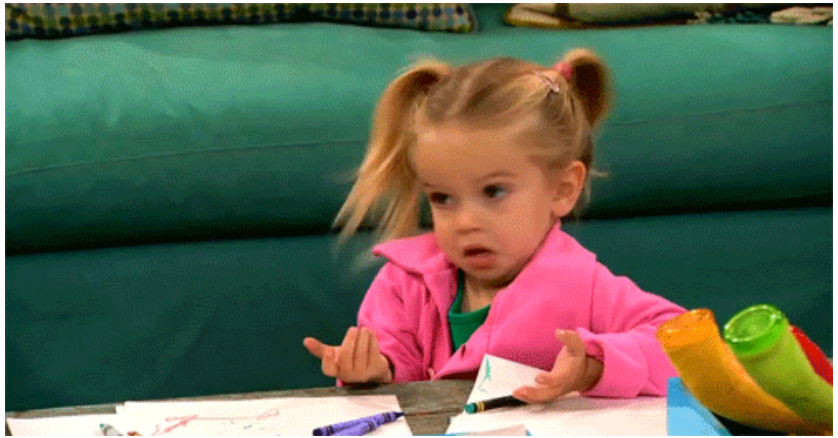
Organizing, documenting and distributing code

ASPP 2022, Bilbao

= How to make your code (more) usable

Why bother?



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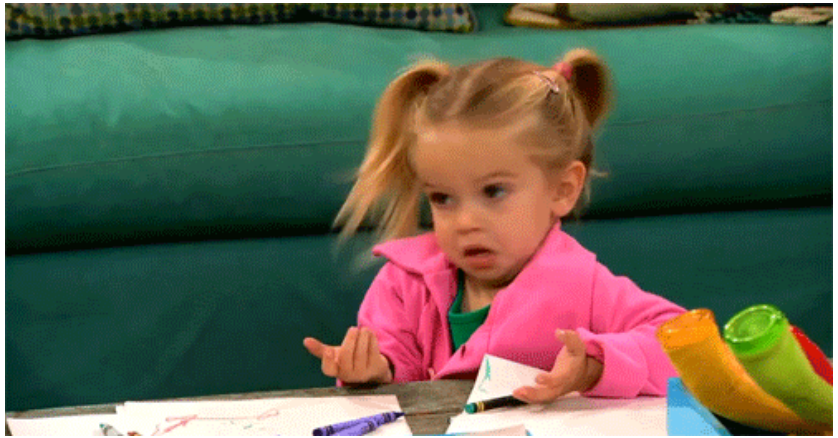

Contents

usability features:

1) folder and file structure

2) error-free importing and installation

3) isolated, protected code

4) readability

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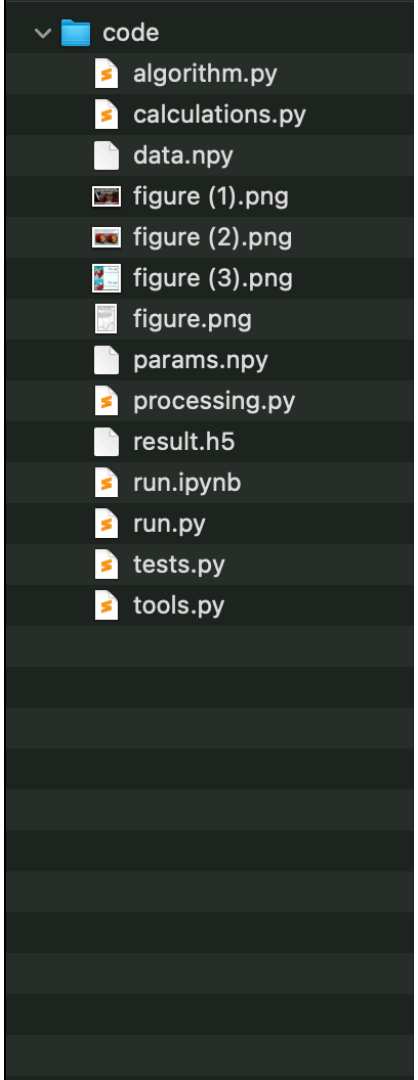
Folder structure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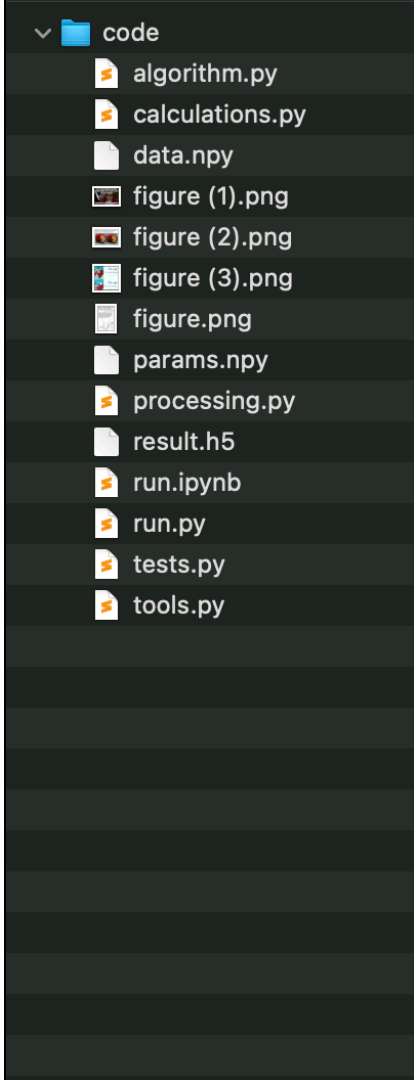
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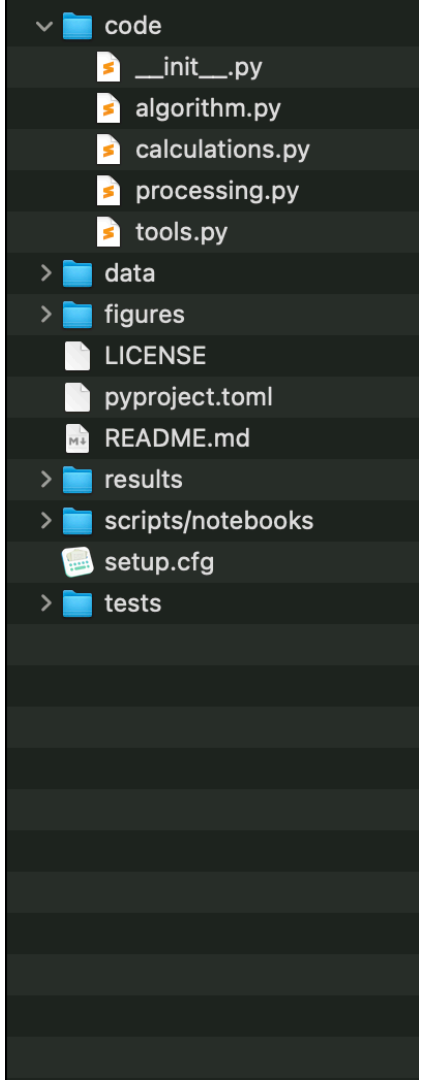
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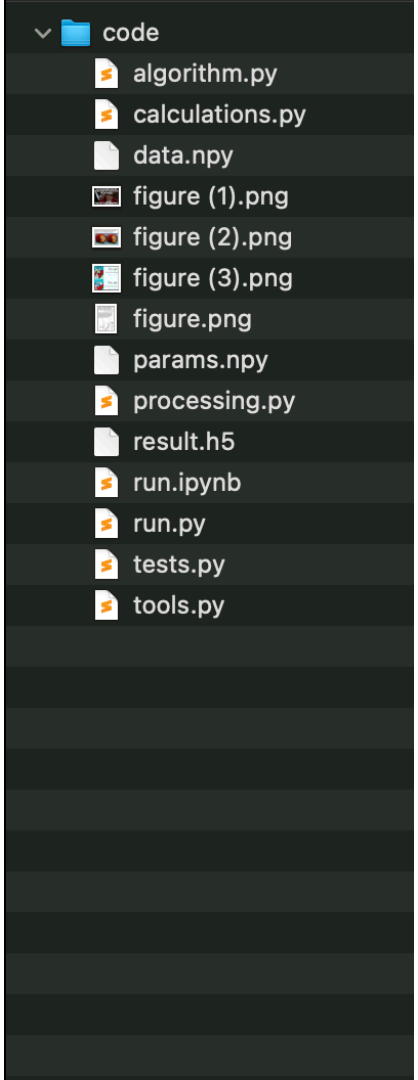
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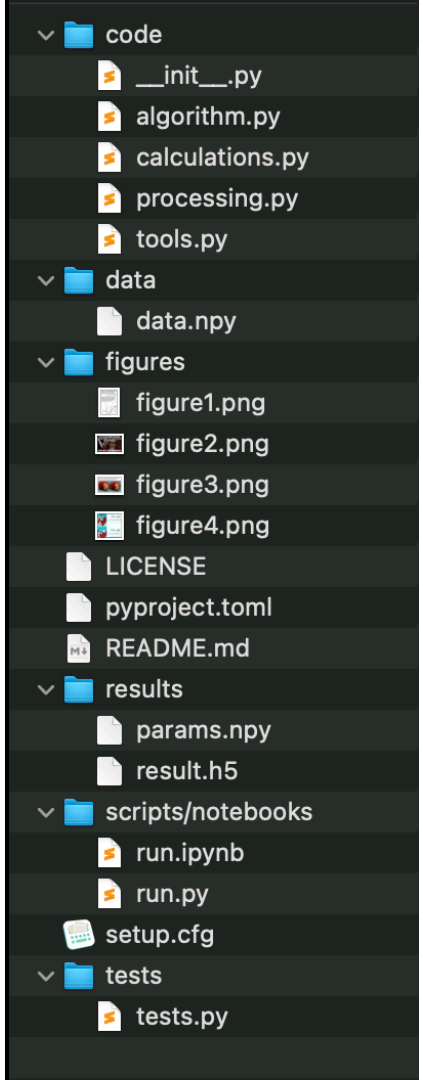
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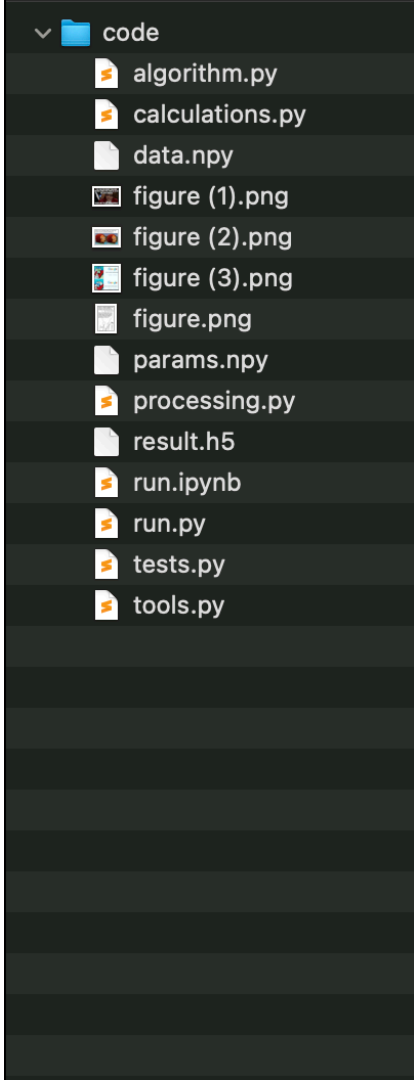
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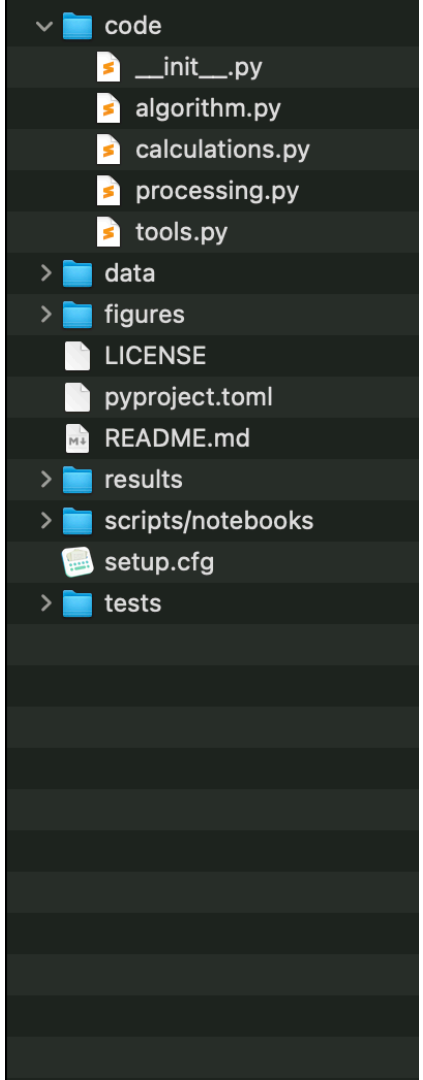
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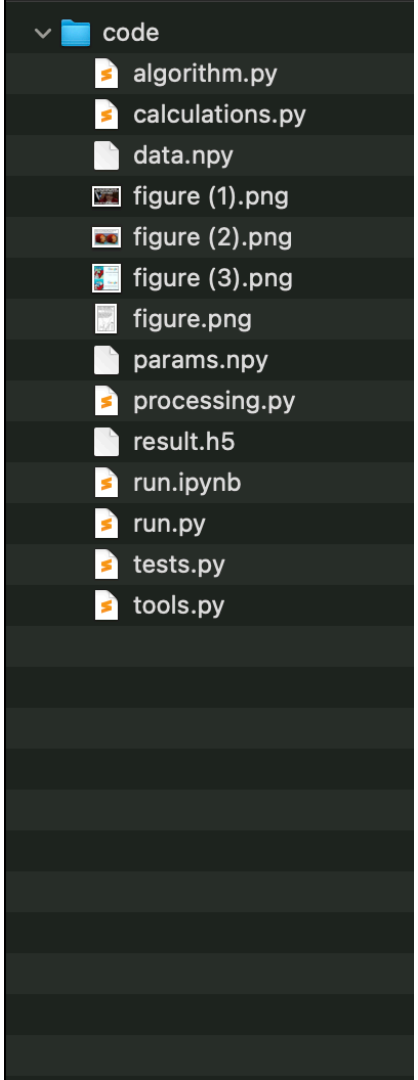
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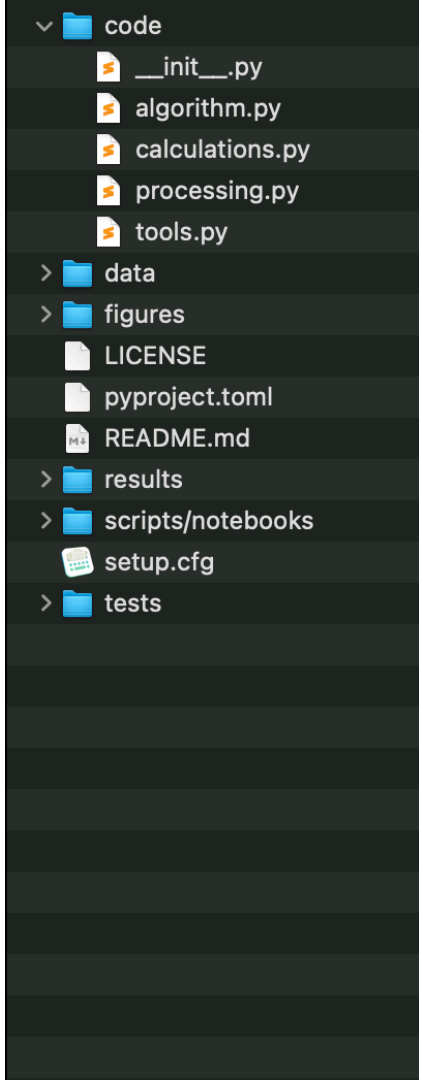
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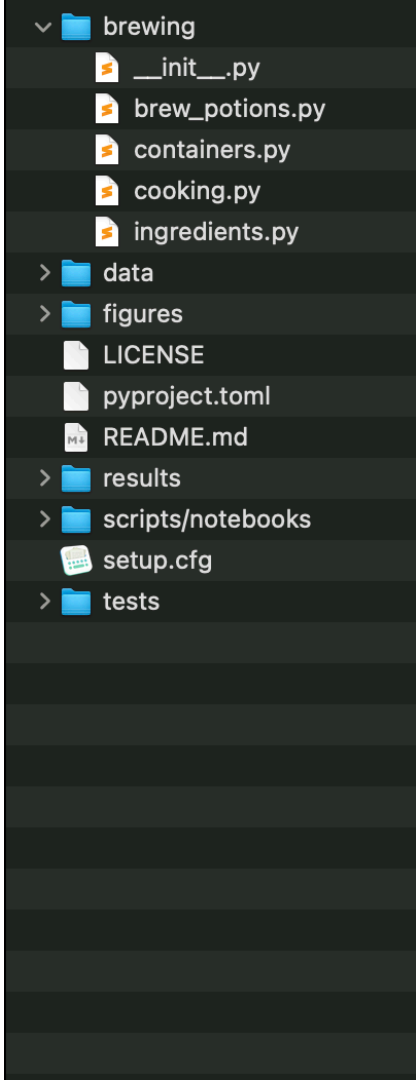
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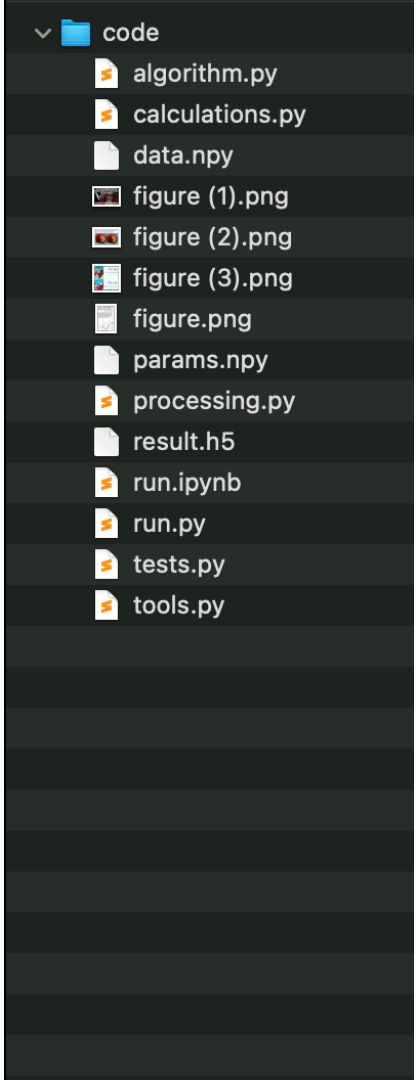
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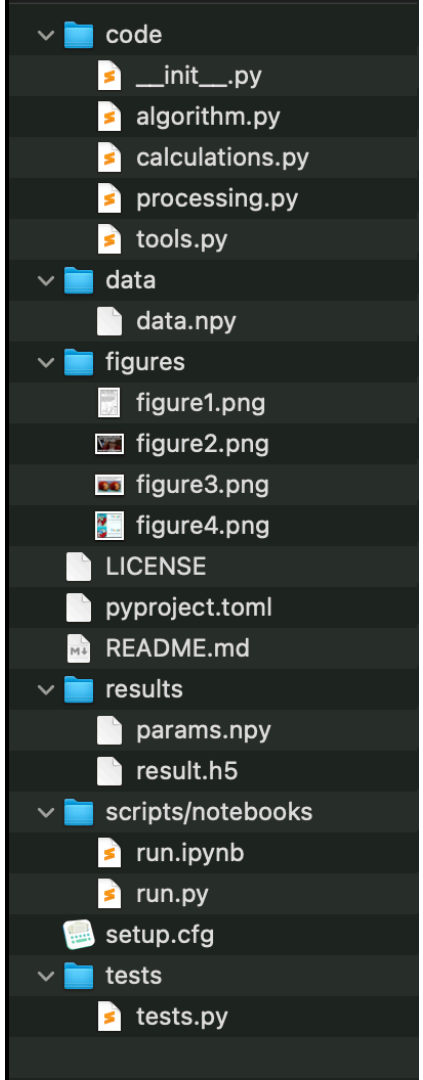
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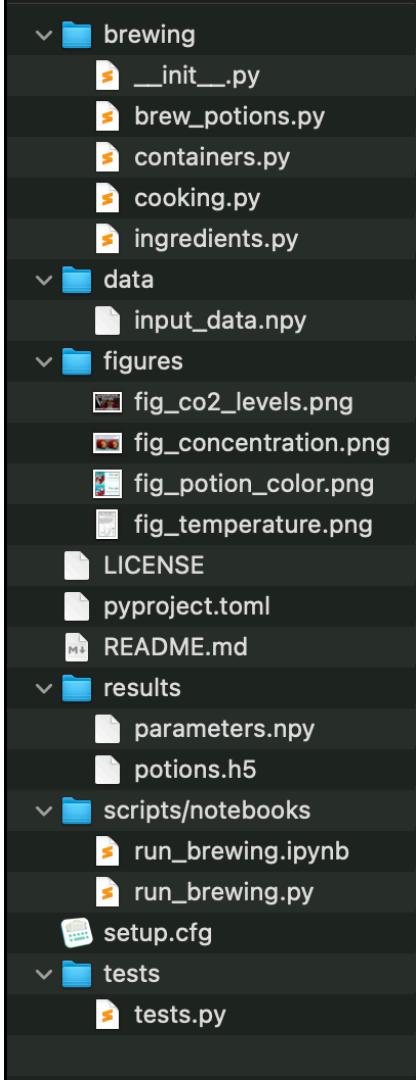
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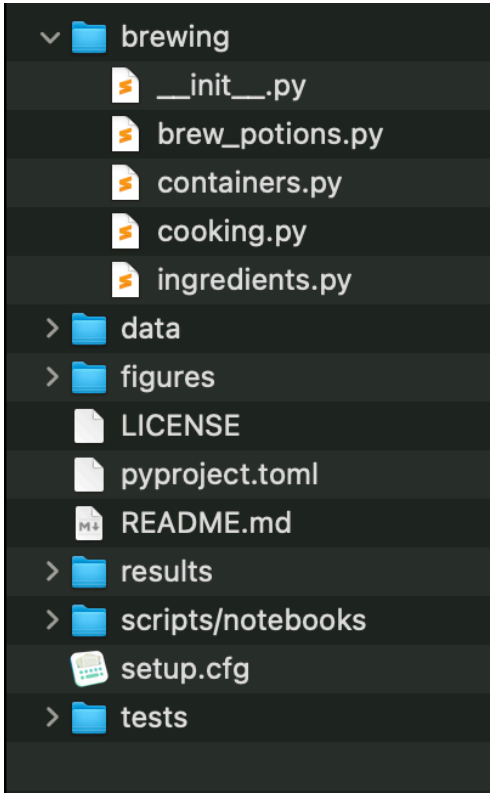
Python package structure



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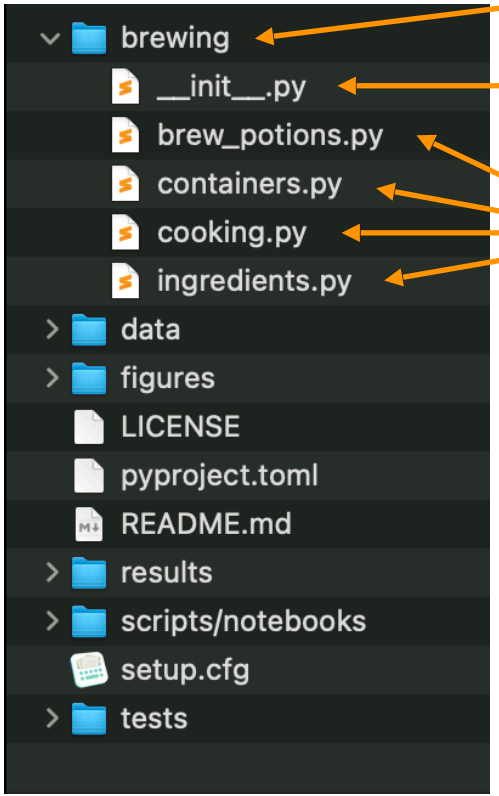

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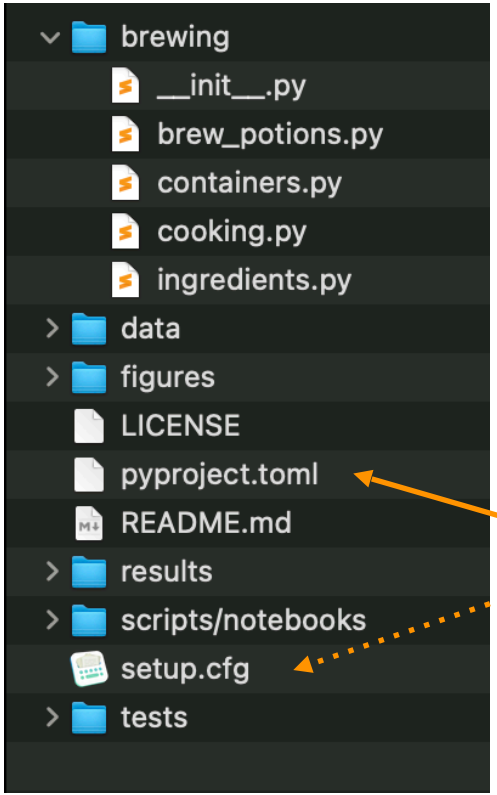

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will explain more later :)

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makes the package (legally) usable.*

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contains more information e.g. instructions on how to use your package.

