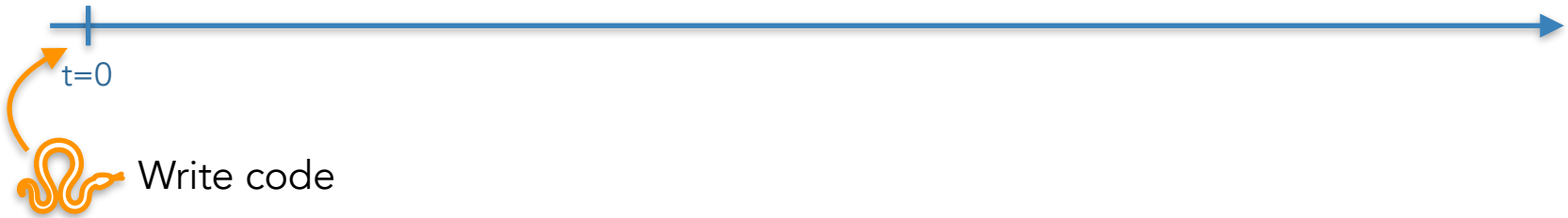
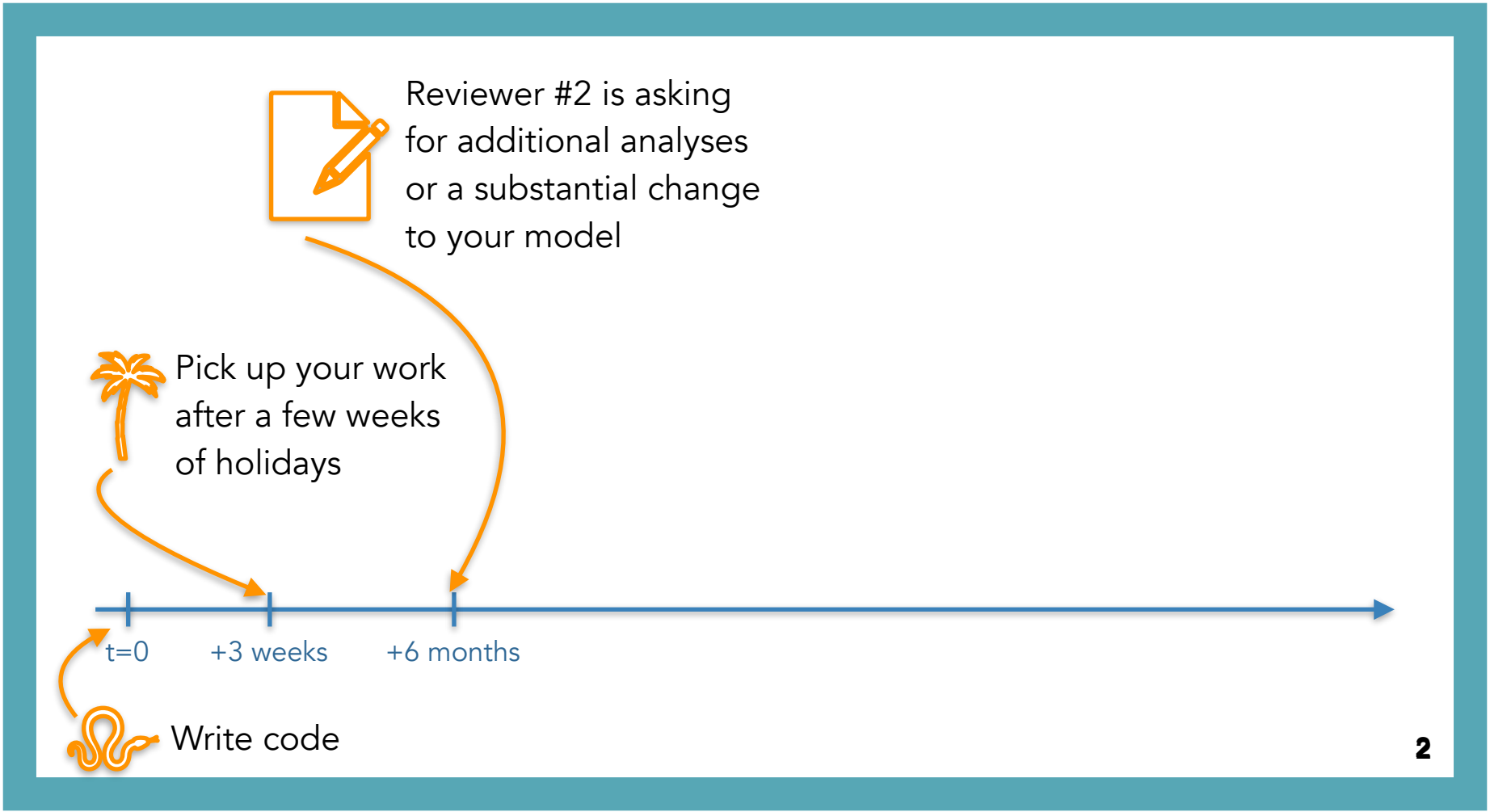
Organizing, documenting and distributing code

ASPP 2021, Bordeaux


t=0
Write code

Pick up your work
after a few weeks
of holidays
t=0
+3 weeks
Write code


Reviewer #2 is asking
for additional analyses
or a substantial change
to your model
Pick up your work
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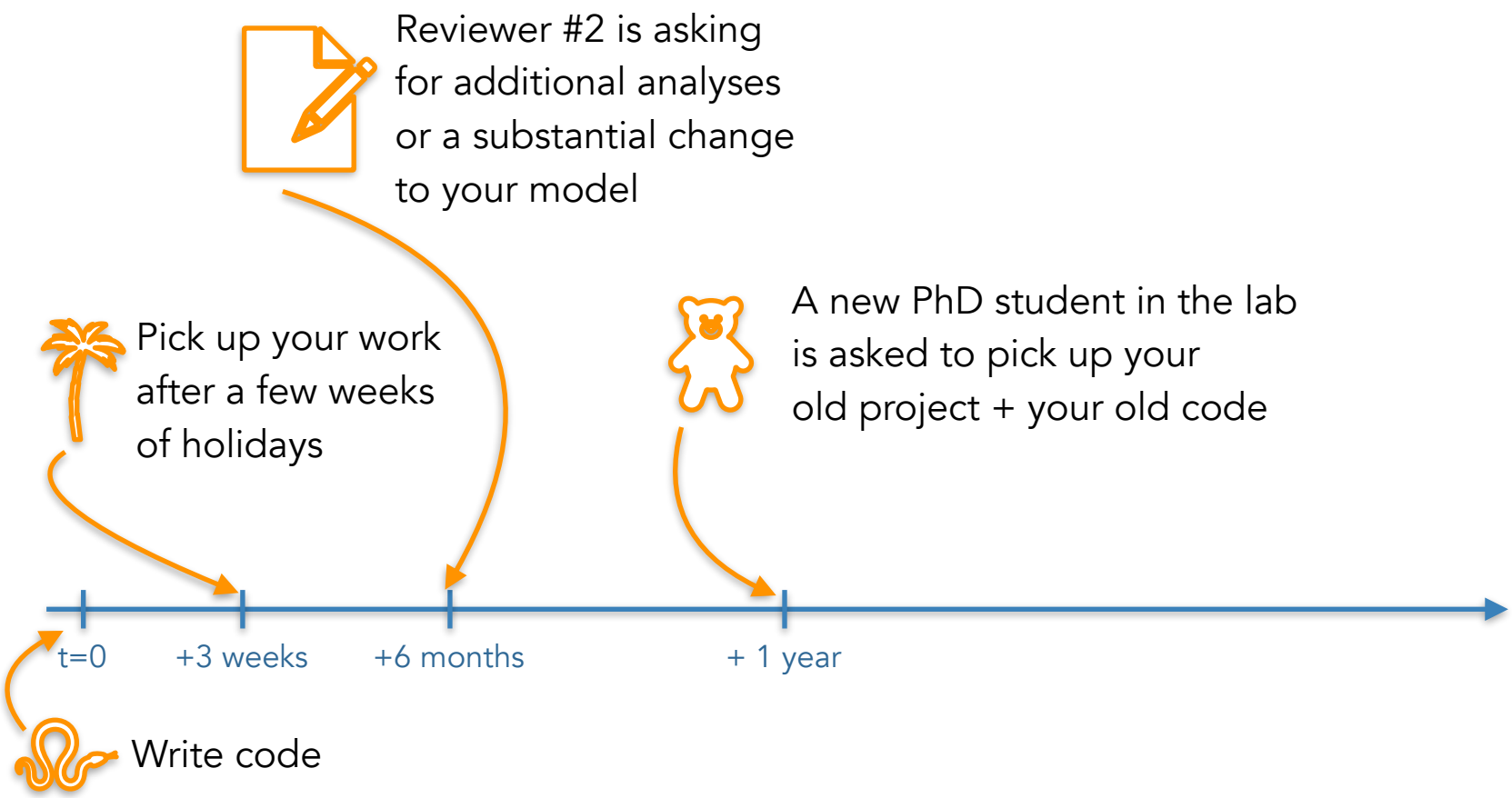
of holidays
t=0
+3 weeks
+6 months
Write code


