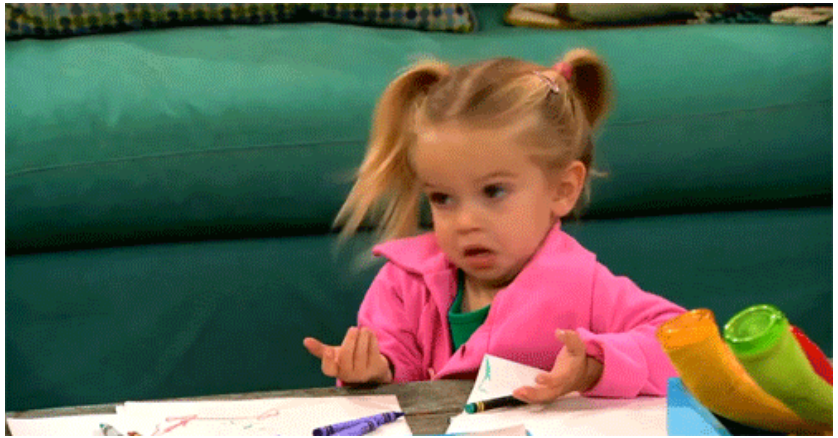
Organising, documenting and distributing code

ASPP 2023, Heraklion

= How to make your code (more) usable

Why bother?



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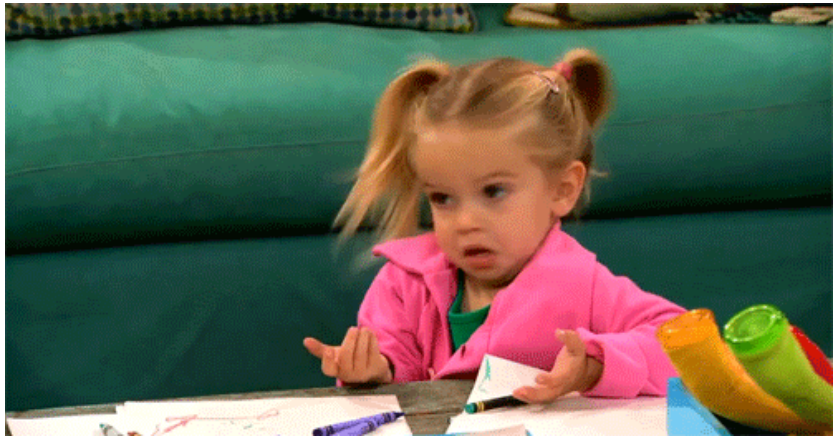

Contents

usability features:

1) separate, individually usable projects

2) clean folder and file structure

3) error-free importing of code

4) readability

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2) clean folder and file structure

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Organise what?

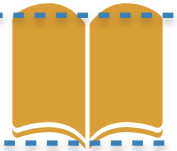
Project 1

packages

documentation

code

other stuff



packages

documentation

code

other stuff

Organise what?

Project 1

packages

numpy = 1.22.0
pandas = 1.2.4

documentation

Readme.md
figure.png

code

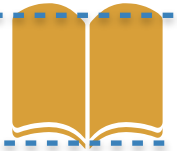
simulation.py
evaluation.py

pip-installable

other stuff

tests/
notebook23.ipynb

Project 2



packages

pandas = 2.0.3
numba = 1.0.2

documentation

Readme.md
figure.png

code

constants.py
training.py

pip-installable

other stuff

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separate your projects

Why environments?

- Blindly updating packages when installing new packages / working on multiple projects will cause problems

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

- 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
```

Why environments?

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```
<stdin>:1: FutureWarning: In a future version of pandas all arguments of
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- code errors
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Previous behavior:

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

