Organizing, documenting and distributing code

ASPP-LatAm 2023, CDMX

= How to make your code (more) usable

Contents

usability features:

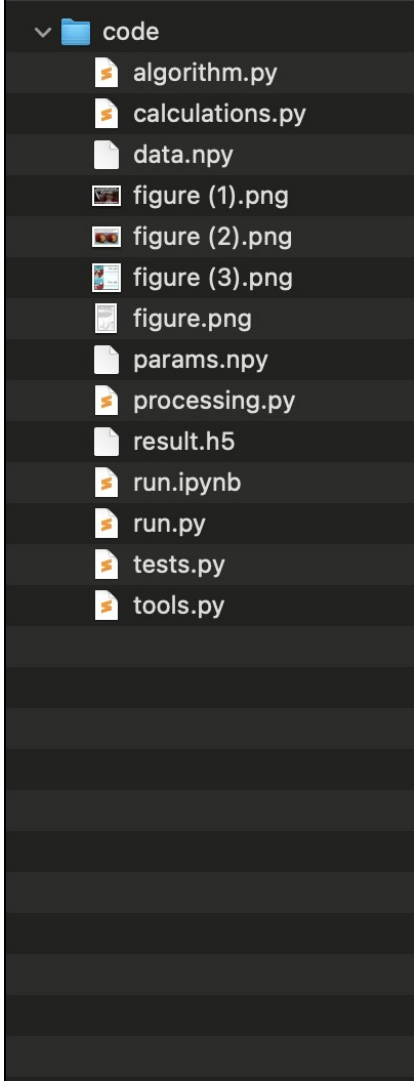
1) folder and file structure

2) error-free importing and installation

3) isolated, protected code

4) readability

Folder structure


code
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data.npy
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figure.png
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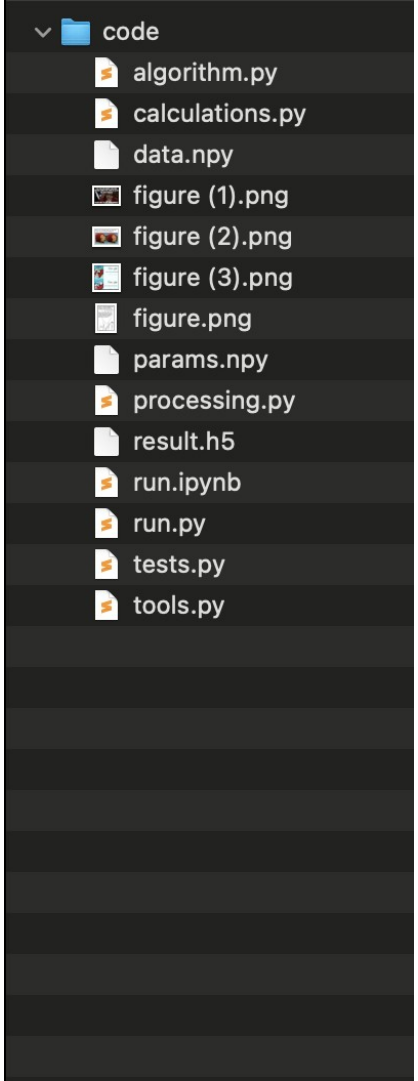
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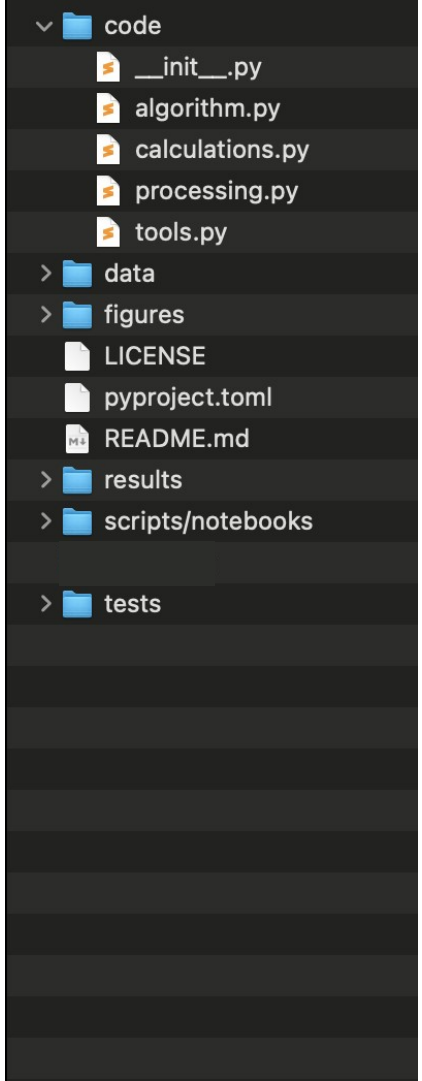
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README.md
results
scripts/notebooks
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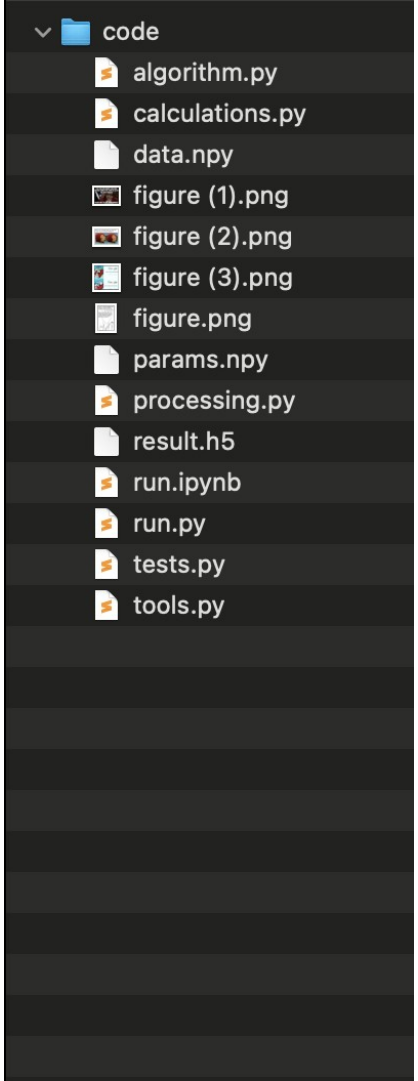
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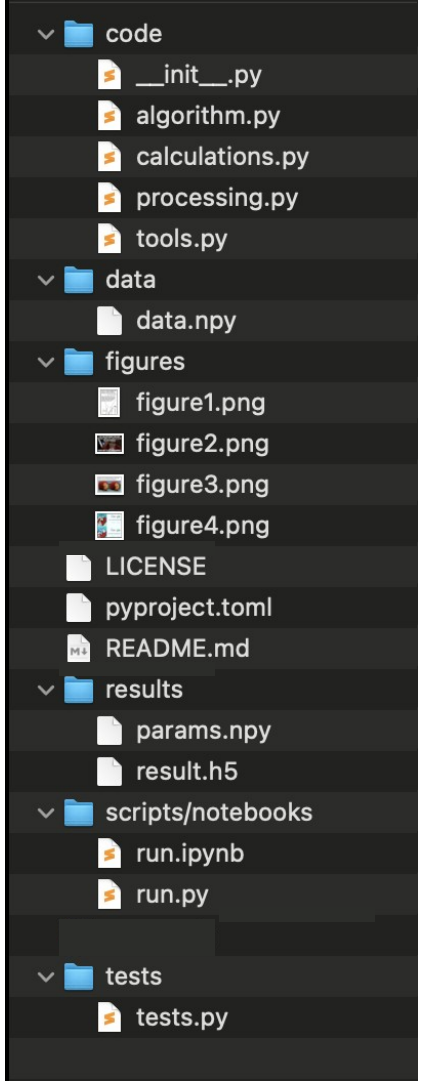
