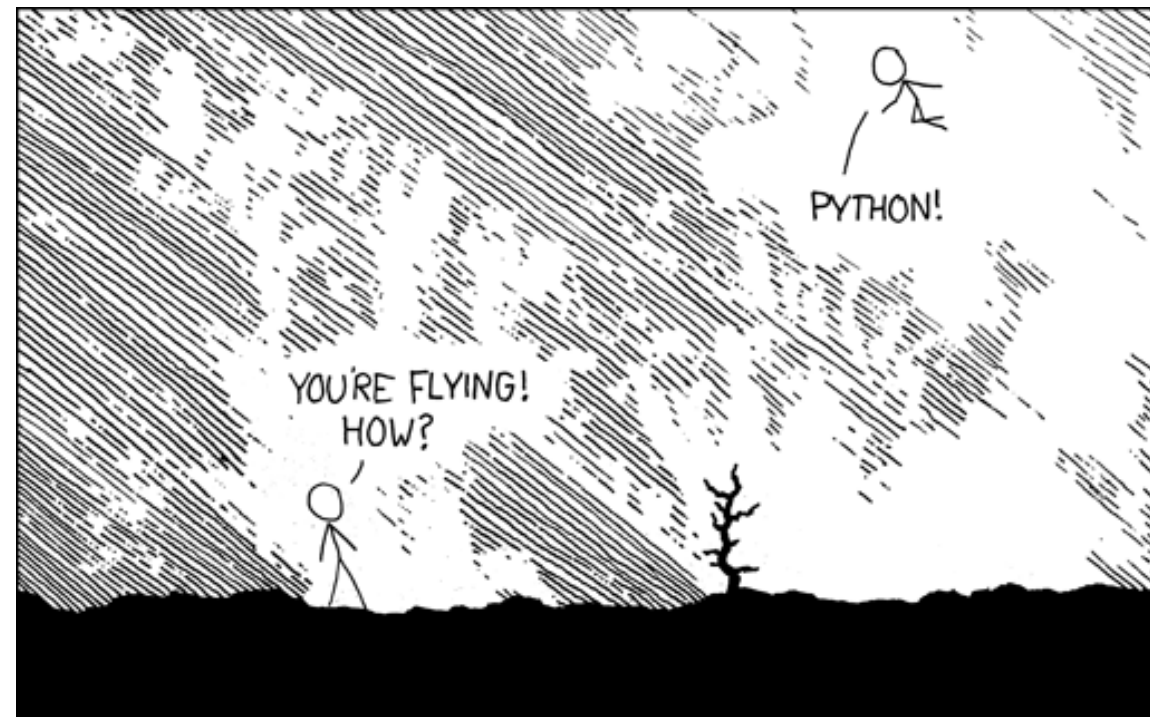


Getting Started running Python

Virtual environments, installing packages, and running code



<https://xkcd.com/353/>



Talley Lambert

 **CITE**
Core for Imaging Technology & Education

 **HARVARD**
MEDICAL SCHOOL



Goals for this Talk

Understand

- 1) What Python is
- 2) Where it "lives" on your computer and where it finds code to run
- 3) What packages are, and how they bring in additional functionality.
- 4) What virtual environments are, and how they help us isolate installed packages.

Know how to

- 1) Use **uv** to manage python, virtual environments, and packages; and use it to run code.

We will not be covering how to actually code in python here





This is an opinionated introduction.

There are many different ways to do this stuff.

I'll occasionally provide my personal preference/recommendation

If you already know and like a different approach,
this doesn't invalidate that :)





What is Python?

"Python is an interpreted, object-oriented, high-level programming language with dynamic semantics."





What is Python?

interpreted

Tl;dr:

With Python, you share and run "regular" text files.
Python does all the OS-specific magic at "runtime".



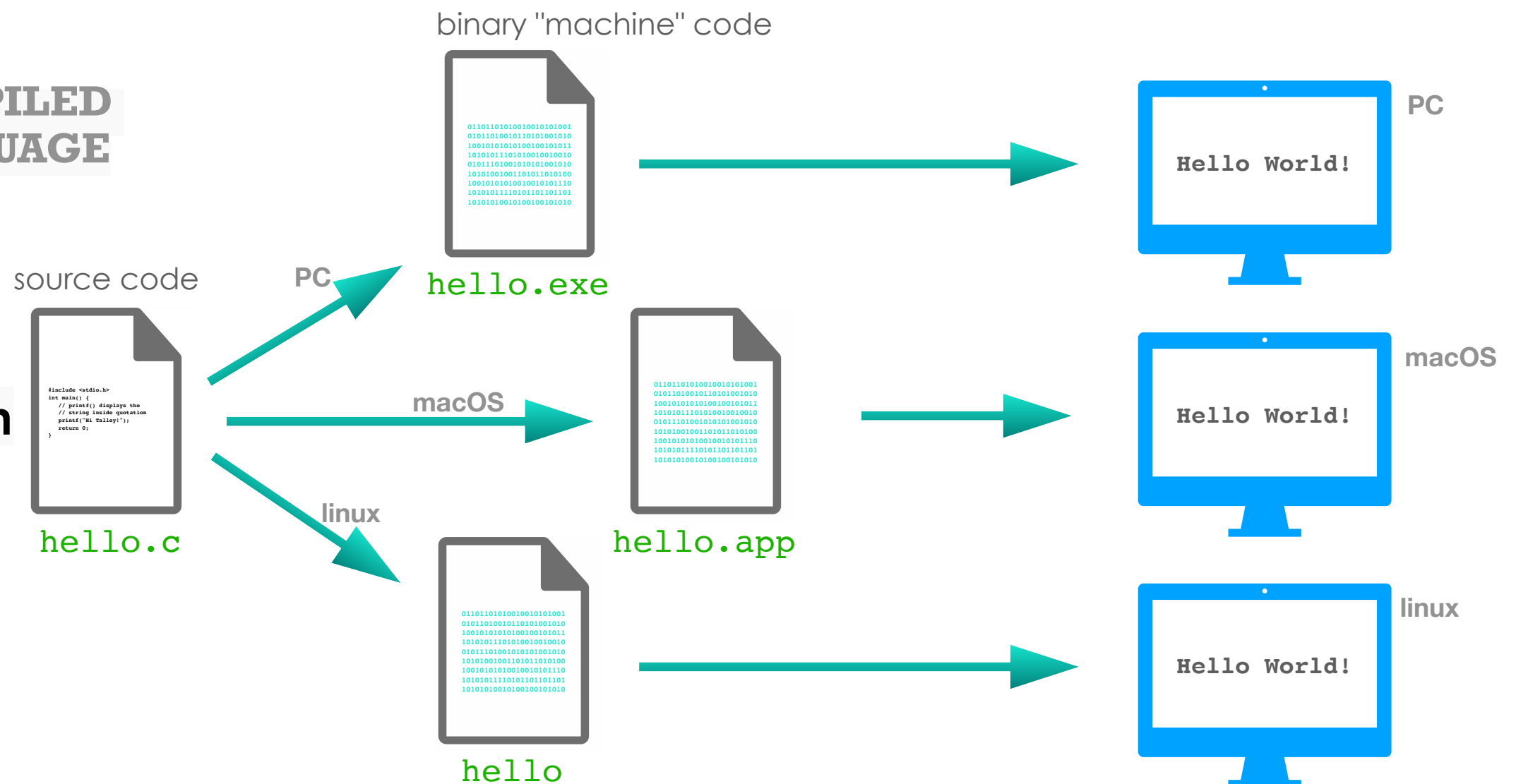


What is Python?