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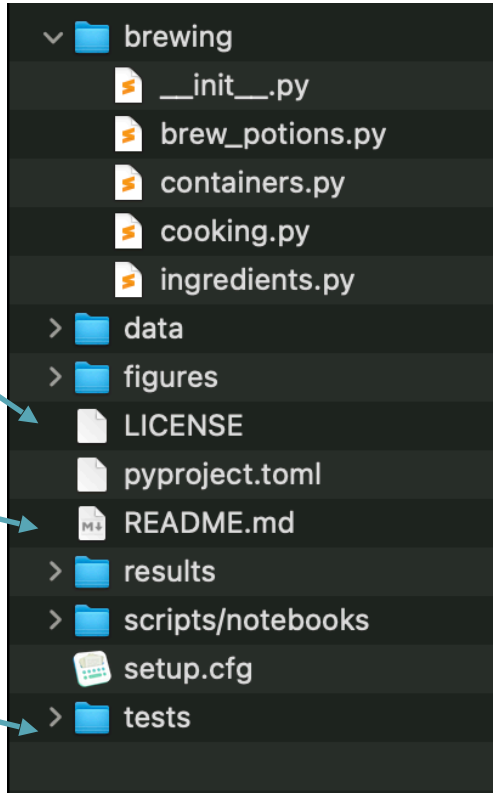

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Advantage 1

—> know where to find items

e.g. wardrobe

- suit, shirts
- towels
- socks

same concept applies to code

—> use meaningful file names

Advantage 2

- it makes all of your code **installable***
- which makes all of your code **importable**

Terminal

```
> pip install brewing
>
> python
>>> import brewing
>>> brewing.brew_a_potion()
```

* (need a few other changes we will go over)

Advantage 2

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Importing

Brewing package

- content of brewing package
  - walk through code
  - run brew_potions.py
  - point out files for exercise

brewing package

Importing

- Follow the instructions in **Exercise 1 Importing.md**

(There is no need to submit a pull request for this exercise)

names & mains

any code running under *if __name__ == "__main__":*

- will be ignored when importing
- will be executed when the module is run as a script

```
if name == "__main__":
    i_will_not_be_imported = True
    print("Not printing when importing")
    print("But printing when run as script")
```

Importing code

- you can always import code from your ***current directory***
  - by calling `import brew_potions`, Python will look for
    - a module called `brew_potions.py` inside the ***current directory***
    - a package called `brew_potions` inside in the ***current directory*** (= folder called brewing with an __init__.py file)

- Importing a module will execute <u>all</u> the code in the module (including imports, print statements)

Importing modules

- you can always import code from other modules (.py files) in your ***current directory***
- Options for e.g. importing *eternal_flame*

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1. `import cooking`

2. `import cooking as cook`

3. `from cooking import eternal_flame`

4. `from cooking import *`

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```
1. import cooking                          + cooking.eternal_flame

2. import cooking as cook                  + cook.eternal_flame

3. from cooking import eternal_flame       + eternal_flame

4. from cooking import *                   + eternal_flame
```

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1. import cooking                          + cooking.eternal_flame
                                           + cooking.fire

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                                           + cook.fire

3. from cooking import eternal_flame       + eternal_flame
                                           X fire

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```

Importing a package

- you can always import a package located in your current directory
- Modules in the package are bound to the package name

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1. import package

2. import package.module

3. from package.module import
   object
```

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Importing

- Thought(?) exercise:
  Exercise 1 Importing.md

Is there a way to get

a) any 2

b) all 3

exercises to work simultaneously?

Importing

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pip editable installation

Knowledge needed

- **what packages are available?**
- what does an editable pip installation do?
- what are the requirements for this?

Available packages

- **core packages** e.g. time, math, os, …
  (come with Python, no installation needed)
- **installed packages** e.g. numpy, scipy, …
  (packages are downloaded to a system location
  e.g. /Library/Frameworks/Python.framework/Versions/3.9/lib/python3.9/site-packages
  which is on the Pythonpath => Python can find it)
- **current directory**

- All packages which fall under these categories can be imported

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Installing other packages

- Options to install a package using **pip**

Option 1: if package is included in PyPI

```
pip install numpy
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Option 2: install from a VCS like git

```
pip install git+https://github.com/<user>/<package-name>.git
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Installing other packages

- You can install Python packages in your terminal using a package manager

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standard package manager for Python

can install packages from PyPI (Python Package Index) or from VCS e.g. github

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open source package manager/ environment manager

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Pip editable install

You can import the package you are currently working on as if it were a package you downloaded.
—> This lets you use your own code as any other package you installed

Advantages:

1. you can **import** the objects in the package **from any directory** (no longer bound to the directory which contains the package)
2. at the same time you can keep your project in your current directory
3. you use your code as someone else would use it, which forces you to write it in a more usable way

Importing own project

- Options to install a package using **pip**

Option 1: if package is included in PyPI

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```

Option 2: install from a VCS like git

```
pip install git+https://github.com/<user>/<package-name>.git
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Option 3: install your package with -e (--editable) option

```
pip install -e <path-to-package>
```

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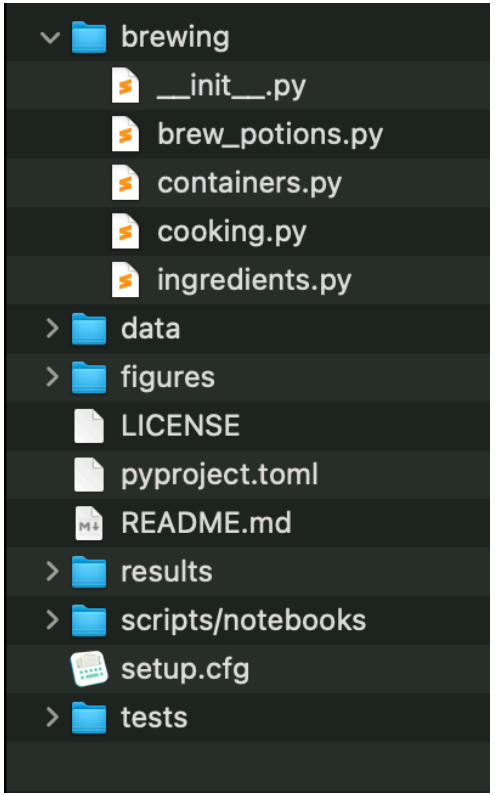

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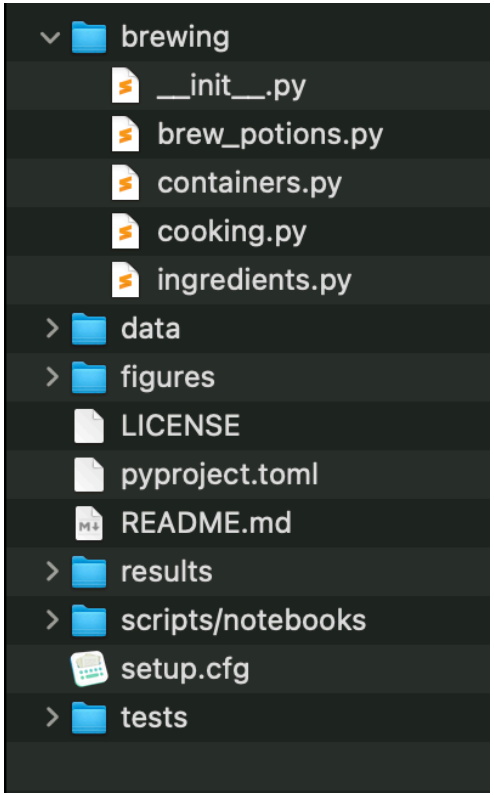

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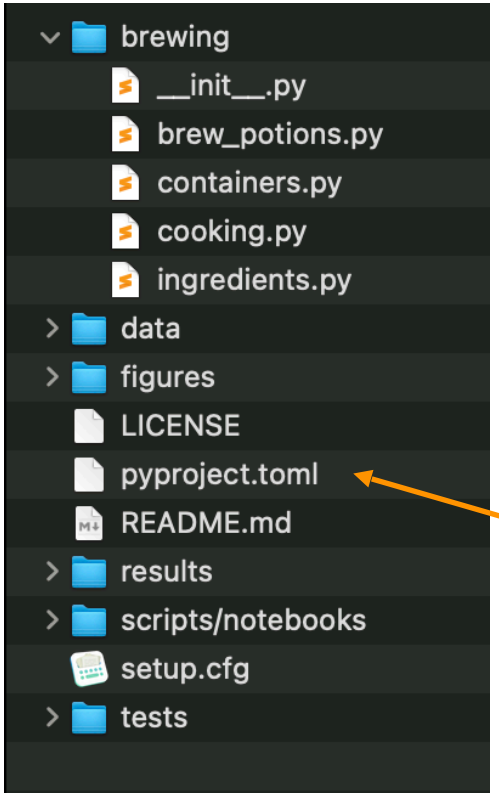

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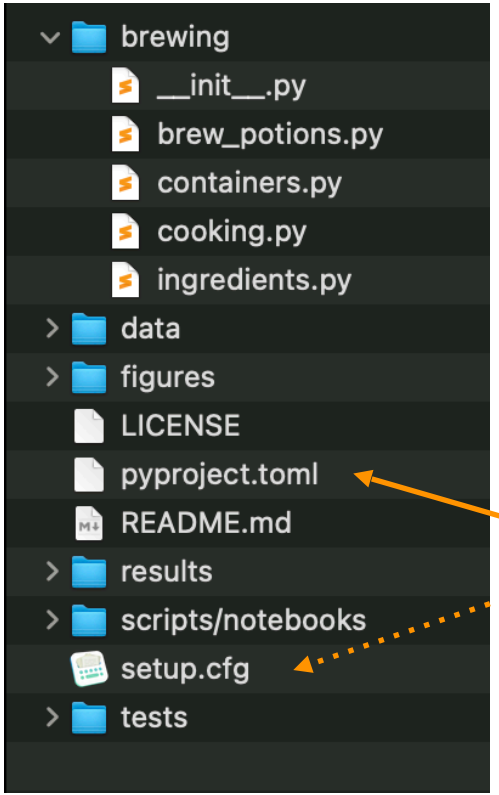

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Project metadata

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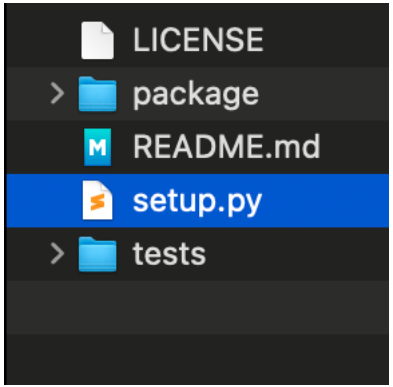

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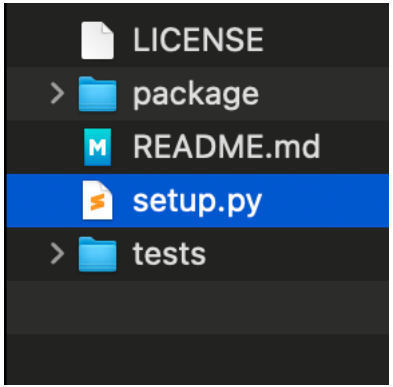

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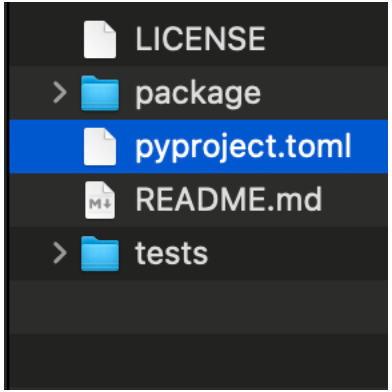
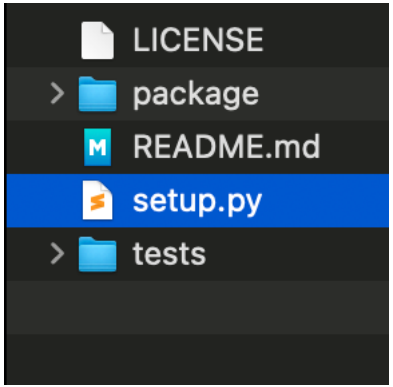
how it should be



the shiny, new recommended way of storing
project metadata and build information

Project metadata

how it started



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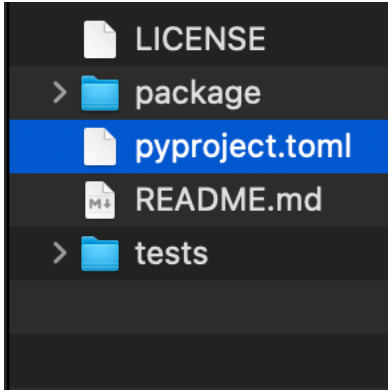

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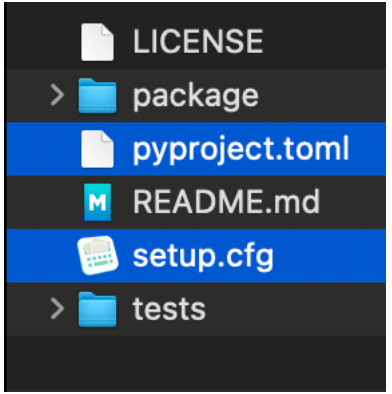

pyproject.toml currently not supported across all systems for editable install, fix by adding an **empty** setup.cfg file

Project metadata

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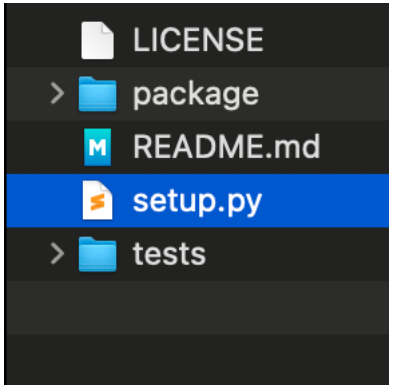

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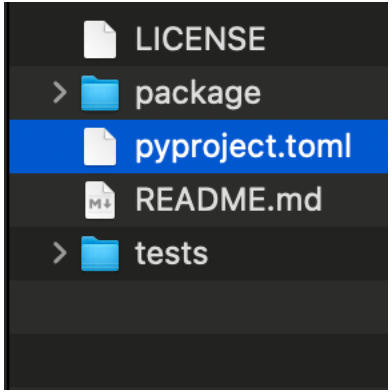

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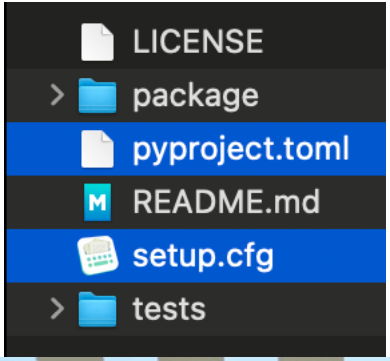

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- Required entries: name, version, description, authors
- **dependencies** not optional if code relies on other packages to work (go through modules and update regularly, don't just copy '> pip freeze')
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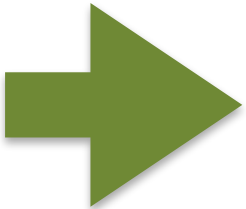

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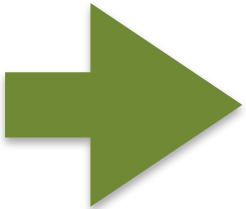

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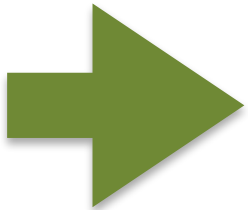

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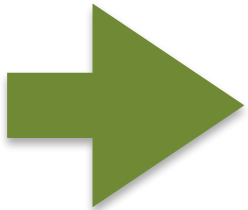

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```

Pip editable installation

- `pip install -e <path-to-folder-above-brewing>`

  or in the directory above `brewing`

  `pip install -e .`

- Follow the instructions in
  Exercise: Editable installation

(There is no need to submit a pull request for this exercise)

how to develop code if it’s in a package

Using the editable installation

- You set your imports once and then never worry about them again
- You have not lost any capability, you only gained usability
- If you absolutely must use notebooks, then you can import your code from your modules into your notebook much easier

Workflow (realistic?)

1 Create

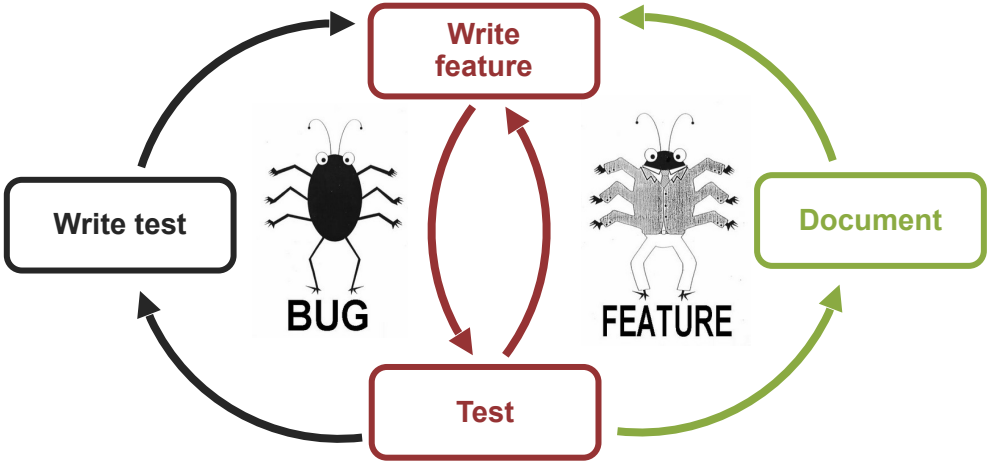
Set up structure

Create files:

```
__init__.py
pyproject.toml
setup.cfg
README
LICENSE
```

Make installable at this point

2 Build & Test



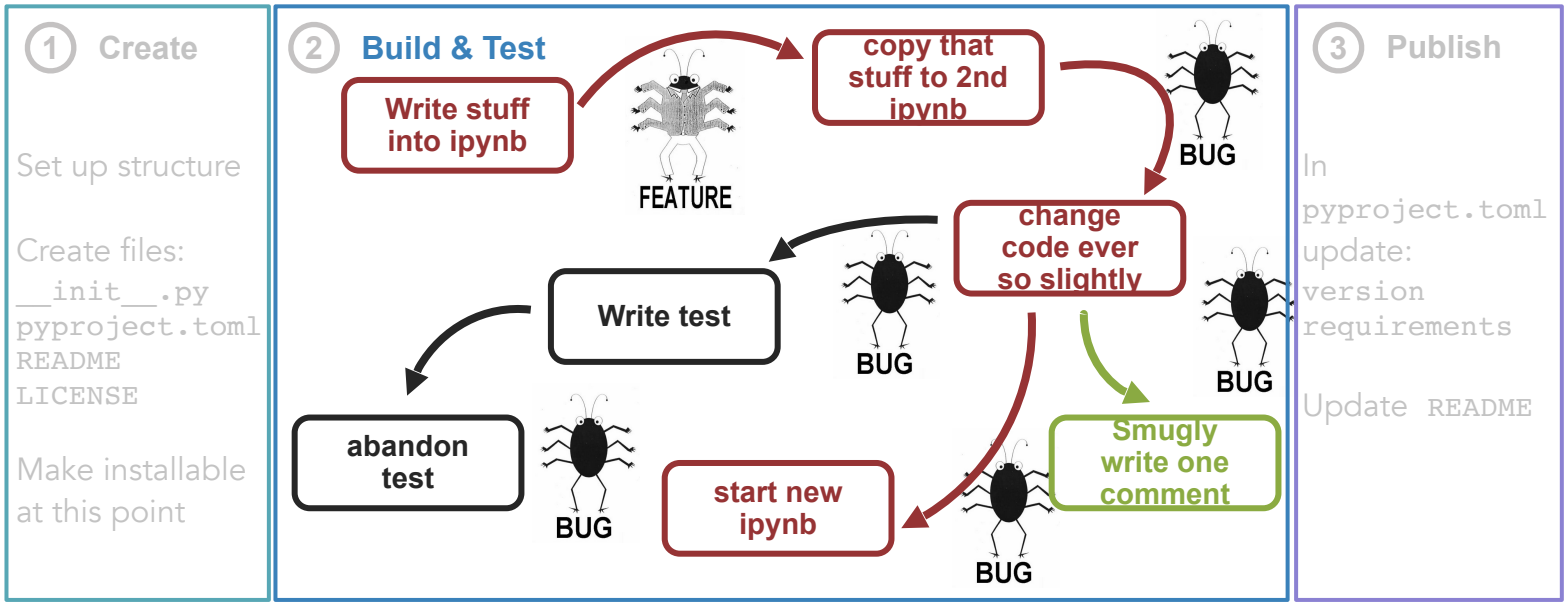
3 Publish

In `pyproject.toml` update:

```
version
requirements
```

Update `README`

Workflow (realistic?)



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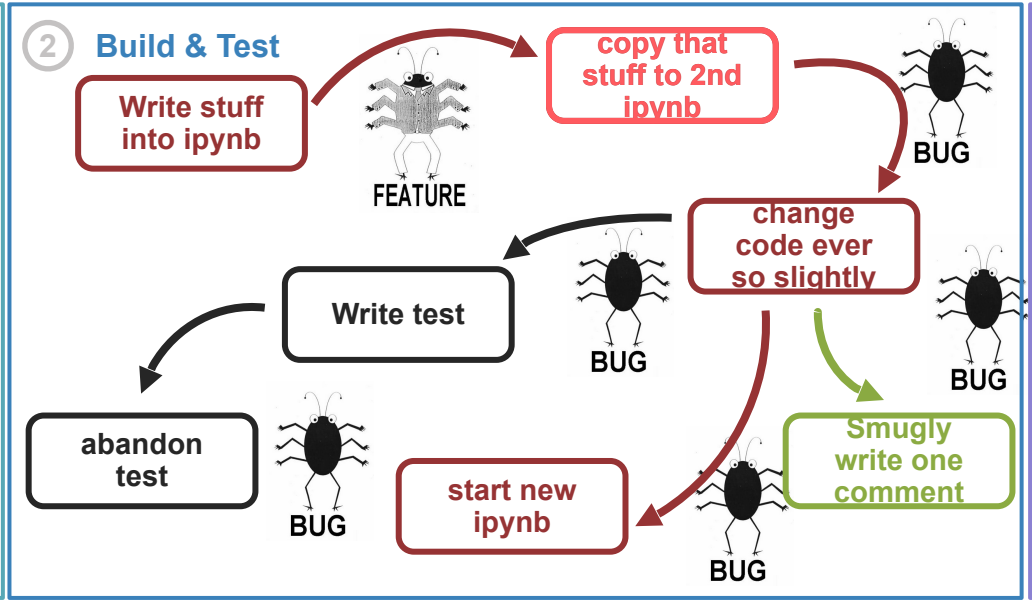

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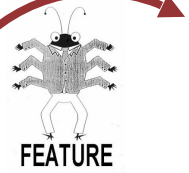
Write stuff into ipynb



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Workflow (realistic?)

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`__init__.py`
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`setup.cfg`
`README`
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Make installable at this point

2 Build & Test

Write stuff into ipynb

Move code to package

3 Publish

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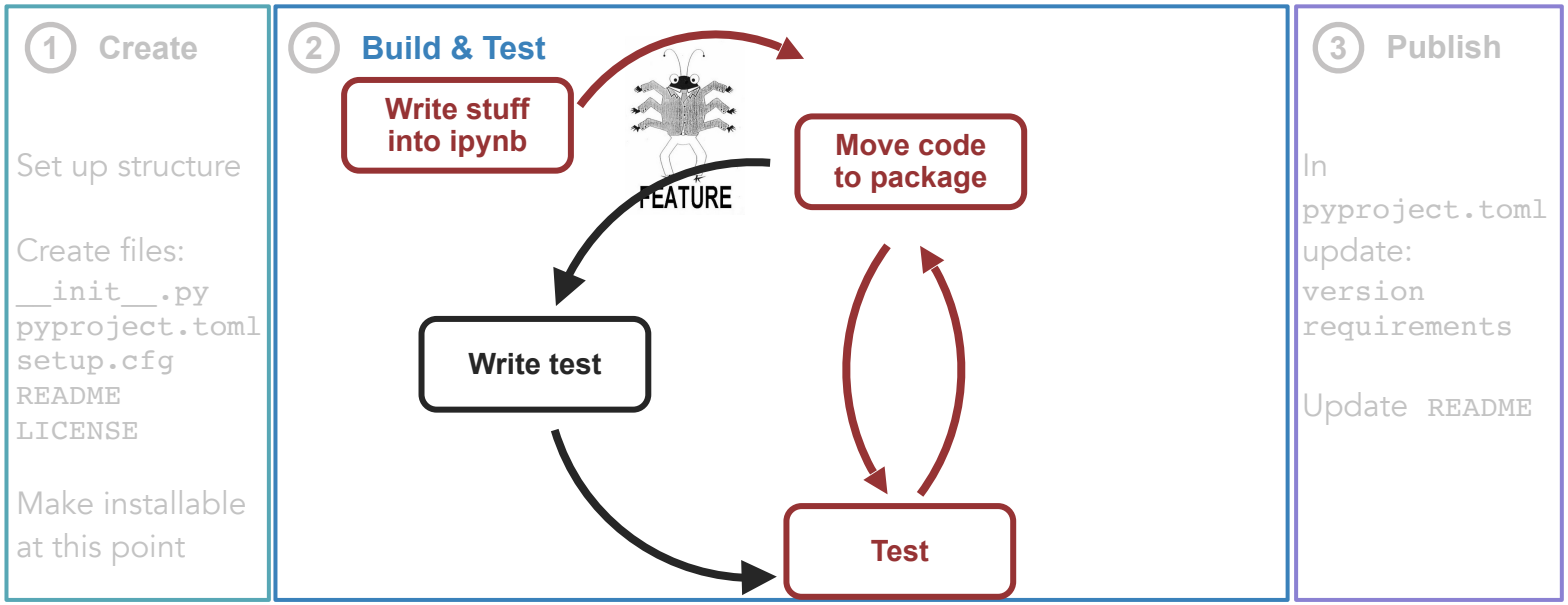
Update `README`

Workflow (realistic?)



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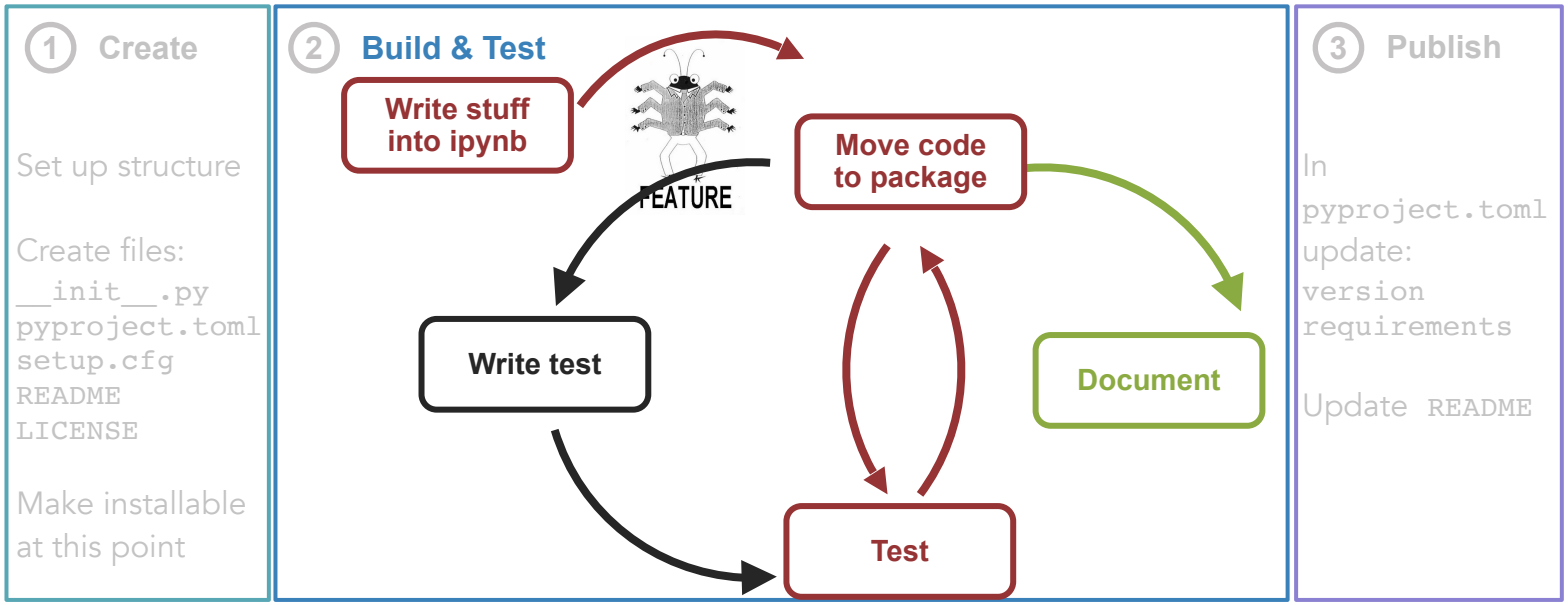

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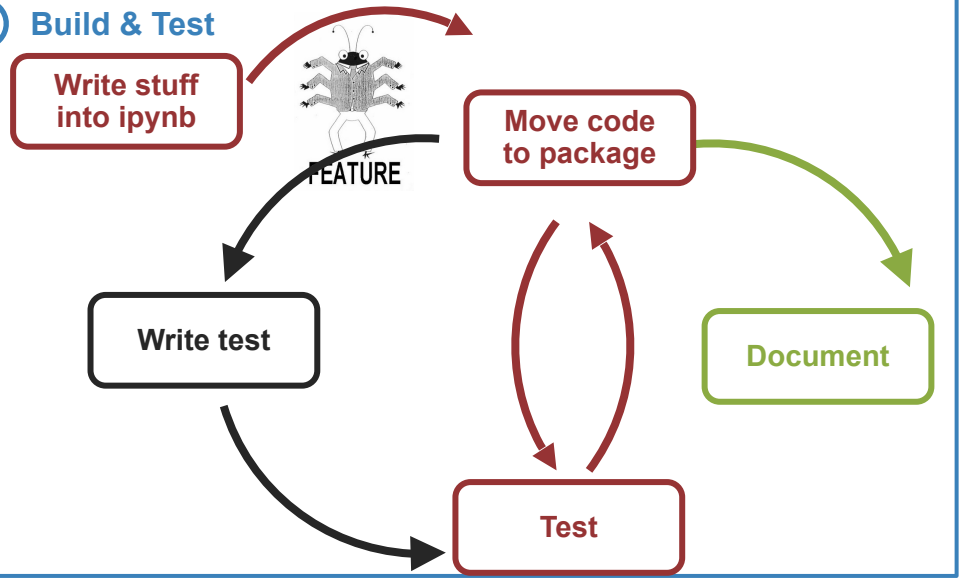

3 Publish

In `pyproject.toml` update:

`version`
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Update `README`

Write your function

- Write the last remaining **potion making function** we need before sharing the package

Exercise:

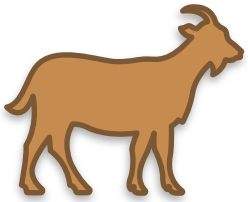
- Create a branch with a unique name
- Follow the instructions in **Exercise 3 Workflow** to write and test a function to make a “Python expert” potion
- Create a Pull Request

defend your code

Why environments?

Project 1

= 1st year
PhD project



Why environments?

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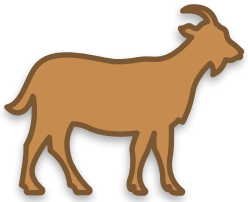

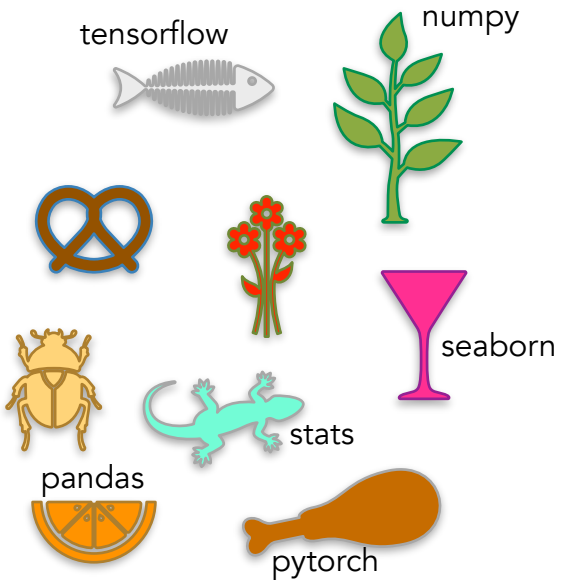

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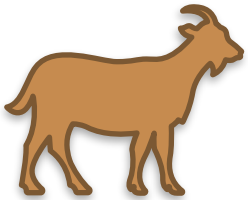
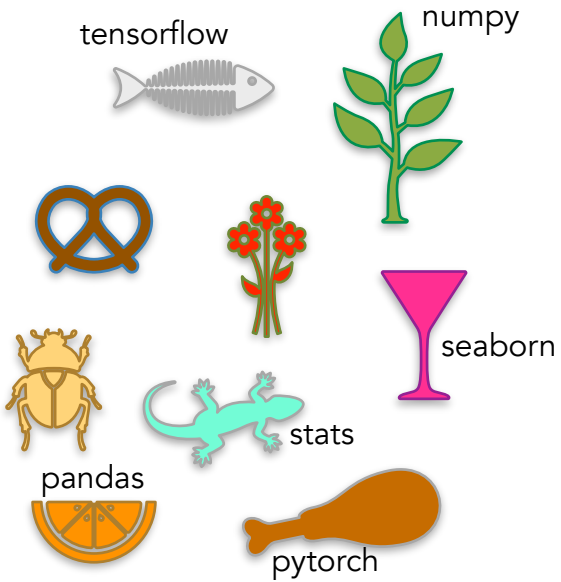
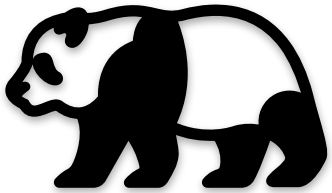




Project 2

= collaboration
with another lab



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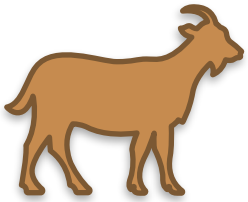

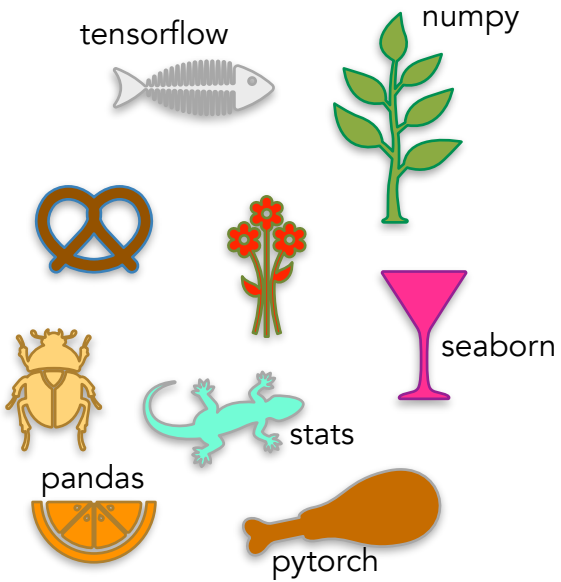

Project 2

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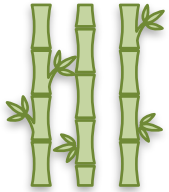
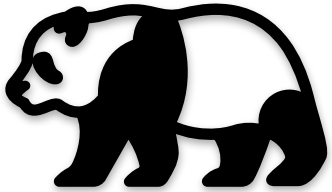
word2vec





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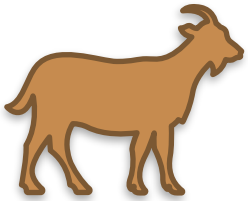

pandas = 1.2.4

dependencies

Why environments?

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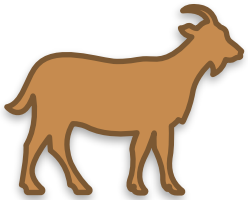
= 1st year
PhD project



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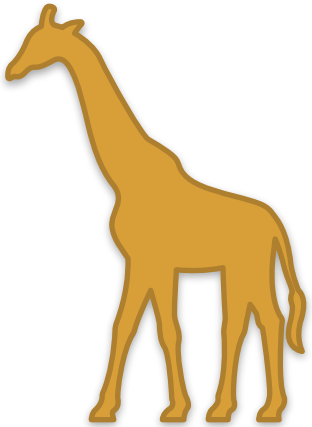
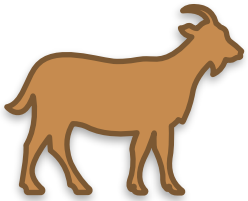


Project 2
= 2nd year
PhD project

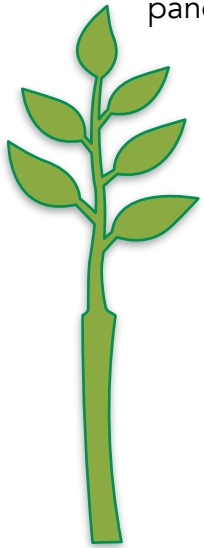
dependencies

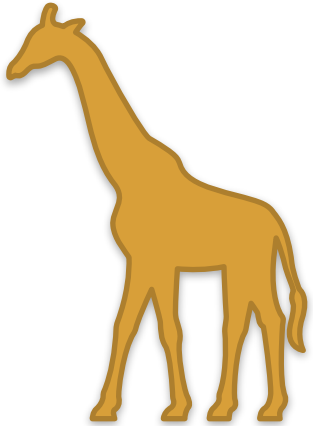
Why environments?

Project 1
= 1st year
PhD project



pandas = 1.3.0



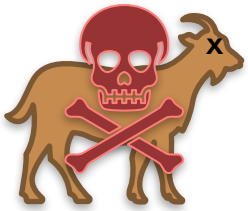


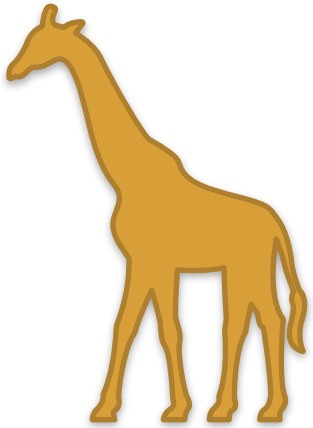
Project 2
= 2nd year
PhD project

dependencies

Why environments?

Project 1
= 1st year
PhD project





Project 2
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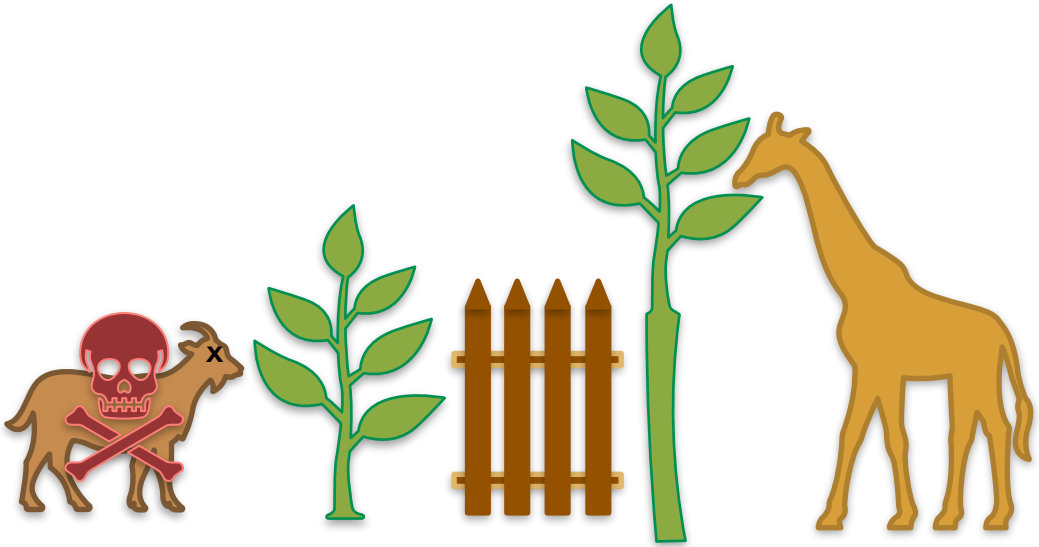
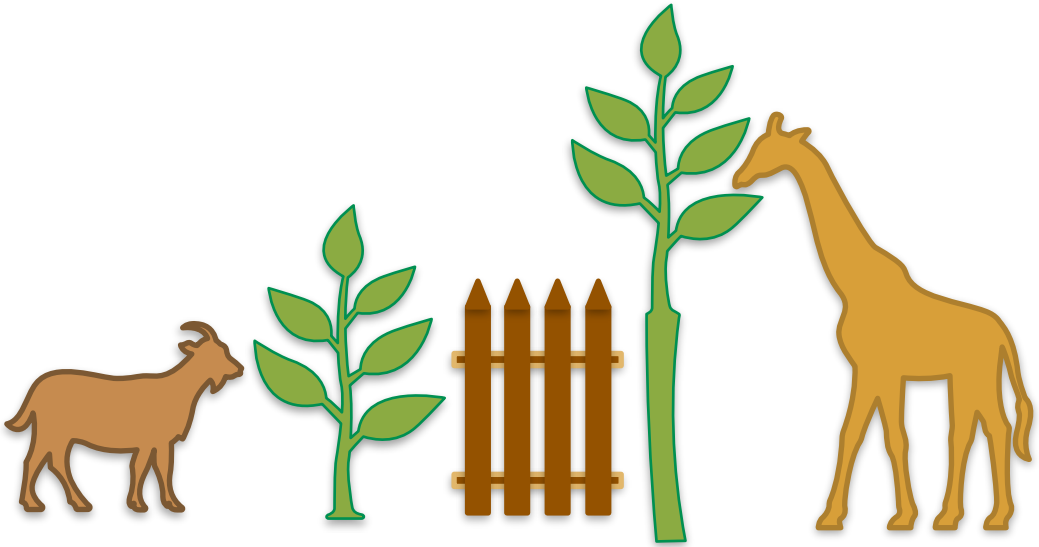


Project 2
= 2nd year
PhD project

dependencies

Why environments?

Project 1
= 1st year
PhD project



Project 2
= 2nd year
PhD project

dependencies

Breaking changes

- Ever ignored a one of these?