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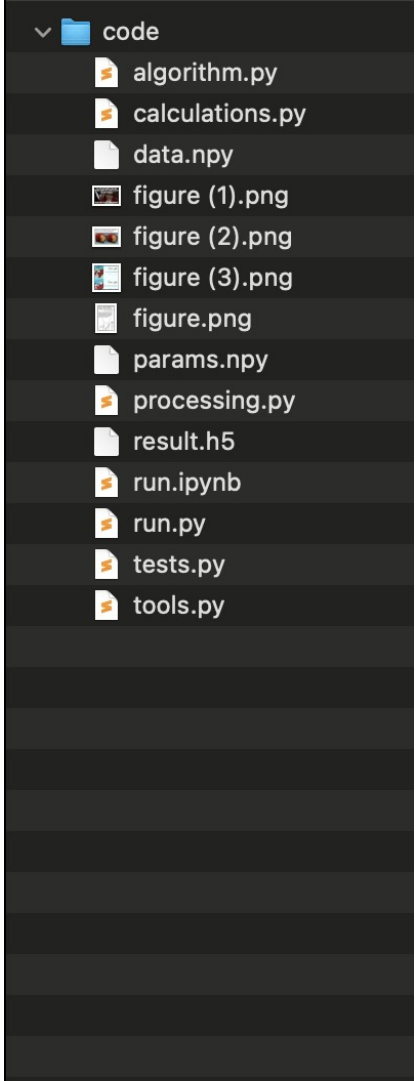
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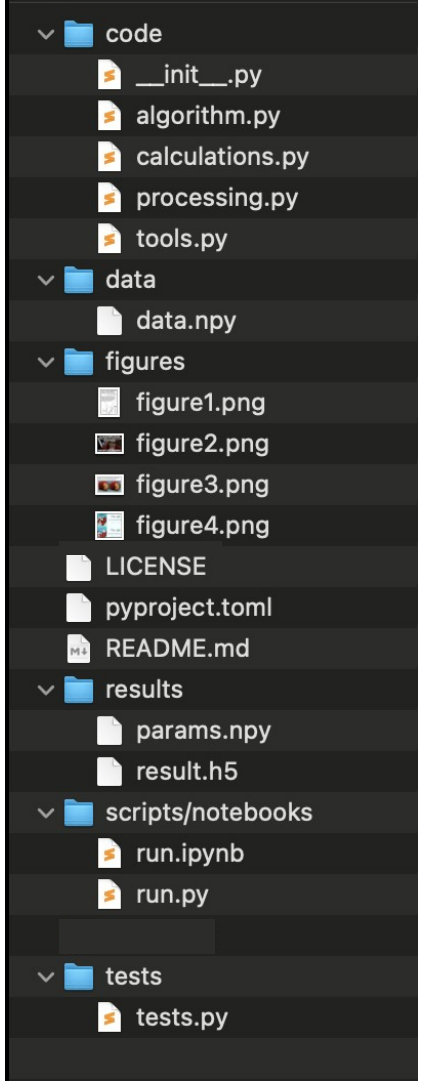
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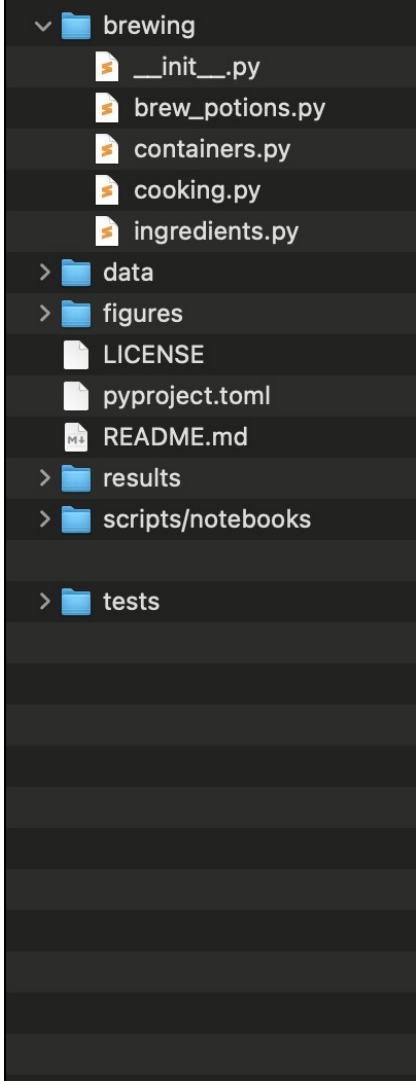
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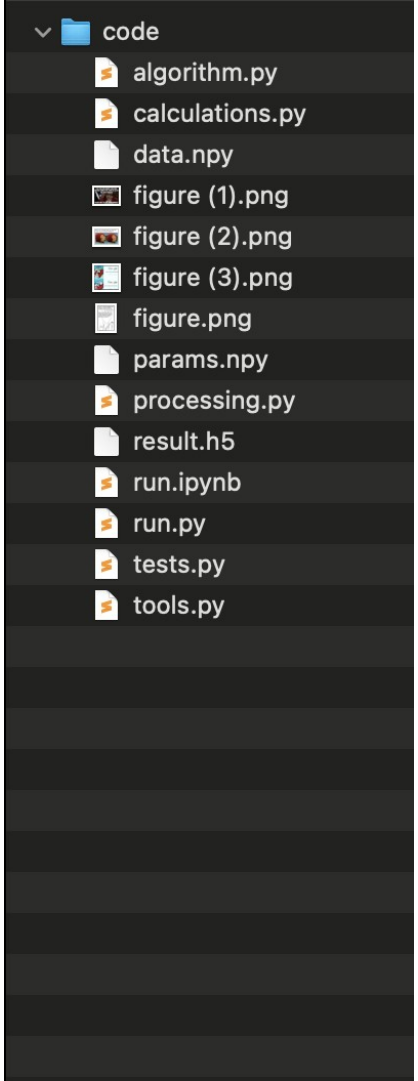
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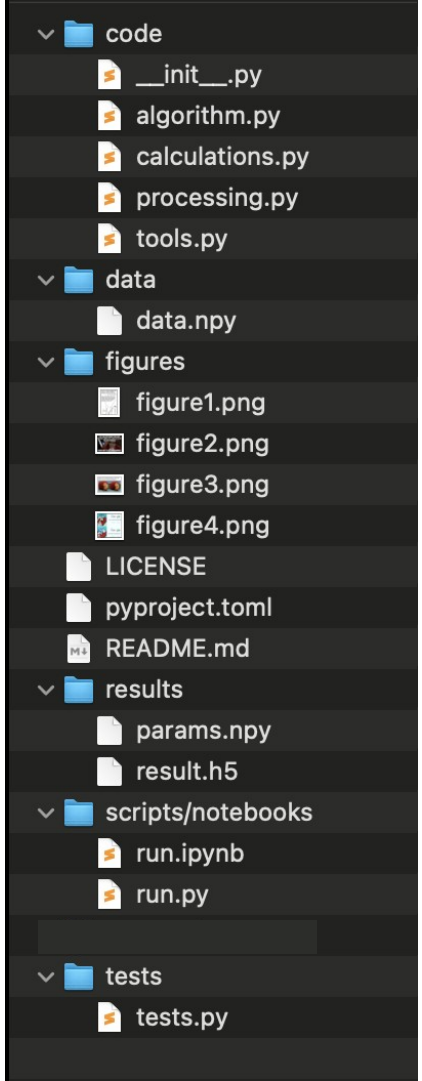
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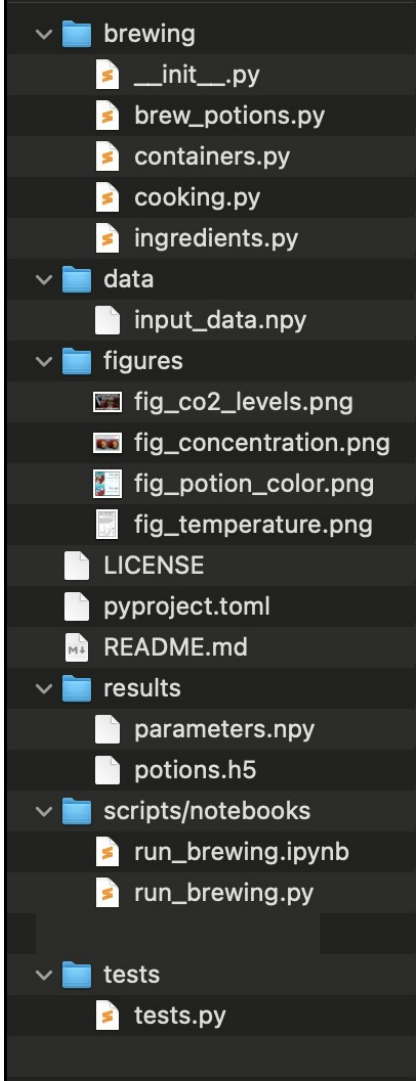
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input_data.npy
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fig_potion_color.png
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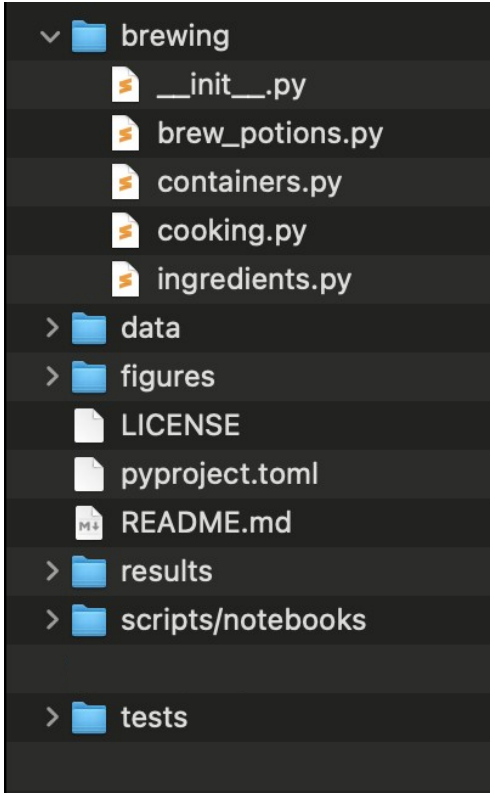
Python package structure