interpreted

COMPILED
LANGUAGE

NOT Python





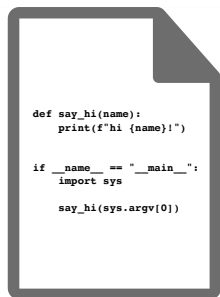
What is Python?

interpreted

INTERPRETED
LANGUAGE

Python

source code



hello.py

compiler



"bytecode"



hello.pyc

python
interpreter



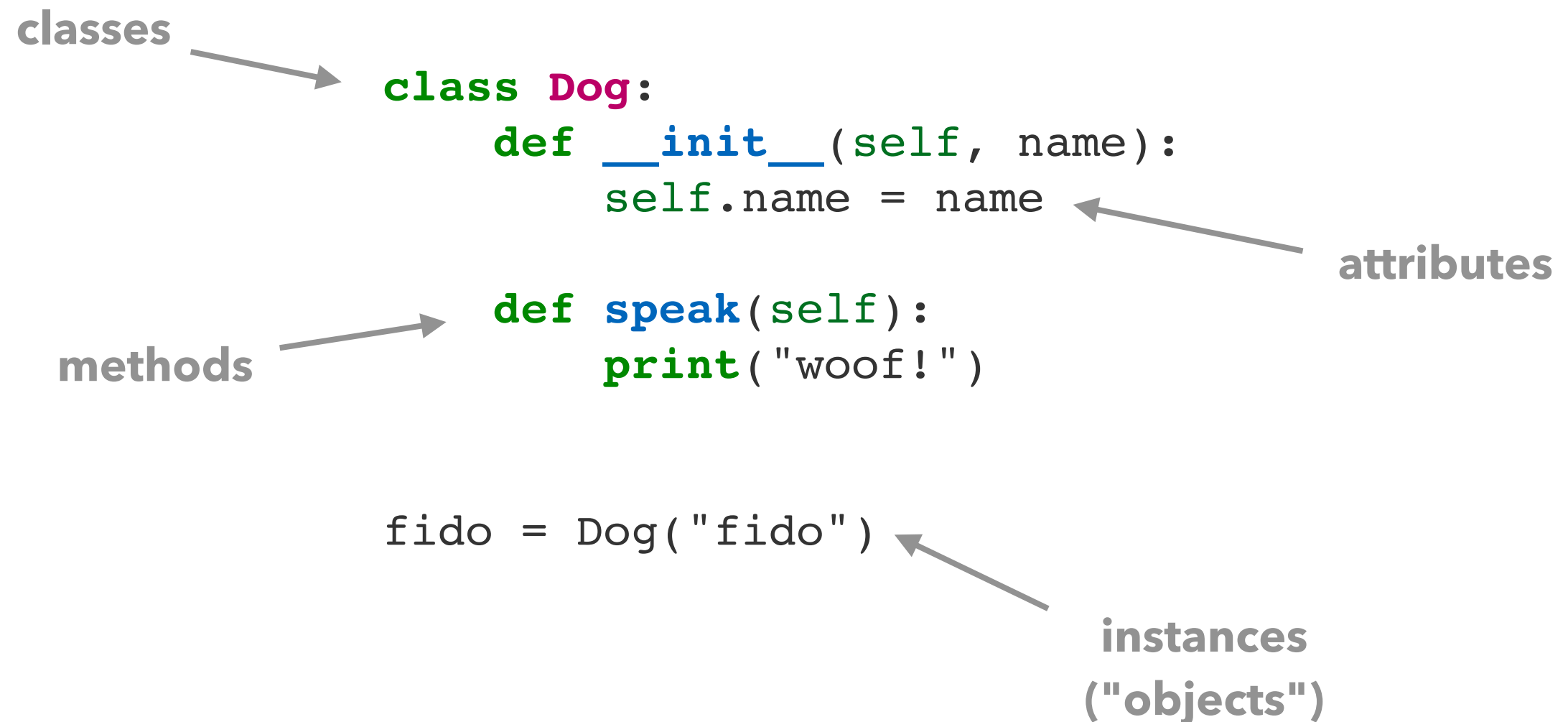
- 👍 Easy **cross-platform** development
- 👍 **Rapid** development
- 👎 Can be slower to execute than compiled languages
(but can be combined with compiled code if necessary)





What is Python?

object-oriented





What is Python?

high-level

"high-level" $\cong$

- easy to understand
- closer to human linguistics
- farther from machine code

👍 Memory management
(you don't have to literally allocate and deallocate memory)

👍 Dynamic typing

👍 Built-in data structures (list, dict, set, tuple, etc...)

<https://docs.python.org/3/tutorial/datastructures.html>





What is Python?

dynamic

```
# make x a string
# no type declaration required!
x = 'hi'

# change it to an integer
# no problem!
x = 2
```

Note: if you *want* types, there are options as well:

<https://docs.python.org/3/library/typing.html>





Strengths

why do scientists use it?

- ✓ Easy to learn, read, and write
- ✓ "Batteries included" (standard library has lots of functionality)
- ✓ Huge community of packages, particularly in data science
- ✓ Rapid development (fast edit-test-debug cycle)
- ✓ Totally free & open-source!
- ✓ "Glue-language" (easy to integrate lower level languages)





Weaknesses

Faster to develop, but can be slower to execute compared to compiled languages

(But... see C-extensions, cython.org, & numba.org, etc...)

