

OpenScience

October 28, 2018

1 Lecture 24: Open Science

CBIO (CSCI) 4835/6835: Introduction to Computational Biology

1.1 Overview and Objectives

At this point, you're ready to dive into data science headfirst. One of the best ways to learn more about specific problems is to see how those problems have been addressed so far; reading through existing code can help immensely. But this touches on an important and emerging area of science called "Open Science." By the end of this lecture, you should be able to

- Define “open science” and its importance to scientific inquiry
- Recall the core strategies for reproducing and replicating results
- Package and release your Python code via distribution channels

1.2 Part 1: What is “Open Science”?

Simply put, Open Science is the **movement to make all scientific data, methods, and materials accessible to all levels of society.**

Why is this a good thing?

- The vast majority of research is publicly funded; it would seem logical that the public have access to it!



openscience

- Open and transparent research makes peer review and replication much easier.
- There is some convincing evidence that Open Science gives projects more downstream impact in the scientific community

Nonetheless, there are some downsides to making everything openly available.

- The deluge of science will overwhelm already heavily-burdened researchers.
- The tools could be used for more nefarious purposes (a good example is a particularly virulent strain of influenza that researchers were experimenting with a few years back that could potentially be used as a bioweapon).

My opinion—as you’ve probably guessed by the title of the lecture—is that the benefits of good Open Science practices outweigh the drawbacks, for the following reason:

I learn best when I can dig in and get my hands dirty.

Reading a paper or even a blog post that vaguely describes a method is one thing. Actually seeing the code, changing it, and re-running it to observe the results is something else entirely and, so I believe, is vastly superior in educational terms.

The scientific deluge is legitimate, though this was already happening even without the addition of open data, open access, and open source. And it would seem that, while we do absolutely need to exercise caution in our research and not pursue the ends by any means necessary, science is the pursuit of knowledge for its own sake and that should also be respected to the highest degree.

To that end, there are **six** main themes that comprise the Open Science guidelines.

1. Open data: all data used in the project should be made available.
2. Open source: all code written in the project should be publicly available.
3. Open methods: the exact procedure of the project is publicly documented.
4. Open review: correspondence between reviewers and authors is public.
5. Open access: resulting publications are publicly available.
6. Open education: all education materials are publicly available.

1.2.1 1: Open Data

If you had to pick the “core” of Open Science, this would probably be it. All of the data used in your study and experiments are published online.

This is definitely a shift from prior precedent; most raw data from scientific experiments remain cloistered.

The situation is further complicated by Terms of Service agreements that prohibit the sharing of data collected. - For example: if you hooked up a Python client to listen to and capture public Twitter posts, you are forbidden from sharing the Twitter data publicly. - Which seems odd, given that the data are public anyway, but there you go.

Repositories and online data banks have sprung up around this idea. Many research institutions host their own open data repositories, as do some large tech companies.

- CERN, the organization behind the Large Hadron Collider, has posted its data online: <http://opendata.cern.ch/about/CMS>
- Amazon has released its own set of large public datasets: <https://aws.amazon.com/public-data-sets/>

