Python Projects and Unit Testing

Structuring Python projects and efficiently testing code with Continuous Integration

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Link to git repository in case you just want to follow along

Why Test Code?

- Following from the debugging talk - half of your time programming is debugging.
- Want to make sure that sensible **output** is given for sensible and insensible **input**.
- Important that all code meets quality standards before deployment.
  - Does the code use the conventions of the programming language (e.g. style guides)?
  - How much of the code can we account for the behaviour of (code coverage)?
  - Does the code behave as intended?
- Frameworks now exist that allow for automated code testing that makes this far less cumbersome.

Topics Covered Today

1. How to set up and structure Python projects.
2. Exporting Python scripts as packages in your local environment.
3. Comprehensive unit testing in Python.
4. Continuous Integration (CI) with *GitHub Actions* to automate the testing procedure and notify you where issues arise.

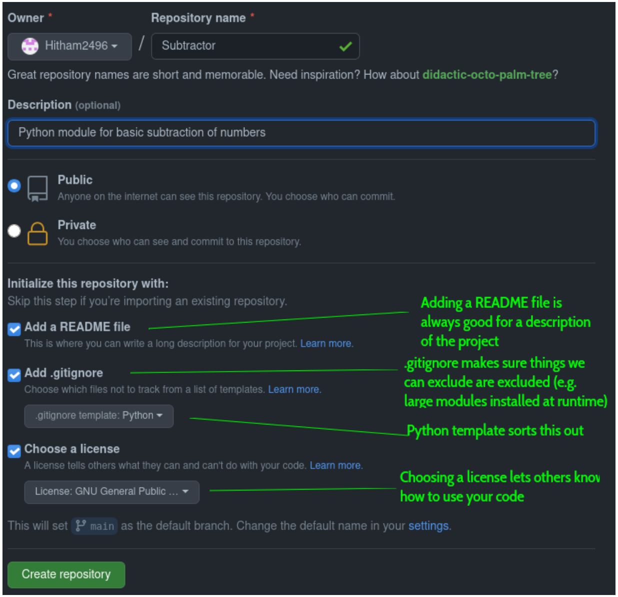
IMPORTANT: These principles can be applied to *any* project in *any* language (within reason) - Python makes for a soft introduction to the topic in this talk.

Today's task: write a 'difference' function `diff(x, y)` that subtracts two numbers[1].

[1] I'm being deliberately vague here

Python Project Structure

Python Project Structure - Create Git Repository



Owner *

Hitham2496 /

Repository name *

Subtractor ✓

Great repository names are short and memorable. Need inspiration? How about didactic-octo-palm-tree?

Description (optional)

Python module for basic subtraction of numbers

● Public
Anyone on the internet can see this repository. You choose who can commit.

○ Private
You choose who can see and commit to this repository.

Initialize this repository with:
Skip this step if you're importing an existing repository.

✓ Add a README file
This is where you can write a long description for your project. Learn more.

✓ Add .gitignore
Choose which files not to track from a list of templates. Learn more.

.gitignore template: Python

✓ Choose a license
A license tells others what they can and can't do with your code. Learn more.

License: GNU General Public ...

This will set `main` as the default branch. Change the default name in your settings.

Adding a README file is always good for a description of the project

.gitignore makes sure things we can exclude are excluded (e.g. large modules installed at runtime)

Python template sorts this out

Choosing a license lets others knov how to use your code

Python Project Structure - Directory Format

Firstly, clone your repository, for me it clones into a directory called `Subtractor`.

Create the following sets of directories in ‘Subtractor‘ (or your equivalent)

Subtractor

- **Subtractor/src** - this is a directory for our source code and modules
  - **Subtractor/src/subtractor** - this is the name I chose for the module we write today
- **Subtractor/tests** - this is for the tests we want to execute

If you create more modules, place them in their own directories in **Subtractor/src**

Python Project Structure - Our Script

- Create a Python script e.g. `diff_calc.py` in **Subtractor/src/subtractor**. These are the contents of mine:

```
#!/usr/bin/env python

def diff(x, y):
    """
    Finds the difference between
    two numbers.
    """
    return x -y
```

- In the same directory create a blank file called `__init__.py`
- This tells Python that we're building a module that we (will) want to import elsewhere in the project.