```
DataFrameGroupBy.sum(numeric_only=False, min_count=0, engine=None,
engine_kwargs=None) #                                          [source]
```

Compute sum of group values.

Parameters: **numeric_only** : *bool, default False*

Include only float, int, boolean columns.

Changed in version 2.0.0: numeric_only no longer accepts `None`.

Why environments?

- Avoid importing errors when working on multiple projects / updating your Python packages

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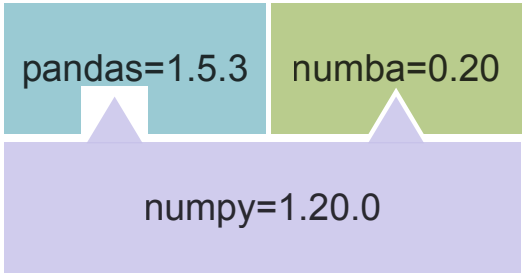

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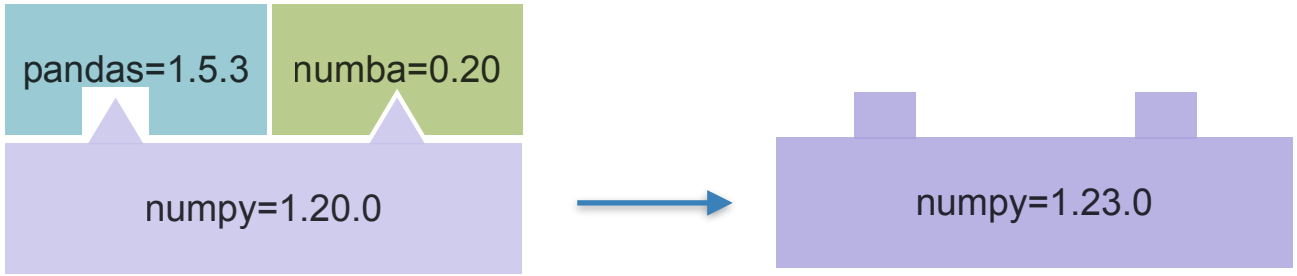

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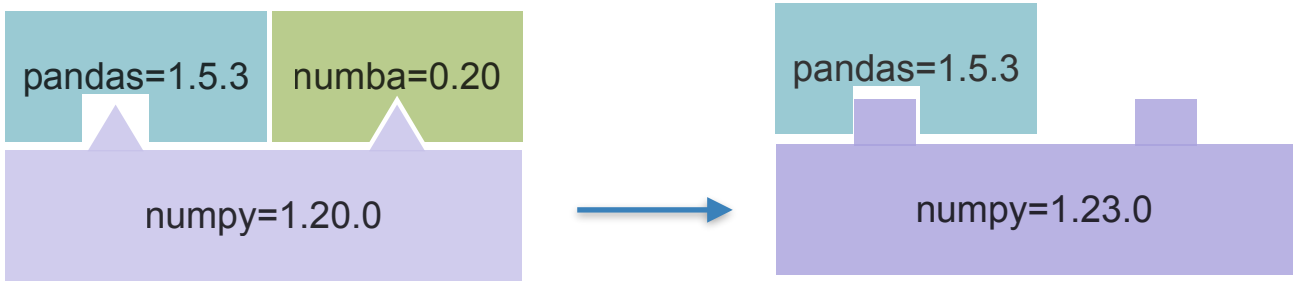

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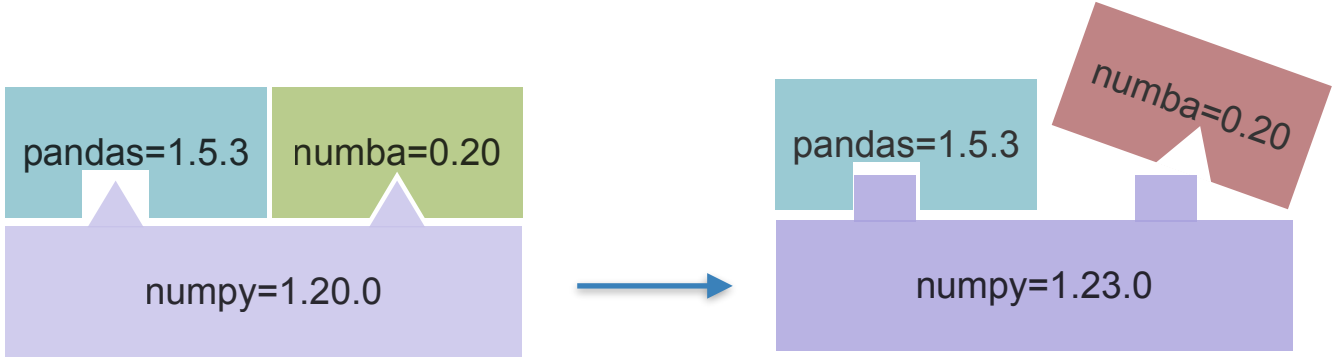


Why environments?

- Avoid importing errors when working on multiple projects / updating your Python packages

- Increased reproducibility: give yourself / other people the exact instructions **and** tools to run your code (cluster, collaboration)

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

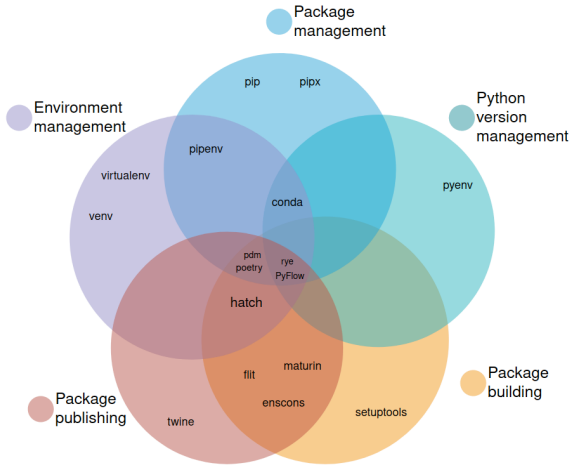
- Create and activate a virtual environment following the directions in **Exercise 1 Virtual Environments.md**

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

Environment Managers

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

- **poetry** - super useful (if it works o.0)
  pyenv - multiple different Pythons
- **etc**



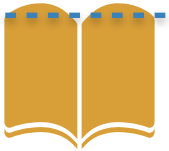
a description of the chaos:

https://chriswarrick.com/blog/2023/01/15/how-to-improve-python-packaging/
https://alpopkes.com/posts/python/packaging_tools/

Organise what?

Project 1

packages



packages

Organise what?

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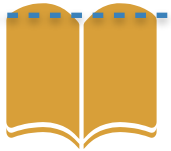
pandas = 1.2.4

Project 2

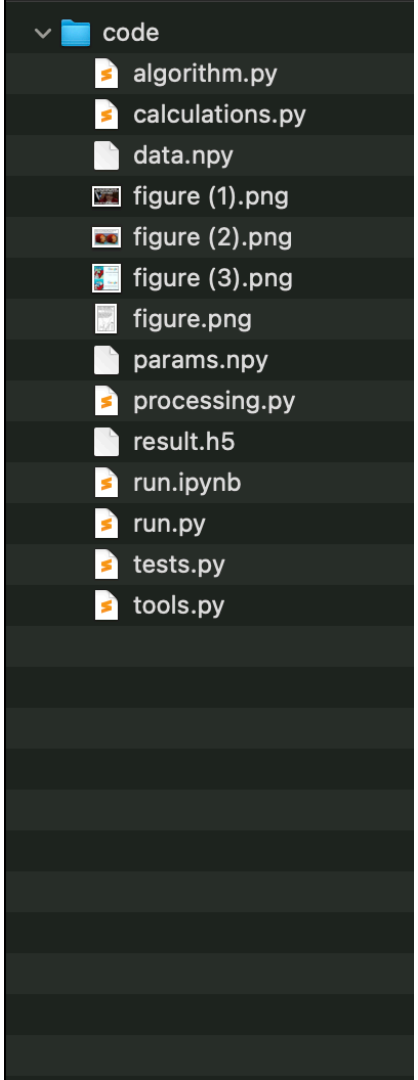


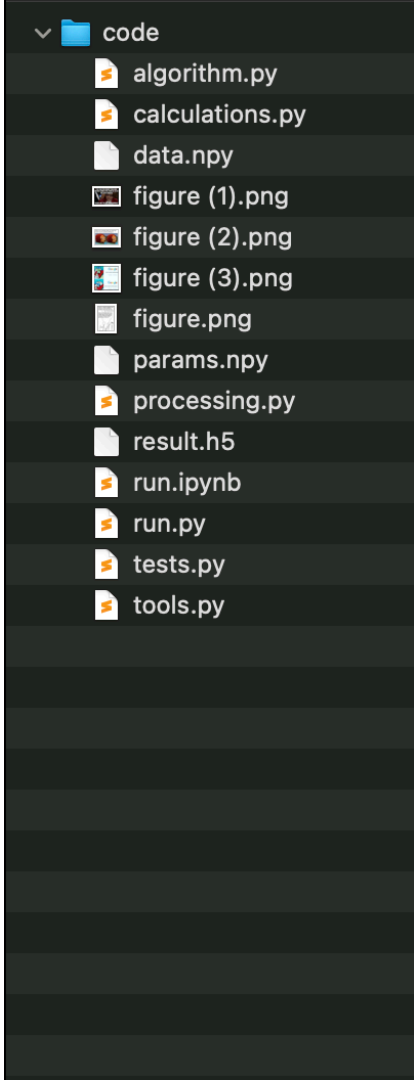
packages

pandas = 2.0.3

numba = 0.21.1

Folder structure


code
algorithm.py
calculations.py
data.npy
figure (1).png
figure (2).png
figure (3).png
figure.png
params.npy
processing.py
result.h5
run.ipynb
run.py
tests.py
tools.py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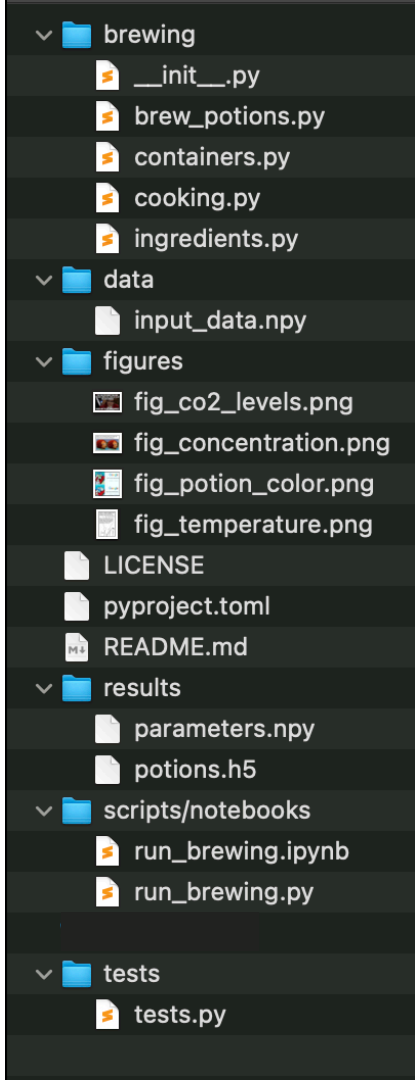
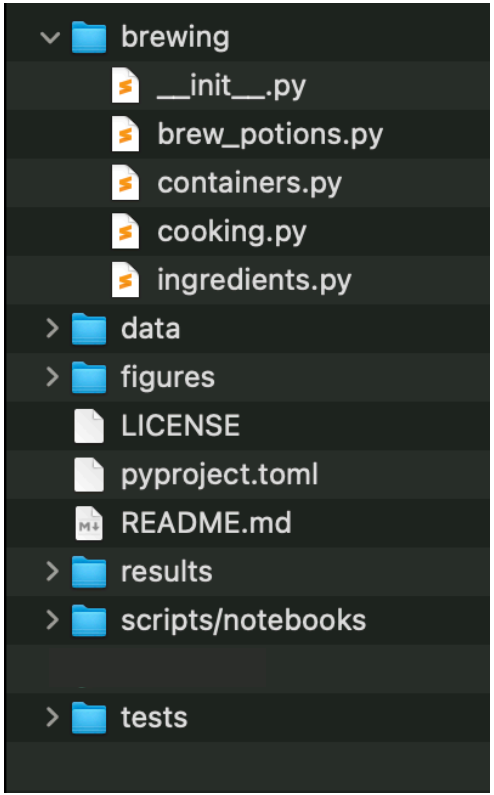

brewing
__init__.py
brew_potions.py
containers.py
cooking.py
ingredients.py
data
input_data.npy
figures
fig_co2_levels.png
fig_concentration.png
fig_potion_color.png
fig_temperature.png
LICENSE
pyproject.toml
README.md
results
parameters.npy
potions.h5
scripts/notebooks
run_brewing.ipynb
run_brewing.py
tests
tests.py

Python package structure



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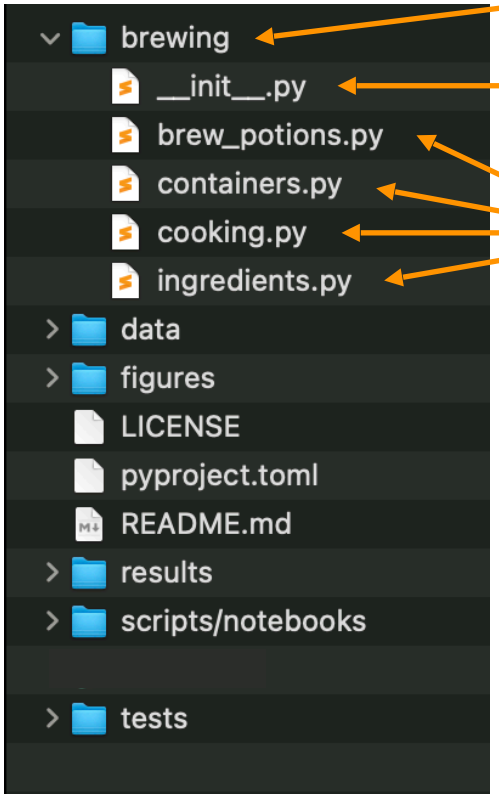
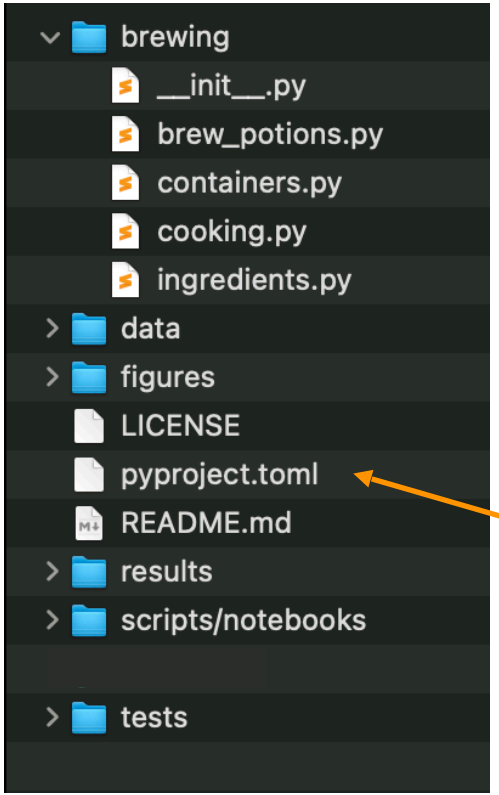


name of package

__init__.py
flags folder as package

modules
your .py files containing your code

Python package structure



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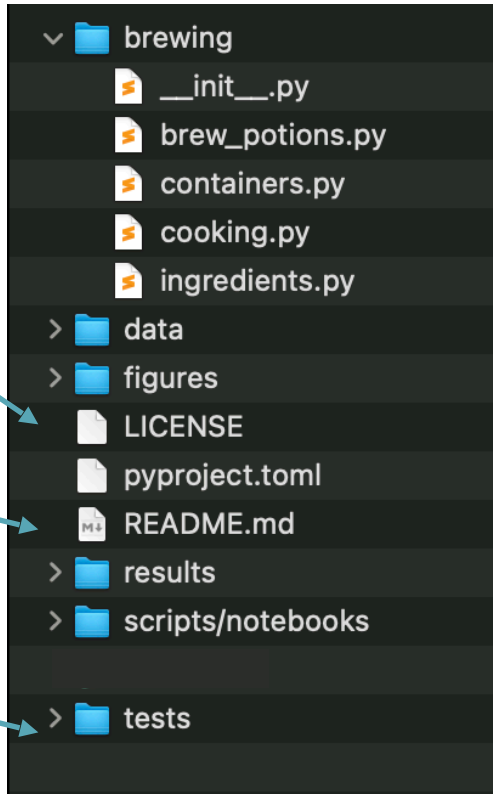
build instructions & package metadata
will explain more later :)

Python package structure



name of package

__init__.py
flags folder as package

modules
your .py files containing your code

build instructions & package metadata
will explain more later :)

LICENSE
makes the package (legally) usable.*

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

tests
you know why :)

* pick one from choosealicense.com

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

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

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Organise what?

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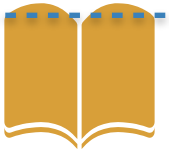
other stuff



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notebook23.ipynb

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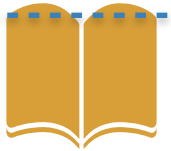

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constants.py
training.py

other stuff

tests/
notebook23.ipynb

Importing

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)

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("Does not print when importing")
    print("Prints when run as script")
```