Reviewer #2 is asking
for additional analyses
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Pick up your work
after a few weeks
of holidays
A new PhD student in the lab
is asked to pick up your
old project + your old code
t=0
+3 weeks
+6 months
+ 1 year
Write code

Reviewer #2 is asking for additional analyses or a substantial change to your model

You are writing your thesis and you need to re-do some figures of your first project

Pick up your work after a few weeks of holidays

A new PhD student in the lab is asked to pick up your old project + your old code

t=0

+3 weeks

+6 months

+ 1 year

+3 years

Write code

Motivation

- **Organising** your code in a standardized way makes it easier to understand and increases **usability** for
  you and **future you** (and **other people**)

Contents

- how to organise your code ==> as a package
  - files and folder structure
  - importing and installing your package
- how to make code understandable ==> documentation
- how to handle requirements ==> virtual environments

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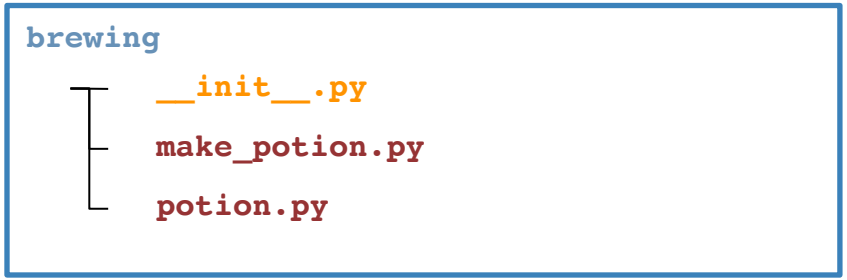
Package structure

Package

- Typically a **package** is a folder (name of folder = name of package) which contains an `__init__.py` file and **modules**.



Modules

- A **module** is a .py file consisting of Python code
  e.g. functions and/or classes and/or variables

- its contents can be imported

File: example_module.py

```
""" This is a module. """


some_constant = 3.14


def some_function(x, y):
    return x + y


def ExampleClass():
    def __init__(self):
        self.greeting = “hello”
    def greet(self):
        print(self.greeting)
```

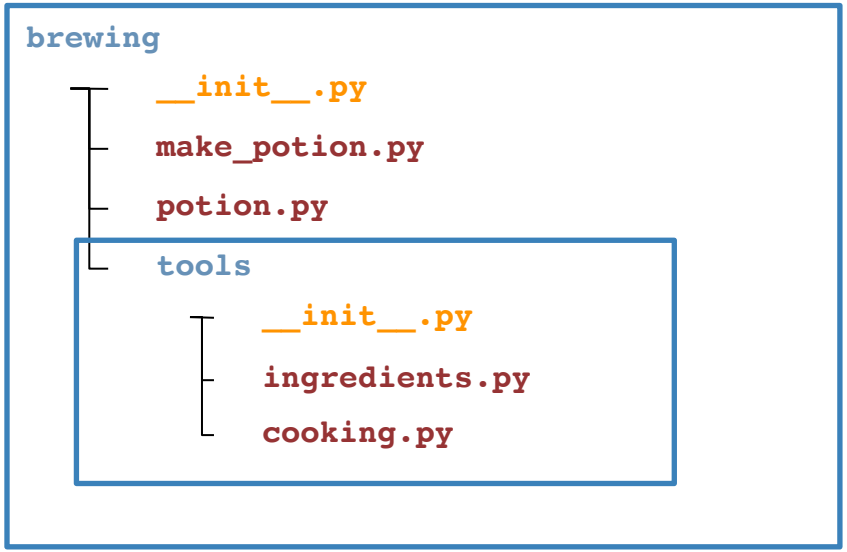
__init__.py

- The **__init__.py** file marks a folder as a package
- can be empty (easiest at the beginning)
- Can be used to control importing

File: __init__.py

Package

- Typically a **package** is a folder (name of folder = name of package) which contains an `__init__.py` file and **modules**.
- A **package** may also contain other **packages**
- the packages you know (numpy, scipy, sklearn, …) follow this structure



Advantage 1

—> know where to find items

e.g. wardrobe

- suit, shirts
- t-shirts
- socks, underwear

same concept applies to code

—> specific module 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***
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Importing code from modules

Importing modules

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

- Importing a module will execute all the code in the module (including print statements, unless you import specific objects)

Importing modules

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

Importing modules

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

1. `import cooking`

2. `import cooking as cook`

3. `from cooking import eternal_flame`

4. `from cooking import *`

Importing modules

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

```
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
```

Importing modules

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

```
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 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 *
```

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 from a package

Order of execution

Terminal

```
> python3 import_pkg.py
```

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

Order of execution

Terminal

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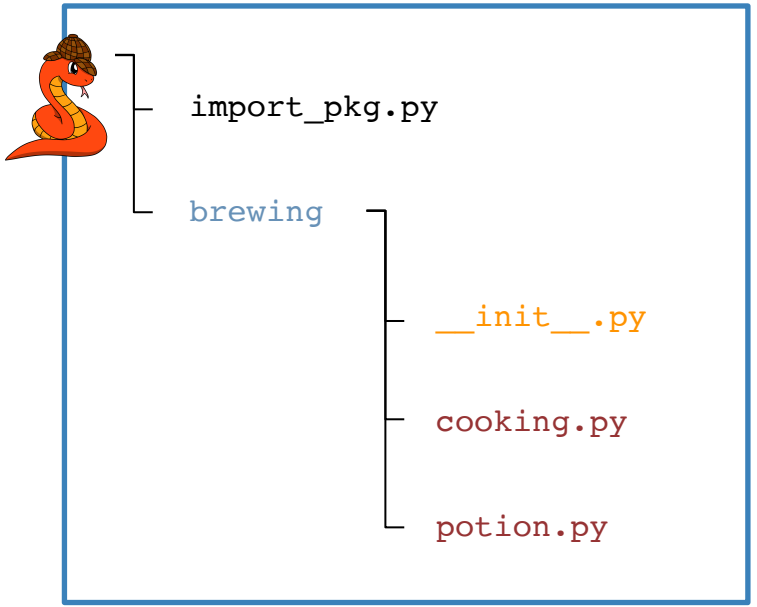

Order of execution

Terminal

```
>  python3 import_pkg.py
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```
# content of import_pkg.py
import brewing
```

import_pkg.py

brewing

__init__.py

cooking.py

potion.py

Order of execution

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# content of import_pkg.py
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```

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

Order of execution

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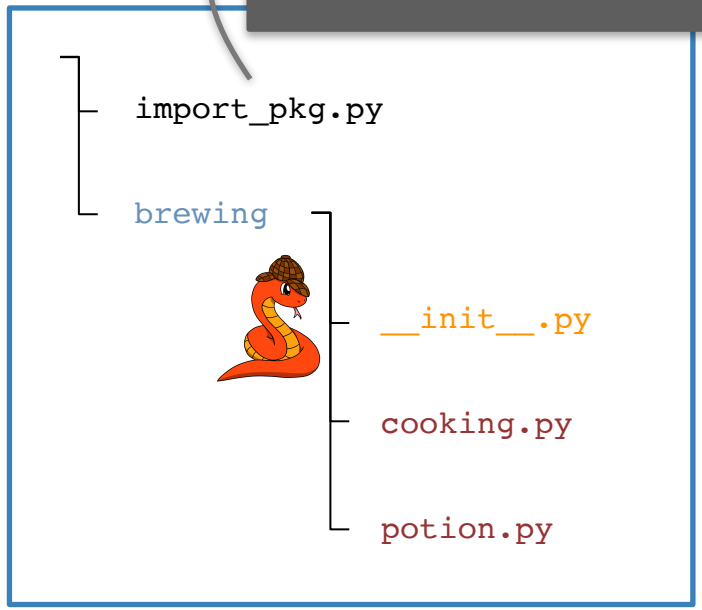