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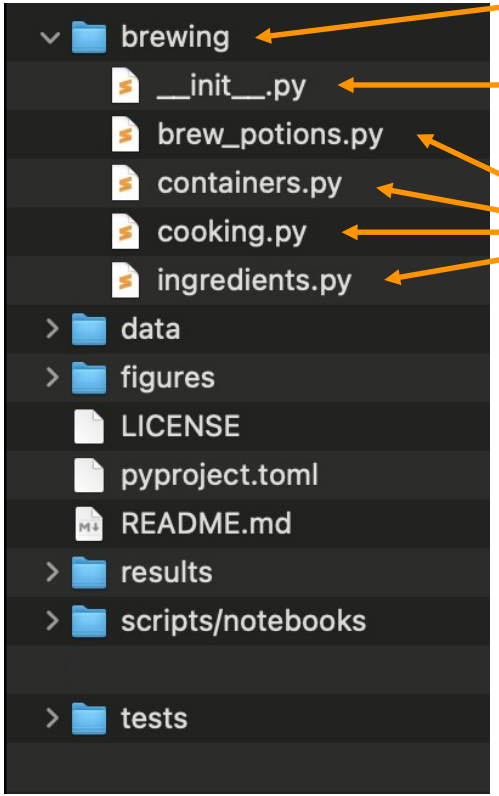
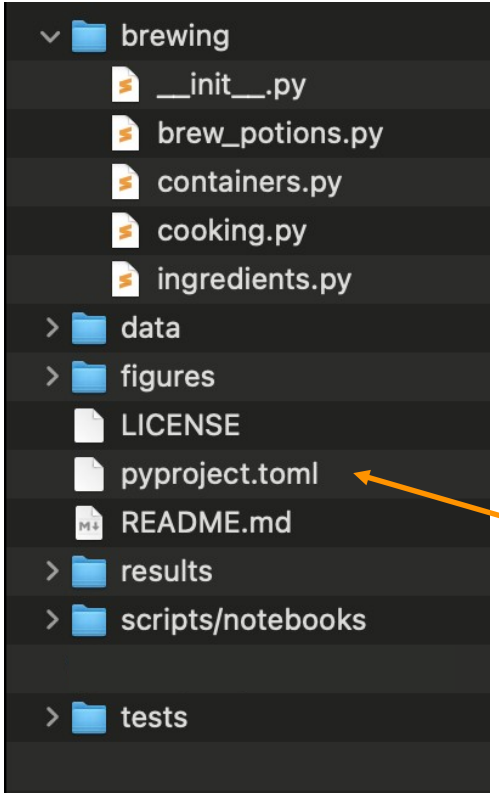