show file & import

Importing modules

- Options for e.g. importing *eternal_flame* from cooking.py

cooking.py

```
# heat sources
fire = 'fire'
eternal_flame = 'eternal_flame'
```

Importing modules

- Options for e.g. importing *eternal_flame* from cooking.py

cooking.py

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# heat sources
fire = 'fire'
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```
1. import cooking
```

Importing modules

- Options for e.g. importing *eternal_flame* from cooking.py

cooking.py

```
# heat sources
fire = 'fire'
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```

1. `import cooking` `+ cooking.eternal_flame`

Importing modules

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1. `import cooking` `+ cooking.eternal_flame`

2. `import cooking as cook`

Importing modules

- Options for e.g. importing *eternal_flame* from cooking.py

cooking.py

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# heat sources
fire = 'fire'
eternal_flame = 'eternal_flame'
```

1. `import cooking` → `cooking.eternal_flame`
2. `import cooking as cook` → `cook.eternal_flame`

Importing modules

- Options for e.g. importing *eternal_flame* from cooking.py

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1. `import cooking` + `cooking.eternal_flame`
2. `import cooking as cook` + `cook.eternal_flame`
3. `from cooking import eternal_flame`

Importing modules

- Options for e.g. importing *eternal_flame* from cooking.py

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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 *`

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1. `import cooking`
   + `cooking.eternal_flame`
   + `cooking.fire`
2. `import cooking as cook`
   + `cook.eternal_flame`
   + `cook.fire`
3. `from cooking import eternal_flame`
   + `eternal_flame`
   X `fire`
4. `from cooking import *`
   + `eternal_flame`
   + `fire`

Importing a package

- Modules in the package are bound to the package name
- How can you call an object inside a module in a package?