Exporting Packages

Exporting Packages - Endless Configuration Files

- To export our code as a module in our local environment, python requires many configuration files, all of these are to be created in **Subtractor**:
  - `pyproject.toml` - this specifies which build tools will be used to create the module.
  - `setup.py` - this will be execute the necessary methods to set up the module compilation.
  - `setup.cfg` - configuration file for `setup.py`
  - `requirements.txt` - other modules we require (e.g. `numPy`) and their specific versions, we don't need any for this project.
  - `requirements_dev.txt` - other modules we require for developing (i.e. testing in out case) and their specific versions, we do need this!
- The `PyPI` documentation provides in-depth guidelines for these - summaries in backup slides.

Interlude - What are we doing again?

- We're trying to get python to run our code in our local environment - this makes using modules that we've written simpler without hardcoding any directories.
- In **Subtractor**, run `pip install -e .`
- This uses `pip` to install the code specified in the configuration files such that we can import it into our code like a normal python package - anywhere.
- Try it! Open a python console anywhere and run:

```
>>> from subtractor.diff_calc import diff
>>> diff(10,2)
8
```

- The `-e` flag in the `pip` command ensures that we install in 'editable' mode, i.e. suited for developing.

Unit Testing in Python

Test Driven Development

- Today we will write appropriate tests after having produced a first attempt of our module - however is this good practice in general?
- Test-driven development is an incredibly useful philosophy for writing intentional code that preempts potential issues - good practice is to **start** by writing tests.
- In producing appropriate tests before writing the bulk of your code, you can make sure to identify limitations/potential pitfalls guided by the constraints of the language you use and the task you are trying to accomplish.
- Important to remain *flexible* during development - allow yourself to develop your tests when the need arises and to let testing instruct the development of your application.

Unit Testing - Sensible Output

What should `diff` return in the following cases:

- `diff(0.1, 0.3)`?
- `diff(1, 0.7)`?
- `diff(3, 2)`?

What about:

- `diff("hi",6)`?
- `diff(4)`?

We can want to ensure that the output is sensible - this includes sensible error messages where the input is insensible.

Unit Testing - Sensible Output

- For `diff(0.1, 0.3)`, the Python subtraction operator allows us to return negative floats (the output is sensible).
- Similarly the subtraction operator allows us to subtract floats and integers (even mixed) so `diff(1, 0,7)` and `diff(3, 2)` work.
- Try `diff("hi", 6)` in the python console you had open - is the error you get very helpful? We can do better.
- What about `diff(4)`? Do we want an error in this case[2]? We can specify a default value for e.g. `y`.

[2] we can still raise an error, this isn't so clear cut

Unit Testing - Let’s upgrade `diff_calc.py`

```
#!/usr/bin/env python

def diff(x, y=0):
    """
    Finds the difference between
    two numbers x and y, default
    value of y is 0.
    """
    if not (isinstance(x, int) or isinstance(x, float)):
        raise TypeError(
                "diff accepts only float or int arguments.")
    if not (isinstance(y, int) or isinstance(y, float)):
        raise TypeError(
                "diff accepts only float or int arguments.")
    return x -y
```

Unit Testing - `unittest` Library

- We specified necessary components for the tests in our configuration file - let's write a test for `diff_calc.py`.
- Convention: in **tests** create a python script called `test_diff_calc.py`. Also create a blank `__init__.py` file in the same place.
- We will use Python's in-built `unittest` package.
- To do this we create a *derived class* of the `unittest.TestCase` type - this will allow us to create an object that contains all of the different tests we want to run.
- These tests will be run by calling the `main()` method in `unittest`.