Order of execution

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```
# content of __init__.py
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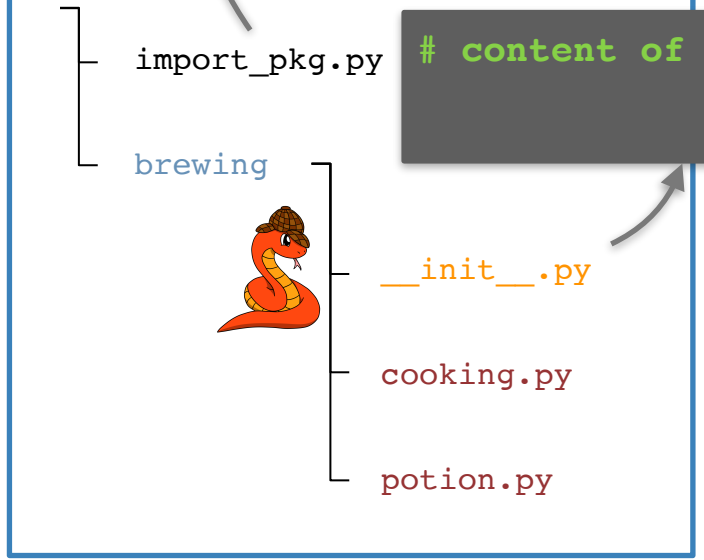

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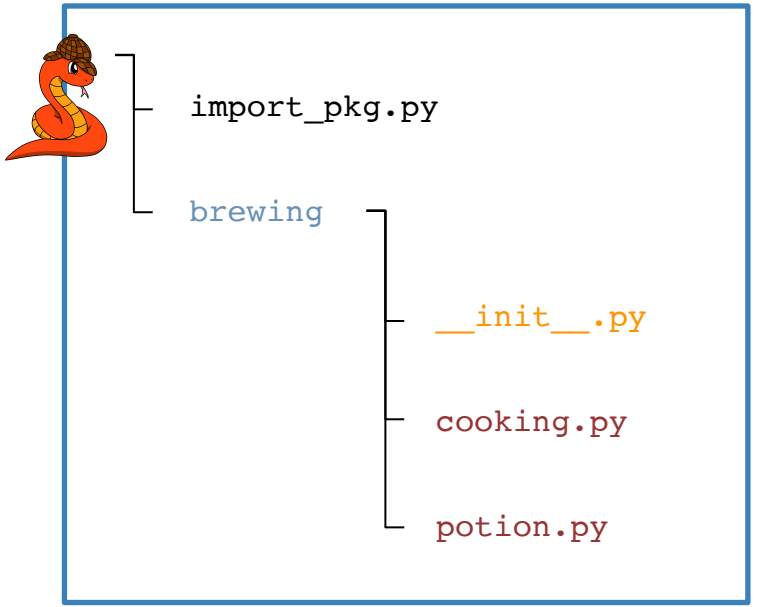

Order of execution

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

import_pkg.py

brewing

__init__.py

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Order of execution

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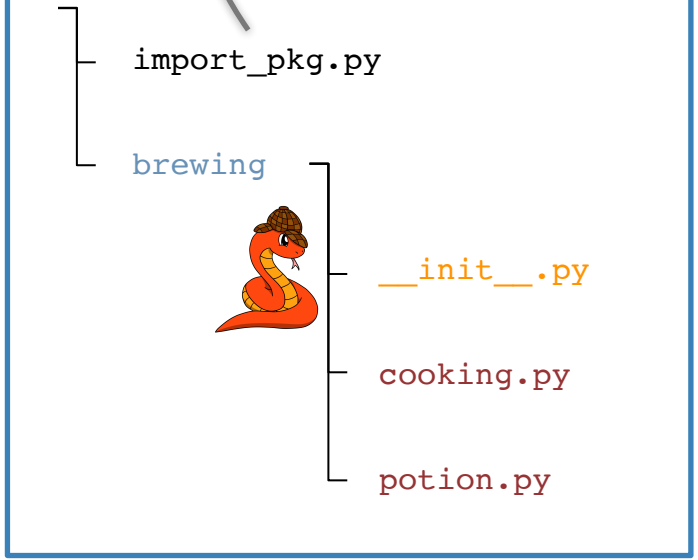

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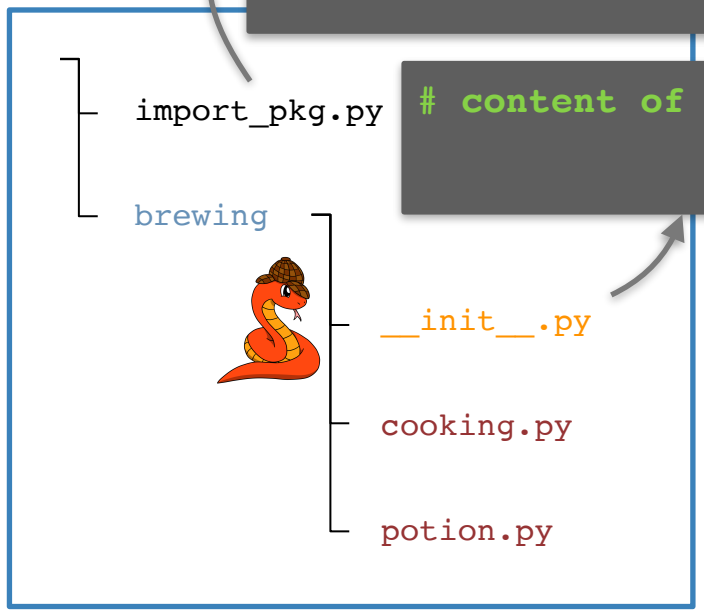

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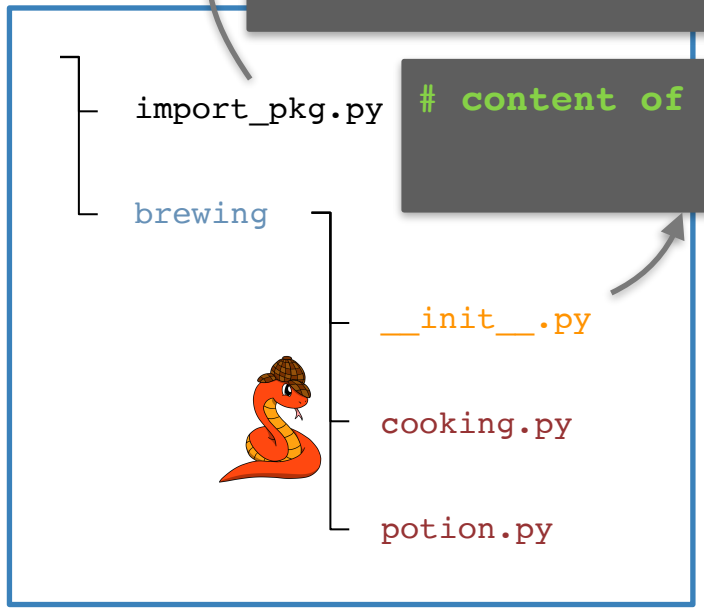

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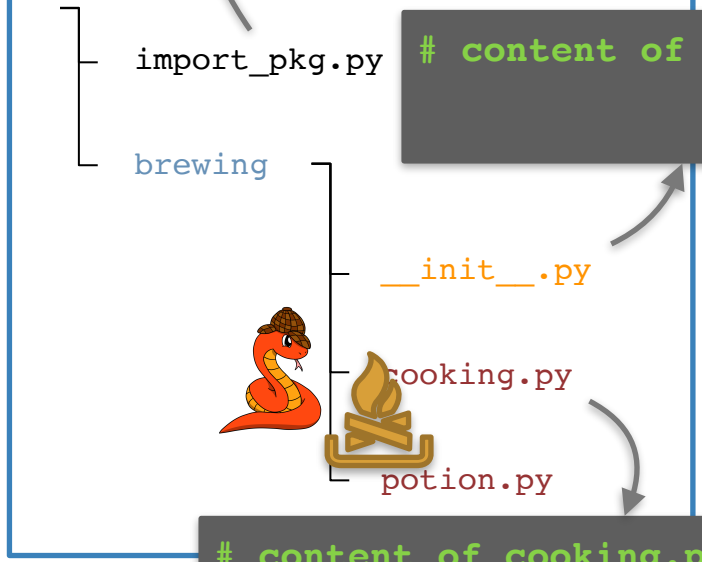


```
# content of cooking.py
eternal_flame = “eternal_flame”
```