OPEN DATA

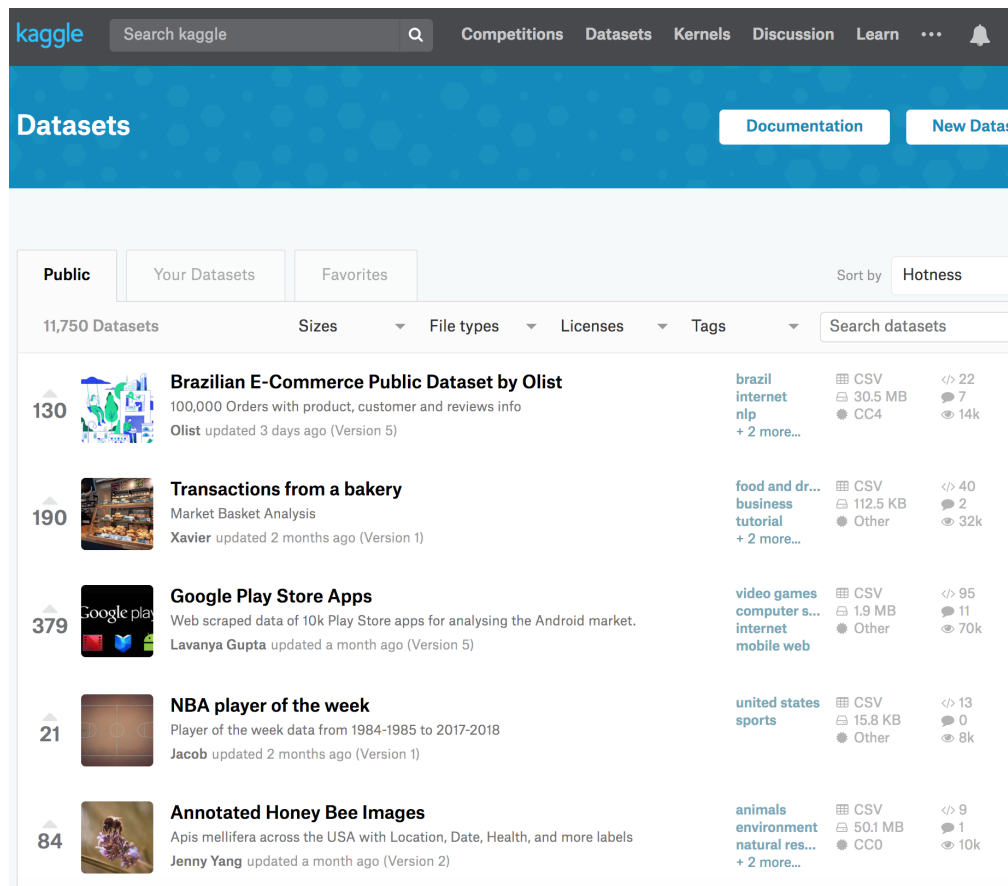
opendata

The screenshot shows the 'opendata CERN' website. It features a search bar at the top with the text 'Search'. Below the search bar, there are filters for 'Dataset' and 'Collision'. The 'Dataset' filter is expanded, showing a list of categories with their respective counts: Dataset (878), Collision (84), Derived (111), Simulated (881), Documentation (38), About (3), Activities (13), Authors (3), Guide (12), Help (2), Policy (2), Report (1), Environment (13), Condition (8), VM (5), Validation (3), News (5), Software (25), Analysis (10), Framework (3), Tool (7), and Validation (5). The search results are sorted by 'Best match' and 'asc.', displaying 20 results. The first three results are listed: 1. /MuOniaParked/Run2012B-22Jan2013-v1/AOD, 2. /HT/Run2011A-12Oct2013-v1/AOD, and 3. /SingleMu/Run2011A-12Oct2013-v1/AOD. Each result includes a brief description and buttons for 'Dataset', 'Collision', and 'CMS'.

cerndata

The screenshot shows the 'Registry of Open Data on AWS' website. It features a search bar at the top with the text 'Search datasets'. Below the search bar, there are filters for 'Dataset' and 'Collision'. The 'Dataset' filter is expanded, showing a list of categories with their respective counts: Dataset (878), Collision (84), Derived (111), Simulated (881), Documentation (38), About (3), Activities (13), Authors (3), Guide (12), Help (2), Policy (2), Report (1), Environment (13), Condition (8), VM (5), Validation (3), News (5), Software (25), Analysis (10), Framework (3), Tool (7), and Validation (5). The search results are sorted by 'Best match' and 'asc.', displaying 20 results. The first three results are listed: 1. /MuOniaParked/Run2012B-22Jan2013-v1/AOD, 2. /HT/Run2011A-12Oct2013-v1/AOD, and 3. /SingleMu/Run2011A-12Oct2013-v1/AOD. Each result includes a brief description and buttons for 'Dataset', 'Collision', and 'CMS'.

awsdata



kaggledata

- Kaggle also has some pretty fantastic open datasets from its competitions:
<https://www.kaggle.com/datasets>
- DataHub is a general-purpose repository for anyone to submit their own datasets.
<https://datahub.io/en/dataset>