```
<stdin>:1: FutureWarning: In a future version of pandas all arguments of
 concat except for the argument 'objs' will be keyword-only
```

- This means that if you keep updating your python packages, you will run into issues at some point
  - code errors
  - unexpected results

Previous behavior:

```
In [1]: df.groupby('label1').rolling(1).sum()
Out[1]:
            a    b
label1
idx1      1.0  2.0
```

New behavior:

```
In [61]: df.groupby('label1').rolling(1).sum()
Out[61]:
                          a    b
label1 label1 label2
idx1   idx1   idx2      1.0  2.0
```

Virtual Environments

What is a virtual environment?

- A semi-isolated python environment -> you cannot access packages (libraries and their dependencies) installed in other environments.
- packages are installed inside a project-specific virtual environment folder (not added to general python path)
- If you break something, you can delete those folders and start over

Virtual Environments

- Create and activate a virtual environment following the directions in **Exercise 5 Virtual Environments.md**

- See what changed with regard to the Python interpreter and the installed packages

Additional advantages

- If you package your code, in your pyproject.toml you will have a record of at least one working combination of the versions of your dependency packages

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Environment Managers

- **venv** - current standard recommended by Python

- **poetry** - super useful (if it works o.0).
  solves dependency conflicts, creates pyproject.toml for you,
  keeps record of all dependency versions in committable file

- **pyenv** - if you need different Python versions in different projects

readability

Documentation

- Documenting your code provides a way of making you code **usable for future you and others**
  - **Comments** (#): describe what a line (or multiple lines of code do); notes to self
  - **Function/method docstring** (''' '''): purpose of function + params / return
  - **Module docstring** (''' '''): what's in this file

```
""" Module docstring """

def add_points(house_points,
    points=0):
    """ Function docstring."""
    # comment
    points += 1000
    return house_points + points
```

NumPy style

- triple double quotes below declaration
- The first line should be a short description
- If more explanation is required, that text should be separated from the first line by a blank line
- Specify Parameters and Returns as
  `name : type`
  `    description`
  (put a line of --- below sections)
- Each line should begin with a capital letter and end with a full stop

- access docs:
  `pydoc3 <module>.<object>`

```
""" This module demonstrates docstrings. """

def add_points(house, house_points, points=0):
    """ Adds up points for house cup.

    If the house is Gryffindor, Dumbledore adds
    1000 points no matter what.

    Parameters
    ----------
    house_points : int
        Current house cup score.
    points : int, optional
        New points to be added/ subtracted.

    Returns
    -------
    int
    """
    if house == "Gryffindor":
       points += 1000
    return house_points + points
```

Typing

- you can declare the type of the function argument
- the package *mypy* checks whether the types make sense

- Be aware that this might be a pain to maintain if you change your functions often and pass complicated objects…
  `tuple[int, dict[str, str]]`

```
""" This module demonstrates docstrings. """

def add_points(house: str,
               house_points: int,
               points: int = 0)
               -> int:
    """ Adds up points for house cup.

    If the house is Gryffindor, Dumbledore adds
    1000 points no matter what.

    Parameters
    ----------
    house_points : Current house cup score.
    points : optional; New points to be added
    """
    if house == "Gryffindor":
       points += 1000
    return house_points + points
```

Variable names

- name your variables so that you can later go back and *read* what the code does (same principle as with module names)

```
x = 10

p = 10

poi = 10

points = 10

points_add = 10

points_to_be_added = 10
```

Variable names

- name your variables so that you can later go back and *read* what the code does (same principle as with module names)

```
x = 10  -> terrible

p = 10  -> just as terrible

poi = 10  -> still terrible

points = 10  -> better, but potentially unspecific

points_add = 10  -> possibly better, possible worse that the one before

points_to_be_added = 10  # clear, but maybe a bit long
```

Variable names

Variable names

```
added_points = [10, 5, 1]
# -> variable names use underscores


def add_points(house, house_points, points=0):
    if house == "Gryffindor":
       points += 1000
    return house_points + points
# -> function names also use underscores

def ScoreKeeper():
    def __init__(self):
        self.house_points = 0
        self._secret_bonus = 5

    def add_points(self, house, points):
        if house == "Gryffindor":
            points += 1000
        return house_points + points
# -> Class names use CamelCase
# -> private variables (intended for use only within the class) prepend "_"
```

Document your function

- Document the function you just wrote according to the instructions in **Exercise 4 Documentation**.

- Use the same Pull Request

Publishing code

- **Github/Gitlab**
  - perfectly fine for publishing publication code
  - perfectly fine for hosting research group code

- **PyPI: Python Package Index**
  - if you want others to use your analysis/model/… you should try to have it on PyPI to make it easier for others to download and use

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Summary

Contents

usability features:

1) folder and file structure
   - standard Python package structure
2) error-free importing and installation
   - editable pip installation
3) isolated, protected code
   - virtual environments
4) readability
   - documentation, typing, naming

Contents

usability features:

1) folder and file structure
   - standard Python package structure
2) error-free importing and installation
   - editable pip installation
3) isolated, protected code
   - virtual environments
4) readability
   - documentation, typing, naming

Mischief Managed

Any questions?

Extra material

Module structure

- constants
- functions
- …

Importing modules

- you can always import code from other modules (.py files) in your ***current directory***
- generally:

```
1. import module-name                    + module-name.object

2. import module-name as abbr            + abbr.object

3. from module-name import object        + object

4. from module-name import *
```

Order of execution

Terminal

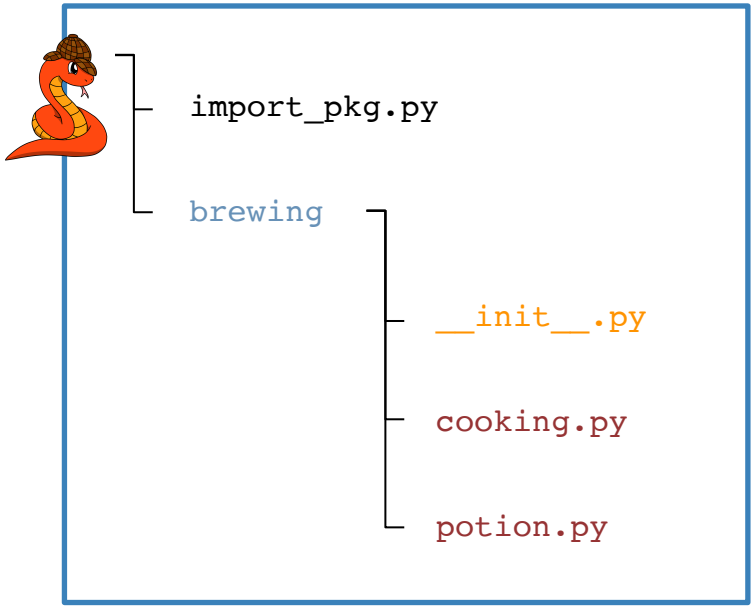
```
> python3 import_pkg.py
```

```
import_pkg.py
brewing
    __init__.py
    cooking.py
    potion.py
```

Order of execution

Terminal

```
>  python3 import_pkg.py
```



Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing
```

import_pkg.py

brewing

__init__.py

cooking.py

potion.py

Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing
```

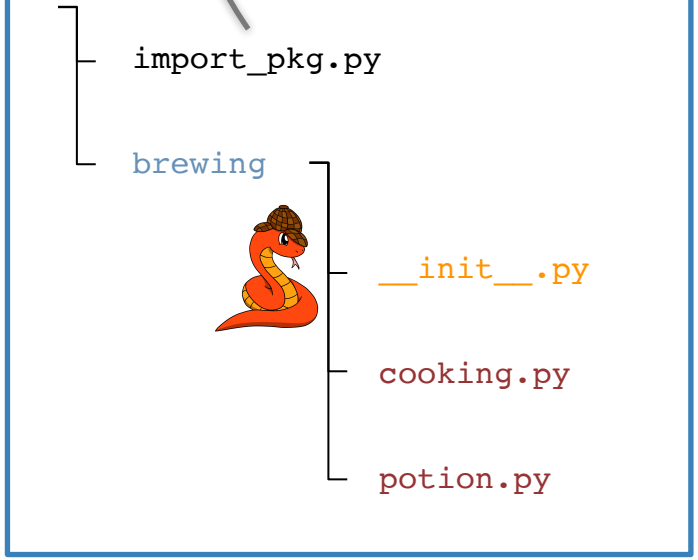
- import_pkg.py
- brewing
  - __init__.py
  - cooking.py
  - potion.py

Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing
```



