more about testing R packages here.

A common challenge in testing is knowing what we should test. Testing every function in a large library is cumbersome and not always needed, while not enough testing can make it harder to find and correct bugs when they arise.

I like the following quote from Martin Fowler regarding when to test:

> "Whenever you are tempted to type something into a print statement or a debugger expression, write it as a test instead." — Martin Fowler

If you prototype applications regularly you'll find yourself writing to the console frequently to see if a piece of code returns what you expect. In data science, writing interactive code is even more common, since machine learning work is highly experimental. On one hand this provides ample opportunity to think about which tests to write. On the other hand, the non-deterministic nature of machine learning code means testing certain aspect of ML can be less than straightforward. As a general rule, look for obvious deterministic pieces of your code that should return the same output every time.

The interactive testing we do in data science is *manual*, but what we are looking for in our packages is **automated testing**. Automated testing means we run a suite of pre-defined tests to ensure our package works end-to-end.

While there are many kinds of tests in software, here we are taking about "**unit tests**." Thinking in terms of unit tests forces us to break up our code into more modular components, which is good practice in software design.

> **NOTE***: If you are used to testing in languages like Python, notice that R is more* ***functional*** *in nature (i.e., methods belong to functions not classes), so there will be some differences.*

There are **2 sub-steps** we will take for testing our R library:

6A: Creating the `tests/testthat` folder;

6B: Writing tests.

— 6A: Creating the `tests/testthat` folder

Just as R expects our R scripts and data to be in specific folders it also expects the same for our tests. To create the tests folder, we run the following in JupyterLab's R console:

```
devtools::use_testthat()
```

You may get the following error:

```
Error: 'testthat' >= 1.0.2 must be installed for this functionality.
```

If so, use the same approach above for installing roxygen2 in Jupyter's terminal.

```
install.packages('testthat')
```

Running `devtools::use_testthat()` will produce the following output:

```
* Adding testthat to Suggests
* Creating `tests/testthat`.
* Creating `tests/testthat.R` from template.
```

There will now be a **new tests folder** in our main directory:

```
datapeek
├── data
├── man
├── R
├── tests
│   └── testthat.R
├── datapeek.Rproj
├── DESCRIPTION
├── NAMESPACE
```

The above command also created a file called `testthat.R` inside the tests folder. This runs all your tests when `R CMD check` runs (we'll look at that shortly). You'll also notice *testthat* has been added under **Suggests** in our `DESCRIPTION` file:

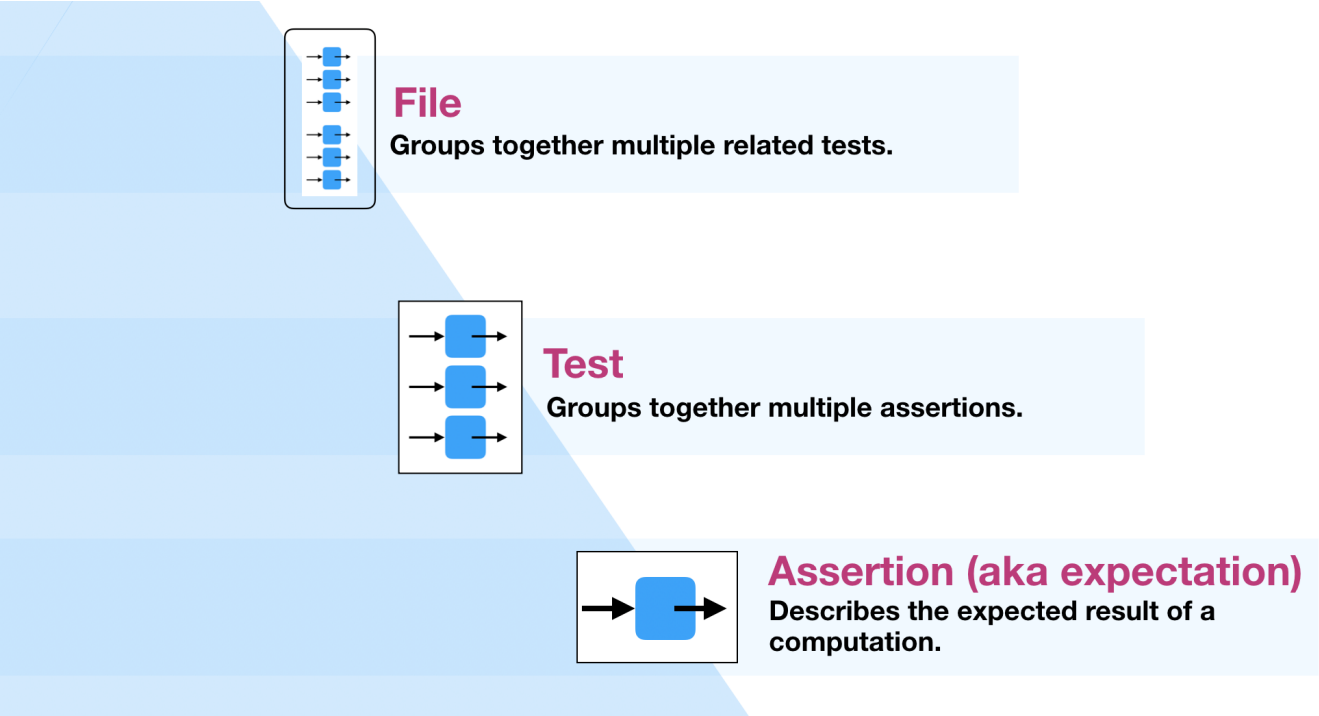
```
Package: datapeek
Title: Provides useful functions for working with raw data.
Version: 0.0.0.1
Authors@R: person("Sean", "McClure", email="sean.mcclure@example.com", role = c('aut','cre'))
Description: The datapeek package helps users transform raw data for machine learning development.
Depends: R (>= 3.5.1)
License: MIT
Encoding: UTF-8
LazyData: true
RoxygenNote: 6.1.1
Imports:
    data.table,
    mltools
Suggests: testthat
```

— 6B: Writing Tests

testthat is the most popular unit testing package for R, used by at least 2,600 CRAN package, not to mention libraries on Github. You can check out the latest news regarding testthat on the Tidyverse page here. Also check out its documentation.

There are 3 levels to testing we need to consider:

- **expectation (assertion):** the expected result of a computation;
- **test:** groups together multiple expectations from a single function, or related functionality from across multiple functions;
- **file:** groups together multiple related tests. Files are given a human readable name with `context()`.



Assertions

Assertions are the functions included in the testing library we choose. We use assertions to check whether our own functions return the expected output. Assertions come in many flavors, depending on what is being checked. In the following section I will cover the main tests used in R programming, showing each one failing so you can understand how it works.

Equality Assertions

- `expect_equal()`
- `expect_identical()`
- `expect_equivalent`

```
# test for equality
a <- 10
expect_equal(a, 14)

> Error: `a` not equal to 14.

# test for identical
expect_identical(42, 2)
```

```
> Error: 42 not identical to 2.

# test for equivalence
expect_equivalent(10, 12)

> Error: 10 not equivalent to 12.
```

There are subtle differences between the examples above. For example, `expect_equal` is used to check for *equality within a numerical tolerance*, while `expect_identical` tests for *exact equivalence*. Here are examples:

```
expect_equal(10, 10 + 1e-7) # true
expect_identical(10, 10 + 1e-7) # false
```

As you write more tests you'll understand when to use each one. Of course always refer to the documentation referenced above when in doubt.