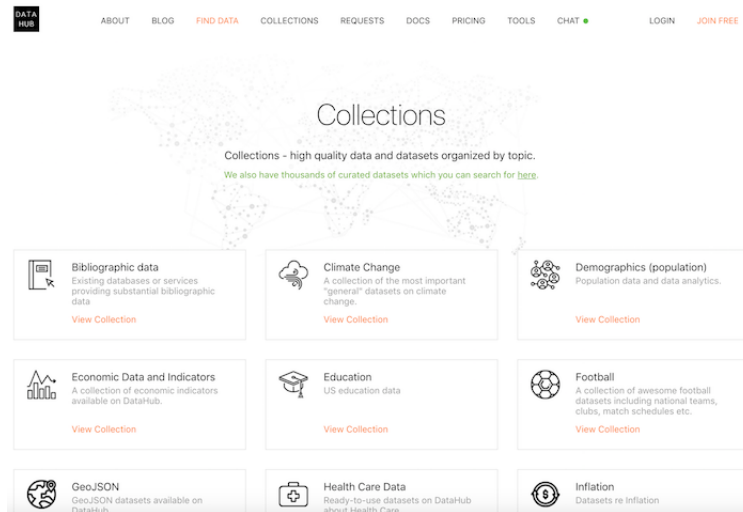
1.2.2 2: Open Source

This is probably the part you're most familiar with. Any (and *all*) code that's used in your project is published somewhere publicly for download.

There are certainly conditions where code can't be fully open sourced—proprietary corporate secrets, pending patents, etc—but to fully adhere to Open Science, the code has to be made completely available for anyone.

Like with open data, there are numerous **repositories** across the web that specialize in providing publicly-available versioning systems for both maintaining and publishing your code.

- GitHub is easily the most popular, and is where the materials for this lecture are published!
<https://github.com/>



datahub



github



- BitBucket is another option that also uses git to manage team codebases
<https://bitbucket.org/>
- SourceForge is one of the oldest and most well-known online repositories
<https://sourceforge.net/>


1.2.3 3: Open Methods


This is probably the trickiest item. How does one make *methods* reproducible?

Open source code is part of it, but even more important is the effort put into making the methods in the code understandable. This takes several forms:

- Documentation, both as accompanying doc files (e.g. JavaDoc) as well as in-code comments
- Proofs of the methods devised if they're novel, or references to their original sources
- Pre-packaged examples that will run with little or no prior configuration on the user's part
- Pre-registered methods *before* any work is conducted
- Self-contained virtual container scripts that satisfy all the prerequisites

Submission: LAS: an integrated language analysis tool for multiple languages #35

 **Open** whedon opened this issue 26 days ago · 8 comments



whedon commented 26 days ago • edited

Submitting author: @jiemakel (Eetu Mäkelä)