name of package

__init__.py
flags folder as package

modules
your .py files containing your code

Python package structure



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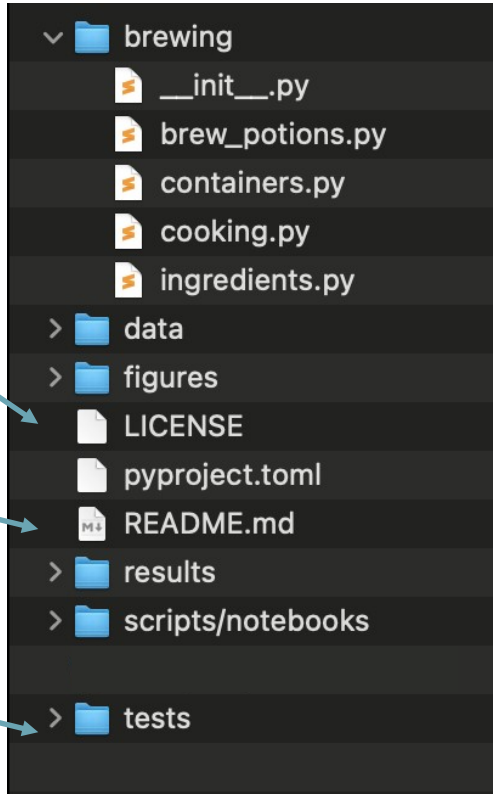
build instructions & package metadata
will explain more later :)

Python package structure



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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

Advantages

- know where to find items
  (use meaningful file names)
- 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)

Importing

Brewing package

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

Importing

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

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

Importing code

- you can always import code from your ***current directory***

  - by calling `import name`, Python will look for

    - a module called `name.py` inside the ***current directory***
    - a package called `name` inside in the ***current directory*** (= folder called `name` with an `__init__.py` file)

- Importing a module will execute all 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("Not printing when importing")
    print("But printing when run as script")
```

Importing modules

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

Importing modules

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```
1. import brew_potions

2. import brew_potions as br

3. from brew_potions import make_example_potion

4. from brew_potions import *
```

Importing modules

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

```
1. import brew_potions                                  + brew_potions.make_example_potion

2. import brew_potions as br                            + br.make_example_potion

3. from brew_potions import make_example_potion         + make_example_potion

4. from brew_potions import *                           + make_example_potion
```

Importing modules

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

```
1. import brew_potions                                  + brew_potions.make_example_potion
                                                        + brew_potions.make_python_expert_potion

2. import brew_potions as br                            + br.make_example_potion
                                                        + br.make_python_expert_potion

3. from brew_potions import make_example_potion         + make_example_potion
                                                        X make_python_expert_potion

4. from brew_potions import *                           + make_example_potion
                                                        + make_python_expert_potion
```

Importing a package

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

```
1. import brewing

2. import brewing.brew_potions

3. from brewing.brew_potions import make_example_potion
```

Importing a package

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```
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```

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

Importing a package

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

```
1. import brewing                                    X

2. import brewing.brew_potions                       + brewing.brew_potions.make_example_potion

3. from brewing.brew_potions import make_example_potion        + make_example_potion
```

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

Importing

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

Is there a way to get
a) *any 2*
b) *all 3*
exercises to work simultaneously?