Testing for **String Matches**

- `expect_match()`

```
# test for string matching
expect_match("Machine Learning is Fun", "But also rewarding.")

> Error: "Machine Learning is Fun" does not match "But also
rewarding.".
```

Testing for **Length**

- `expect_length`

```
# test for length
vec <- 1:10
expect_length(vec, 12)

> Error: `vec` has length 10, not length 12.
```

Testing for **Comparison**

- `expect_lt`
- `expect_gt`

```
# test for less than
a <- 11
expect_lt(a, 10)

> Error: `a` is not strictly less than 10. Difference: 1

# test for greater than
a <- 11
expect_gt(a, 12)

> Error: `a` is not strictly more than 12. Difference: -1
```

Testing for **Logic**

- `expect_true`
- `expect_false`

```
# test for truth
expect_true(5 == 2)

> Error: 5 == 2 isn't true.

# test for false
expect_false(2 == 2)

> Error: 2 == 2 isn't false.
```

Testing for **Outputs**

- `expect_output`
- `expect_message`

```
# testing for outputs
expect_output(str(mtcars), "31 obs")

> Error: `str\(mtcars\)` does not match "31 obs".

# test for warning
f <-function(x) {
  if(x < 0) {
    message("*x* is already negative")
  }
}

expect_message(f(1))

> Error: `f(1)` did not produce any messages.
```

There are many more included in the testthat library. If you are new to testing, start writing a few simple ones to get used to the process. With time you'll build an intuition around what to test and when.

Writing Tests

A **test** is a *group of assertions*. We write tests in testthat as follows:

```
test_that("this functionality does what it should", {
    // group of assertions here
})
```

We can see we have both a **description** (the *test name*) and the **code** (containing the assertions). The description completes the sentence, "test that ...."

Above, we are saying "*test that* this functionality does what it should."

The assertions are the outputs we wish to test. For example:

```
test_that("trigonometric functions match identities", {
      expect_equal(sin(pi / 4), 1 / sqrt(2))
      expect_equal(cos(pi / 4), 1 / sqrt(10))
      expect_equal(tan(pi / 4), 1)
    })

> Error: Test failed: 'trigonometric functions match identities'
```

> **NOTE**: *It is worth considering the balance between cohesion and coupling with our test files. As stated in Hadley's book, "the two extremes are clearly bad (all tests in one file, one file per test). You need to find a happy medium that works for you. A good starting place is to have one file of tests for each complicated function."*

Creating Files

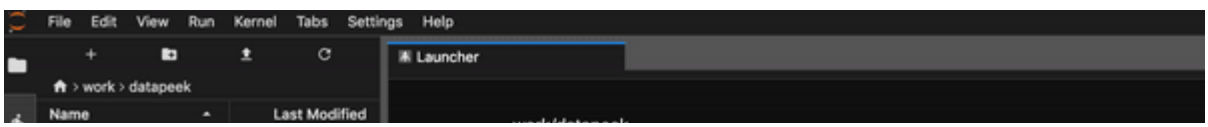
The last thing we do in testing is create files. As stated above, a"file" in testing is a group of tests covering a related set of functionality. Our test file must live inside the `tests/testthat/` directory. Here is an example test file for the *stringr* package on GitHub:

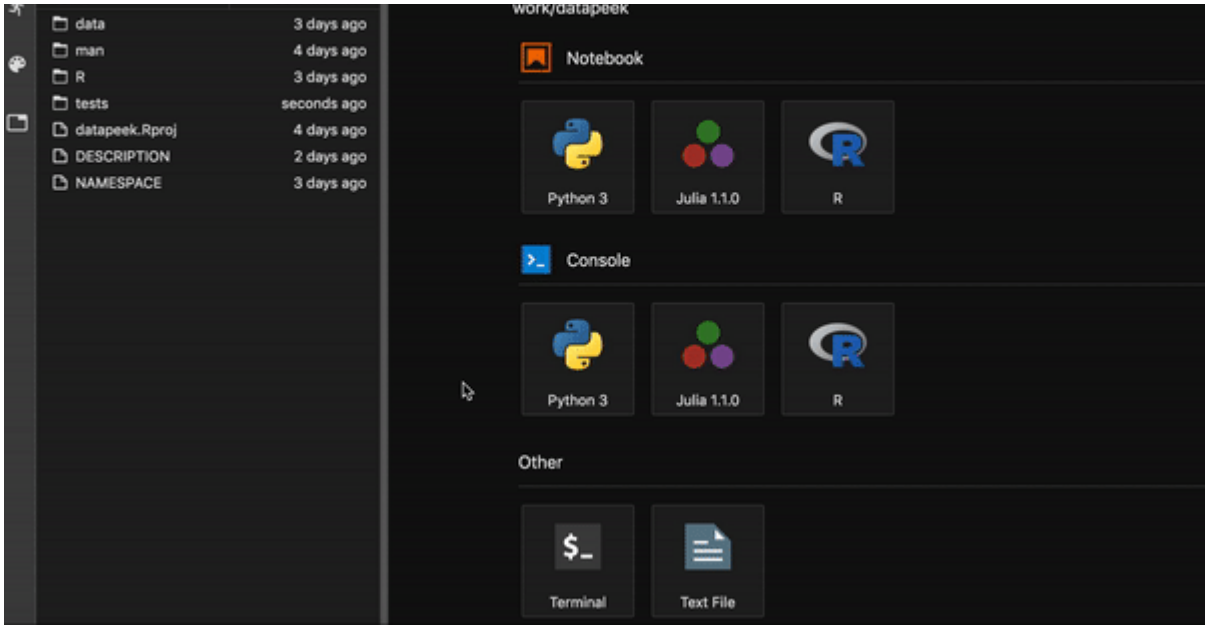
```
context("case")

x <- "This is a sentence."

test_that("to_upper and to_lower have equivalent base versions", {
  expect_identical(str_to_upper(x), toupper(x))
  expect_identical(str_to_lower(x), tolower(x))
})

test_that("to_title creates one capital letter per word", {
  expect_equal(str_count(x, "\\W+"), str_count(str_to_title(x), "[[:upper:]]"))
})

test_that("to_sentence capitalizes just the first letter", {
  expect_identical(str_to_sentence("a Test"), "A test")
})
```

Example Test File from the stringr package on GitHub.

The file is called test-case.R (starts with "test") and lives inside the `tests/testthat/` directory. The *context* at the top simply allows us to provide a simple description of the file's contents. This appears in the console when we run our tests.

Let's **create our test file**, which will contain tests and assertions related to our 4 functions. As usual, we use JupyterLab's Text File in Launcher to create and rename a new file:





Creating a Test File in R

Now let's add our tests:

For the first function I am going to **make sure a data frame with the correct number of features is returned**:

```
context('utility functions')

library(data.table)
library(mltools)

load('../../data/iris.rda')

test_that("data frame with correct number of features is returned", {
    res <- encode_and_bind(iris, 'Species')
    expect_equal(dim(res)[2], 8)
})
```

test-utilities.R hosted with ♡ by GitHub view raw

Notice how we called our `encode_and_bind` function, then simply checked the equality between the dimensions and the expected output. We run our automated tests at any point to ensure our test file runs and we get the expected output. Running `devtools::test()` in the console runs our tests:

```
devtools::test()
```

```
Loading datapeek
Testing datapeek
✔ | OK F W S | Context
✔ |  1       | utility functions

══ Results ═══════════════════════════════════════════════════════════════════
OK:       1
Failed:   0
Warnings: 0
Skipped:  0

:)
```

We get a smiley face too!