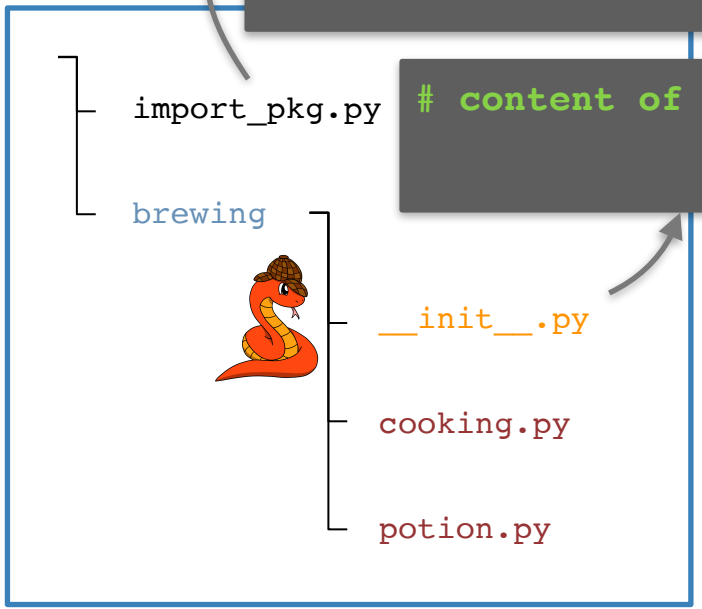
Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing
```

```
# content of __init__.py
```



Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing
```

```
# content of __init__.py
```

import_pkg.py

brewing

__init__.py

cooking.py

potion.py

Order of execution

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> python3 import_pkg.py
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```
import_pkg.py
brewing
    __init__.py
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    potion.py
```

Order of execution

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```
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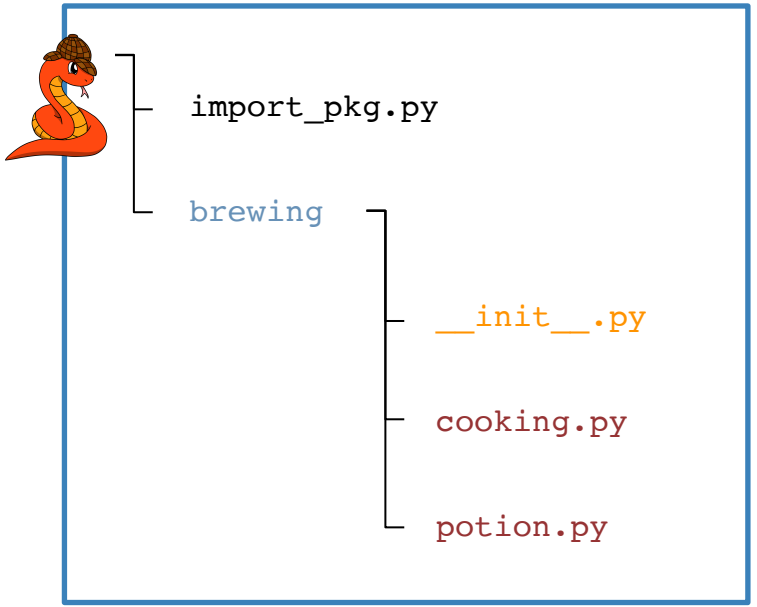
```



Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```

```
import_pkg.py
brewing
    __init__.py
    cooking.py
    potion.py
```

Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```

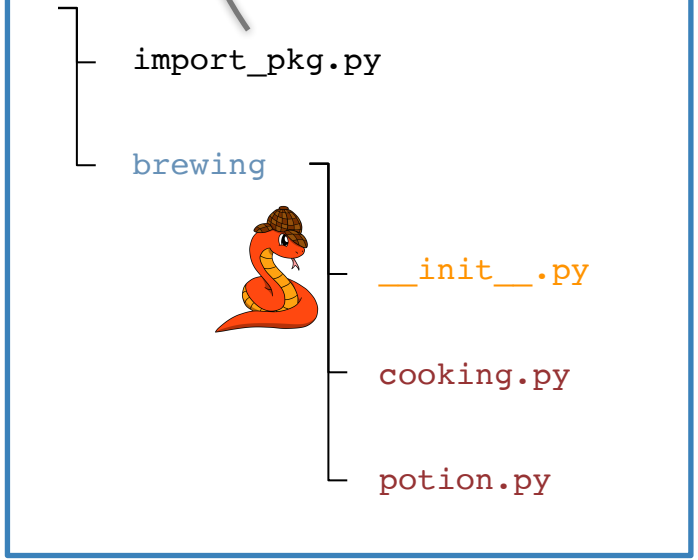
- import_pkg.py
- brewing
  - __init__.py
  - cooking.py
  - potion.py

Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```



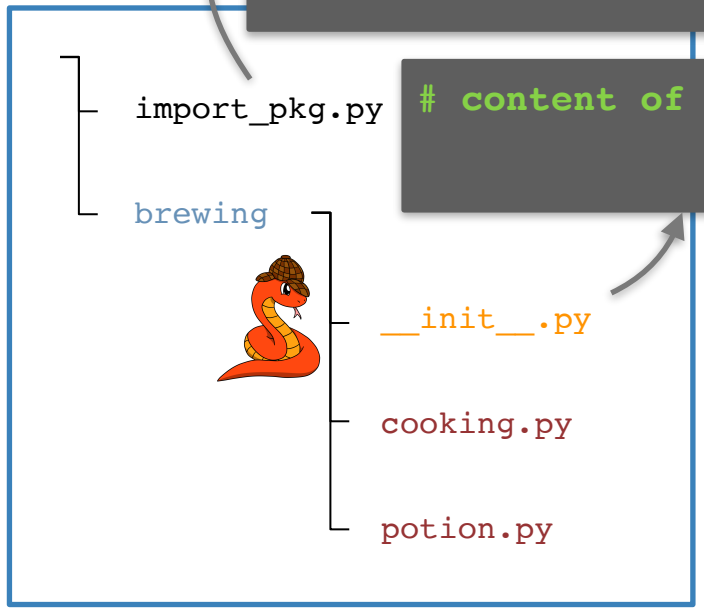
Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```

```
# content of __init__.py
```



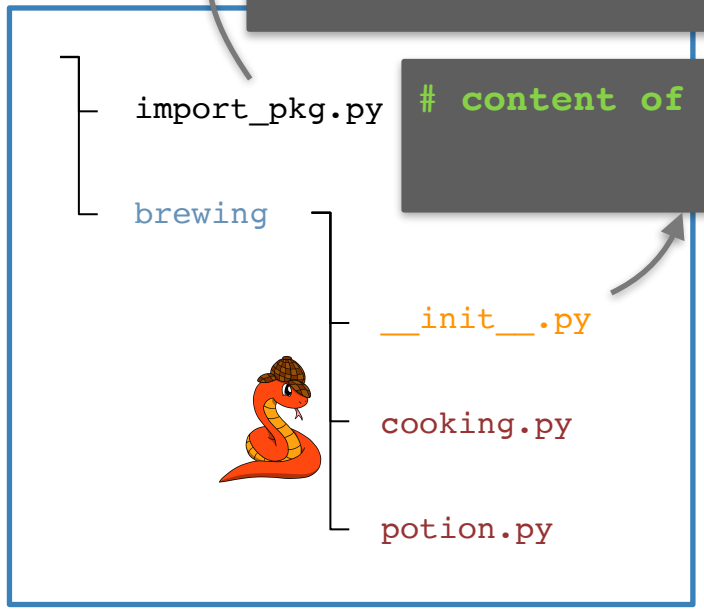
Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```

```
# content of __init__.py
```



Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```

```
# content of __init__.py
```

```
import_pkg.py
brewing
    __init__.py
    cooking.py
    potion.py
```

```
# content of cooking.py
eternal_flame = “eternal_flame”
```

Order of execution

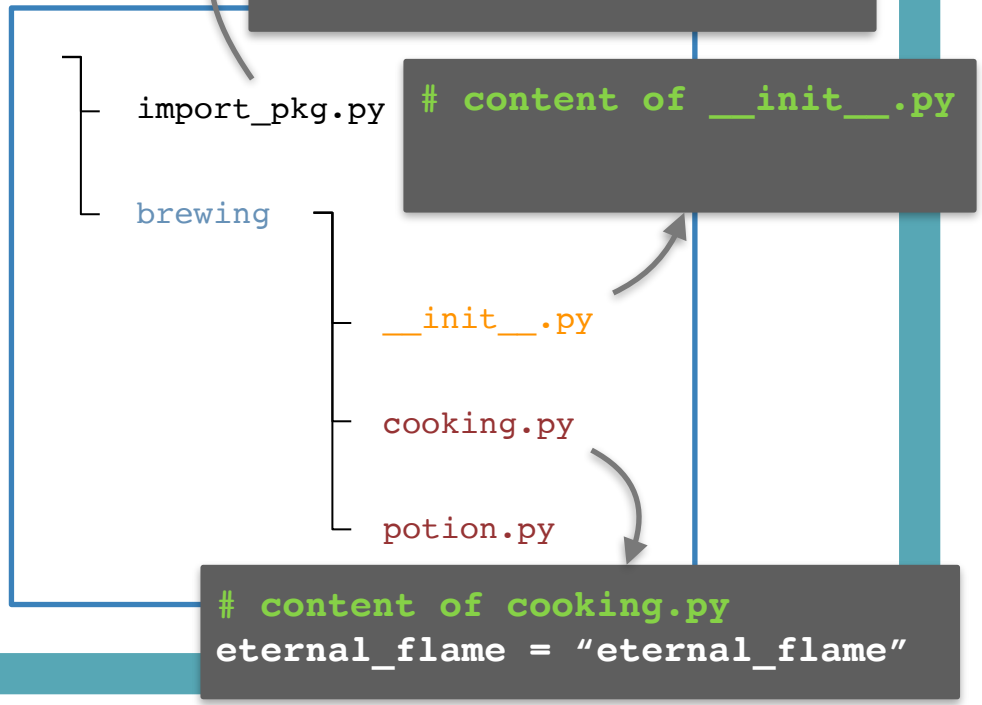
Terminal

```
>  python3 import_pkg.py
```

```
# content of import_pkg.py
import brewing.cooking
```

```
# content of __init__.py
```

```
# content of cooking.py
eternal_flame = "eternal_flame"
```



Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
import_pkg.py
brewing
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    make_potion.py
```

Order of execution

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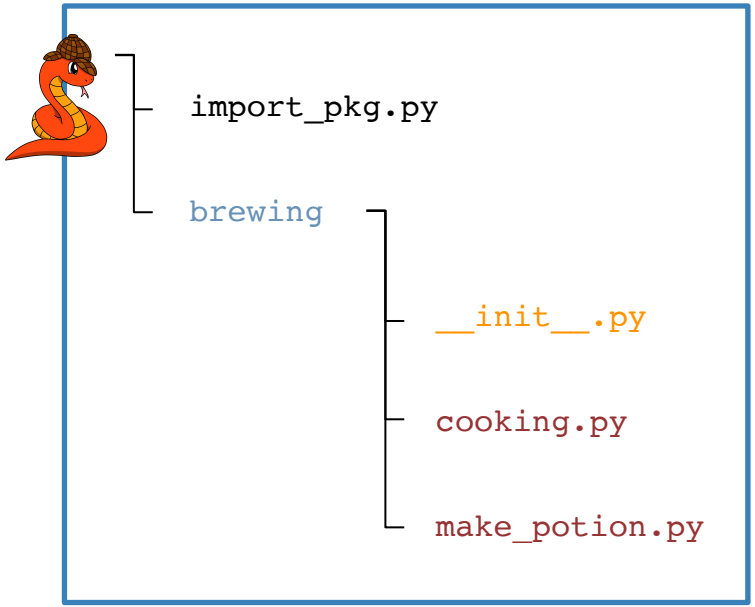
```