Order of execution

Terminal

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```

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

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import_pkg.py
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    __init__.py
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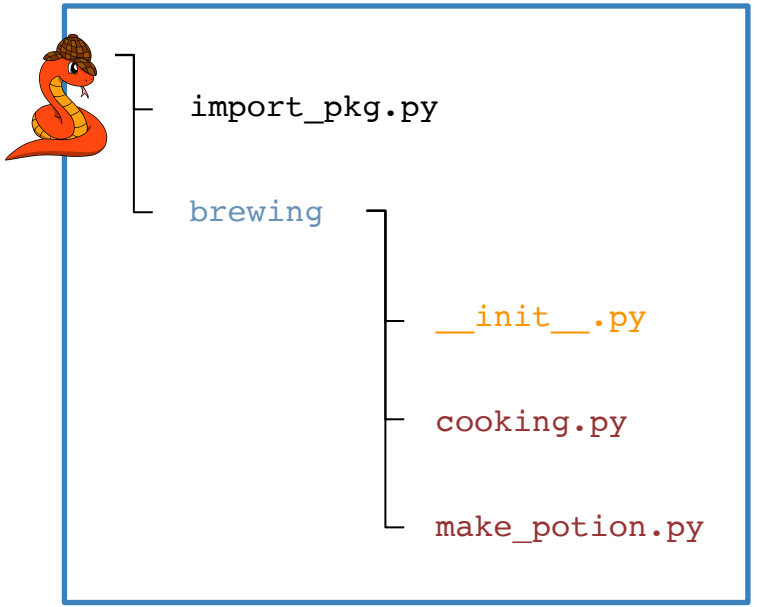

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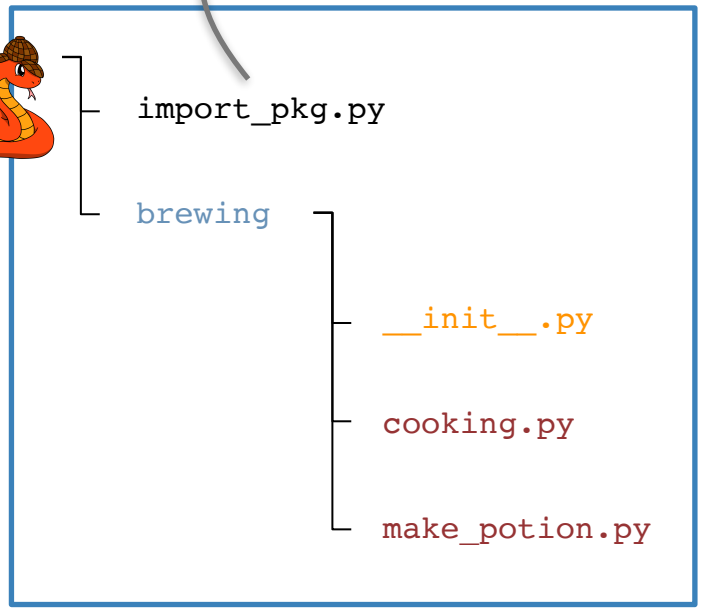

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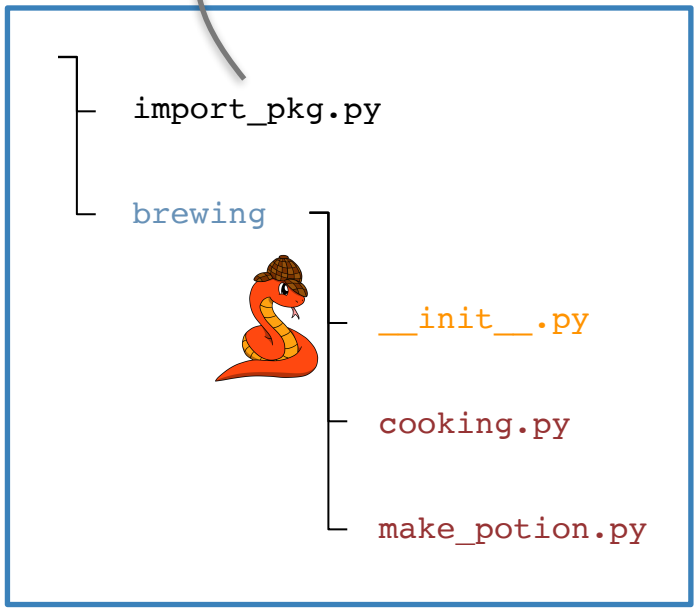

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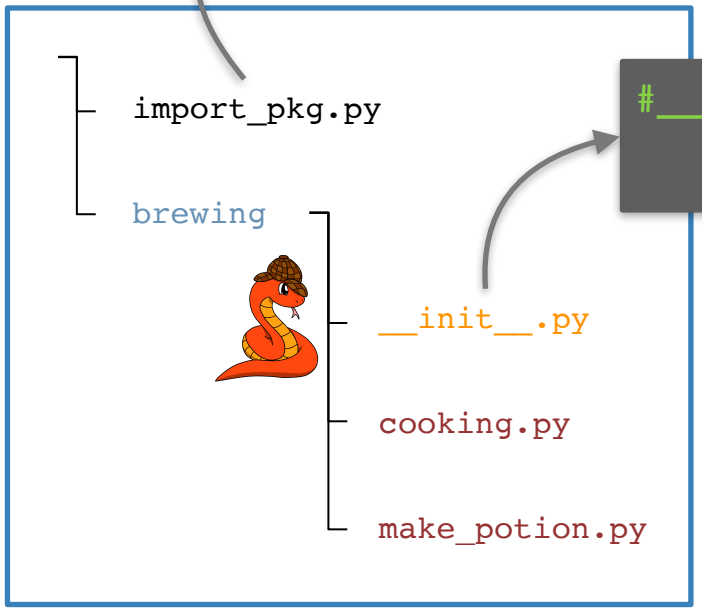


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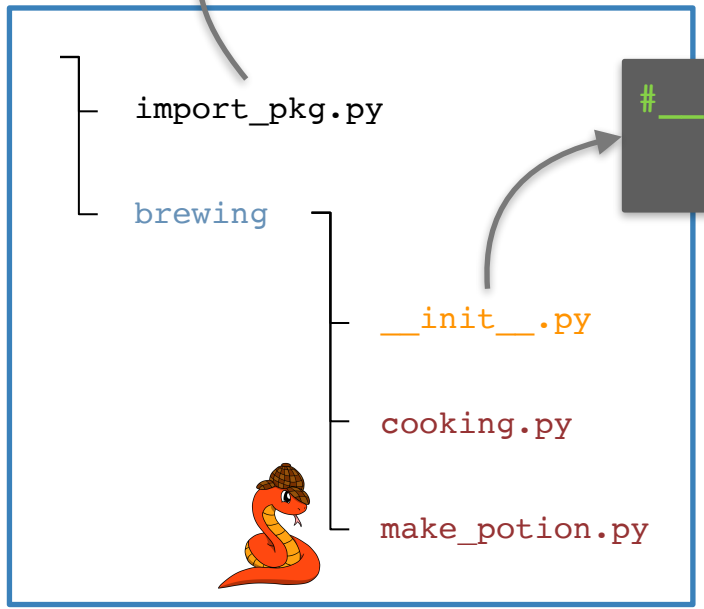