Since our **second function** removes a specified feature I will use the same test as above, checking for the dimensions of the returned frame. Our **third function** applies a specified function to a chosen column, so I will write a test that checks the result of given specified function. Finally, our **fourth function** returns the closest matching string, so I will simply check the returned string for the expected result.

Here is our full test file:

```
context('utility functions')

library(data.table)
library(mltools)

load('../../data/iris.rda')

test_that("data frame with correct number of features is returned", {
    res <- encode_and_bind(iris, 'Species')
    expect_equal(dim(res)[2], 8)
})

test_that("data frame with correct number of features is returned", {
    res <- remove_features(iris, 'Species')
    expect_equal(dim(res)[2], 4)
})

test_that("newly created columns return correct sum", {
    res <- apply_function_to_column(iris, "Sepal.Width, Sepal.Length", "new_col1, new_col2", "x*
    expect_equal(sum(res$new_col1), 2293)
    expect_equal(sum(res$new_col2), 4382.5)
})
```

```
23
24  test_that("closest matching string is returned", {
25      res <- get_closest_string(c("hey there", "we are here", "howdy doody"), "doody")
26      expect_true(identical(res, 'howdy doody'))
27  })
```

test-utilities.R hosted with ♡ by GitHub view raw

> **NOTE**: *Notice the relative path to the data in the test file.*

Testing our Package

As we did above, we run our tests using the following command:

```
devtools::test()
```

This will run *all tests* in any test files we placed inside the testthat directory. Let's check the result:

```
devtools::test()

Loading datapeek
Testing datapeek
✔ | OK F W S | Context
✔ |  5       | utility functions

══ Results ═══════════════════════════════════════════════════════════════════
OK:       5
Failed:   0
Warnings: 0
Skipped:  0

Way to go!
```

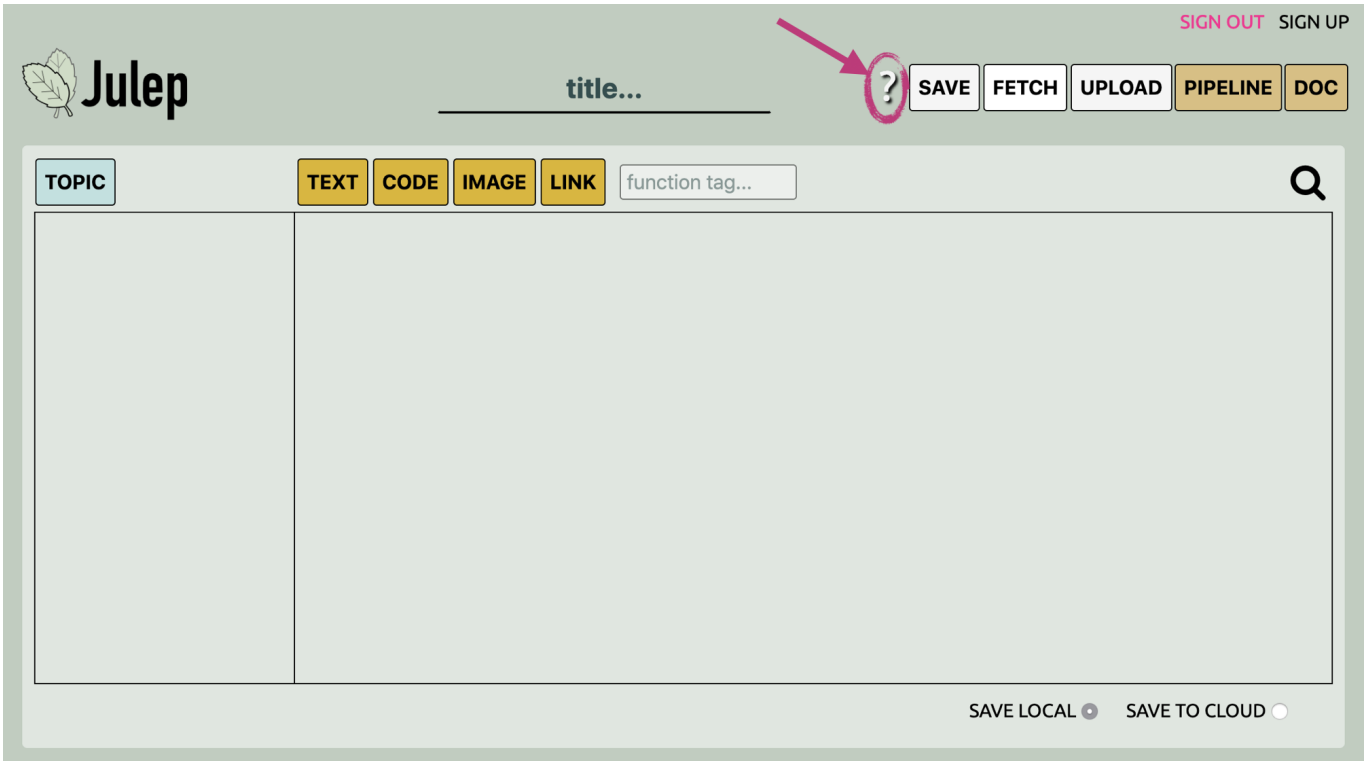
We had 5 assertions across 4 unit tests, placed in one test file. Looks like we're good. If any of our tests failed we would see this in the above printout, at which point we would look to correct the issue.

STEP 7: Create Documentation

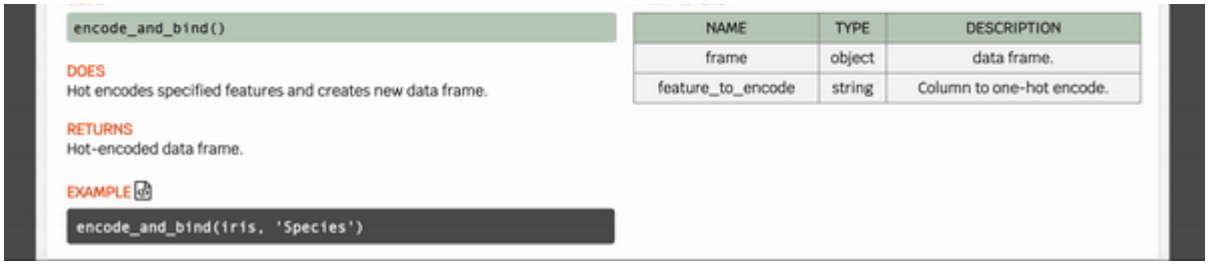
This has traditionally been done using "Vignettes" in R. You can learn about creating R vignettes for your R package here. Personally, I find this a dated approach to

documentation. I prefer to use things like **Sphinx** or **Julep**. Documentation should be easily **shared**, **searchable** and **hosted**.

Click on the question mark at julepcode.com to learn how to use Julep.



I created and hosted some simple documentation for our R datapeek library, which you can find here.