Decreased memory efficiency

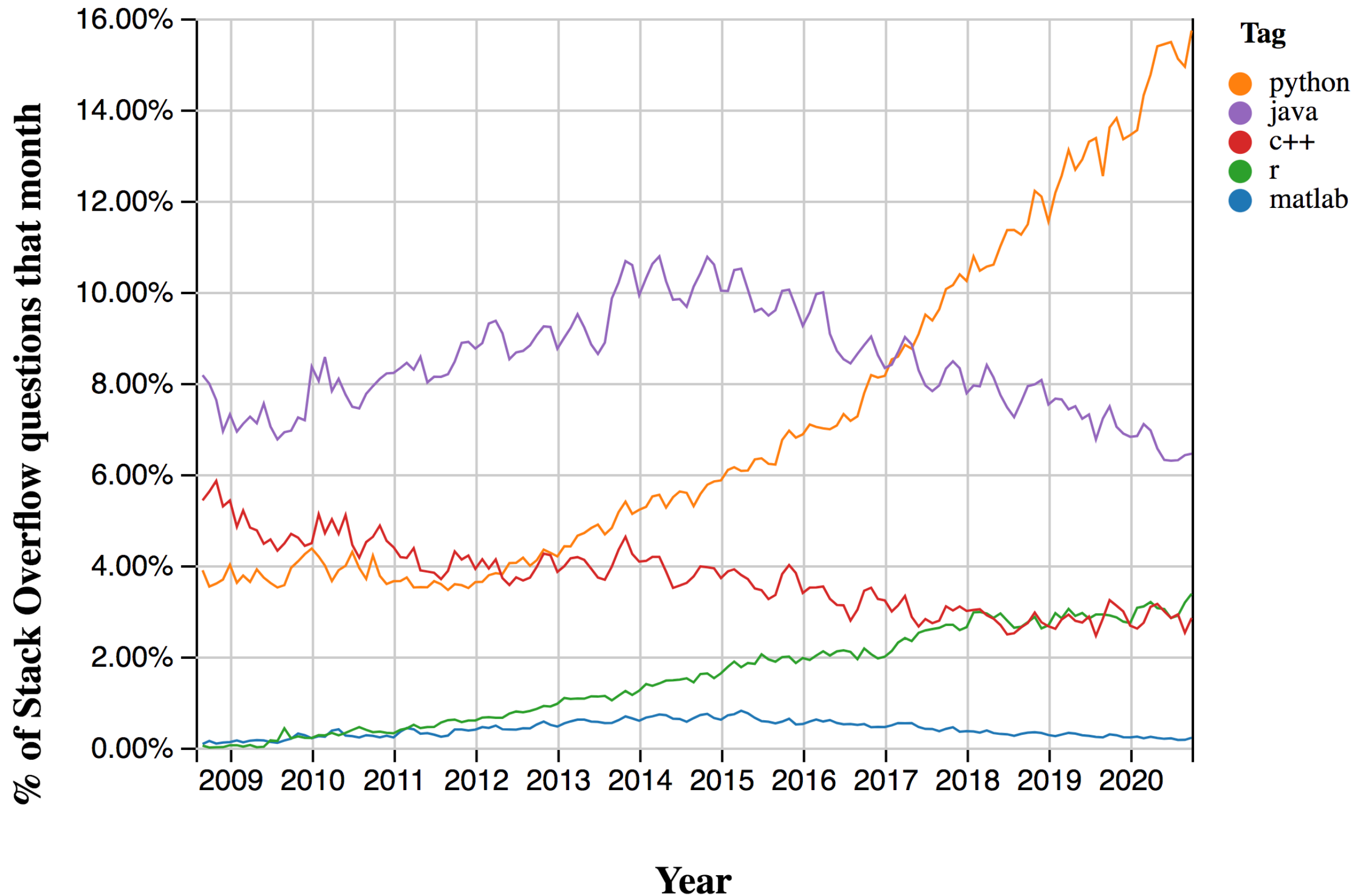
Parallelism & concurrency requires some workarounds

(But: many solutions exist... see dask.org)





So hot right now...





Terms

python interpreter

The **program** that actually "runs" (i.e. parses, compiles, interprets) python code. (ex: "CPython 3.8")

module

An organizational unit of python code. Usually a **single file** ending in `.py` that contains python definitions and expressions,

package

A collection of modules. Usually, this is a **folder** of python modules that also contains an `__init__.py` file. "Package" also frequently refers to an installable python library/application (e.g. numpy, matplotlib, pandas...)

package manager

A **program** that automates the installation, updating and removal of packages (e.g. pip, conda)

virtual environment

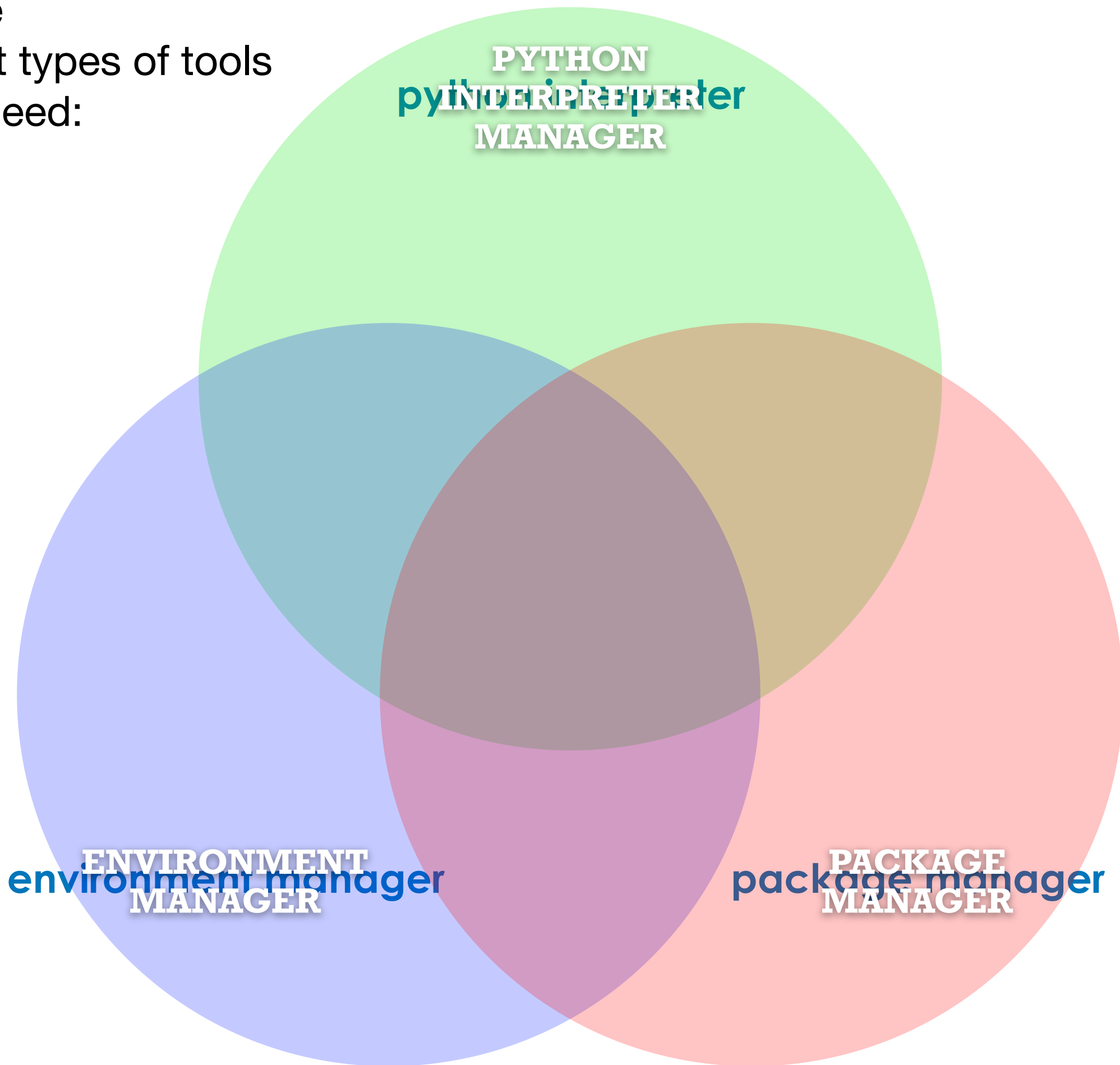
An **isolated collection** of packages, settings, and an associated python interpreter, that allows multiple different collections to exist on the same system

environment manager

A **program** that automates the creation and deletion of virtual environments (e.g. conda, virtualenv, venv)