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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- All packages which fall under these categories can be imported

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 Inc

Knowledge needed

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

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
```

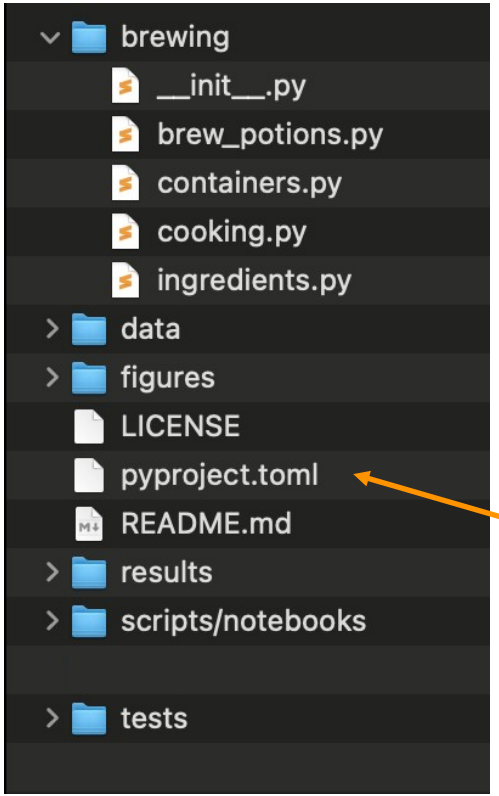
Option 3: install your package with -e (--editable) option

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

Knowledge needed

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

Python package structure



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...

LICENSE
makes the package (legally) usable.*

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

tests
you know why :)

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Python package structure

orange file = required in order to make the package installable

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makes the package (legally) usable.*

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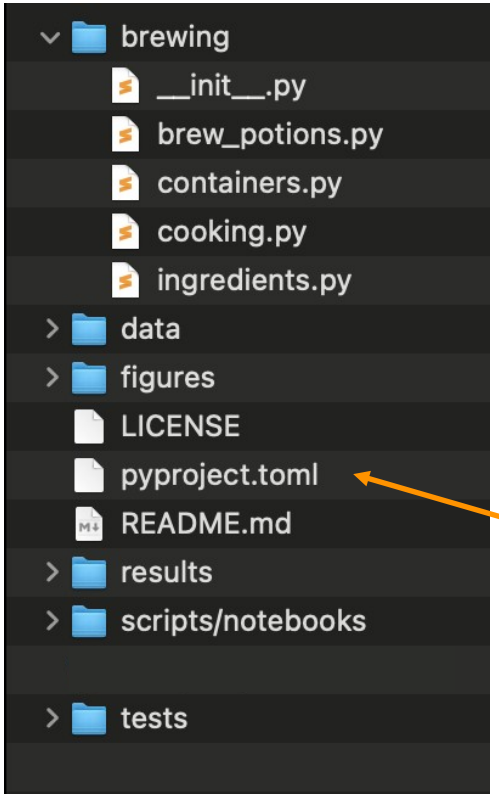

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pyproject.toml

- 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

```toml
[project]
name = "brewing"
version = "0.1.0"
description = "a python package for brewing potions"
authors = [{ name = "H. Granger", email = "h.granger@hogwarts.ac.uk" }]
license = { file = "LICENSE" }
requires-python = ">=3.7"
dependencies = ["numpy", "matplotlib >= 3.0.0", "pytest"]

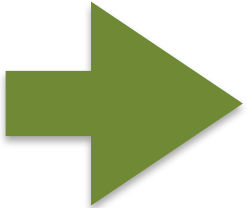
[tool.setuptools]
packages = ["brewing"]

[project.urls]
“Homepage” = ["https://github.com/ASPP/2023-heraklion-ODD"]

[build-system]
requires = ["setuptools>=42"]
build-backend = "setuptools.build_meta"
```

pyproject.toml

- dependencies should be kept minimal (only what you actually import in your module files)



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[build-system]
requires = ["setuptools>=42"]
build-backend = "setuptools.build_meta"
```

- When possible don’t depend on a specific version of a package. Conflicting version requirements between packages are annoying to handle as a user.
- When possible don’t depend on a specific version of Python. It is usually not necessary.

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 (ideal)