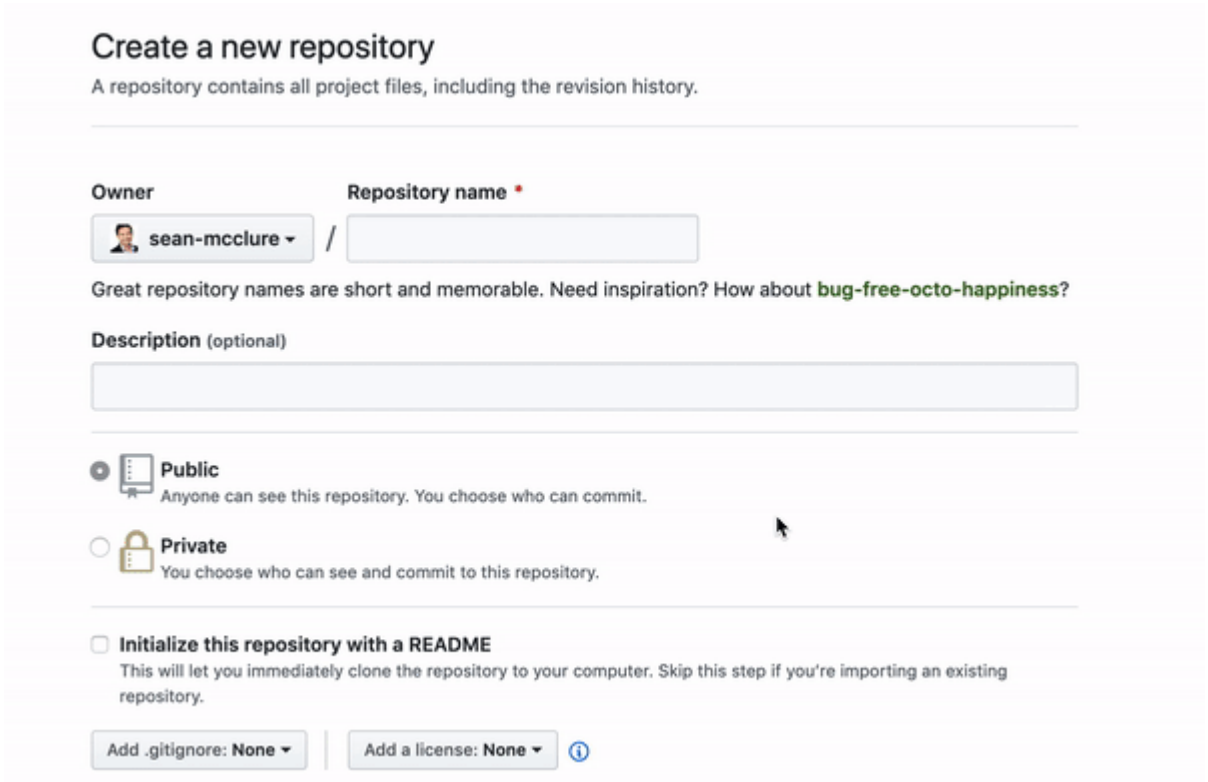
Of course we will also have the library on **GitHub**, which I cover below.

STEP 8: Share your R Library

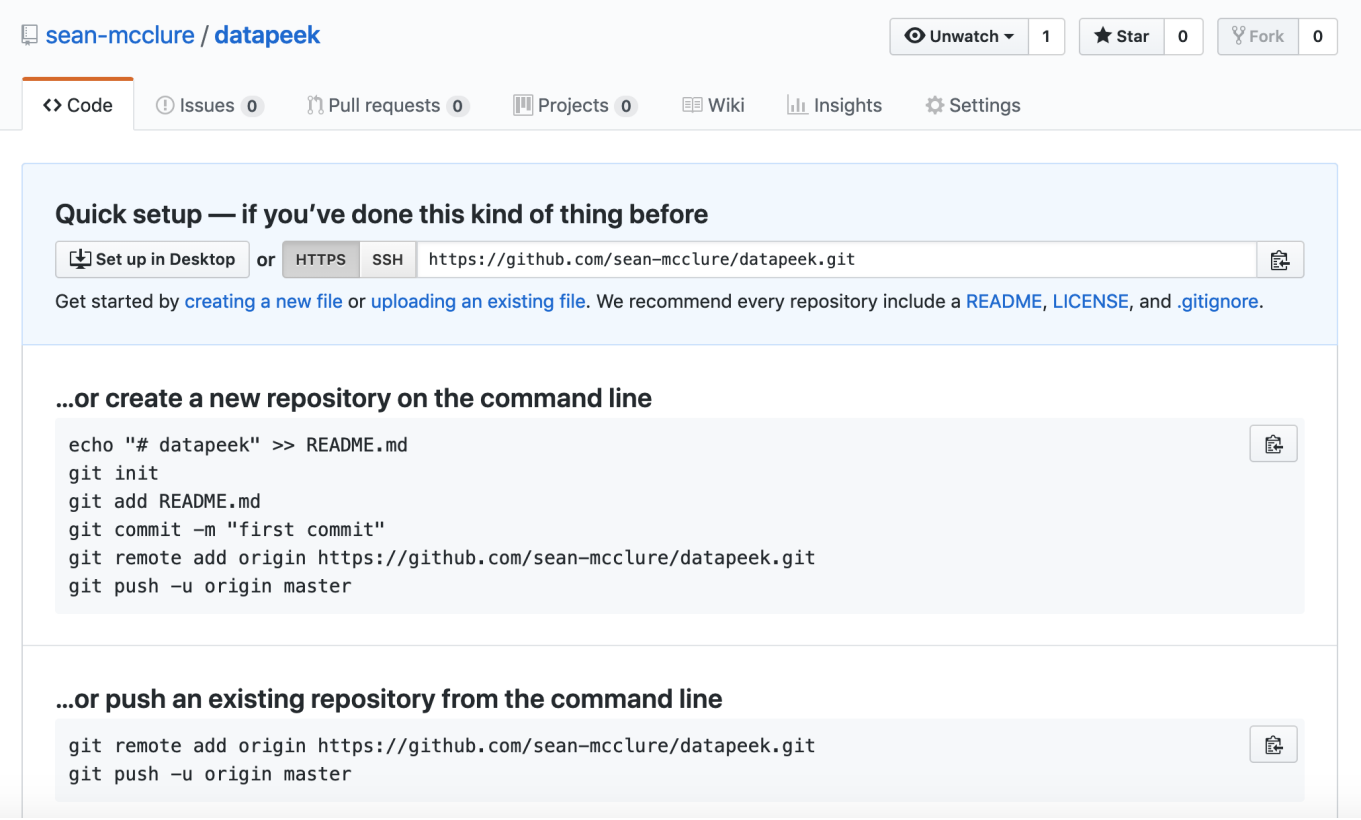
As I mentioned in the introduction we should be creating libraries on a regular basis, so others can benefit from and extend our work. The best way to do this is through **GitHub**, which is the standard way to distribute and collaborate on open source software projects.

In case you're new to GitHub here's a quick tutorial to get you started so we can push our datapeek project to a remote repo.

Sign up/in to GitHub and **create a new repository**.



…which will provide us with the usual screen:



With our remote repo setup we can initialize our **local repo** on our machine, and send our first commit.

Open Terminal in JupyterLab and change into the datapeek directory:

```
data  datapeek.Rproj  DESCRIPTION  man  NAMESPACE  R  tests
jovyan@b61d208e1c0c:~/work/datapeek$
```

Initialize the local repo:

```
git init
```

```
Initialized empty Git repository in /home/jovyan/work/datapeek/.git/
jovyan@b61d208e1c0c:~/work/datapeek$
```

Add the remote origin (your link will be different):

```
git remote add origin https://github.com/sean-mcclure/datapeek.git
```

Now run `git add .` to add all modified and new (untracked) files in the current directory and all subdirectories to the **staging** area:

```
git add .
```

Don't forget the "dot" in the above command. Now we can **commit** our changes, which adds any new code to our local repo.