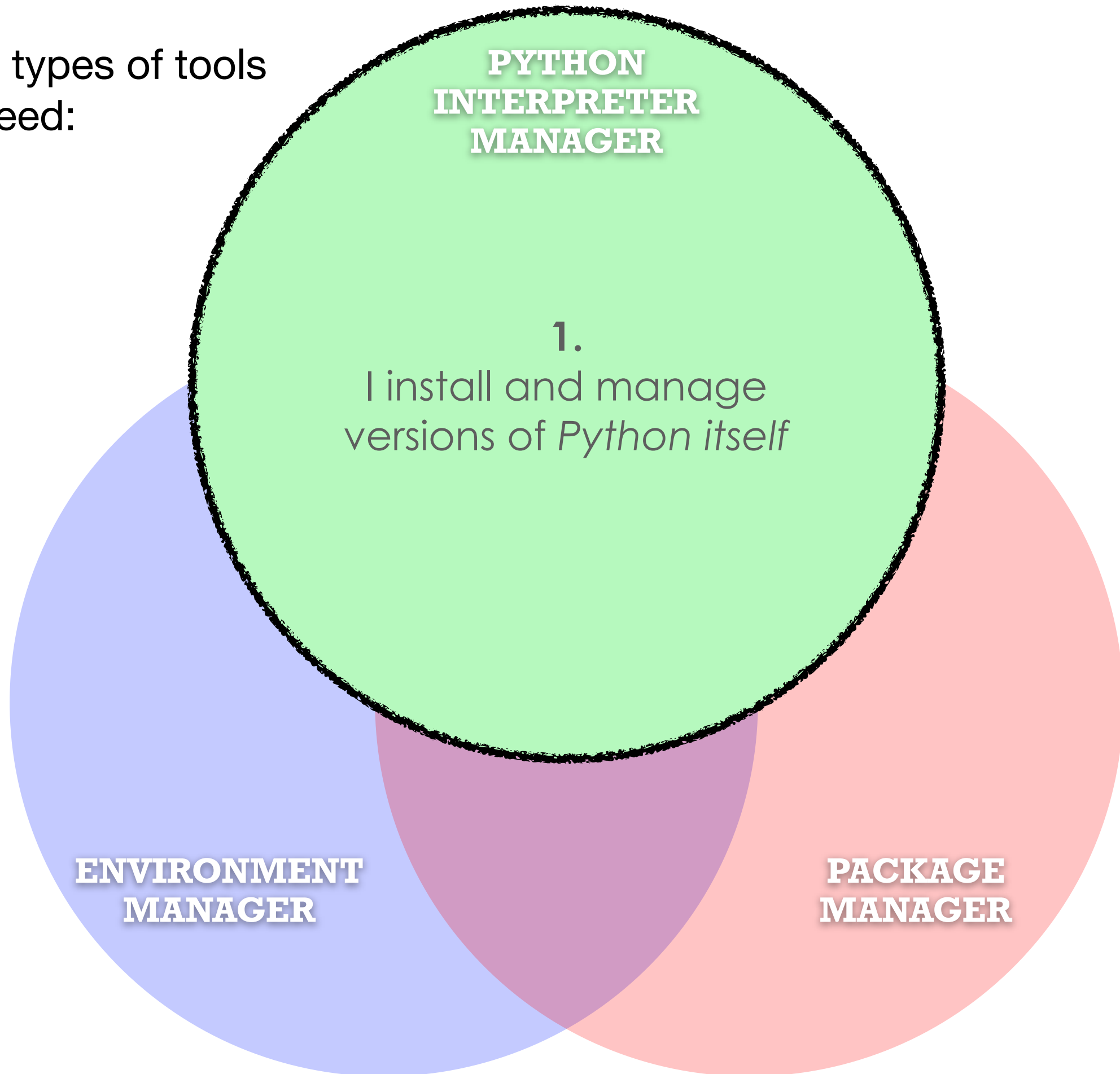


The three
important types of tools
you will need:



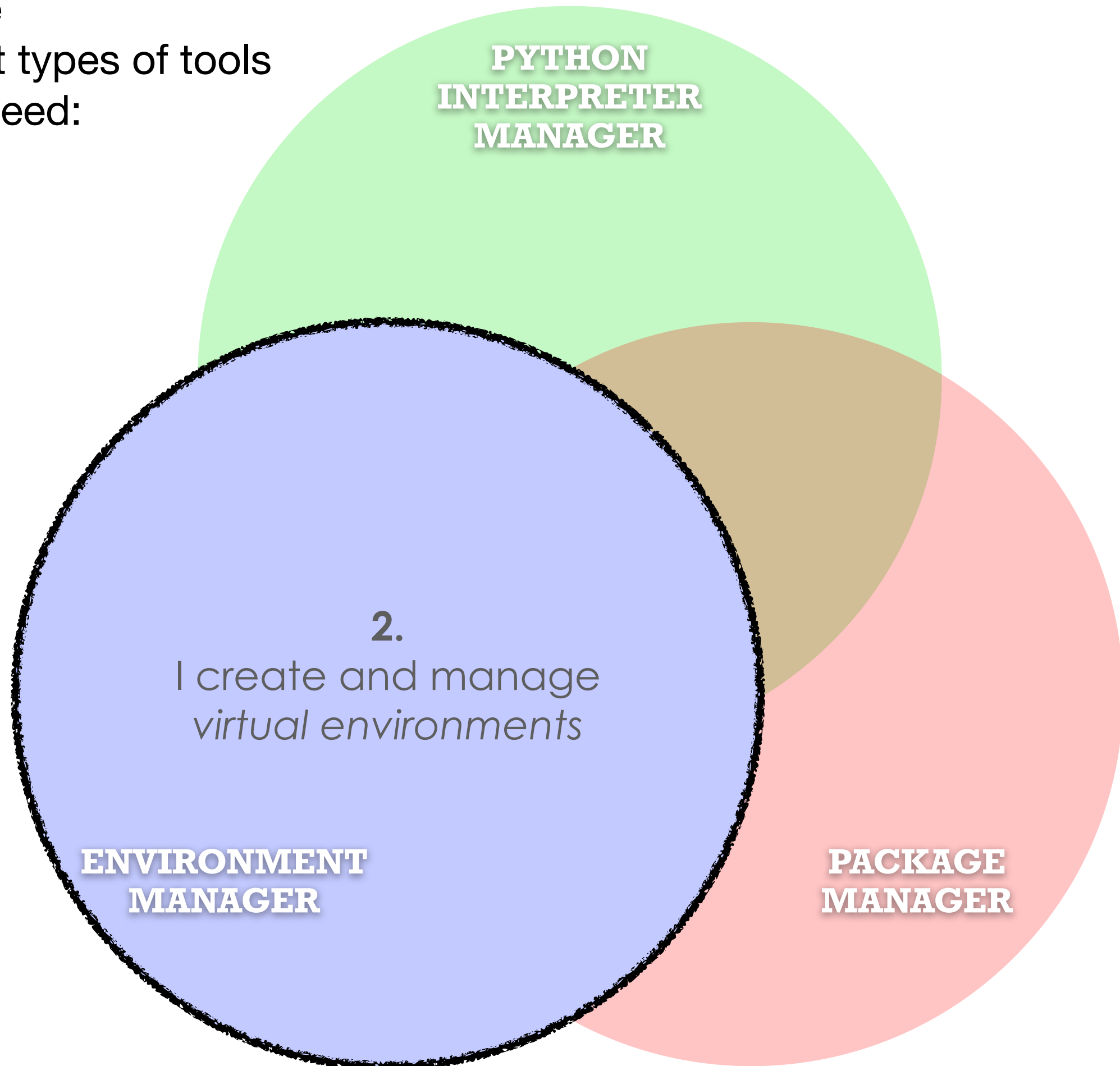


The three
important types of tools
you will need:



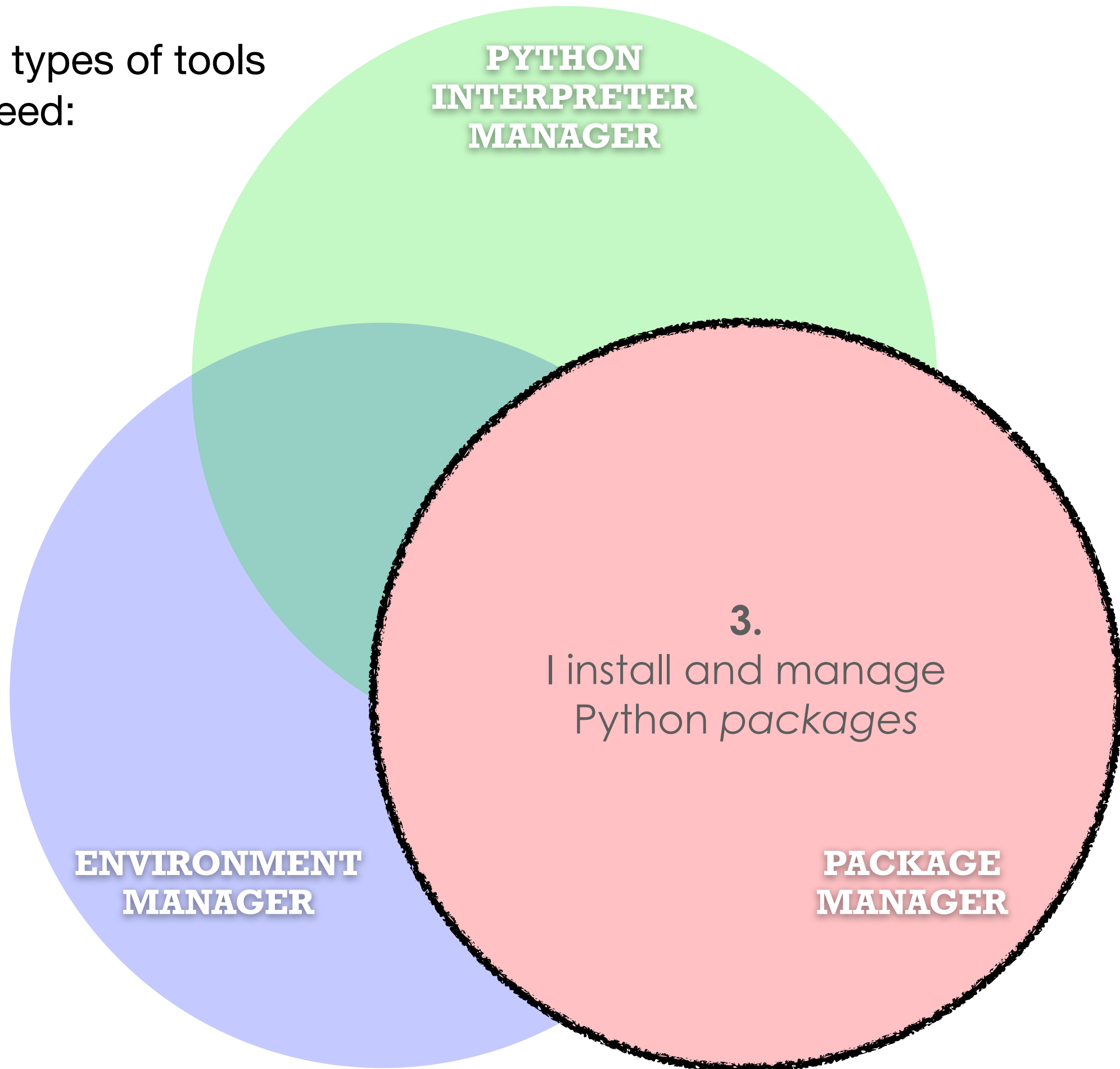


The three
important types of tools
you will need:





The three
important types of tools
you will need:





What does it mean to run code in python?

Executing a script/program/file

```
# ~/Desktop/hi.py  
print("hello world!")
```

```
$ python ~/Desktop/hi.py  
hello world!
```

Using an interactive console or notebook

```
$ python  
Python 3.13.5 (main, Jul 8 2025,  
20:55:53) [Clang 20.1.4] on darwin  
  
>>> print("hello world!")  
hello world!
```





Python is modular

One Python module (file) can **import** functionality from another module (file)

```
# ~/Desktop/do_math.py  
  
from numpy import add  
  
print(add(1, 2))
```

```
$ python ~/Desktop/do_math.py  
3
```