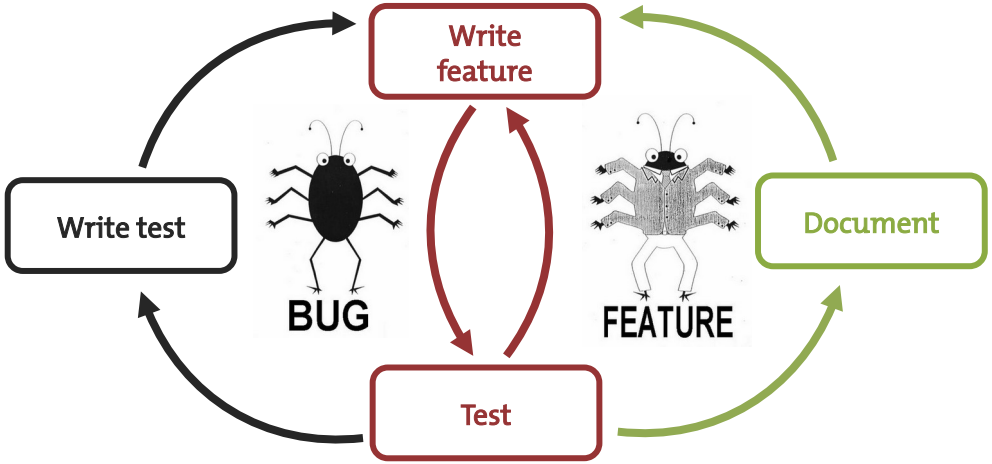
1 Create

Set up structure

Create files:
`__init__.py`
`pyproject.toml`
`README`
`LICENSE`

Make installable at this point

2 Build & Test

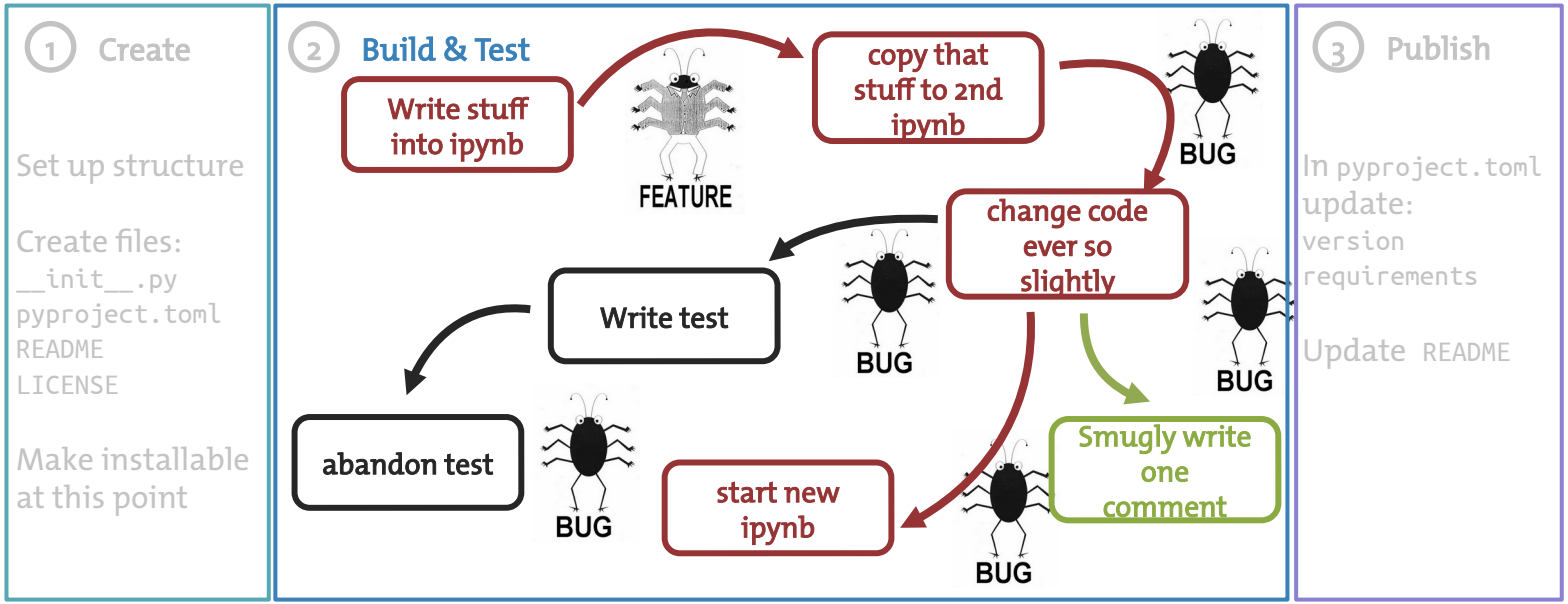


3 Publish

In `pyproject.toml` update:
`version`
`requirements`

Update `README`

Workflow (realistic)



Workflow (pragmatic)

1 Create

Set up structure

Create files:
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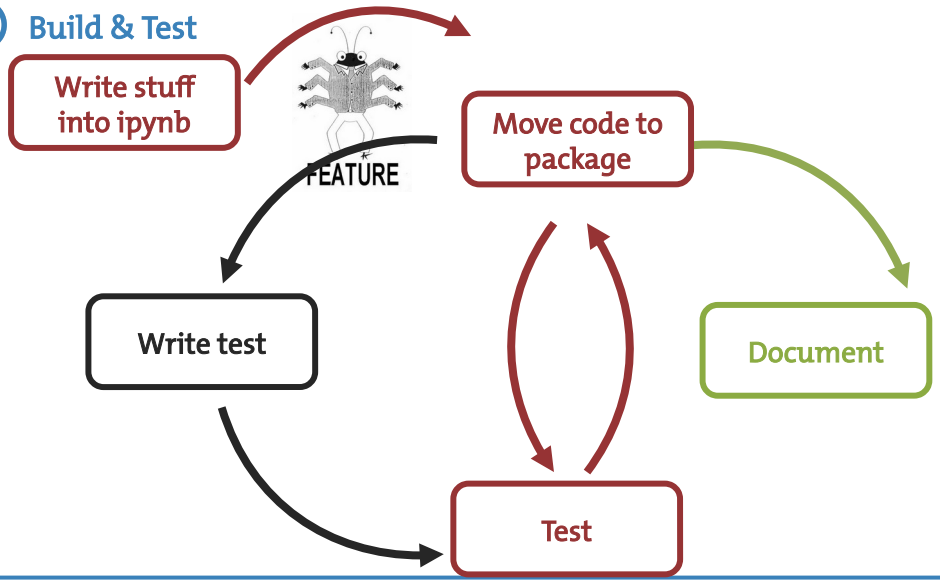
`README`
`LICENSE`

Make installable at this point

2 Build & Test



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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 it on PyPI to make it easier for others to download and use

Write your function

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

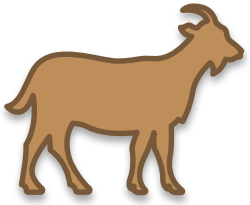
Exercise:

- 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

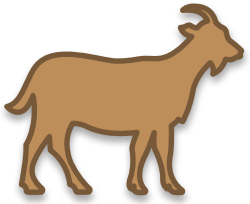
Why environments?

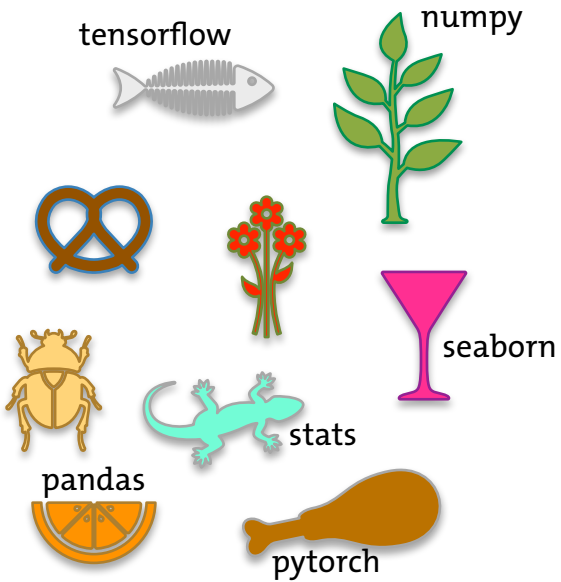
Project 1
= 1st year
PhD project



Why environments?