But, since we are working inside a Docker container the **username** and **email** associated with our local repo cannot be autodetected. We can **set these** by running the following in terminal:

```
git config --global user.email {emailaddress}
git config --global user.name {name}
```

Use the email address and username you use to sign into GitHub.

Now we can commit:

```
git commit -m 'initial commit'
```

With our new code committed we can do our push, which transfers the last commit(s) to our *remote* repo:

```
git push origin master
```

> **NOTE***: Since we are in Docker you'll likely get asked again for* ***authentication****. Simply add your GitHub username and password when prompted. Then run the above command again.*

Some readers will notice we didn't place a `.gitignore` file in our directory. It is usually fine to push all files inside smaller R libraries. For larger libraries, or libraries containing

large datasets, you can use the site **gitignore.io** to see what common gitignore files look like. Here is a common R .gitignore file for R:

```
### R ###
# History files
.Rhistory
.Rapp.history

# Session Data files
.RData

# User-specific files
.Ruserdata

# Example code in package build process
*-Ex.R

# Output files from R CMD build
/*.tar.gz

# Output files from R CMD check
/*.Rcheck/

# RStudio files
.Rproj.user/

# produced vignettes
vignettes/*.html
vignettes/*.pdf

# OAuth2 token, see https://github.com/hadley/httr/releases/tag/v0.3
.httr-oauth

# knitr and R markdown default cache directories
/*_cache/
/cache/

# Temporary files created by R markdown
*.utf8.md
*.knit.md

### R.Bookdown Stack ###
# R package: bookdown caching files
/*_files/
```

```
41  /*_files/
```

.gitignore hosted with ♡ by GitHub view raw

Example .gitignore file for an R package

To recap, git **add** adds all modified and new (untracked) files in the current directory to the **staging** area. **Commit** adds any changes to our *local* repo, and **push** transfers the last commit(s) to our *remote* repo. While `git add` might seem superfluous, the reason it exists is because sometimes we want to only commit certain files, this we can stage files selectively. Above, we staged *all* files by using the "dot" after `git add .`

You may also notice we didn't include a **README** file. You should indeed include this, however for the sake of brevity I have left this step out.

Now, **anyone can use our library**. 👍 Let's see how.

STEP 9: Install your R Library

As mentioned in the introduction I will not be discussing CRAN in this article. Sticking with GitHub make it easier to share our code frequently, and we can always add CRAN criteria later.

To install a library from GitHub, users can simply run the following command on their local machine:

```
devtools::install_github("yourusername/mypackage")
```

As such, we can simply instruct others wishing to use datapeek to run the following command on their local machine:

```
devtools::install_github("sean-mcclure/datapeek")
```

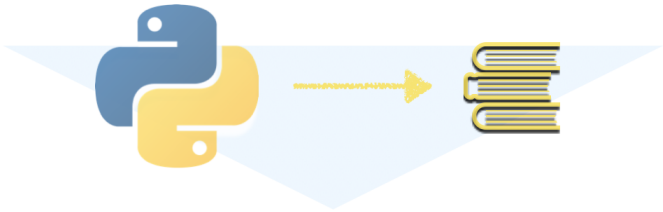
This is something we would include in a README file and/or any other documentation we create. This will install our package like any other package we get from CRAN:

Users then load the library as usual and they're good to go:

```
library(datapeek)
```

I recommend trying the above commands in a new R environment to confirm the installation and loading of your new library works as expected.

CREATING LIBRARIES IN PYTHON



Creating Python libraries follows the same high-level steps we saw previously for R. We require a basic **directory structure** with proper **naming** conventions, **functions** with **descriptions**, **imports**, specified **dependencies**, added **datasets**, **documentation**, and the ability to **share** and allow others to **install** our library.

We will use **JupyterLab** to build our Python library, just as we did for R.

Library vs Package vs Module

In the beginning of this article I discussed the difference between a "**library**" and a "**package**", and how I prefer to use these terms interchangeably. The same holds for Python libraries. "**Modules**" are another term, and in Python simply refer to any file containing Python code. Python libraries obviously contain modules as scripts.

Before we start:

I stated in the introduction that we will host and install our libraries on and from GitHub. This encourages rapid creation and sharing of libraries without getting bogged down by publishing criteria on popular package hosting sites for R and Python.

The most popular hosting site for Python is the Python Package Index (PyPI). This is a place for **finding**, **installing** and **publishing** python libraries. Whenever you run `pip install <package_name>` (or `easy_intall`) you are fetching a package from PyPI.

While we won't cover hosting our package on PyPI it's still a good idea to see if our library name is *unique*. This will minimize confusion with other popular Python libraries and improve the odds our library name is distinctive, should we decide to someday host it on PyPI.

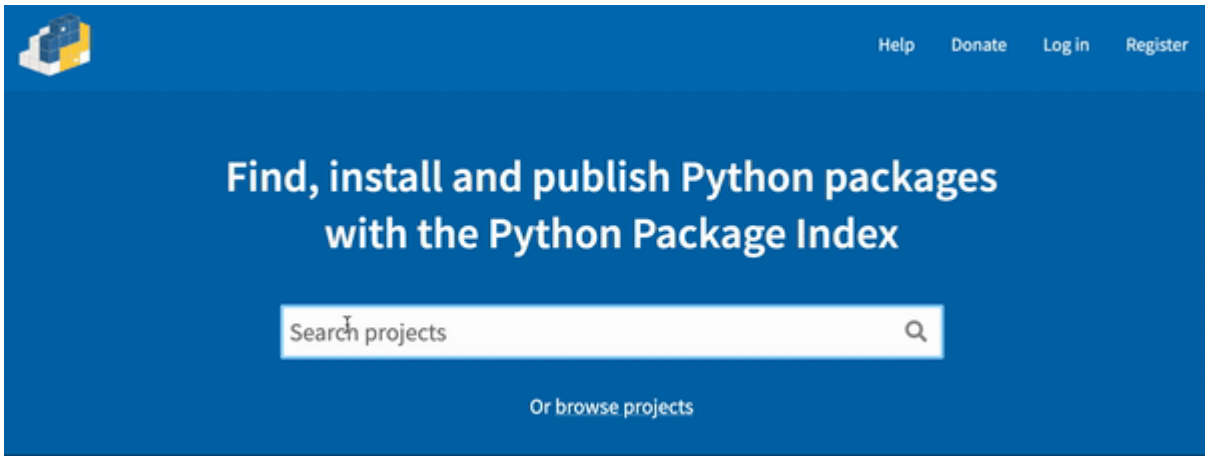
First, we should follow a few naming conventions for Python libraries.

Python Library Naming Conventions

- Use all **lowercase**;
- Make the name **unique** on PyPI (search for name on PyPI)

- No **hyphens** (you can use underscore to separate words)

Our library name is **datapeek**, so the first and third criteria are met; let's check PyPI for *uniqueness*:



All good. 👍

We're now ready to move through each step required to create a Python library.

STEP 1: Create Package Framework

JupyterLab should be up-and-running as per the instructions in the **setup section** of this article.