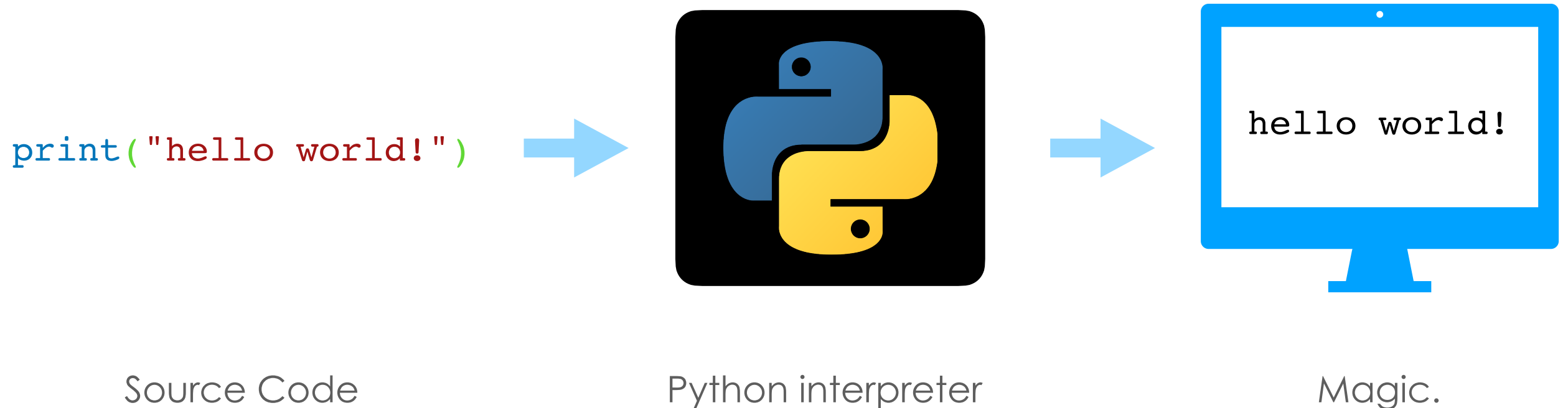




What is the Python interpreter?

```
$ python
```

The **Python interpreter** is a program that parses and compiles source code (human readable code) into "bytecode" (a lower level representation) that is then "interpreted" (executed) by the python "virtual machine"





What is the Python interpreter?

```
$ python
```

The **Python interpreter** is a program that parses and compiles source code (human readable code) into "bytecode" (a lower level representation) that is then "interpreted" (executed) by the python "virtual machine"

Where does it live?

(It can live almost anywhere)

```
$ which python
python not found
```

```
python is /usr/bin/python # mac ≤ Catalina 10.15
```

```
$ python --version
Python 2.7.16
```



Python 3 has been out since 2008

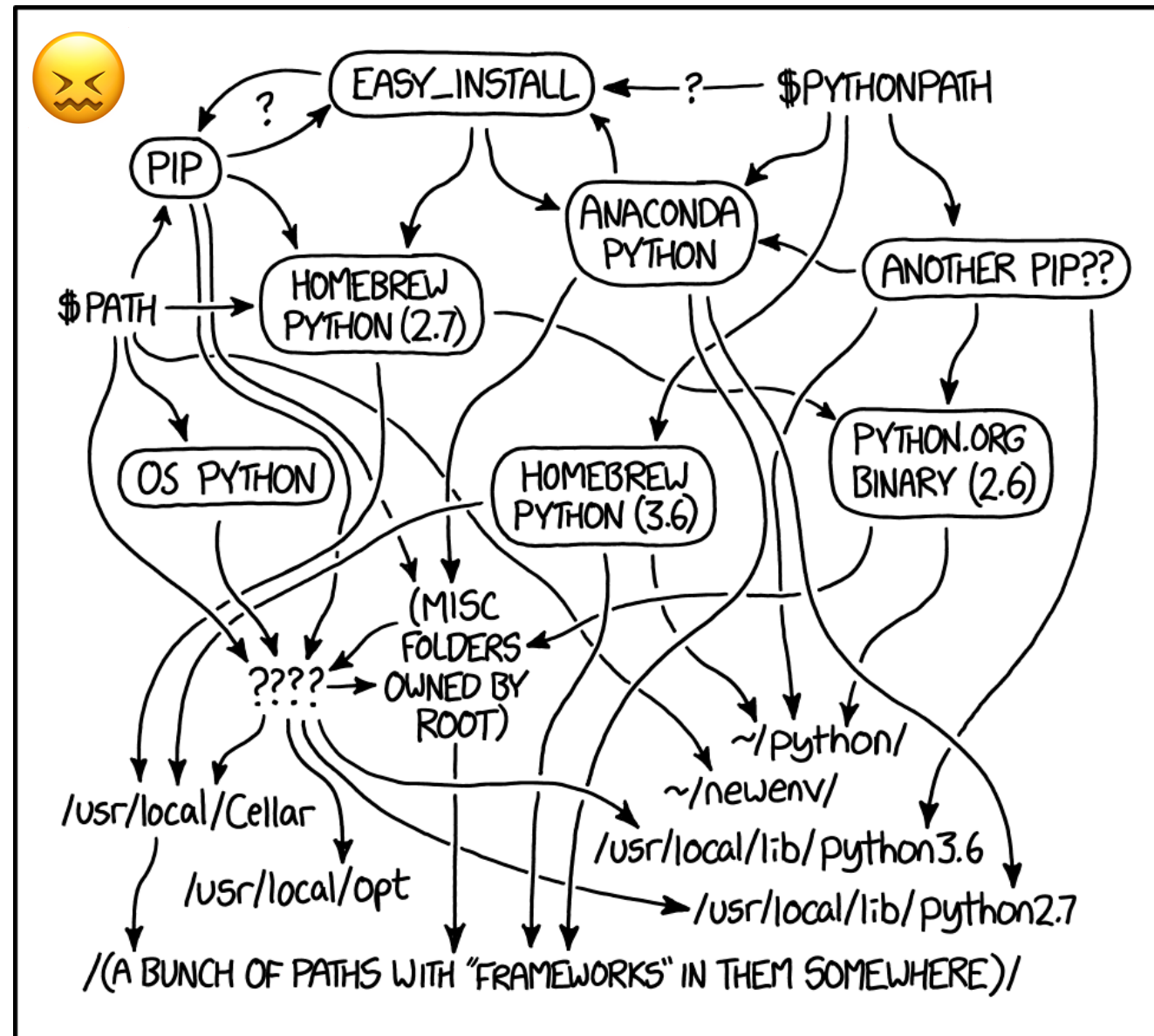
Python 2 is end-of-life as of Jan. 2020

For this and many other reasons... don't use your system python (if you have one)!





OK, then how should I get Python?