```
1. import package

2. import package.module

3. from package.module import
   object
```

Importing a package

- Modules in the package are bound to the package name
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1. `import package`	–
2. `import package.module`	+ `package.module.object`
3. `from package.module import object`	+ `object`

Importing a package

- Modules in the package are bound to the package name
- How can you call an object inside a module in a package?

1. `import package`	– *
2. `import package.module`	+ `package.module.object`
3. `from package.module import object`	+ `object`

* this is how it works when the __init__.py file is empty, which it usually is

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 2 Importing.md**

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

Order of execution

Terminal

```
> python3 ex_outside.py
```

```
ex_outside.py
brewing
    __init__.py
    cooking.py
    potion.py
```

Order of execution

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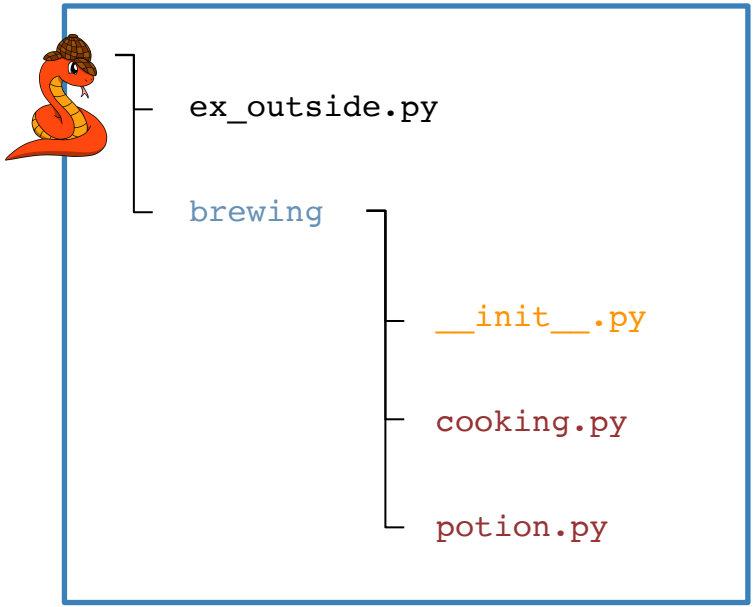

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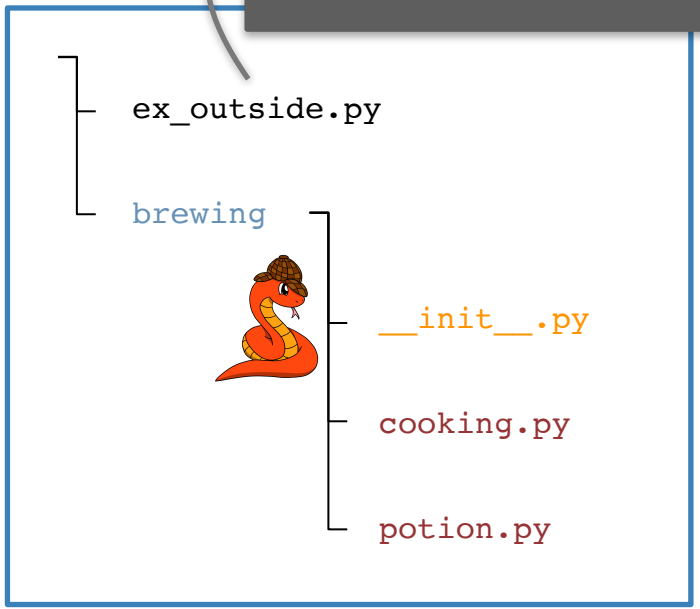

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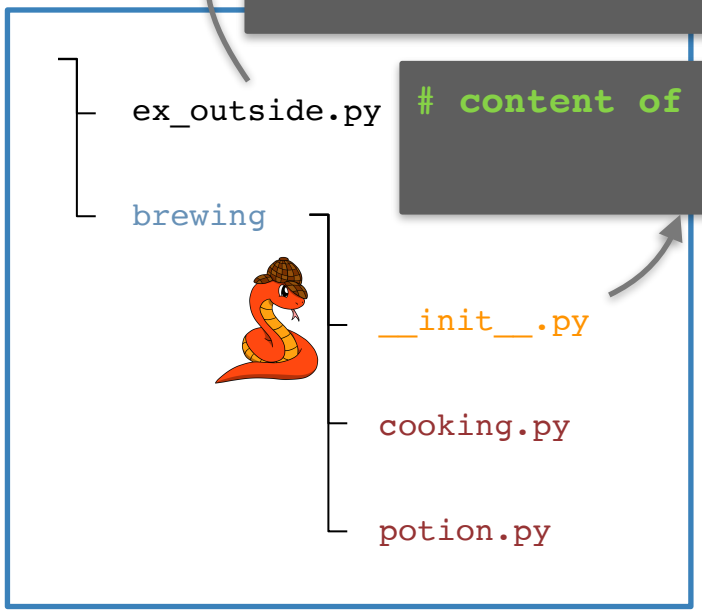

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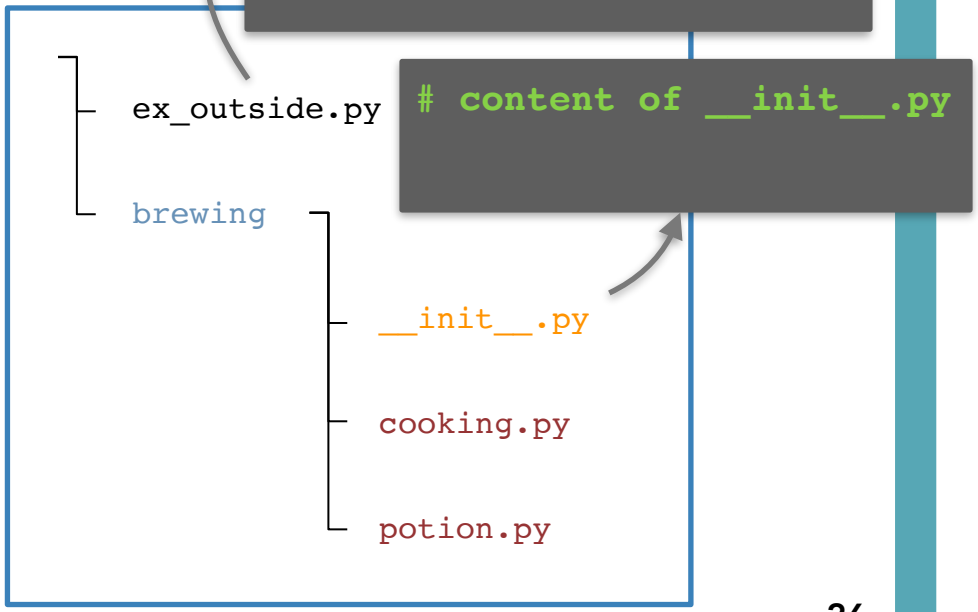

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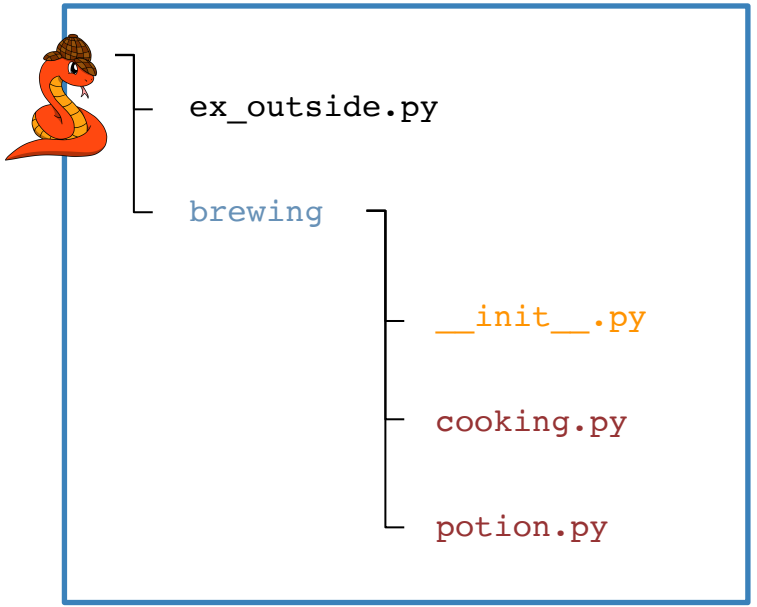

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import brewing.cooking
```

ex_outside.py

brewing

__init__.py

cooking.py

potion.py

Order of execution

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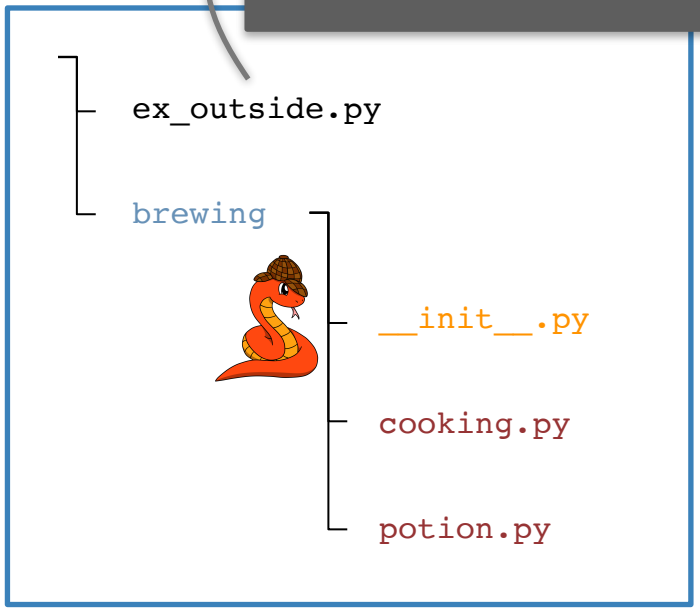