Repository: <https://github.com/jiemakel/las>

Version: v1.4.8

Status

JOSS Under Review

Status badge code:

```
HTML: <a href="http://joss.theoj.org/papers/87f0093e30a01b1078d8dea41476a08a">, which collates the papers you want to read and helps filter out all the others.

Preprints have become *so* popular, that versions of arXiv have popped up for almost every

OpenReview.net
Search ICLR 2019 Conference

## ICLR 2019

### International Conference on Learning Representations

New Orleans, Louisiana, United States
May 6 - May 9, 2019
<https://iclr.cc/Conferences/2019>

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- ICLR 2019 Conference submissions are now closed.
- For more details refer to the ICLR 2019 - Call for Papers.

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Please contact the ICLR 2019 Program Chairs at [iclr2019programchairs@googlegroups.com](mailto:iclr2019programchairs@googlegroups.com) with any questions or concerns about conference administration.

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Anonymous

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#### Learning to Separate Domains in Generalized Zero-Shot and Open Set Learning: a probabilistic perspective

Anonymous

27 Sep 2018 ICLR 2019 Conference Blind Submission Readers: Everyone 4 Replies

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arxiv



## Preprint servers are appearing in many disciplines



preprints

area!

### 1.2.6 6: Open Education

This and Open Methods are closely related. In this sense, any course materials that come from research that is done are made available for others.

**MIT OpenCourseWare** is probably the best example of open education at work, but these types of sites are proliferating.

- Many courses ([including this one!](#)) are making their materials freely available on GitHub.
- Tech companies such as GitHub (aptly named: [GitHub Classroom](#)) are developing educational tools specifically aimed at student classrooms. Amazon Web Services [provides a similar platform](#) for course materials, often bundled with its cloud compute services.

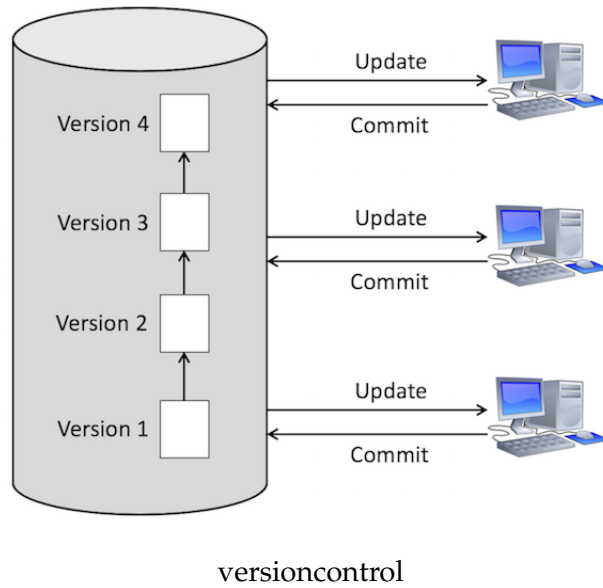
**Note:** This does not by default include MOOCs. If MOOCs make their materials freely available online, then and only then would it fall under this section.

So that's all great! But...

**What can I do? Where do I start?**

### 1.3 Part 2: Open Science Best Practices

In the previous section we went over the absolute essentials for an Open Science project or research endeavor. It included some examples of real-world services and tools to help expedite the process.



Here, we'll go into a bit more detail as to exactly how you should tweak your projects to be truly Open Science. It's not really something you can just "tack on" at the end; rather, you'll need to design your projects from the onset to be part of the Open Science initiative.

When you invent the next [TensorFlow](#), we'll all be thanking you for following these best practices!

### 1.3.1 Version control

This is a good starting point for any project.

Version control keeps track of changes within your code base.

It's a lot like Google docs, but for code.

You all know Dropbox? Has it ever saved your life? If so, the next time you start a coding project, use some form of *version control*.

There are several different version control systems out there for code, depending on what you like.

I personally prefer `git`, but I've used all of these before.

### 1.3.2 Anatomy of an open source project

There are some common files and folder hierarchies to implement at the very start of a new project. The [shablona](#) GitHub repository has all this documented very well, but here are the highlights:

- Your `src` folder, containing all your source code. Surprise!
- A directory of tests for your code. Always always always *always* write tests!
- A README file of some kind. This is your introduction that summarizes your project, gives a basic overview of how to use it, what the prerequisites are, links to further (more detailed) documentation, and any problems that are known.



vcsystems

- A doc folder containing *detailed* documentation about every aspect of your project, including any examples.
- A build script of some sort: a script you can run which automates the majority of the install process.
- Continuous integration (CI). This is bit more advanced, but the idea of continuous integration is to have your code exported out to an auto-compiler every time you update the code, so that you know *immediately* whether or not it builds successfully.
- A LICENSE file. This is often overlooked (like clicking through a EULA), but in the age of open source and Open Science it is *absolutely essential* to have a license of some sort.

### 1.3.3 Document, document, document

This is drilled into computer science students from day 1, and yet one constant across every software project is that the *documentation sucks*. To meet basic adequacy standards, documentation should include

- **The code itself.** This is the [radical notion](#) that code should be easy to understand, especially if read by someone who did NOT write it. Save [code golf](#) for the competitions!
- **Comments in the code.** Invariably there will be some logic in the code that doesn't make sense at first glance. This should be explained with clear comments. Not comments like `# loop through the array`, but useful comments like `# Because the array is already sorted, we only loop through parts of it to search for the value we want.`

What does this code do?

```

shablona/
|- README.md
|- shablona/
 |- __init__.py
 |- shablona.py
 |- due.py
 |- data/
 |- ...
 |- tests/
 |- ...
|- doc/
 |- Makefile
 |- conf.py
 |- sphinxext/
 |- ...
 |- _static/
 |- ...
|- setup.py
|- .travis.yml
|- .mailmap
|- appveyor.yml
|- LICENSE
|- Makefile
|- ipynb/
 |- ...

```

shablona

```

In [1]: def do(a, b):
 c = a + " " + b
 return c

```

What if I'd written it this way:

```

In [2]: def full_name(first_name, last_name):
 name = first_name + " " + last_name
 return name

```

Or even this way:

```

In [3]: def full_name(first_name, last_name):
 """
 Helper function, to concatenate the first name and the last name
 into a single full name.
 """