Unit Testing - test_diff_calc.py

```
import unittest
from subtractor.diff_calc import diff


class TestSubtract(unittest.TestCase):
    def test_something(self):
        ...
    def test_something_else(self):
        ...
    .
    .
    .


if __name__ == "__main__":
    unittest.main(verbosity=2)
```

Unit Testing - `unittest` Library

- The scope for testing in Python is huge, would encourage looking up what you can do.
- For our purposes the test functions we use will be void and undecorated, we will make use of the simple `assert` methods available in `unittest`
  - `assert(some_bool)` - the test will pass iff `some_bool==True`
  - `assertEqual(x, y)` - the test will pass iff `x==y`
  - `assertRaises(some_exception, some_method, *args)` - the test will pass iff `some_method(*args)` raises `some_exception`
- Once we have made our tests (look at the example on GitHub if you want inspiration), we can run them by executing `pytest` in **Subtractor**.

Unit Testing - What Could Go Wrong?

- Since we are only subtracting two numbers, it's hard to see what could go wrong. However if you execute the example on GitHub you should get an error.
- The `verbose` option in the test file gives some comprehensive output, the key lines are:

```
>       self.assertEqual(diff(1.2, 1.0), 0.2)
E       AssertionError: 0.19999999999999996 != 0.2
```

- Python uses floating point numbers which - to high precision - can lead to inaccuracies. Try `1.2 - 0.2` in a Python console!
- We need to decide a course of action - is the accuracy of `0.19999999999999996` enough for us? If so we can add a tolerance.

Unit Testing - Upgrade `diff_calc.py` Again

```
#!/usr/bin/env python

def diff(x, y=0, TOL=9):
    """
    Finds the difference between
    two numbers x and y, default
    value of y is 0.
    """
    if not (isinstance(x, int) or isinstance(x, float)):
        raise TypeError(
                "diff accepts only float or int arguments.")
    if not (isinstance(y, int) or isinstance(y, float)):
        raise TypeError(
                "diff accepts only float or int arguments.")
    return round(x -y, TOL)
```

Unit Testing - Style Guides and Linter

- `PEP8` is seen as the most universal Python style guide; it has many rules regarding how code is laid out (e.g. whitespace, comments, variable names, etc.).
- Rather than manually checking against the conditions required to accord with the style guide we can use a *linter*.
- `flake8` is a Python linter, running `flake8 somefile.py` will tell you where the style guide is not followed in `somefile.py`.
- Running it on our module shows that we have a whitespace issue in our return statement, adding a space: `x -y` to `x - y` fixes the issue.

Continuous Integration

Continuous Integration

- Manually running these tests every time is cumbersome - if we have many tests and source files we may forget to run on all of them.
- We can use *Continuous Integration* (CI) to build and test our project every time we make a small change.
- GitHub Actions makes this very convenient - allows us to create a *workflow* that executes certain tasks (e.g. building, testing, linting ...) in an order and configuration we specify.
- Uses `YAML` configuration scripts - lots of templates available!
- Go to Actions -> Continuous Integration -> {choose whatever you like!}

Continuous Integration

- For our script, we are treating it as a module so choose *Python package*, looking at the script we see that it builds our project, tests all modules and lints all scripts!
- We can customise certain aspects:
  - do we want to run this script whenever we commit to any branch, or just main?
  - which versions of Python do we want to test with? Which operating systems?
  - we can add e.g. `requirements_dev.txt` to the script in case we have other test libraries that are needed.
- When we commit a change to the main branch (for instance), a workflow will be sent to the queue where it will wait until a compatible *runner* is free to run it.
- You can inspect the output of these workflows to see where the errors occur - our linter and rounding error would be picked up here!