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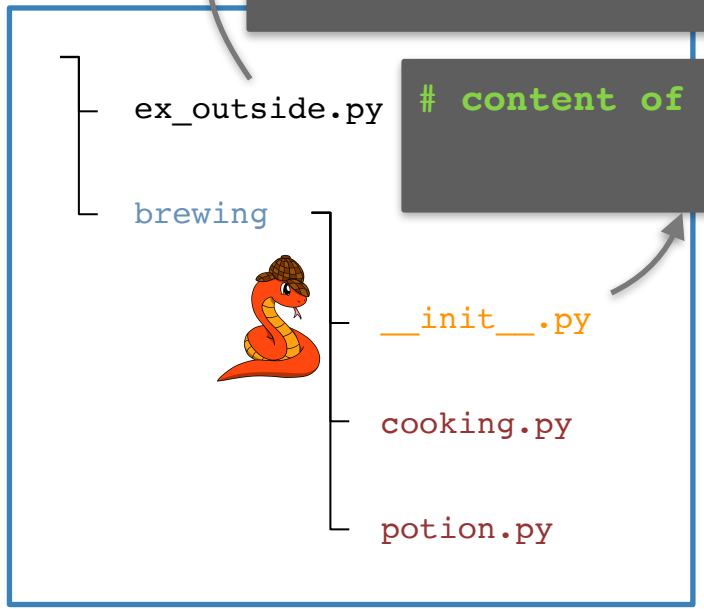

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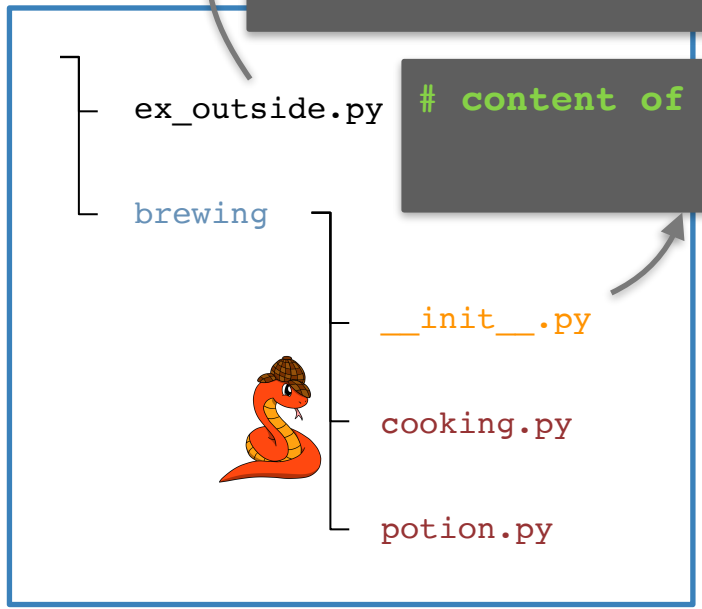

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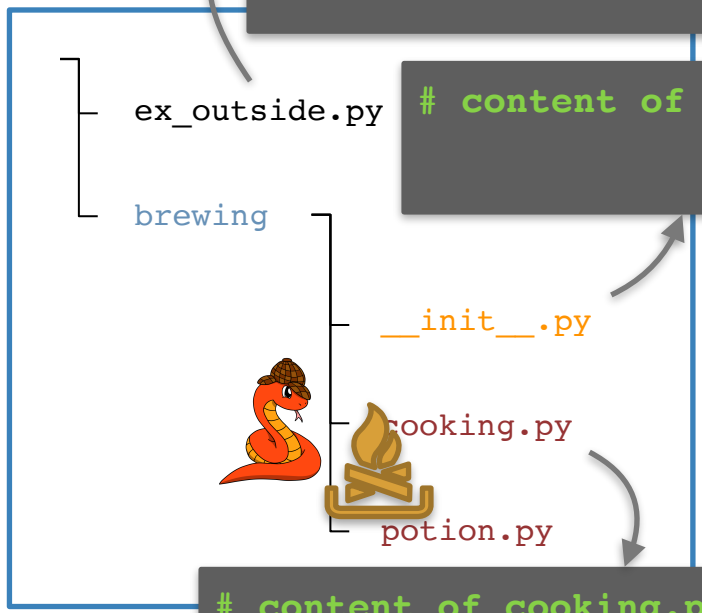


```
# content of cooking.py
eternal_flame = “eternal_flame”
```

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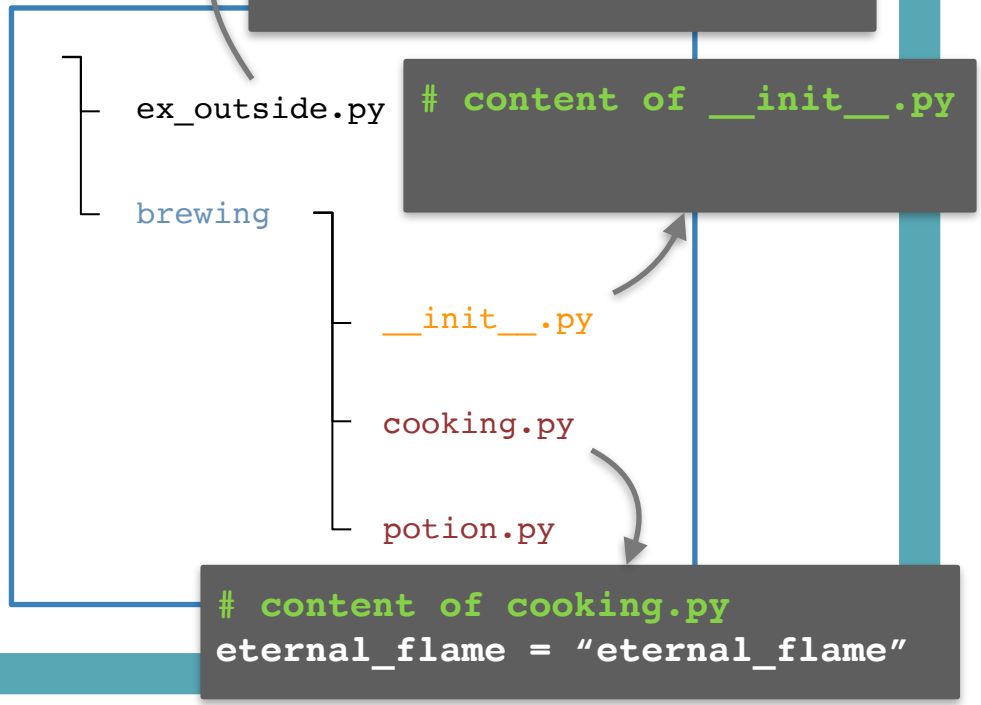