Project 1
= 1st year
PhD project

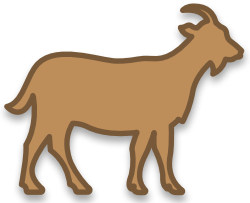


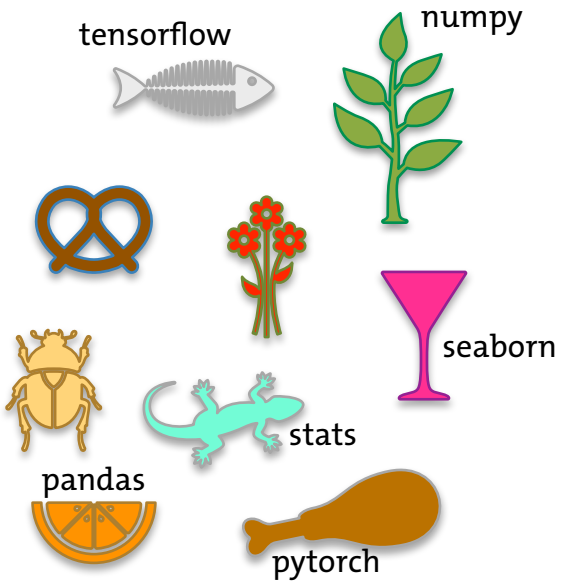


dependencies

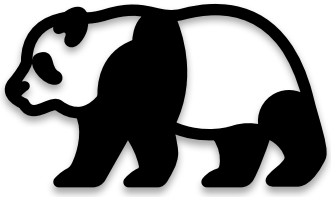
Why environments?

Project 1
= 1st year
PhD project





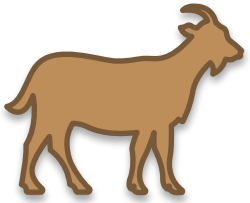
Project 2
= collaboration
with another lab

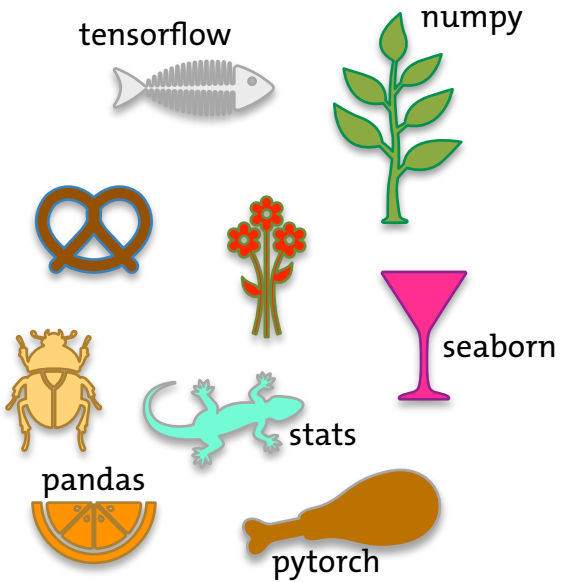


dependencies

Why environments?

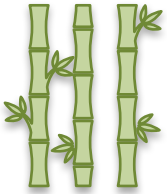
Project 1
= 1st year
PhD project

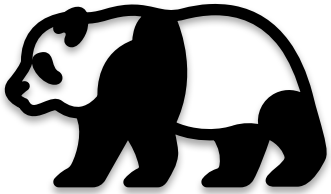




Project 2
= collaboration
with another lab

word2vec

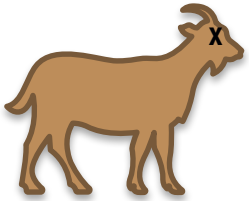




dependencies

Why environments?

Project 1
= 1st year
PhD project

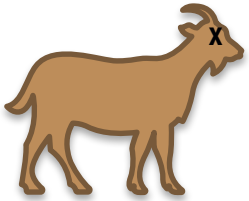


pandas = 1.2.4

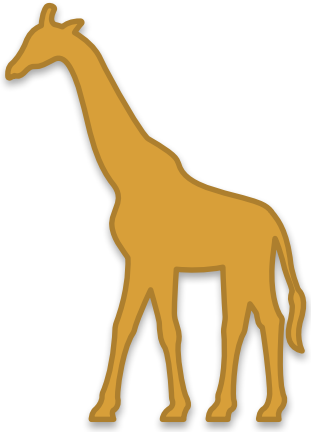
dependencies

Why environments?

Project 1
= 1st year
PhD project



pandas = 1.2.4

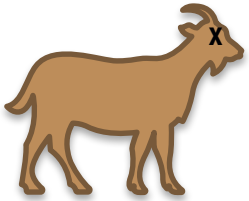


Project 2
= 2nd year
PhD project

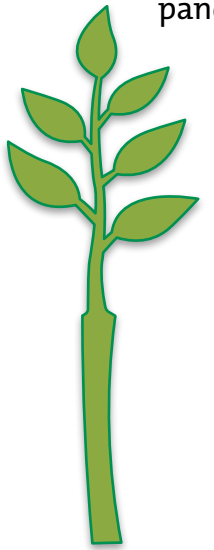
dependencies

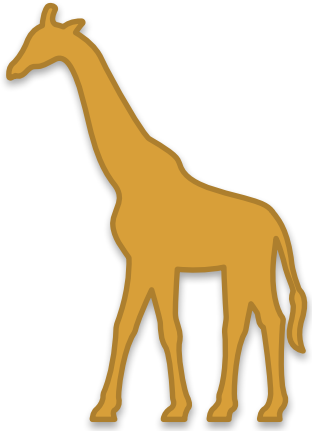
Why environments?