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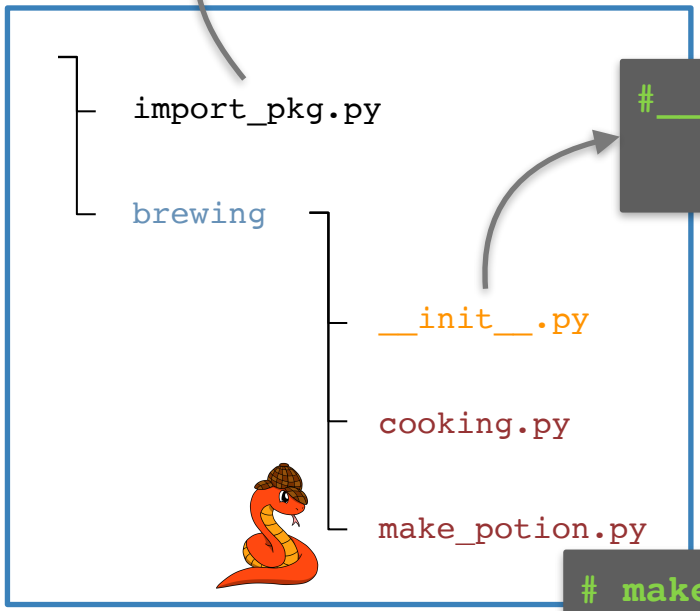


```
#__init__.py
```

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

Order of execution

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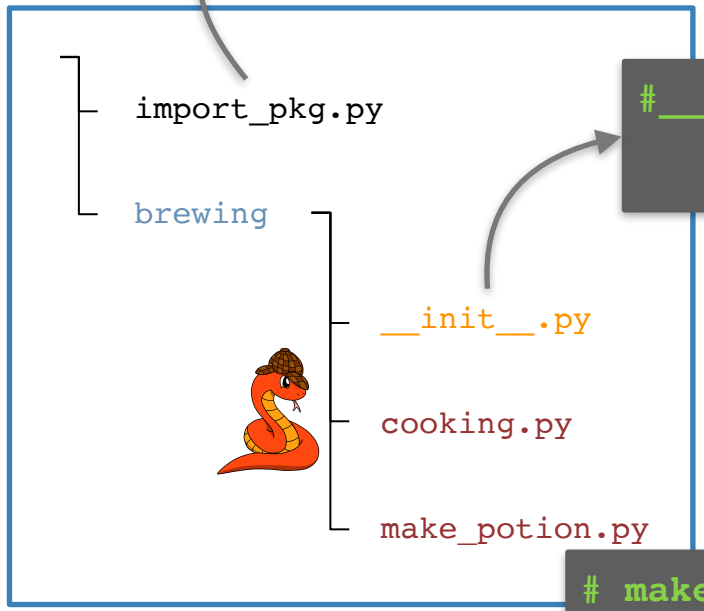


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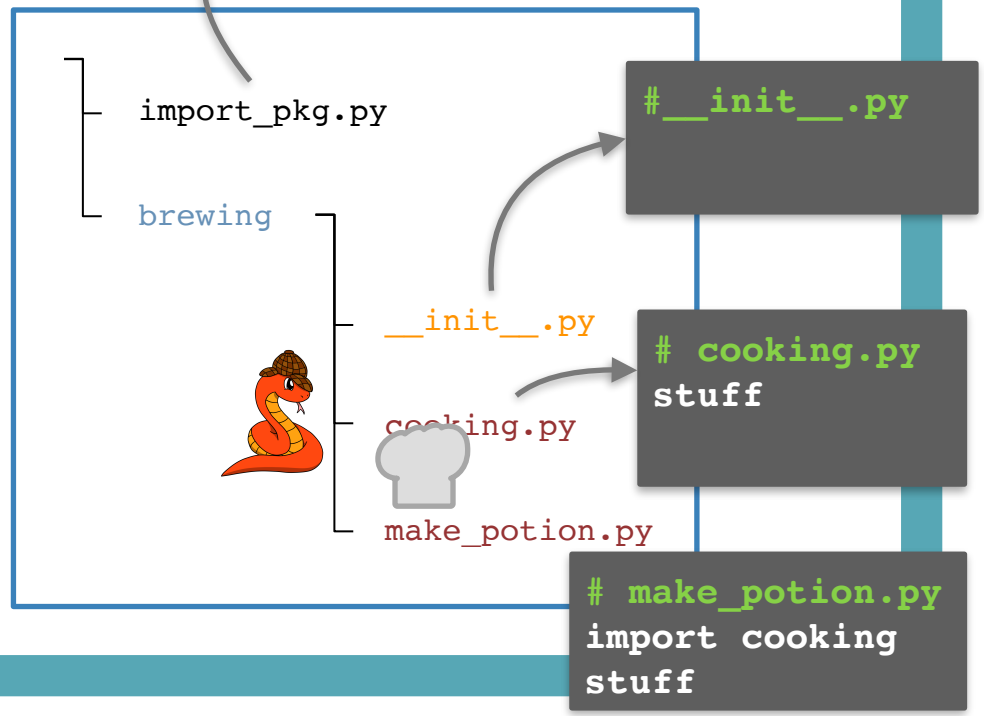

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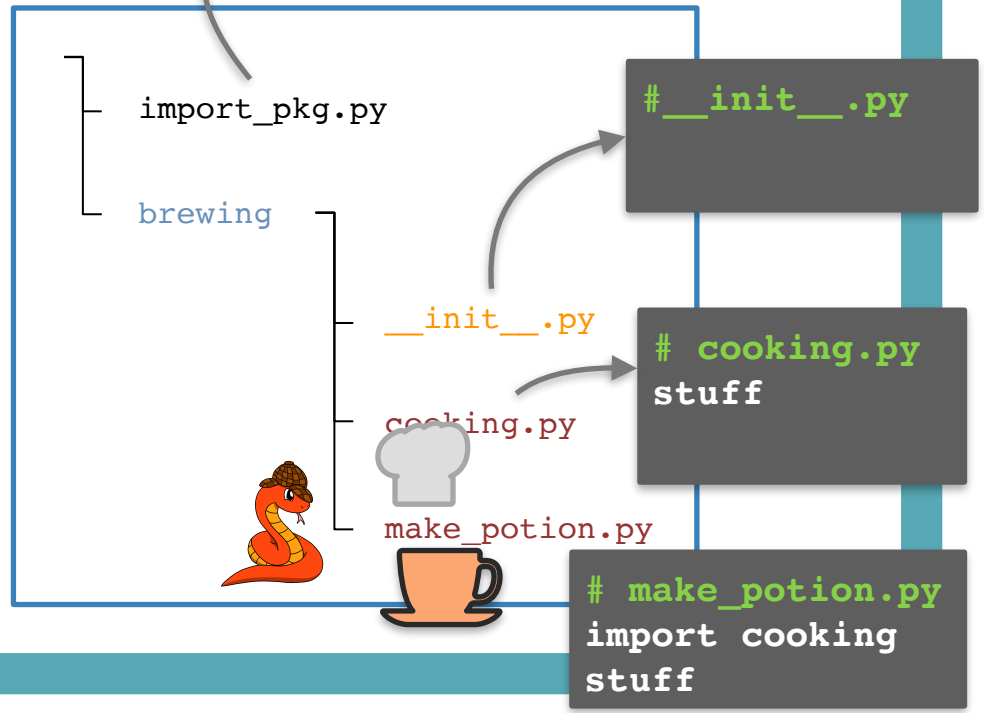

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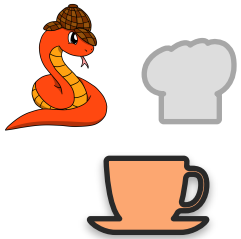

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import_pkg.py
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    cooking.py
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```

```
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```

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

Importing a package

- you can always import a package that is located in the directory the script is located in
- Modules in the package are bound to the package name
- If the __init__.py file is empty

```
1. import package                          -

2. import package.module                   + package.module.object

3. from package.module import object       + object

4. from package.subpackage.module          + object
   import object
```

Importing

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

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

?

pip editable installation

Knowledge needed

- what happens when a package is installed?
- 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

Available packages

brewing package

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- **current directory**

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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

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- what happens when a package is installed?
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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>
```