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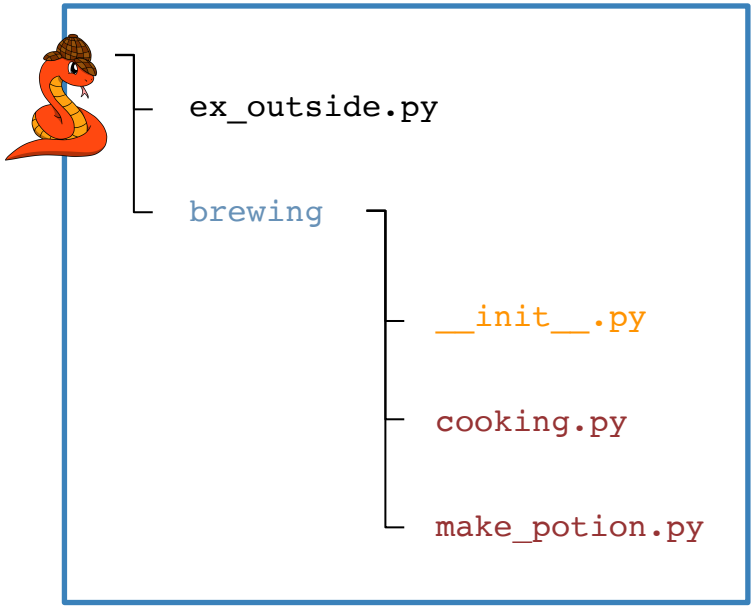

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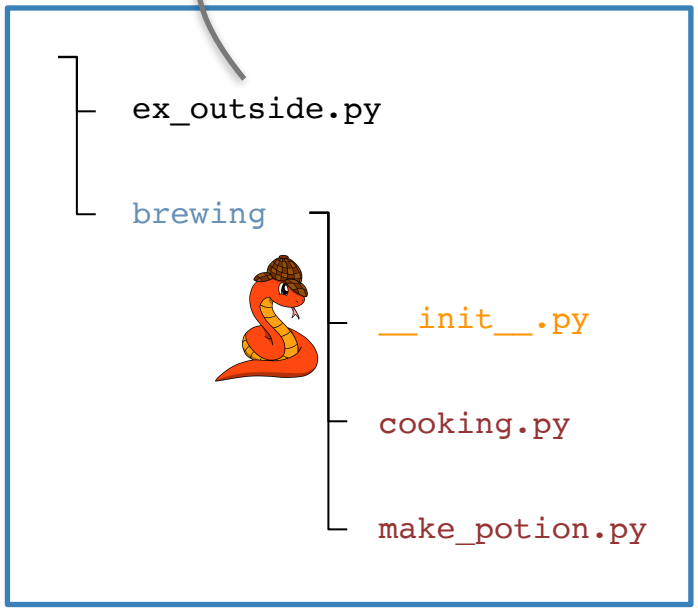

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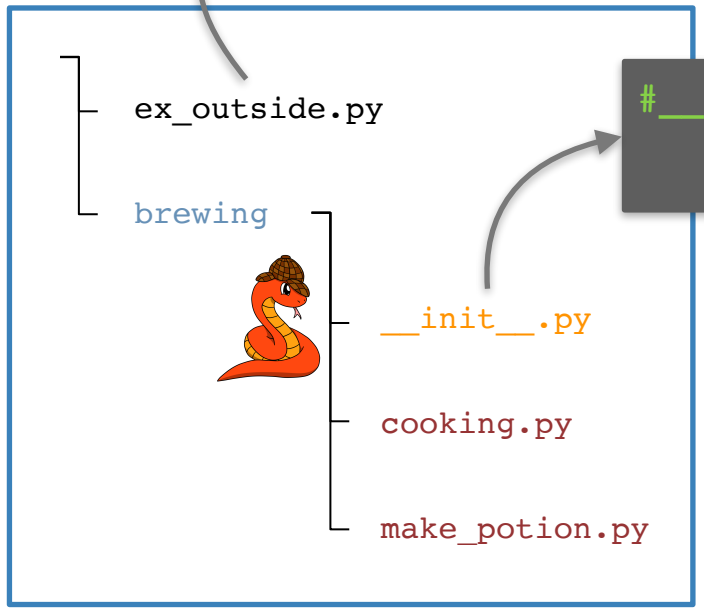


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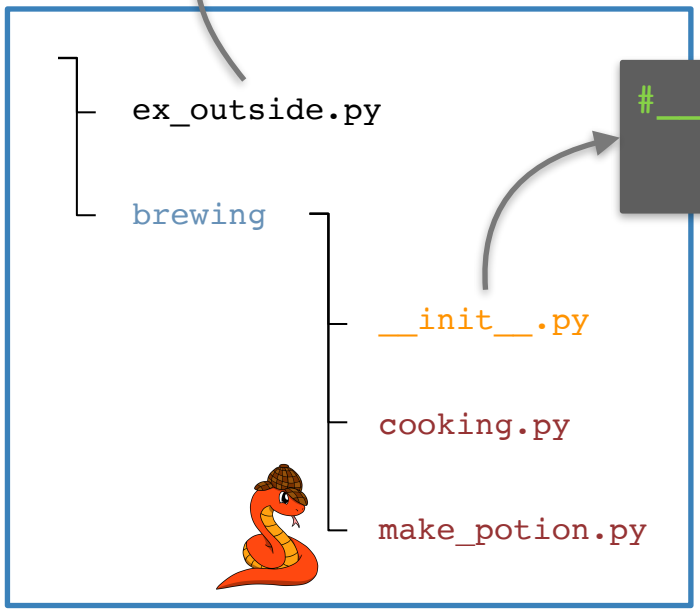


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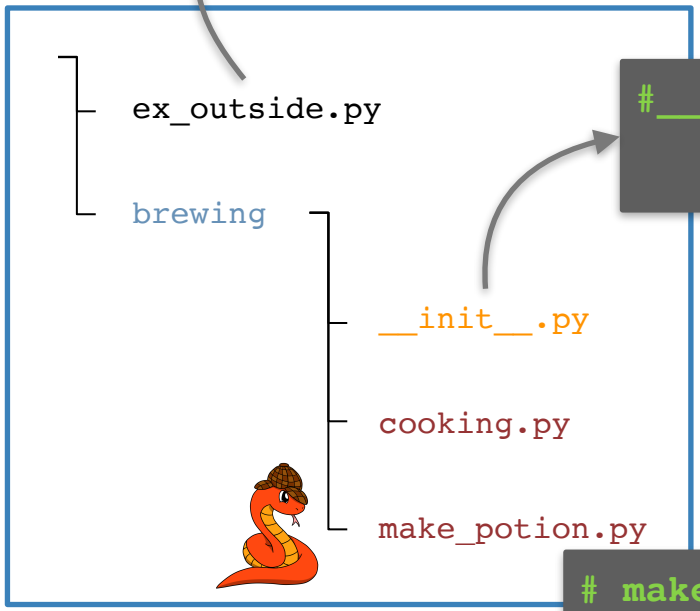


```
#__init__.py
```

```
# make_potion.py
import cooking
def coffee():
```

Order of execution

Terminal

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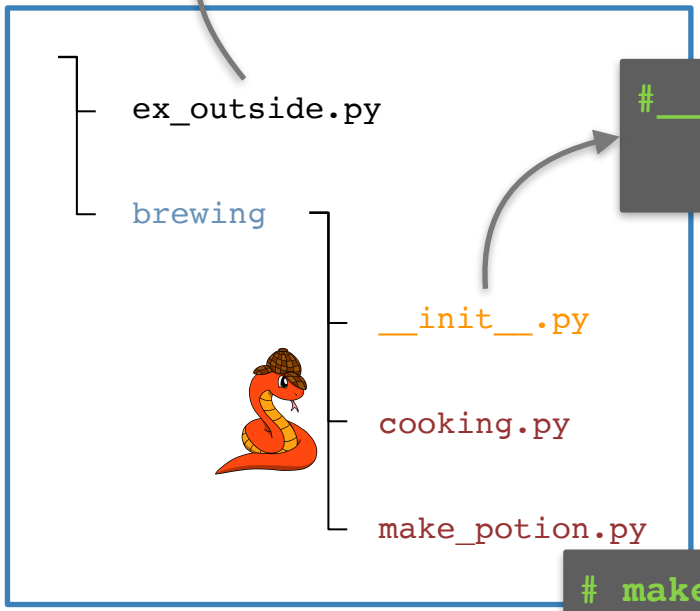