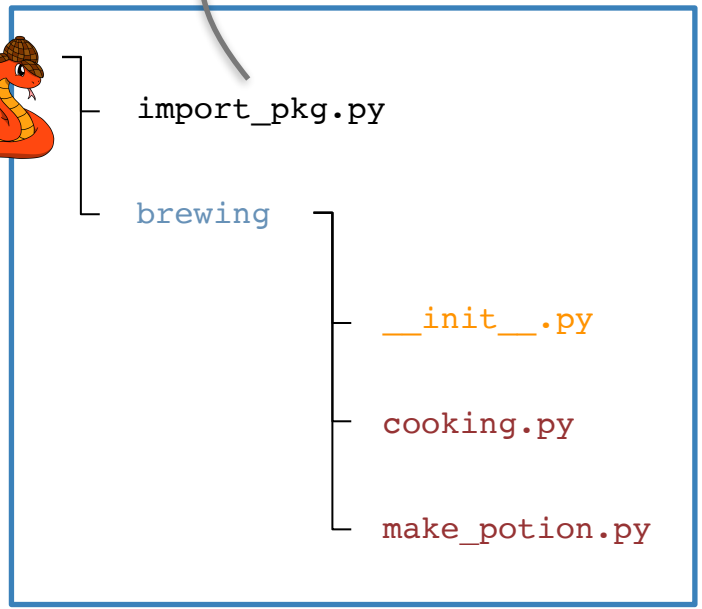


Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py
import brewing.make_potion
```



Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py
import brewing.make_potion
```

```
import_pkg.py
brewing
    __init__.py
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```

Order of execution

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# import_pkg.py
import brewing.make_potion
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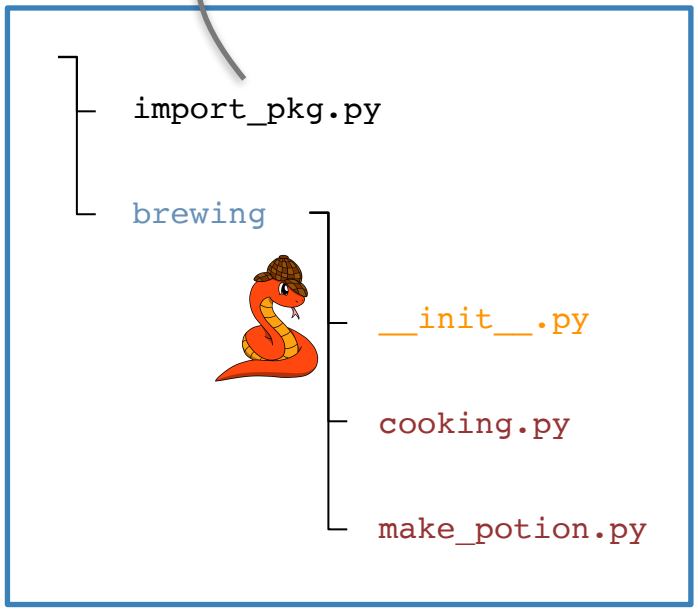

Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# import_pkg.py
import brewing.make_potion
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```
import_pkg.py
brewing
    __init__.py
    cooking.py
    make_potion.py
```

```
#__init__.py
```

Order of execution

Terminal

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>  python3 import_pkg.py
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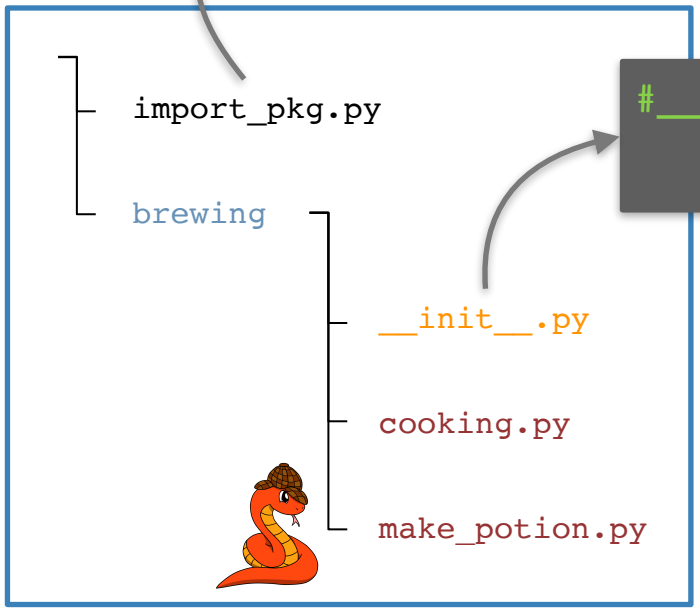
```
# import_pkg.py
import brewing.make_potion
```




```
#__init__.py
```

Order of execution

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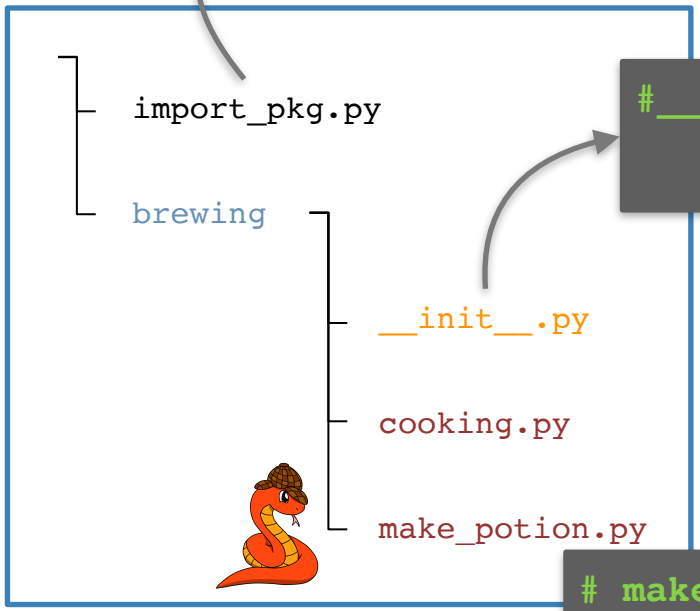
```
# import_pkg.py
import brewing.make_potion
```




```
#__init__.py
```

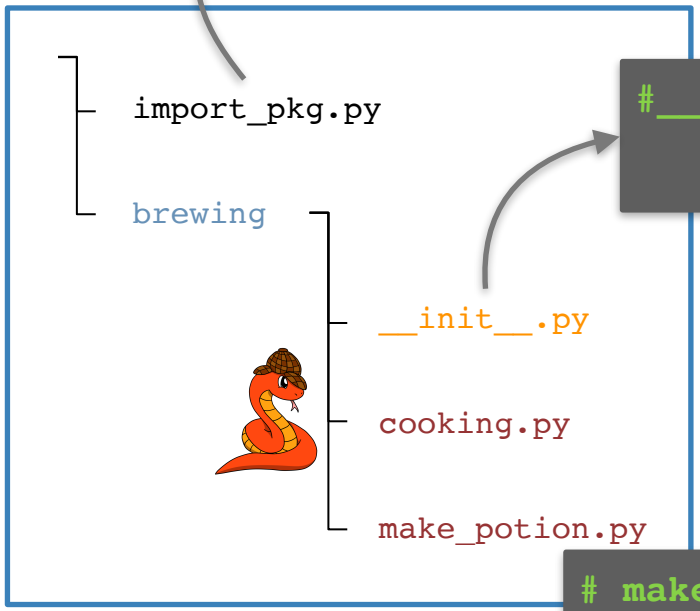
```
# make_potion.py
import cooking
stuff
```

Order of execution

Terminal

```
>  python3 import_pkg.py
```

```
# import_pkg.py
import brewing.make_potion
```




```
#__init__.py
```

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stuff
```

Order of execution

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import brewing.make_potion
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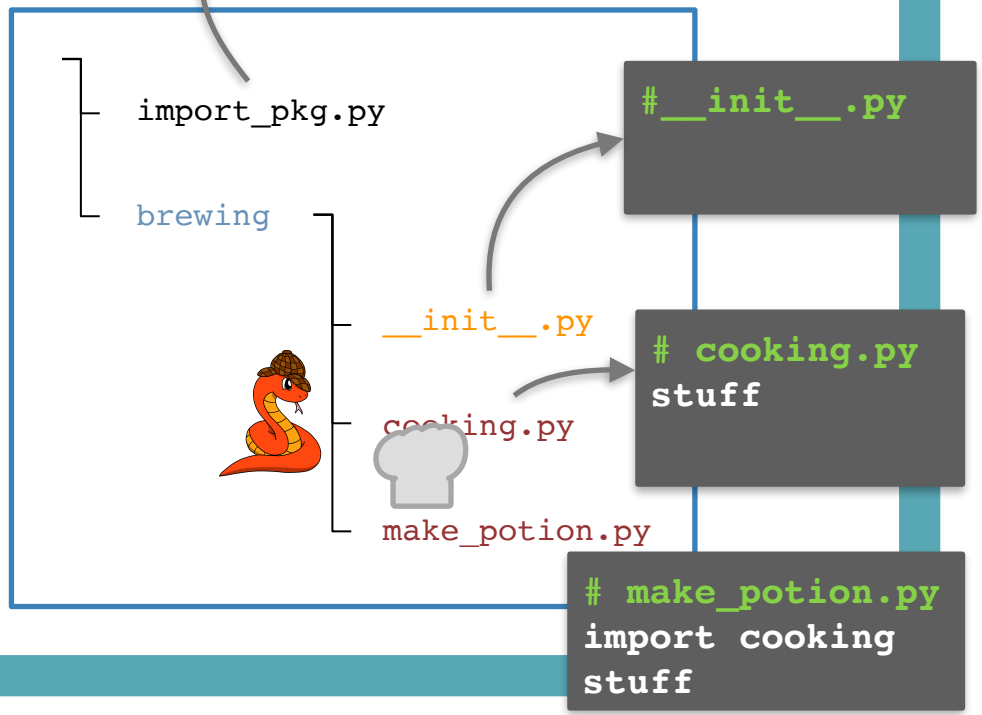

Order of execution

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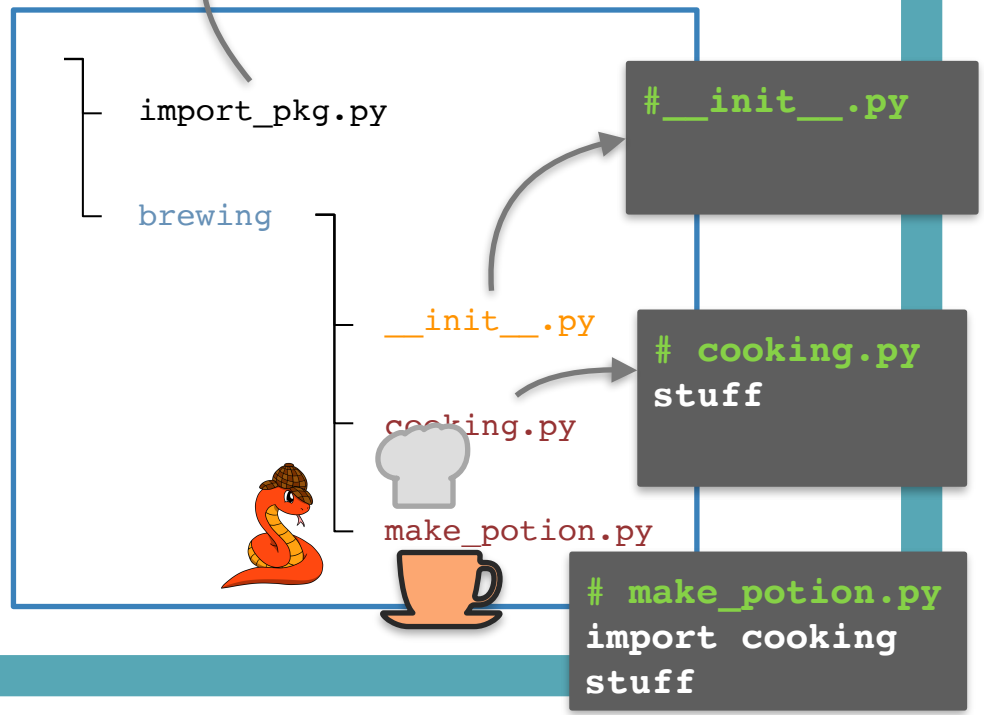
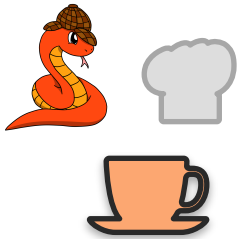
```



Order of execution

Terminal

```
>  python3 import_pkg.py
```



```
# import_pkg.py
import brewing.make_potion
```

```
import_pkg.py
brewing
    __init__.py
    cooking.py
    make_potion.py
```

```
#__init__.py
```

```
# cooking.py
stuff
```

```
# make_potion.py
import cooking
stuff
```

Keeping track of docstrings

- Most commonly used hosting websites: facilitate building, versioning, and hosting
  - github.io
  - readthedocs.org
- Automate documentation
  - Sphinx: a package to collect docstrings and create a nicely formatted documentation website