Project 1
= 1st year
PhD project



pandas = 1.3.0



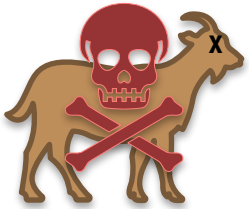


Project 2
= 2nd year
PhD project

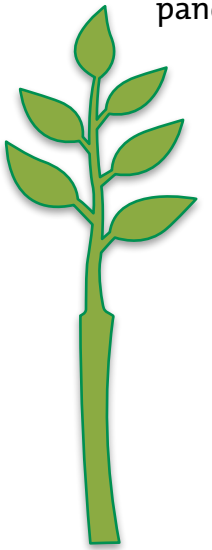
dependencies

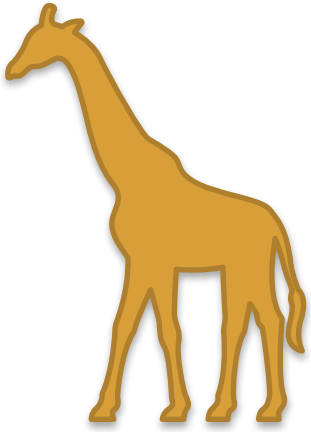
Why environments?

Project 1
= 1st year
PhD project



pandas = 1.3.0

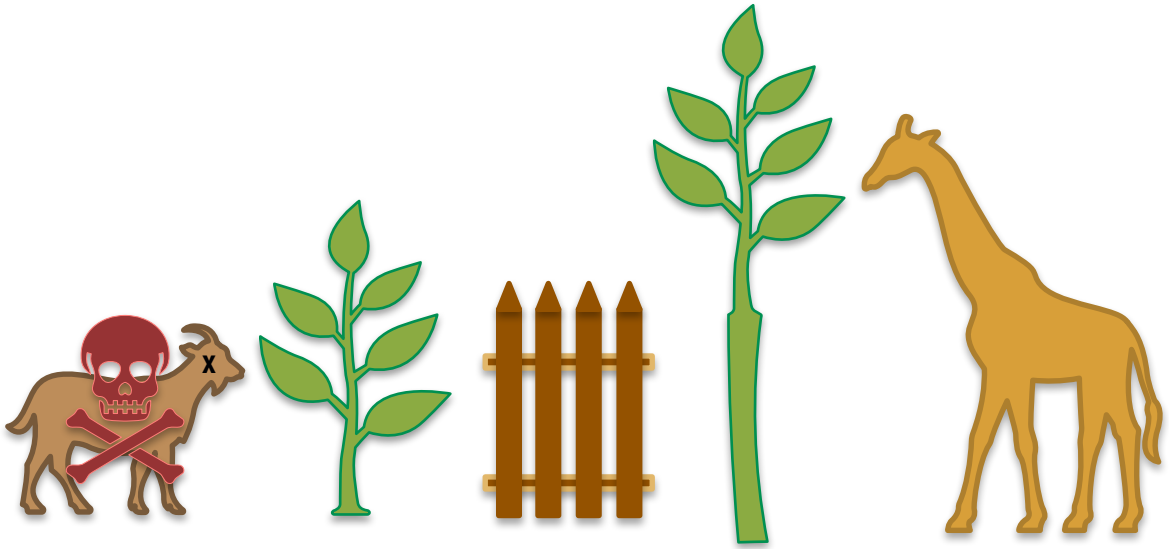




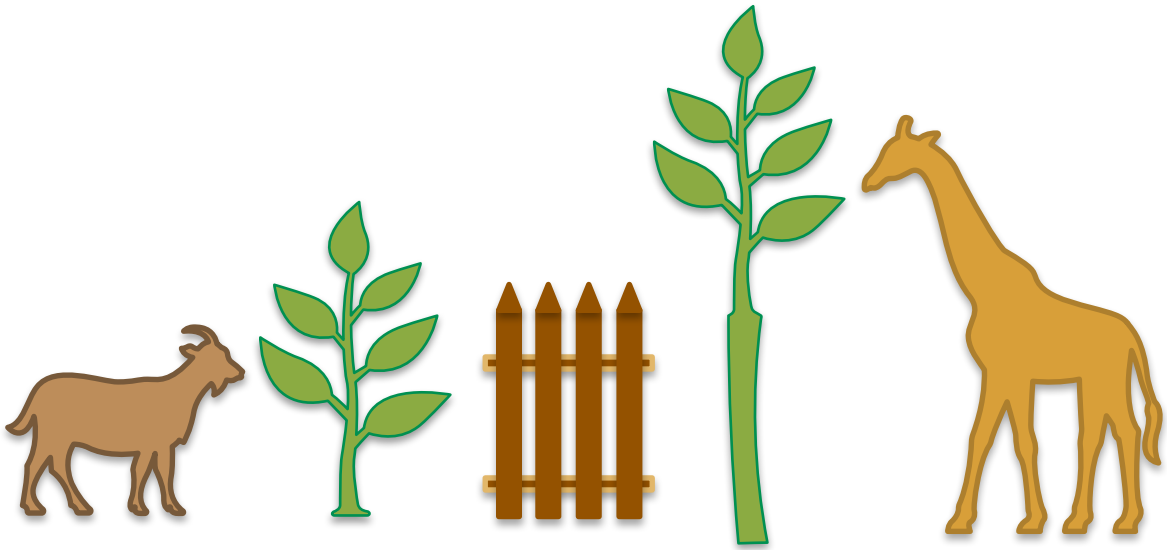
Project 2
= 2nd year
PhD project

dependencies

Why environments?



Why environments?



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 4 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

Environment Managers

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

  Million others*:
  conda, virtualenv-wrapper, pipenv, poetry, flit, hatch, PDM

* a description of the chaos:

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

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 from the Python prompt:
  help `<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 (overkill?)

- 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

```
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
# -> 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

Summary

Contents

usability features:

1) folder and file structure
   - standard Python package structure
2) error-free importing and installation and publishing
   - how to make a package installable
3) isolated, protected code
   - virtual environments
4) readability
   - documentation, typing, naming