 # Concatenates the two names with a space in between.
 name = first_name + " " + last_name

 # Return the full name.
 return name

```

Python (and *any other* programming language) will have a “style” of documenting the code whereby other utilities can take those comments and turn them into documentation.



## Welcome

Sphinx is a tool that makes it easy to create intelligent and beautiful documentation, written by Georg Brandl and licensed under the BSD license.

It was originally created for [the Python documentation](#), and it has excellent facilities for the documentation of software projects in a range of languages. Of course, this site is also created from reStructuredText sources using Sphinx!

sphinx

Java pioneered this approach in the 1990s with “Javadocs” and every language since has emulated that in some way.

Python’s version is “Sphinx” <http://www.sphinx-doc.org/en/master/>

- **README.** This is usually the user’s first introduction to a new software package (GitHub makes this file the default landing page of a repository!). It should clearly state the purpose of the software, how to install and run it, and some basic usage examples before pointing the user to where they can go to learn more.

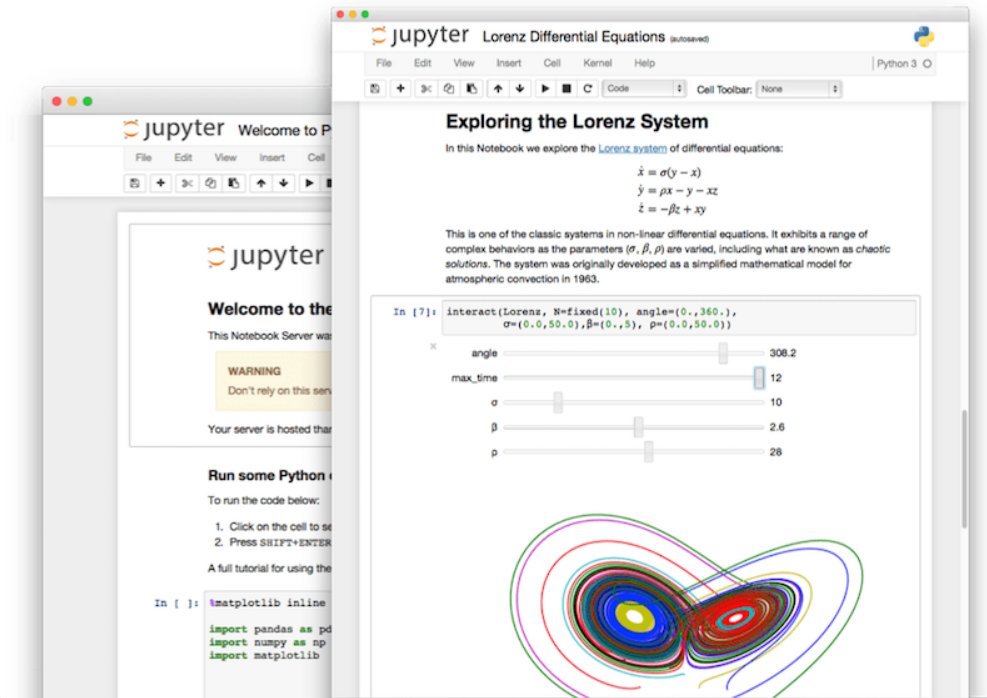
### 1.3.4 Examples and tests

Right after the README, this is the next place the user will go: examples for how to run the code. Is it command line? What options are there? What kind of data can I run through it? What should I expect for output? These sorts of questions can be addressed with

- **Quickstart.** This is file that is dedicated to getting the user up and running with the software as quickly as possible with an example. The goal is to put the user in the driver’s seat as quickly as possible, and let them ask questions later.
- **Examples.** This usually takes the form of a bash script, written to invoke the code and have it run on a sample dataset that’s provided. Alternatively, you can give a step-by-step guide of what commands to run, what inputs to give, and what the expected output should be.
- **Unit tests.** You’ll learn more about this as you take higher-level software engineering courses, but the main idea is you want to write code that *tests* your main code. The user can also go here to get a feel for how the code should be used.
- **Containers.** This is a very advanced topic that we won’t cover in this course, but the “wave of the future” is to build your software inside *containers* (e.g. [Docker](#)). Think of containers as super-lightweight virtual machines that anyone can build from a simple script. Using containers, you can package your software in such a way that you don’t have to worry about operating systems or clashing software dependencies.

### 1.3.5 Scientific Notebooks

If you’re an R or Python user, you’ve probably heard of “scientific notebooks”.



jupyterpreview



Turn a Git repo into a collection of interactive notebooks

mybinder

They're interactive, usually web-based applications that blur the lines between - written documents - code modules - figures and tables by interleaving all three within the same medium.

**\*\*These very slides were built entirely in Jupyter, a multi-language scientific notebook platform!**

While these slides were built in Jupyter, they were exported into HTML and PDF, so the code isn't technically live anymore.

However, through platforms like mybinder, you can turn any GitHub repository into a collection of active notebooks! You can do this yourself with these slides—all you need is a web browser!

### 1.3.6 Containers

**WARNING: This is super-advanced.**

Has anyone ever - tried to run code that is 6+ months old? - tried to install an old(er) video game on a new computer? - tried to install a new app on an old smartphone OS?