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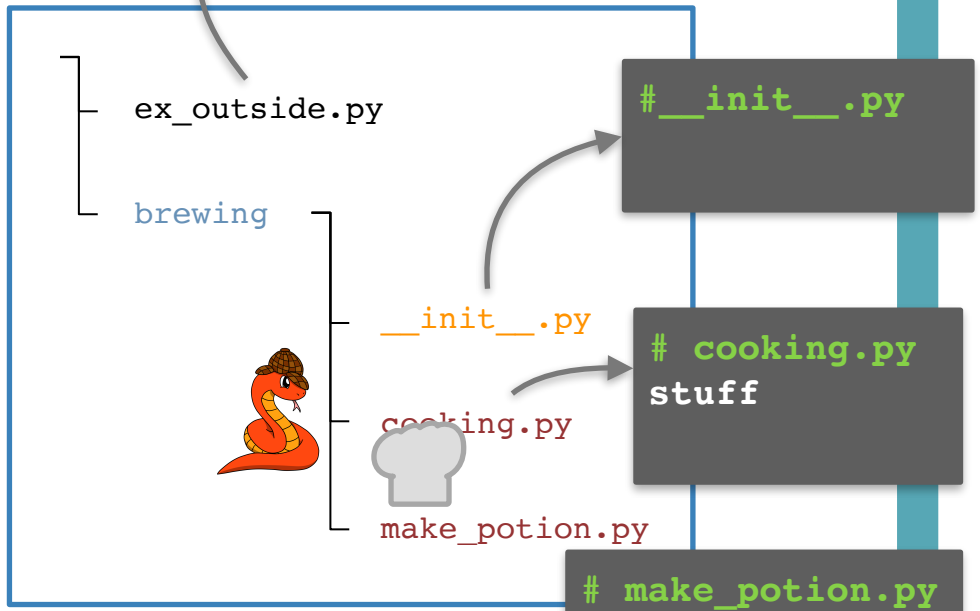


```
#__init__.py
```

```
# cooking.py
stuff
```

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```

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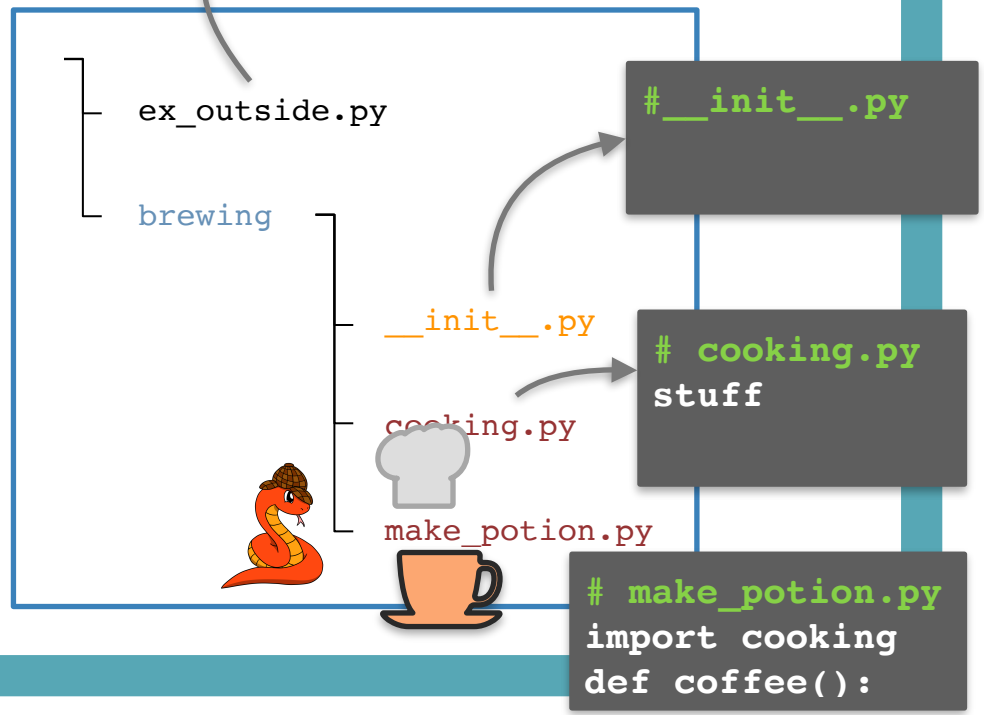


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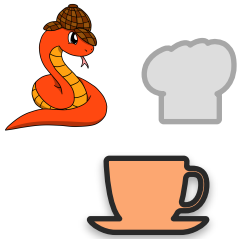

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Importing

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

Is there a way to get

a) any 2

b) all 3

exercises to work simultaneously?

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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. /usr/lib64/python3.11/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
```

Option 2: install from a VCS like git

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

Installing other packages

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

pip

standard package manager for Python

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

conda

open source package manager/ environment manager

can install packages which were reviewed by Anaconda (not all)

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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

```
pip install numpy
```

Option 2: install from a VCS like git

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

Option 3: install your package with -e (--editable) option