Continuous Integration and Delivery - Ideas

- For Python we can do many things - build applications, build modules, ...
- We can equally organise a *Continuous Delivery* (CD) system - something that publishes or deploys our work in some way.
- We can use CD (which works similarly through GitHub Actions) to publish our package to `PyPI` so that anyone can install it with `pip`!
- Can provide sensitive information e.g. login info for `PyPI` that can be stored securely in *GitHub Secrets* for use in these workflows.
- Using API (Application Programming Interface) keys is preferred over keeping passwords stored - `PyPI` grants the option to create these for all your projects!

Continuous Integration and Delivery - Ideas

The scope of CI/CD extends *well* beyond testing Python modules, here are just a few off-the-cuff examples:

- Build and deploy a website.
- Build a paper with LaTeX and host it online.
- Execute the same code in a `docker` container to mimic an environment that is difficult to set up correctly by hand (this is really useful for HEP software).

What will you do?

Backup

Some Notes on Security

- Brief important note with PyPI - anyone can upload code to be installed via `pip` so make sure you never use `pip` with `sudo`!
- Similarly, if you want to provide e.g. login details for a CD system you can upload these to GitHub secrets where they are securely kept.
- It is better practice where available to use API (Application Programming Interface) keys for authentication.
- For Python packages, you can generate these online in PyPI for each project you create and add them to GitHub secrets.

Code Coverage

- When writing code, you want to make sure that as many of the possible branches that can be followed has behaviour that is accounted for.
- For example, with lots of `if, else` statements, your tests should ensure that all possible combinations receive testing - this is code coverage.
- `pytest-cov` allows you to test for code coverage - will give a percentage of your code that is covered by your tests (lots of cool visualisation tools can be used with this).
- Philosophy: This can be a tool to instruct your testing which in turn instructs your development, but these factors are all inter-related aspects of your project, make sure you adapt your testing as your project progresses and vice versa!

Exporting Packages - `__init__.py`

- This file is the initialisation file for the package - when we run: `import module`, the code we put in here will be executed.
- For our project we left this blank (there is not much initialisation that needs to be done).
- If you have certain tasks that need to be done exactly once at the start when importing a library - it can be a good idea to add these in the initialisation file.
- E.g. you may have a database of (for a particle physics calculation) matrix elements evaluated at certain phase space points - you can set the module to open a connection to the database as soon as it is imported by adding the appropriate code here.

Exporting Packages - `pyproject.toml`

- This file contains instructions for which build tools to use and is fairly standard - will be applicable as is to most basic projects. These are the contents:

  ```
  [build-system]
  requires = ["setuptools>=42.0", "wheel"]
  build-backend = "setuptools.build_meta"
  ```

- The build tools (e.g. `pip` and `build`) used by Python require this file to understand how the module is supposed to be built.

Exporting Packages - `setup.py`

- Previously, *dynamic* configuration was the favoured approach - all the setup commands are executed in `setup.py`.
- This can be problematic - can lead to security issues.
- This is one reason why you should **NOT** use `pip` with `sudo`
- Now we use *static* configuration, we provide the settings for `setup.py` in a configuration file. `setup.py` looks like:

```
from setuptools import setup

if __name__ == "__main__":
    setup()
```

Exporting Packages - `setup.py` - Common Issue

- If you are having permission issues, specify the `-user` option when installing your module.
- To enable this compatibility you may need to modify your `setup.py` such that it looks like:

```
from setuptools import setup
import site
import sys

site.ENABLE_USER_SITE = "--user" in sys.argv[1:]

if __name__ == "__main__":
    setup()
```

Exporting Packages - `setup.cfg`

- This is the configuration file for `setup.py`
- The format is simple, we have three main sections:
    - `[metadata]` - basic information about the module e.g. name, author, version, license, description, etc.
    - `[options]` - options that need to be set for correct installation, e.g. which packages need to be build, what packages the install requires, where the packages are stored, etc.
    - `[options.extras_require]` - extra requirements for development, for our purposes this is where we will list the modules needed for testing.
- Please base this on the version available on the repo, altering names etc. where necessary.