Knowledge needed

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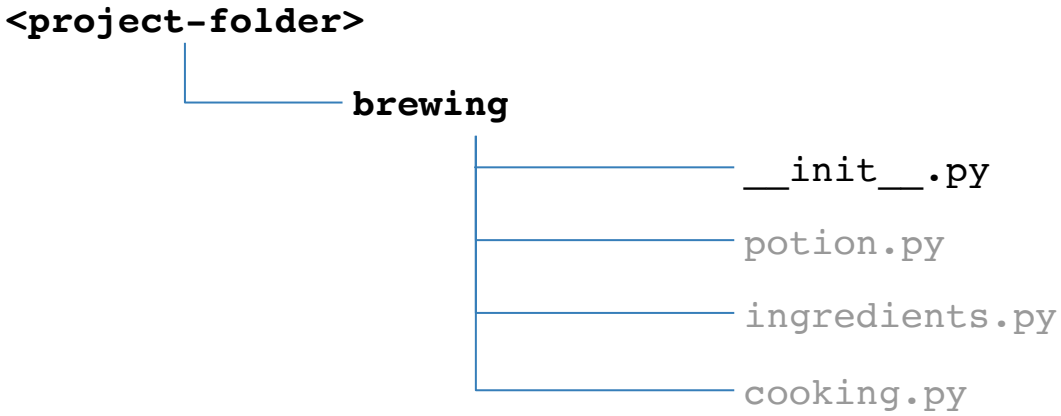
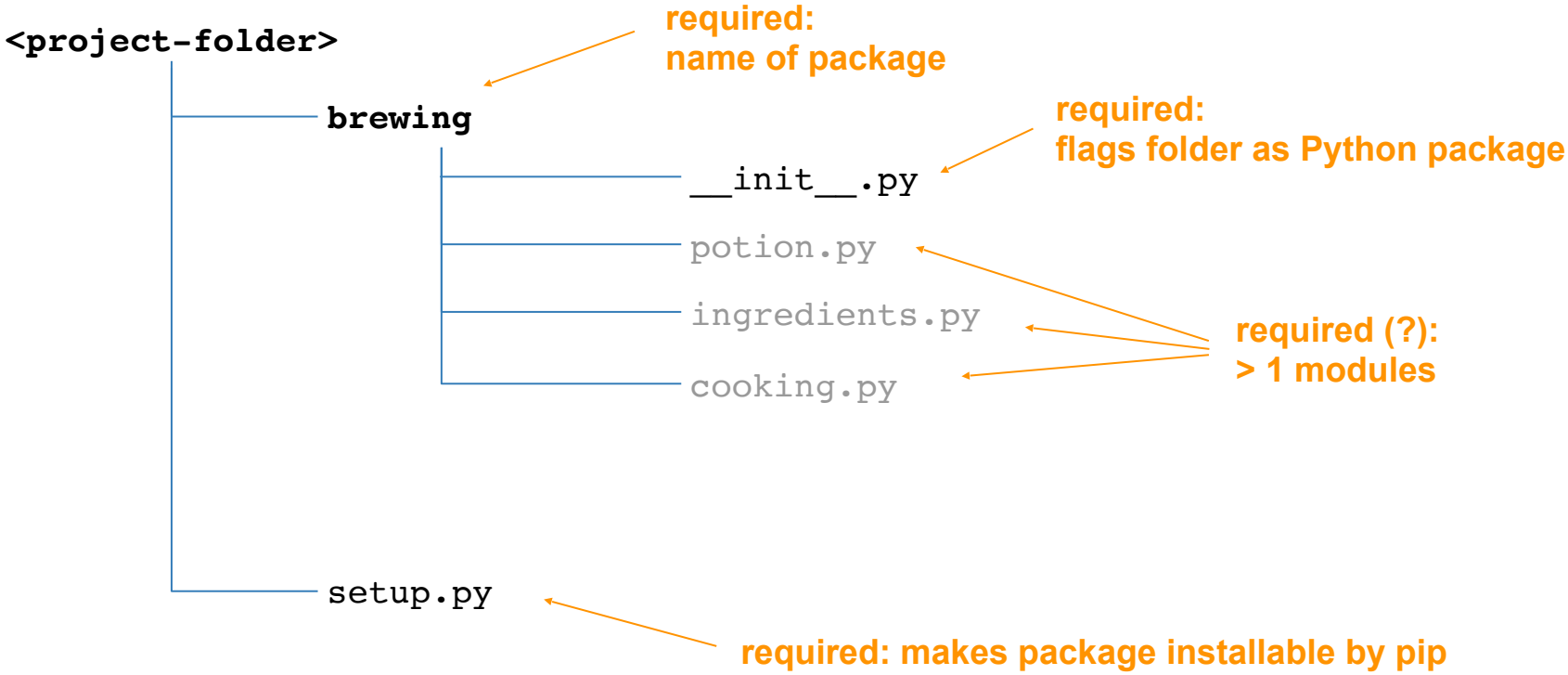
Requirements



* pick one from choosealicense.com

Requirements



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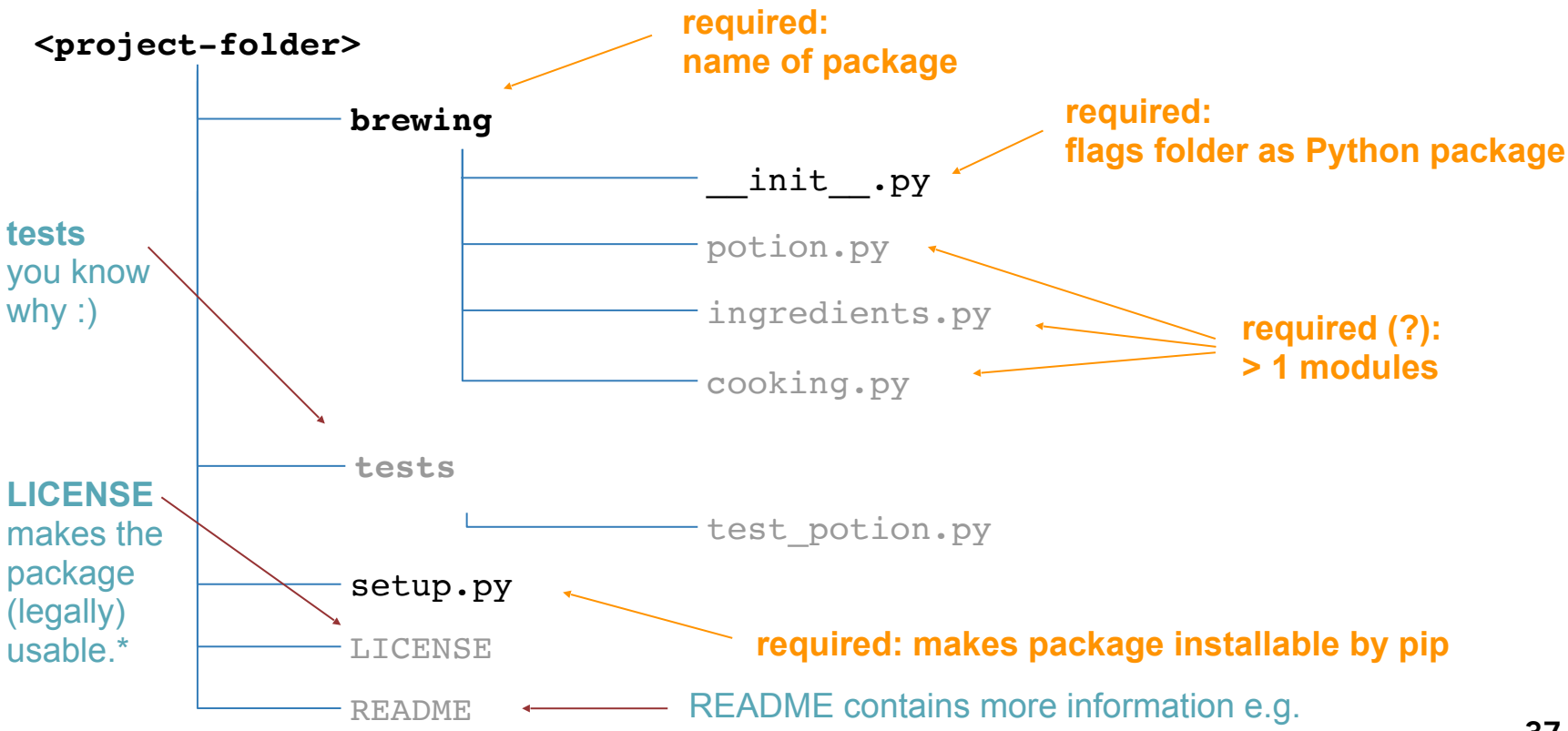