Use JupyterLab's **New Folder** and **Text File** options to create the following **directory structure** and **files**:

```
datapeek
├── datapeek
    └── __init__.py
    └── utilities.py
├── setup.py
```

> **NOTE**: ***Bold*** *names are* ***folders*** *and* ***light*** *names are* ***files****. We will refer to the* ***inner*** *datapeek folder as the "module directory" and the* ***outer*** *datapeek directory as the "root directory."*

The following video shows me creating our datapeek directory in JupyterLab:

Network error

A network hiccup interrupted playback. Please reload the player and try again.

There will be files we do not want to commit to source control. These are files that are created by the Python build system. As such, let's also add the following **.gitignore file** to our package framework:

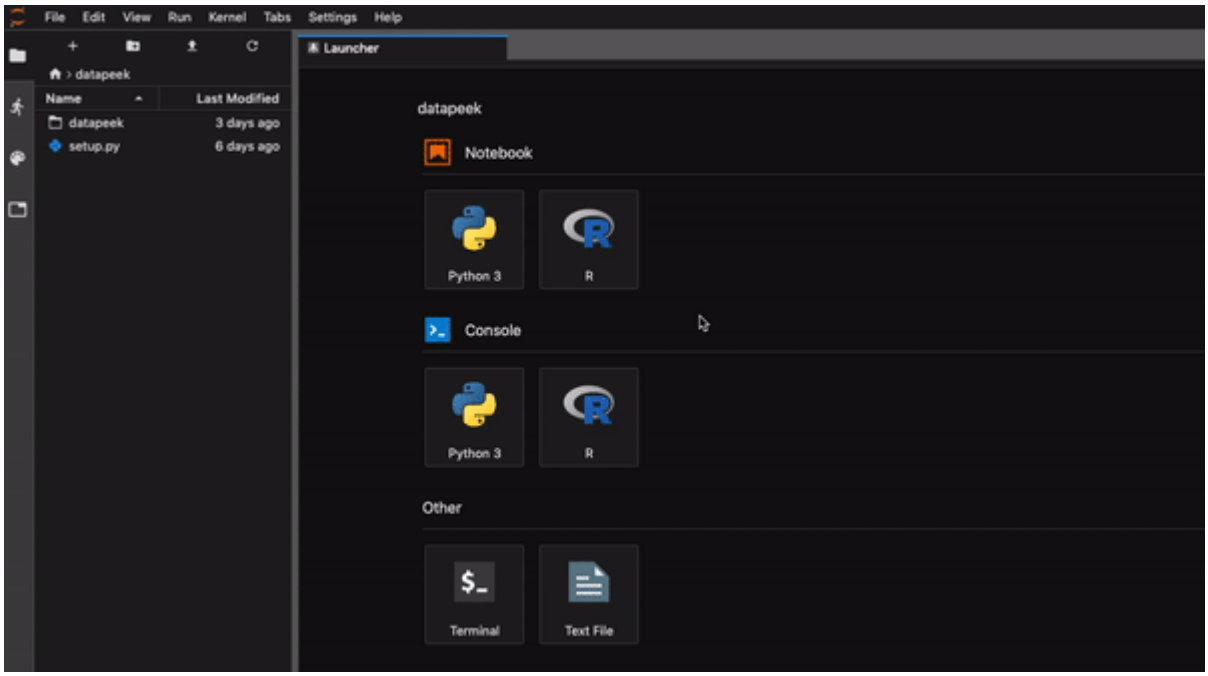
```
# Compiled python modules.
*.pyc

# Setuptools distribution folder.
/dist/

# Python egg metadata, regenerated from source files by setuptools.
/*.egg-info
```

gitignore hosted with ♡ by GitHub view raw

> **NOTE**: *At the time of this writing JupyterLab lacks a front-end setting to toggle hidden files in the browser. As such, we will simply name our file gitignore (no preceding dot); we will change it to a hidden file later prior to pushing to GitHub.*

Add your gitignore file as a simple text file to the **root directory:**

```
datapeek
├── datapeek
    └── __init__.py
    └── utilities.py
├── setup.py
├── gitignore
```



STEP 2: Fill Out Description Details

Just as we did for R, we should add *metadata* about our new library. We do this using **Setuptools**. Setuptools is a Python library designed to facilitate packaging Python projects.

Open setup.py and add the following details for our library:

```
from setuptools import setup

setup(name='datapeek',
      version='0.1',
      description='A simple library for dealing with raw data.',
      url='https://github.com/sean-mcclure/datapeek_py',
      author='Sean McClure',
      author_email='sean.mcclure@example.com',
      license='MIT',
      packages=['datapeek'],
      zip_safe=False)
```

```
        zip_safe=False)
```

setup.py hosted with ♡ by GitHub view raw

Of course you should change the authoring to your own. We will add more details to this file later. The keywords are fairly self-explanatory. `url` is the URL of our project on GitHub, which we will add later; unless you've already created your python repo, in which case add the URL now. We talked about licensing in the R section. `zip_safe` simply means our package can be run safely as a zip file which will usually be the case. You can learn more about what can be added to the setup.py file here.

STEP 3: Add Functions

Our library obviously requires *functions* to be useful. For larger libraries we would organize our modules so as to balance cohesion/coupling, but since our library is small we will simply keep all functions inside a single file.

We will add the same functions we did for R, this time written in Python:

```python
import pandas as pd
from fuzzywuzzy import fuzz

def encode_and_bind(frame, feature_to_encode):
    dummies = pd.get_dummies(frame[[feature_to_encode]])
    res = pd.concat([frame, dummies], axis=1)
    res = res.drop([feature_to_encode], axis=1)
    return(res)

def remove_features(frame, list_of_columns):
    res = frame.drop(frame[list_of_columns],axis=1)
    return(res)

def apply_function_to_column(frame, list_of_columns, new_col, funct):
    frame[new_col] = frame[list_of_columns].apply(lambda x: eval(funct))
    return(frame)

def get_closest_string(list_of_strings, search_string):
    all_dists = []
    all_strings = []
    for string in list_of_strings:
        dist = fuzz.partial_ratio(string, search_string)
        all_dists.append(dist)
```

```
            all_strings.append(string)
        top = max(all_dists)
        ind=0
        for i, x in enumerate(all_dists):
            if x == top:
                ind = i
        return(all_strings[ind])
```

utilities.py hosted with ♡ by GitHub view raw

Add these functions to the `utilities.py` module, inside datapeek's module directory.

STEP 4: List External Dependencies

Our library will often require other packages as *dependencies*. Our user's Python environment will need to be aware of these when installing our library (so these other packages can also be installed). **Setuptools** provides the `install_requires` keyword to list any packages our library depends on.