```
pip install -e <path-to-package>
(cd <path-to-package>; conda develop .)
```

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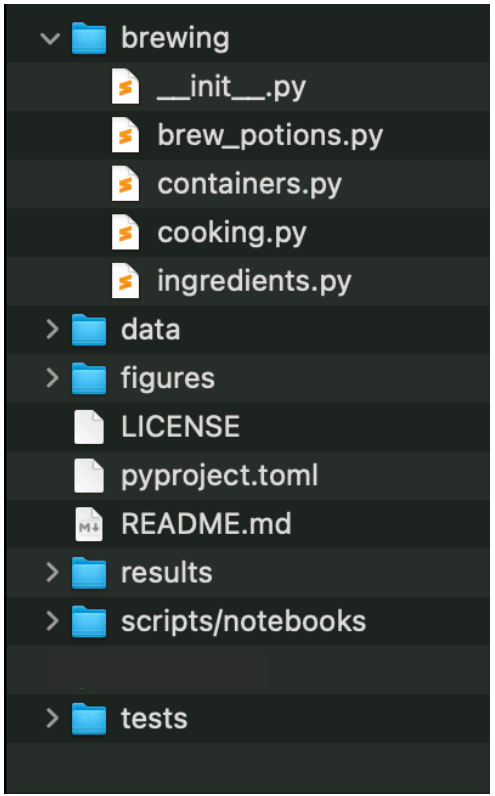
Python package structure

LICENSE
makes the package (legally) usable.*

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

tests
you know why :)



name of package

__init__.py
flags folder as package

modules
your .py files containing your code

build instructions & package metadata
the time has come to explain this…

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orange files = required in order to do an editable pip installation

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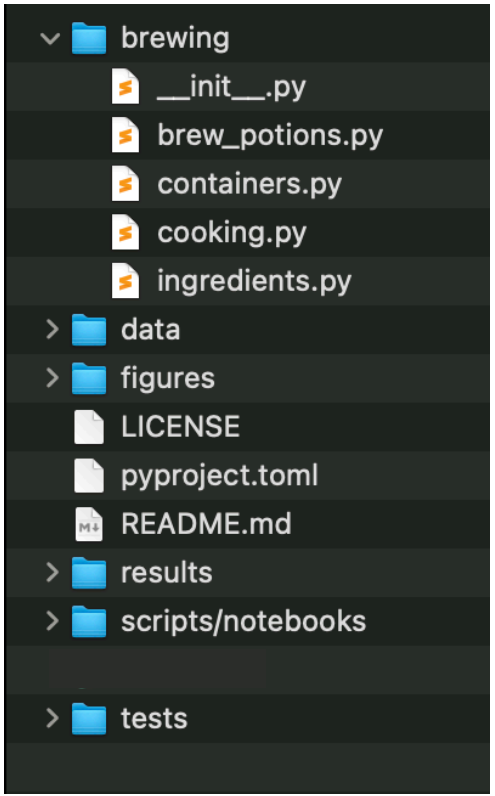

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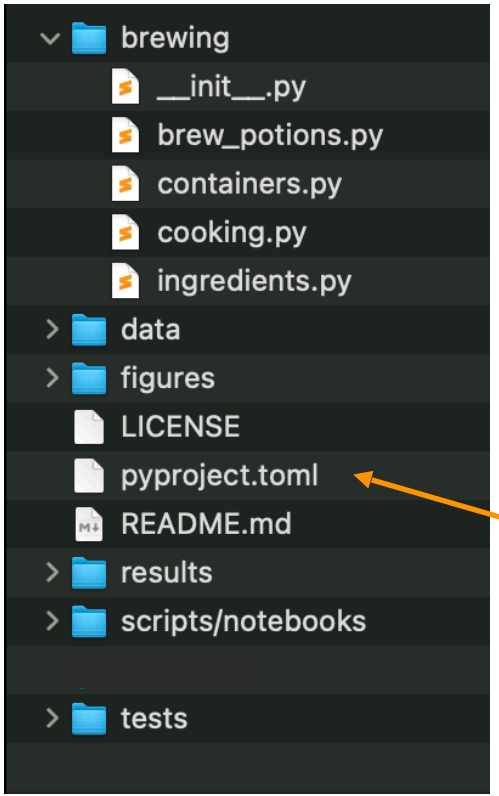

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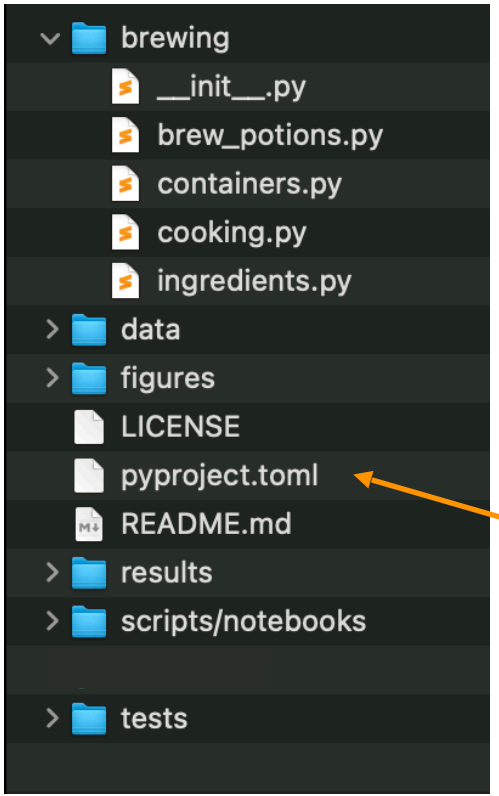

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(with Python <3.10(?) you need an empty setup.cfg file)

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pyproject.toml

- The pyproject.toml file holds static information about the package = meta data
- 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')
  -> can also go into separate requirements.txt file

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[project]
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version = "0.1.0"
description = "a python package for brewing potions"
authors = [{ name = "H. Granger", email =
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license = { file = "LICENSE" }
readme = "README.md"
requires-python = ">=3.7"
dependencies = ["numpy", "matplotlib >= 3.0.0",
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classifiers = [
    "Programming Language :: Python :: 3",
    "License :: OSI Approved :: BSD License",
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[tool.setuptools]
packages = ["brewing"]

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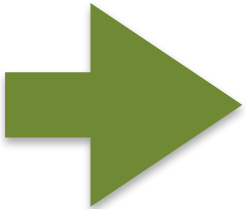

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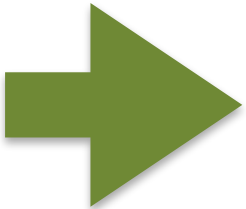

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Pip editable installation

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

  or in the directory above `brewing`

  `pip install -e .`

- Follow the instructions in
  Exercise 3: Editable installation

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

Additional advantages

- if your code is pip-installable, you can put your tests into a separate folder (-> more organised)
- your pyproject.toml file acts as a record of the necessary packages to run your code

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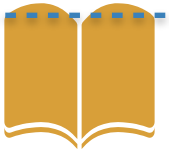
Organise what?

Project 1

packages

code

other stuff



packages

code

other stuff

Organise what?

Project 1

packages

numpy = 1.22.0
pandas = 1.2.4

code

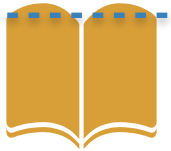
simulation.py
evaluation.py

pip-installable

other stuff

tests/
notebook23.ipynb

Project 2



packages

pandas = 2.0.3
numba = 1.0.2

code

constants.py
training.py

pip-installable

other stuff

tests/
notebook23.ipynb

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 can use the code as before just without worrying about imports

- You have not lost any capability, you only gained usability

- If you are using notebooks for teaching/demos, then importing your code from your modules makes it much cleaner

Workflow (ideal)

1 Create

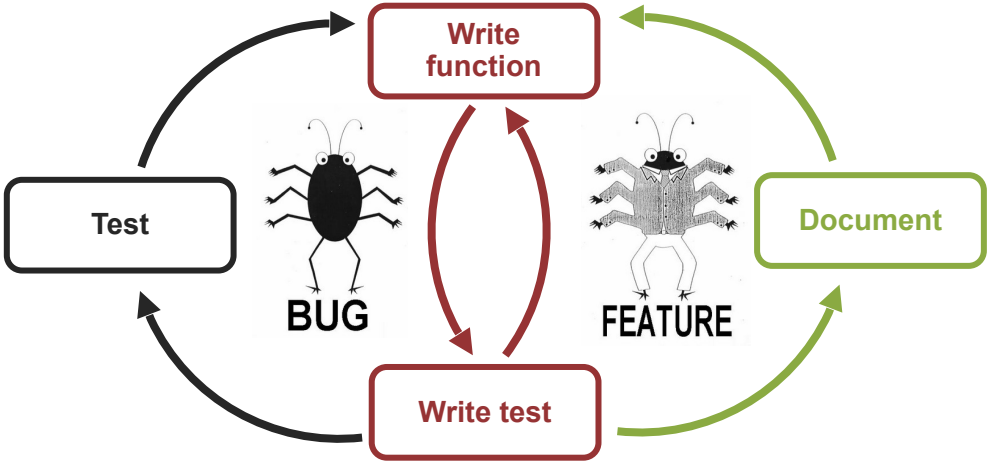
Set up structure

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`

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 4 Workflow** to write and test a function to make a “Python expert” potion
- Create a 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 library, you must have your code on PyPi to make it easier for others to download and use it

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
```

~~NumPy~~ style

- *personal* suggestion:
  if you work with pandas, it is easy to forget the shape of DataFrames.

- Add the format into docstring (and keep up to date!)
  OR
  Write proper tests, you can always check the DataFrame format there

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

def some_function(df):
    """ If it helps, you can add a DF example.

    Parameters
    ----------
    df : pd.DataFrame
        Historical house cup scores.
                      house      points
            year
            1999    Slytherin         100
            2020   Hufflepuff        2800
    """

    return df
```

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

class 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
```

Document your function

- Document the function you just wrote according to the instructions in **Exercise 5 Documentation**.

- Use the same Pull Request

Organise what?

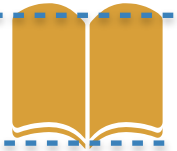
Project 1

packages

documentation

code

other stuff



packages

documentation

code

other stuff

Organise what?

Project 1

packages

numpy = 1.22.0
pandas = 1.2.4

documentation

Readme.md
figure.png

code

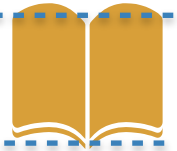
simulation.py
evaluation.py

pip-installable

other stuff

tests/
notebook23.ipynb

Project 2



packages

pandas = 2.0.3
numba = 1.0.2

documentation

Readme.md
figure.png

code

constants.py
training.py

pip-installable

other stuff

tests/
notebook23.ipynb

Summary

Contents

usability features:

1) separate, individually usable projects
   - virtual environments
2) clean folder and file structure
   - standard Python package structure
3) error-free importing of code
   - editable pip installation
4) readability
   - documentation, typing, naming

Contents

usability features:

1) separate, individually usable projects
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4) readability
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References

https://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.1001745

https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1005510#pcbi.1005510.ref001

https://goodresearch.dev/

Mischief Managed

Any questions? - - feel free to give feedback

Extra material

Module structure

- constants
- functions
- …

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