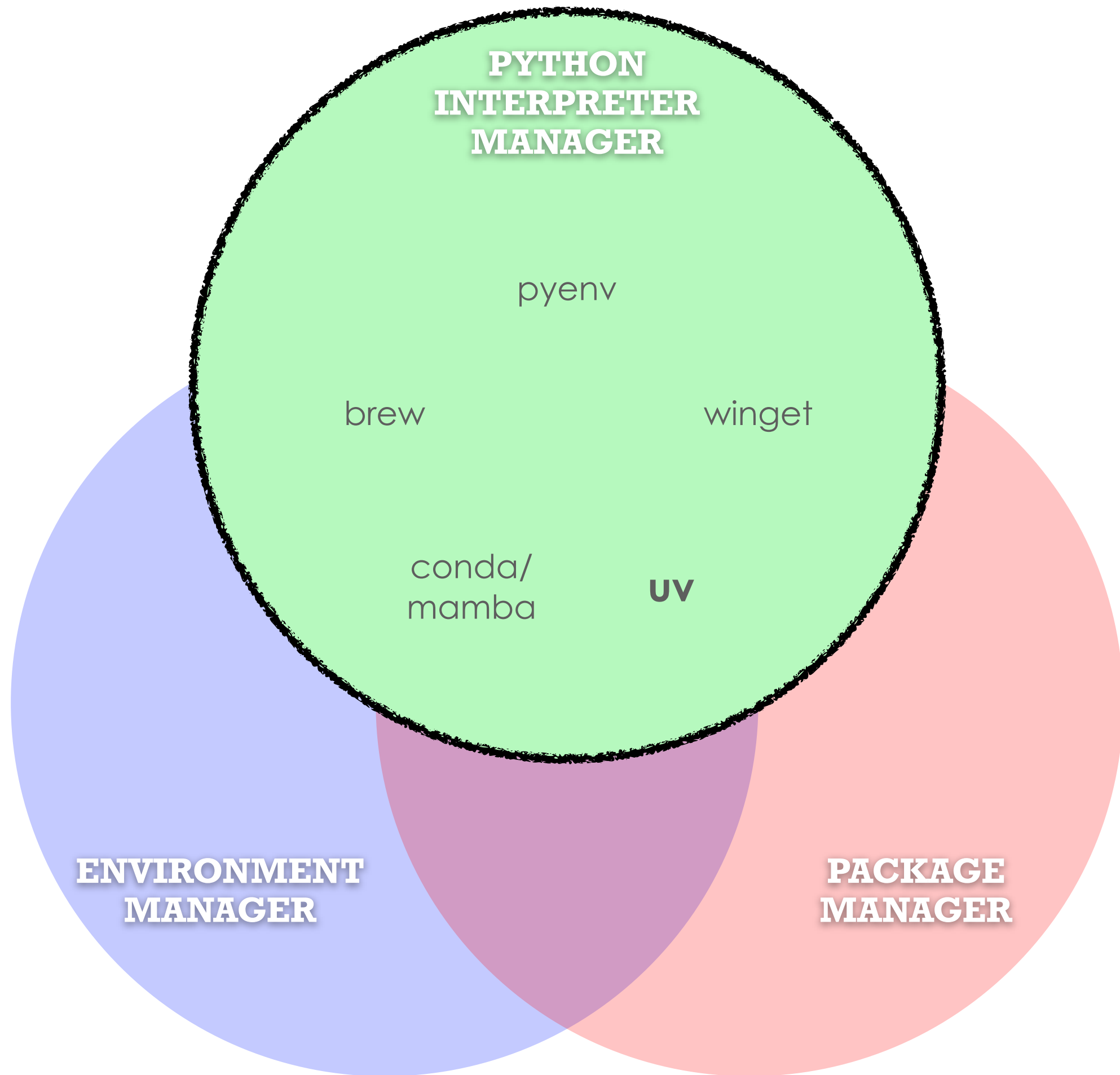


MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED
THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

tl;dr: install uv

<https://docs.astral.sh/uv/getting-started/installation/>







Installing uv



Instructions at <https://docs.astral.sh/uv/getting-started/installation/>

```
curl -LsSf https://astral.sh/uv/install.sh | sh
```

```
powershell -ExecutionPolicy Bypass -c "irm https://astral.sh/uv/install.ps1 | iex"
```





Installing uv



Instructions at <https://docs.astral.sh/uv/getting-started/installation/>

```
~/Desktop/project  
→ curl -LsSf https://astral.sh/uv/install.sh | sh
```





Running Python with uv

```
uv run [COMMAND]
```

Ensures that the command or script is run in a Python "environment"
(more on that in a moment).

Will download Python for you if needed.

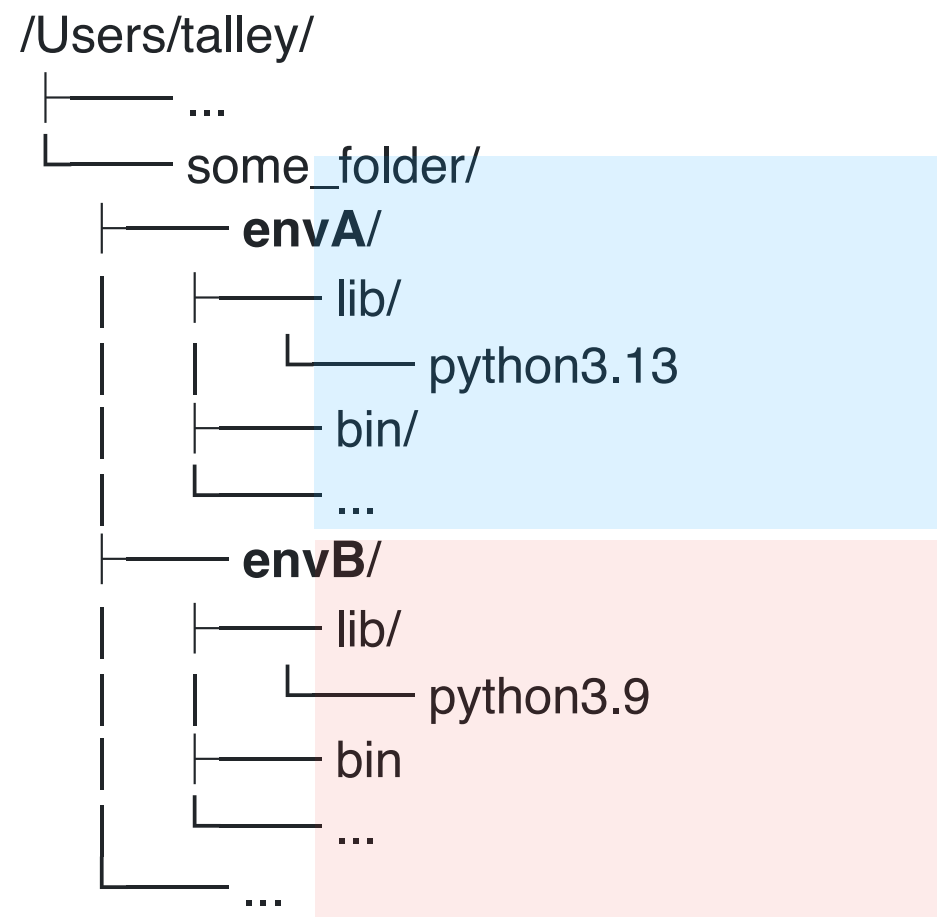




What is a python virtual environment?