Our datapeek library depends on the **fuzzywuzzy** package for fuzzy string matching, and the **pandas** package for high-performance manipulation of data structures. To specify our dependencies, **add** the following to your setup.py file:

```
install_requires=[
    'fuzzywuzzy',
    'pandas'
]
```

Your setup.py file should currently look as follows:

```
from setuptools import setup

setup(name='datapeek',
      version='0.1',
      description='A simple library for dealing with raw data.',
      url='https://github.com/sean-mcclure/datapeek_py',
      author='Sean McClure',
      author_email='sean.mcclure@example.com',
      license='MIT',
      packages=['datapeek'],
```

```
        install_requires=[
            'fuzzywuzzy',
            'pandas'
        ],
        zip_safe=False)
```

setup.py hosted with ♡ by GitHub view raw

We can **confirm** all is in order by running the following in a JupyterLab **terminal** session:

```
python setup.py develop
```

> **NOTE**: *Run this in datapeek's root directory.*

After running the command you should see something like this:

```
Installed /Users/seanmcclure/Desktop/datapeek/datapeek
Processing dependencies for datapeek==0.1
Searching for fuzzywuzzy==0.17.0
Best match: fuzzywuzzy 0.17.0
Adding fuzzywuzzy 0.17.0 to easy-install.pth file

Using /Users/seanmcclure/anaconda3/lib/python3.5/site-packages
Finished processing dependencies for datapeek==0.1
```

…with an ending that reads:

```
Finished processing dependencies for datapeek==0.1
```

If one or more of our dependencies is not available on PyPI, but is available on GitHub (e.g. *a bleeding-edge machine learning package is only available on Github…or it's another one of our team's libraries hosted only on GitHub*), we can use `dependency_links` inside our setup call:

```
setup(
    ...
    dependency_links=
['http://github.com/user/repo/tarball/master#egg=package-1.0'],
    ...
)
```

If you want to add additional metadata, such as **status**, **licensing**, **language version**, etc. we can use `classifiers` like this:

```
setup(
    ...
    classifiers=[
        'Development Status :: 3 - Alpha',
        'License :: OSI Approved :: MIT License',
        'Programming Language :: Python :: 2.7',
        'Topic :: Text Processing :: Linguistic',
      ],
    ...
)
```

To learn more about the different classifiers that can be added to our setup.py file see here.

STEP 5: Add Data

Just as we did above in R we can add data to our Python library. In Python these are called **Non-Code Files** and can include things like **images**, **data**, **documentation**, etc.

We **add data** to our library's module directory, so that any code that requires those data can use a *relative path* from the consuming module's `__file__` variable.

Let's add the Iris dataset to our library in order to provide users a quick way to test our functions. First, use the **New Folder** button in JupyterLab to **create a new folder called data** inside the module directory:

```
datapeek
├── datapeek
    └── __init__.py
    └── utilities.py
    └── data
├── setup.py
├── gitignore
```

…then **make a new Text File** inside the data folder called iris.csv, and **paste** the data from here into the new file.

If you close and open the new csv file it will render inside JupyterLab as a proper table:

	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
7	4.6	3.4	1.4	0.3	setosa
8	5.0	3.4	1.5	0.2	setosa
9	4.4	2.9	1.4	0.2	setosa
10	4.9	3.1	1.5	0.1	setosa
11	5.4	3.7	1.5	0.2	setosa
12	4.8	3.4	1.6	0.2	setosa
13	4.8	3.0	1.4	0.1	setosa
14	4.3	3.0	1.1	0.1	setosa
15	5.8	4.0	1.2	0.2	setosa
16	5.7	4.4	1.5	0.4	setosa
17	5.4	3.9	1.3	0.4	setosa
18	5.1	3.5	1.4	0.3	setosa
19	5.7	3.8	1.7	0.3	setosa
20	5.1	3.8	1.5	0.3	setosa
21	5.4	3.4	1.7	0.2	setosa
22	5.1	3.7	1.5	0.4	setosa

CSV file rendered in JupyterLab as formatted table.

We specify Non-Code Files using a `MANIFEST.in` file. **Create another Text File** called `MANIFEST.in` placing it inside your root folder:

```
datapeek
├── datapeek
    └── __init__.py
    └── utilities.py
    └── data
├── MANIFEST.in
├── setup.py
├── gitignore
```

…and **add this line** to the file:

```
include datapeek/data/iris.csv
```

> **NOTE**: *The MANIFEST.in is often not needed, but included in this tutorial for completeness. See here for more discussion.*

We also need to **include the following line** in setup.py:

```
include_package_data=True
```

Our setup.py file should now look like this:

```
from setuptools import setup

setup(name='datapeek',
      version='0.1',
      description='A simple library for dealing with raw data.',
      url='https://github.com/sean-mcclure/datapeek_py',
      author='Sean McClure',
      author_email='sean.mcclure@example.com',
      license='MIT',
      packages=['datapeek'],
      install_requires=[
          'fuzzywuzzy',
          'pandas'
      ],
      include_package_data=True,
      zip_safe=False)
```

setup.py hosted with ♡ by GitHub view raw

STEP 6: Add Tests

As with our R library we should add tests so others can extend our library and ensure their own functions do not conflict with existing code. **Add a test folder** to our library's module directory:

```
datapeek
├── datapeek
    └── __init__.py
    └── utilities.py
    └── data
    └── tests
├── MANIFEST.in
├── setup.py
├── gitignore
```

Our test folder should have its own `__init__.py` file as well as the test file itself. **Create** those now using JupyterLab's Text File option:

```
datapeek
├── datapeek
    └── __init__.py
    └── utilities.py
    └── data
    └── tests
        └──__init__.py
        └──datapeek_tests.py
├── MANIFEST.in
├── setup.py
├── gitignore
```

Our datapeek directory structure is now set to house test functions, which we will write now.

Writing Tests

Writing tests in Python is similar to doing so in R. Assertions are used to check the expected outputs produced by our library's functions. We can use these "unit tests" to check a variety of expected outputs depending on what might be expected to fail. For example, we might want to ensure a data frame is returned, or perhaps the correct number of columns after some known transformation.

I will add a simple test for each of our 4 functions. Feel free to add your own tests. Think about what should be checked, and keep in mind Martin Fowler's quote shown in the R section of this article.

We will use **unittest**, a popular unit testing framework in Python.

Add unit tests to the datapeek_tests.py file, ensuring the unittest and datapeek libraries are imported:

```
from unittest import TestCase
from datapeek import utilities
import pandas as pd

use_data = pd.read_csv('datapeek/data/iris.csv')

def test_encode_and_bind():
    s = utilities.encode_and_bind(use_data, 'sepal_length')
    assert isinstance(s, pd.DataFrame)

def test_remove_features():
    s = utilities.remove_features(use_data, ['sepal_length','sepal_width'])
    assert s.shape[1] == 3

def test_apply_function_to_column():
    s = utilities.apply_function_to_column(use_data, ['sepal_length'], 'times_4', 'x*4')
    assert s['sepal_length'].sum() * 4 == 3506.0

def test_get_closest_string():
    s = utilities.get_closest_string(['hey there','we we are','howdy doody'], 'doody')
    assert s == 'howdy doody'
```

test.py hosted with ♡ by GitHub view raw

To run these tests we can use **Nose**, which extends unittest to make testing easier. **Install nose** using a **terminal** session in JupyterLab:

```
$ pip install nose
```

We also need to **add** the following lines to setup.py:

```
setup(
    ...
    test_suite='nose.collector',
    tests_require=['nose'],
)
```

Our setup.py should now look like this:

```
from setuptools import setup

setup(name='datapeek',
      version='0.1',
      description='A simple library for dealing with raw data.',
      url='https://github.com/sean-mcclure/datapeek_py',
      author='Sean McClure',
      author_email='sean.mcclure@example.com',
      license='MIT',
      packages=['datapeek'],
      install_requires=[
          'fuzzywuzzy',
          'pandas'
      ],
      test_suite='nose.collector',
      tests_require=['nose'],
      include_package_data=True,
      zip_safe=False)
```

setup.py hosted with ♡ by GitHub view raw

Run the following from the root directory to run our tests:

```
python setup.py test
```

Setuptools will take care of installing nose if required and running the test suite. After running the above, you should see the following:

```
datapeek.tests.datapeek_tests.test_encode_and_bind ... ok
datapeek.tests.datapeek_tests.test_remove_features ... ok
datapeek.tests.datapeek_tests.test_apply_function_to_column ... ok
datapeek.tests.datapeek_tests.test_get_closest_string ... ok

----------------------------------------------------------------------
Ran 4 tests in 0.352s

OK
```

All our tests have **passed!**

If any test should fail, the unittest framework will show which functions did not pass. At this point, check to ensure you are calling the function correctly and that the output is indeed what you expected. It can also be good practice to purposely write tests to fail first, then write your functions until they pass.