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Setup.py

- The setup function receives package information and package meta data
- required entries: name, version, packages(/modules)
- **install_requires** 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

```
from setuptools import setup, find_packages

with open('README.txt', 'r') as fh:
    long_description = fh.read()

setup(
    name = 'potions',
    version = '0.1.0',
    packages = find_packages(),
    author = 'ASPP 2021',
    author_email = 's.snape@hogwarts.ac.uk',
    description = 'an example python package',
    long_description = long_description,
    license = 'MIT',
    url = 'https://github.com/ASPP/2021-bordeaux-
ODD.git',
    install_requires = ['numpy >= 1.13.0',
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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

Workflow (realistic?)

1 Create

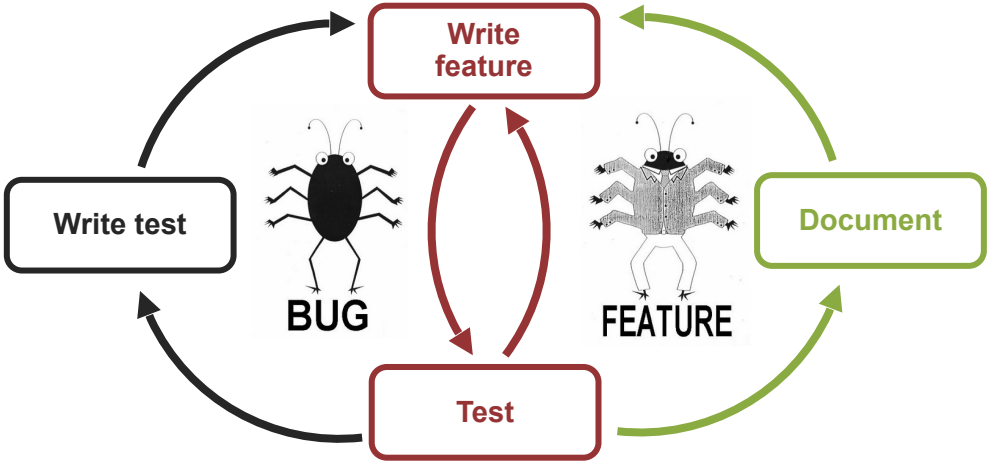
Set up folder structure

Create files:

```
__init__.py
setup.py
README
LICENSE
```

Make installable at this point

2 Build & Test



3 Publish

In `setup.py` 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 Workflow** to write and test a function to make a “Python expert” potion
- Create a Pull Request

?

documentation

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 doctring """

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
```

Document your function

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

- Use the same Pull Request

Keeping track of your docstrings

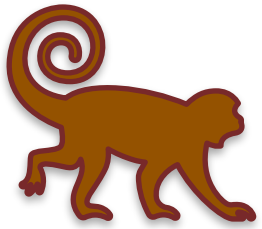
- Most commonly used hosting websites: facilitate building, versioning, and hosting
  - github.io
  - readthedocs.org
- Automate documentation
  - Sphinx: a package to collect docstrings and create a nicely formatted documentation website

?

virtual environments

Why environments?

Project 1



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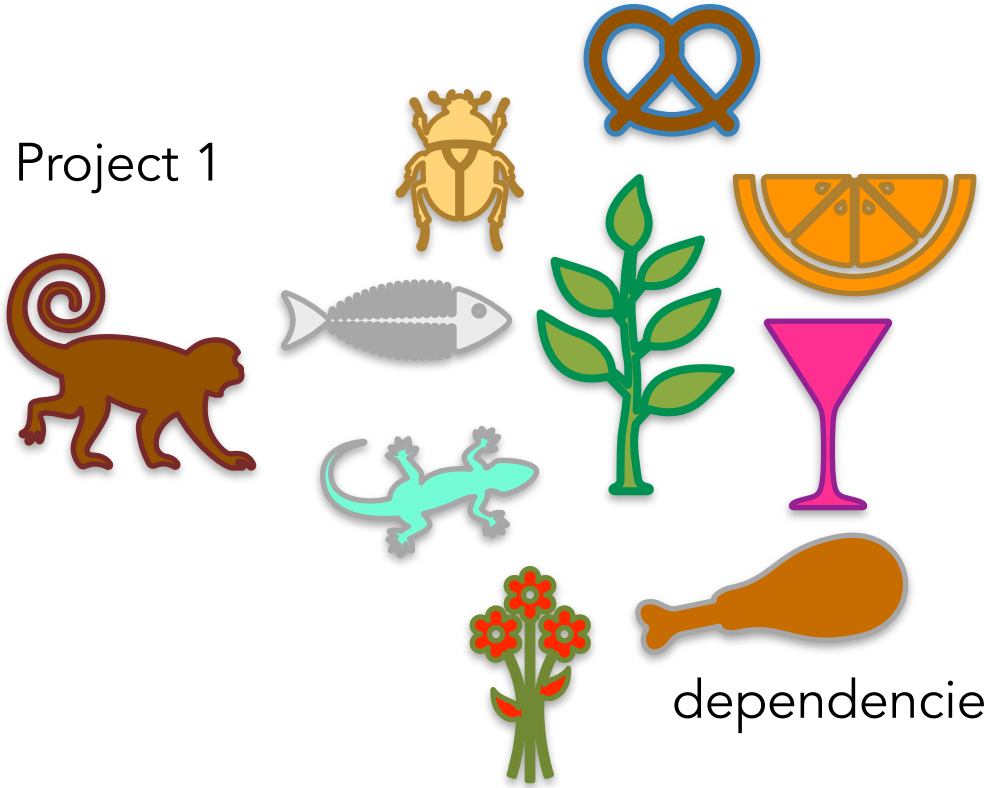

dependencies

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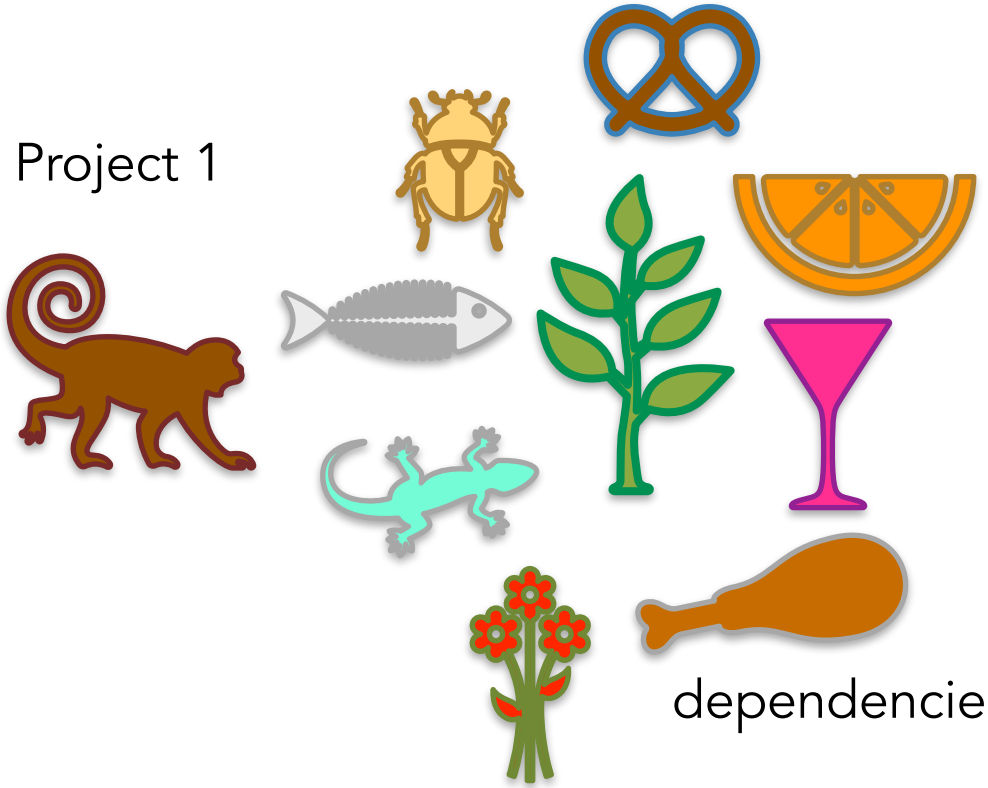
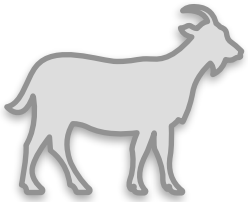


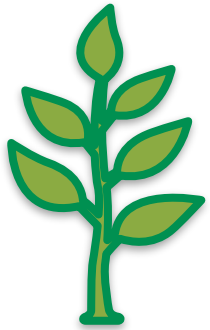
dependencies

Project 2

Why environments?