```
(py27) Apollo:OpenScience squinn$ ipython
Python 2.7.15 |Anaconda custom (64-bit)| (default, May 1 2018, 18:37:05)
Type "copyright", "credits" or "license" for more information.

IPython 5.6.0 -- An enhanced Interactive Python.
? -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.

In [1]: division = 5 / 2

In [2]: print division
2

In [3]:
```

python2



docker

Did it run?

Here's a great example: Python 2 versus Python 3.

Python 2 was the *de facto* Python version for over a decade (it's kind of the Windows XP of Python). When Python 3 was introduced in the late 2000s, nobody upgraded.

What should this code output?

```
In [4]: division = 5 / 2
```

```
In [5]: print(division)
```

2.5

This notebook is running Python 3. Let's run it in Python 2, shall we?

Containers, such as **Docker**, allow you to create bash-script-like *recipes* that build the precise environment you want.

This has *huge* implications in reproducibility: you can provide others with an exact set of instructions—even a pre-built image!—of the environment in which you conducted your work.



pypi



protocols

### 1.3.7 Python Package Index (pypi) is your friend

PyPI is the [Python Package Index](#), and is where the *vast* majority of external Python packages are hosted (over 85,000 as of this lecture!). In addition to publishing your code on GitHub, you can also package your code to be automatically installed via a package manager like `pip` or `easy_install`.

Provided you're already adhering to the anatomy of an open source project, there are only a few other steps needed to get your code ready for publishing on PyPI: in particular, writing the `setup.py` script that will tell the package managers of people who want to install your package exactly *how* to install your package.

Then you just upload the code to PyPI! <http://peterdowns.com/posts/first-time-with-pypi.html>

### 1.3.8 Pre-registration

Pre-registration means *publishing your methods publicly BEFORE any work has been done*.

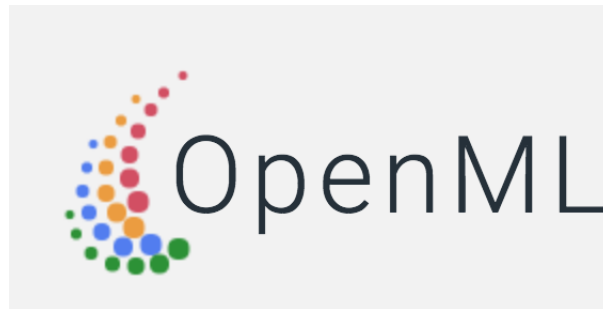
Why is this important?

Sites like Protocols.io <https://www.protocols.io/> and OSF <https://osf.io/prereg/> have pre-registration modules, sometimes linked with certain journals who agree to publish the results of the methods, regardless of whether they're positive or negative.



osf





openml

This makes sense for wet lab / life sciences or even theory-driven statistics, but what about empirical or computational studies like applied machine learning?

Turns out, there are a number of pre-registration sites for those too, including OpenML.

### 1.3.9 Licensing

Yes, this is super boring, I agree. Fortunately, the wonderful folks at GitHub have created an awesome resource for you to use.

**Choose a License:** It provides a handy choose-your-adventure flowchart for picking the perfect open software license for your project. I highly recommend it.

However, if you're just looking for a **tl;dr version** and want the basic lay of the land, GitHub's default licenses for new projects include

- MIT License (pretty much the “no warranty whatsoever, use at your own risk” license)
- Apache 2.0 License (almost exactly like the MIT, but allows for patents and trademarks)
- GPLv3 License (requires anyone who modifies your code to publish those modifications under GPLv3 too)

## 1.4 Final Thoughts

In my view, Open Science and its practices will only become more important. - Replicating previous results - Providing hands-on tools to the upcoming generation of scientists

Six major areas of Open Science - These have to be addressed from the beginning, not tacked on after the fact

Already lots of great open source tools and repositories to encourage Open Science practices - data repositories - tools for method replication and testing - standards for code structure, results presentation, and method preregistration

## 1.5 Additional Resources

**These slides!** <https://github.com/quinngroup/open-science-2018>

1. GitHub template for open source Python projects <https://github.com/uwescience/shablona>
2. Mozilla Open Science Lab <https://science.mozilla.org/>
3. Open Science Framework (OSF) for all phases of the scientific pipeline <https://osf.io/>
4. The Center for Open Science (COS), which supports OSF <https://cos.io/>
5. Docker <https://www.docker.com/>