STEP 7: Create Documentation

As I mentioned in the R section, I use **Julep** to rapidly create sharable and searchable documentation. This avoids writing cryptic annotations and provides the ability to immediately host our documentation. Of course this doesn't come with the IDE hooks that other documentation does, but for rapidly communicating it works.

You can find the documentation I create for this library here.

STEP 8: Share Your Python Library

The standard approach for sharing python libraries is through PyPI. Just as we didn't cover CRAN with R, we will not cover hosting our library on PyPI. While the requirements are fewer than those associated with CRAN there are still a number of steps that must be taken to successfully host on PyPI. The steps required to host on sites other than GitHub can always be added later.

GitHub

We covered the steps for adding a project to GitHub in the R section. The same steps apply here.

I mentioned above the need to **rename our gitignore file** to make it a hidden file. You can do that by running the following in **terminal**:

```
mv gitignore .gitignore
```

You'll notice this file is no longer visible in our JupyterLab directory (it eventually disappears). Since JupyterLab still lacks a front-end setting to toggle hidden files simply run the following in terminal at anytime to see hidden files:

```
ls -a
```

We can make it visible again should we need to view/edit the file in JupyterLab, by running:

```
mv .gitignore gitignore
```

Here is a quick **recap** on pushing our library to GitHub (change git URL to your own):

- **Create** a new repo on GitHub called datapeek_py
- **Initialize** your library's directory using `git init`
- **Configure** your local repo with your GitGub email and username (if using Docker) using:

```
git config --global user.email {emailaddress}
git config --global user.name {name}
```

- **Add** your new remote origin using `git remote add origin https://github.com/sean-mcclure/datapeek_py.git`
- **Stage** your library using `git add .`
- **Commit** all files using `git commit -m 'initial commit'`
- **Push** your library to the remote repo using `git push origin master` (authenticate when prompted)

Now, **anyone can use our python library**. 👍 Let's see how.

STEP 9: Install your Python Library

While we usually install Python libraries using the following command:

```
pip install <package_name>
```

… this requires hosting our library on PyPI, which as explained above is beyond the scope of this article. Instead we will learn how to install our Python libraries from GitHub, as we did for R. This approach still requires the `pip install` command but uses the GitHub URL instead of the package name.

Installing our Python Library from GitHub

With our library hosted on GitHub, we simply use `pip install git+` followed by the URL provided on our GitHub repo (available by clicking the *Clone or Download* button on the GitHub website):

```
pip install git+https://github.com/sean-mcclure/datapeek_py
```

Now, we can **import our library** into our Python environment. For a single function:

```
from datapeek.utilities import encode_and_bind
```

…and for **all functions**:

```
from datapeek.utilities import *
```

Let's do a quick check in a new Python environment to ensure our functions are available. Spinning up a new Docker container, I run the following:

Fetch a dataset:

```
iris = pd.read_csv('https://raw.githubusercontent.com/uiuc-cse/data-fa14/gh-pages/data/iris.csv')
```

Check functions:

```
encode_and_bind(iris, 'species')
```

	sepal_length	sepal_width	petal_length	petal_width	species_setosa	species_versicolor	species_virginica
0	5.1	3.5	1.4	0.2	1	0	0
1	4.9	3.0	1.4	0.2	1	0	0
2	4.7	3.2	1.3	0.2	1	0	0
3	4.6	3.1	1.5	0.2	1	0	0
4	5.0	3.6	1.4	0.2	1	0	0
5	5.4	3.9	1.7	0.4	1	0	0
6	4.6	3.4	1.4	0.3	1	0	0
7	5.0	3.4	1.5	0.2	1	0	0
8	4.4	2.9	1.4	0.2	1	0	0
9	4.9	3.1	1.5	0.1	1	0	0
10	5.4	3.7	1.5	0.2	1	0	0

```
remove_features(iris, ['petal_length', 'petal_width'])
```

	sepal_length	sepal_width	species
0	5.1	3.5	setosa
1	4.9	3.0	setosa
2	4.7	3.2	setosa
3	4.6	3.1	setosa
4	5.0	3.6	setosa
5	5.4	3.9	setosa
6	4.6	3.4	setosa
7	5.0	3.4	setosa
8	4.4	2.9	setosa

```
apply_function_to_column(iris, ['sepal_length'], 'times_4', 'x*4')
```

	sepal_length	sepal_width	petal_length	petal_width	species	times_4
0	5.1	3.5	1.4	0.2	setosa	20.4
1	4.9	3.0	1.4	0.2	setosa	19.6
2	4.7	3.2	1.3	0.2	setosa	18.8
3	4.6	3.1	1.5	0.2	setosa	18.4
4	5.0	3.6	1.4	0.2	setosa	20.0
5	5.4	3.9	1.7	0.4	setosa	21.6
6	4.6	3.4	1.4	0.3	setosa	18.4
7	5.0	3.4	1.5	0.2	setosa	20.0

```
get_closest_string(['hey there','we we are','howdy doody'], 'doody')
```

```
'howdy doody'
```

Success!

SUMMARY

In this article we looked at how to create both R and Python libraries using JupyterLab running inside a Docker container. Docker allowed us to leverage Docker Stacks such that our environment was easily controlled and common packages available. This also made it easy to use the same high-level interface to create libraries through the browser for 2 different languages. All files were written to our local machine since we mounted a volume inside Docker.

Creating libraries is a critical skill for any machine learning practitioner, and something I encourage others to do regularly. Libraries help isolate our work inside useful abstractions, improves reproducibility, makes our work shareable, and is the first step towards designing better software. Using a lightweight approach ensures we can prototype and share quickly, with the option to add more detailed practices and publishing criteria later as needed.

As always, please ask **questions** in the comments section should you run into issues. Happy coding.

If you enjoyed this article you might also enjoy:

Learn to Build Machine Learning Services, Prototype Real Applications, and Deploy your Work to...

In this post I show readers how to expose their machine learning models as RESTful web services, prototype real...

towardsdatascience.com

Graduating from Toy Visuals to Real Applications with D3.js

Too often we learn about technology and methods in isolation, disconnected from the true goal of data science; to...

towardsdatascience.com

GUI-fying the Machine Learning Workflow: Towards Rapid Discovery of Viable Pipelines

PREFACE

towardsdatascience.com

FURTHER READING AND RESOURCES

- R Packages by Hadley Wickham
- Testing by Hadley Wickham
- Python Packaging by Scott Torborg
- Jupyter Data Science Notebook
- Docker — Orientation and Setup

- JupyterLab Documentation
- Available CRAN Packages By Date of Publication
- Documenting Functions in R
- Julep
- gitignore.io
- The Python Package Index
- Setuptools Documentation
- Iris Dataset on GitHub
- Unit Tests — Wikipedia Article
- unitest — A Unit Testing Framework
- Nose — Nicer Testing for Python
- Test-Driven Development — Article on Wikipedia
- Docker Run Reference

Machine Learning Artificial Intelligence Python R Language Development

About Help Legal