Project 1





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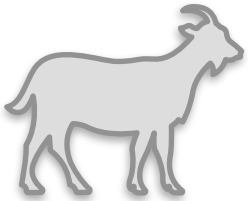
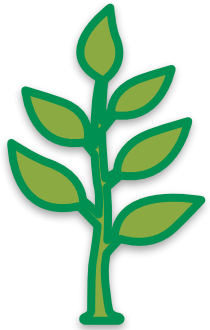
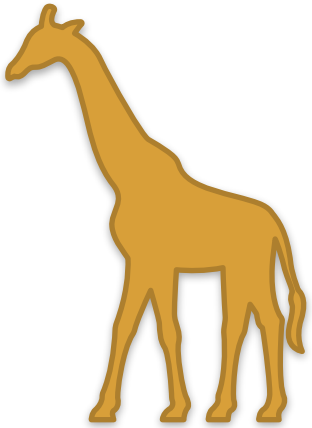




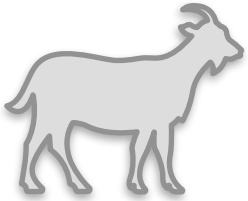


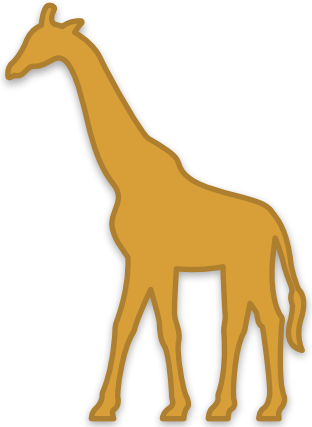
Project 2

dependencies

Why environments?

Project 1





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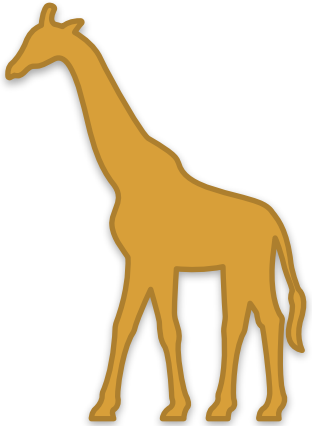

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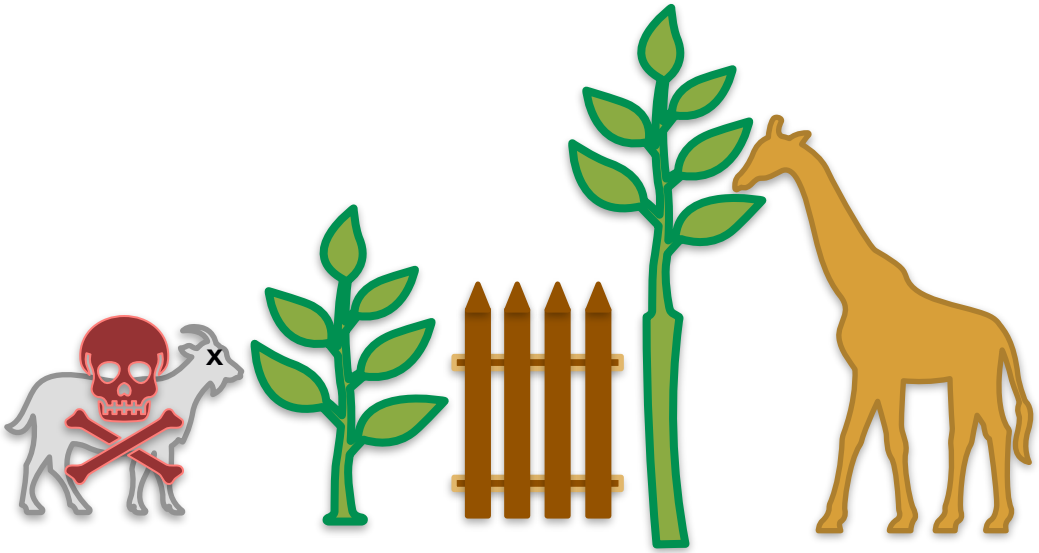

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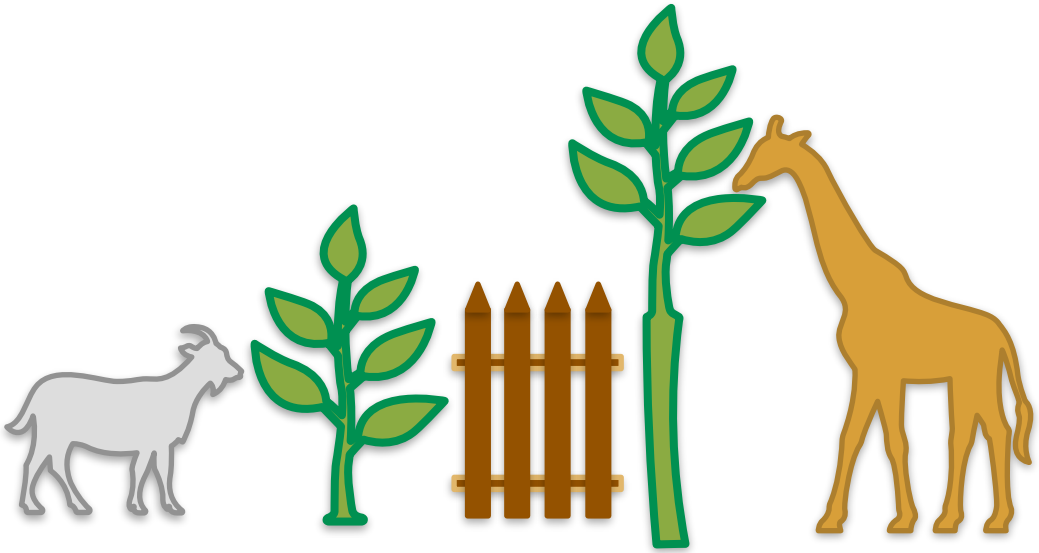


Project 2

dependencies

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 start over easily

Virtual Environments

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

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

?

Summary

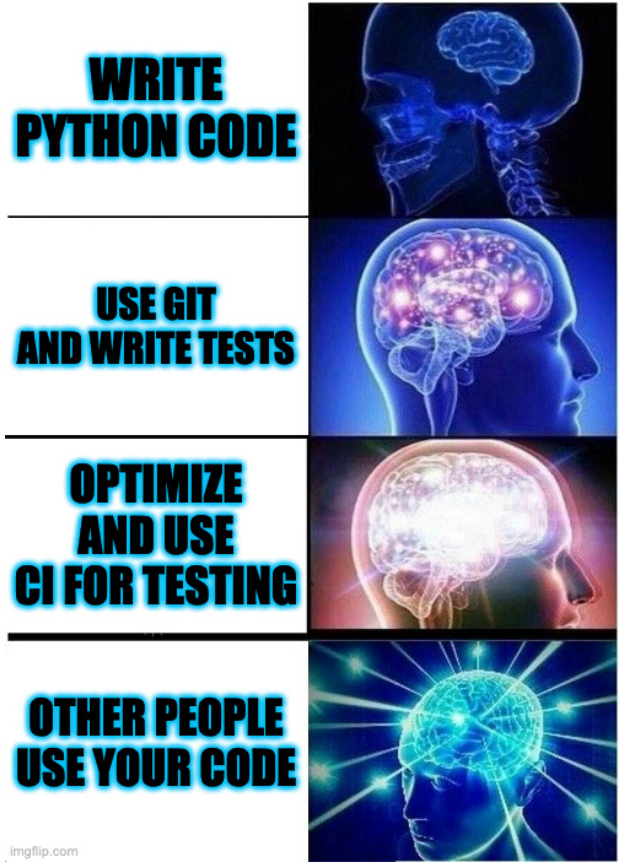
Circle back

- **Organising** helps **you** and **future you** (and **other people**)

- following a **package folder structure** makes it easy to find objects
- creating a package will standardise the **import** statements
- doing an **editable install** will enable you to use it as you would do any package (e.g. from any directory) -> as another person would
- **documenting** your code will let anyone read your code more easily
- Using **virtual environments** will isolate your projects from each other and increase your chances of having your code work properly

Mischief Managed

Any questions?


WRITE
PYTHON CODE
USE GIT
AND WRITE TESTS
OPTIMIZE
AND USE
CI FOR TESTING
OTHER PEOPLE
USE YOUR CODE
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X