An isolated collection of **packages**, **settings**, and a **python interpreter**,
... that allows multiple different collections to exist on the same system

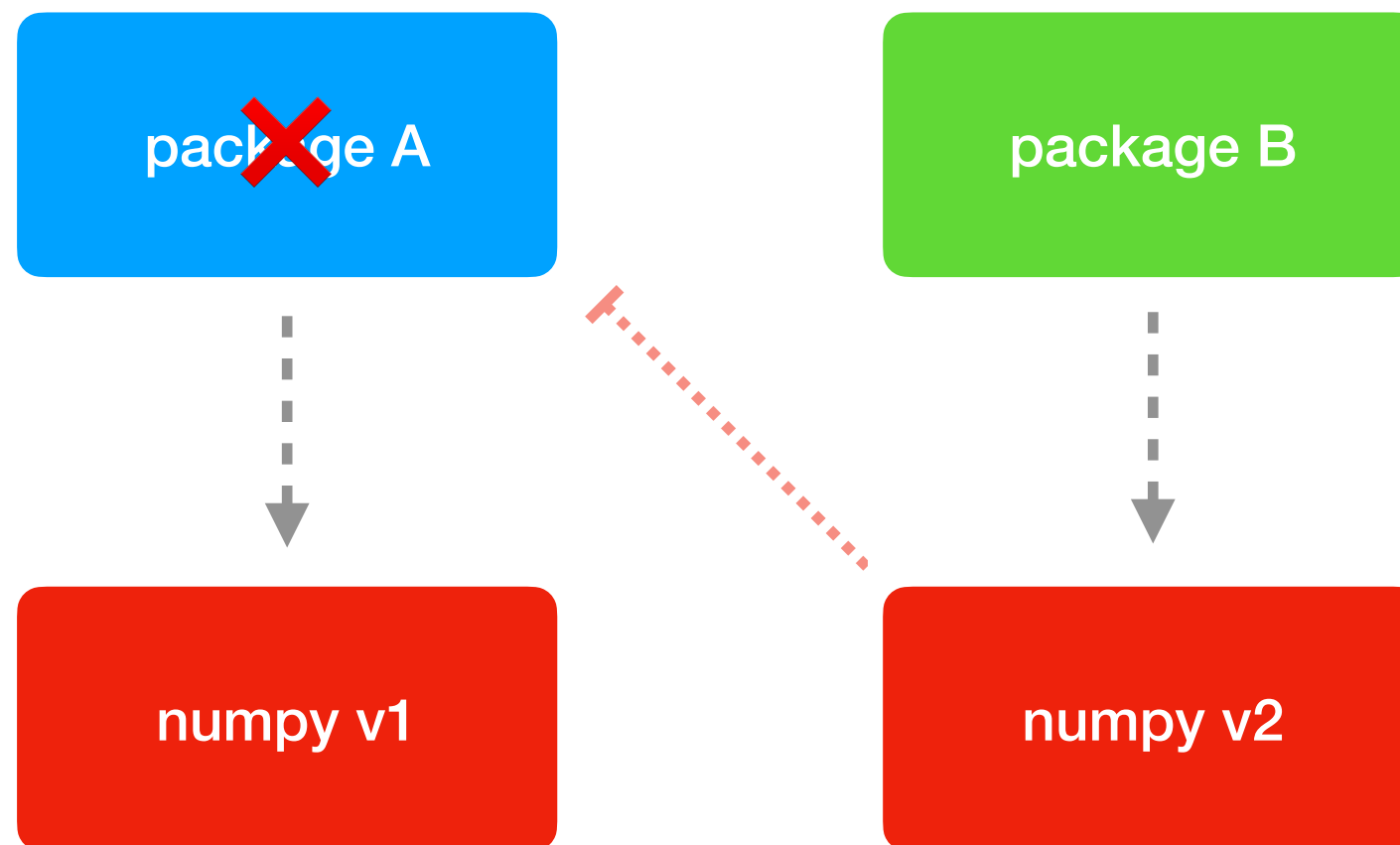
... (It's usually a literal folder somewhere on your computer...)





Why would I need more than 1 environment?

Problem 1: conflicting package dependencies



Tip! you can only have one version of any given package installed in an environment



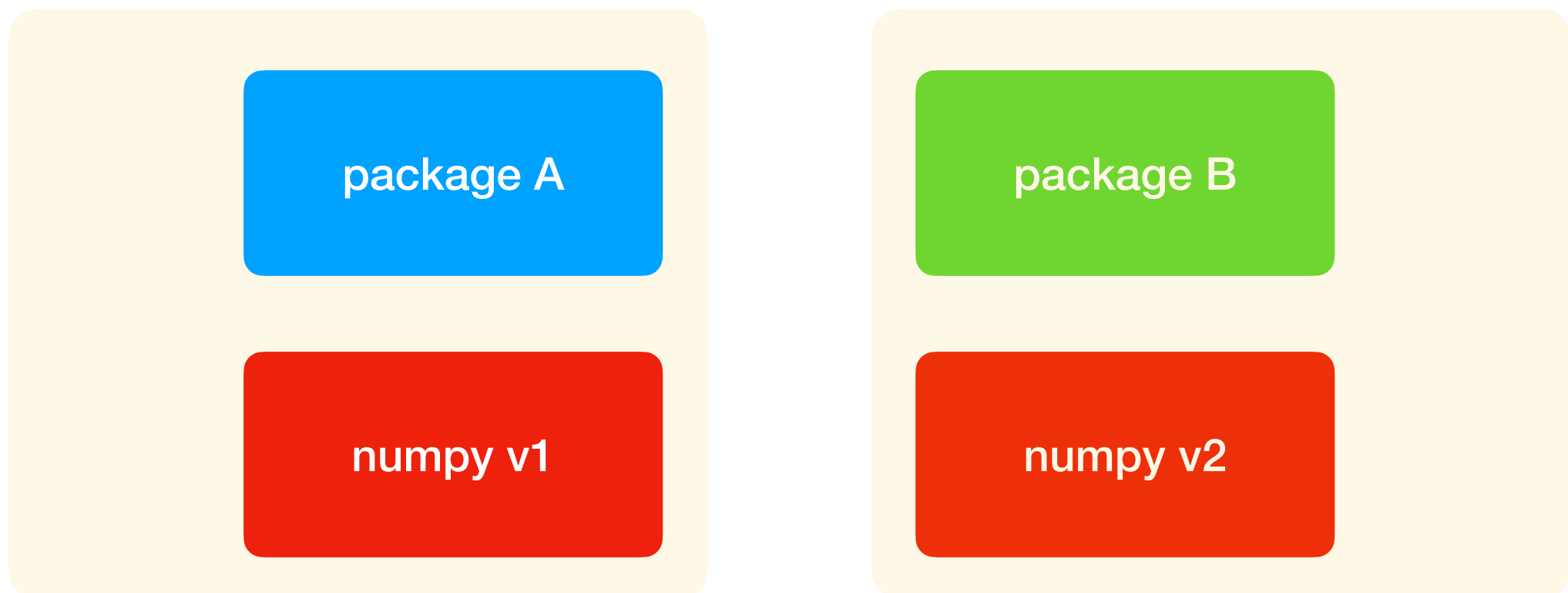


Why would I need more than 1 environment?

Solution:

Create **multiple** "virtual" environments

each one contains all of the dependencies and requirements for a particular application





Why would I need more than 1 environment?

Problem 2: "It worked fine on *my* computer!" 🤔

Using environments also keeps your "globally" installed packages to a minimum, and makes your project dependencies much clearer





Why would I need more than 1 environment?

Try to avoid having one big "base" environment
where you install everything!

Think of environments as disposable!

Don't get "attached" to an environment...
Learn to recreate them quickly





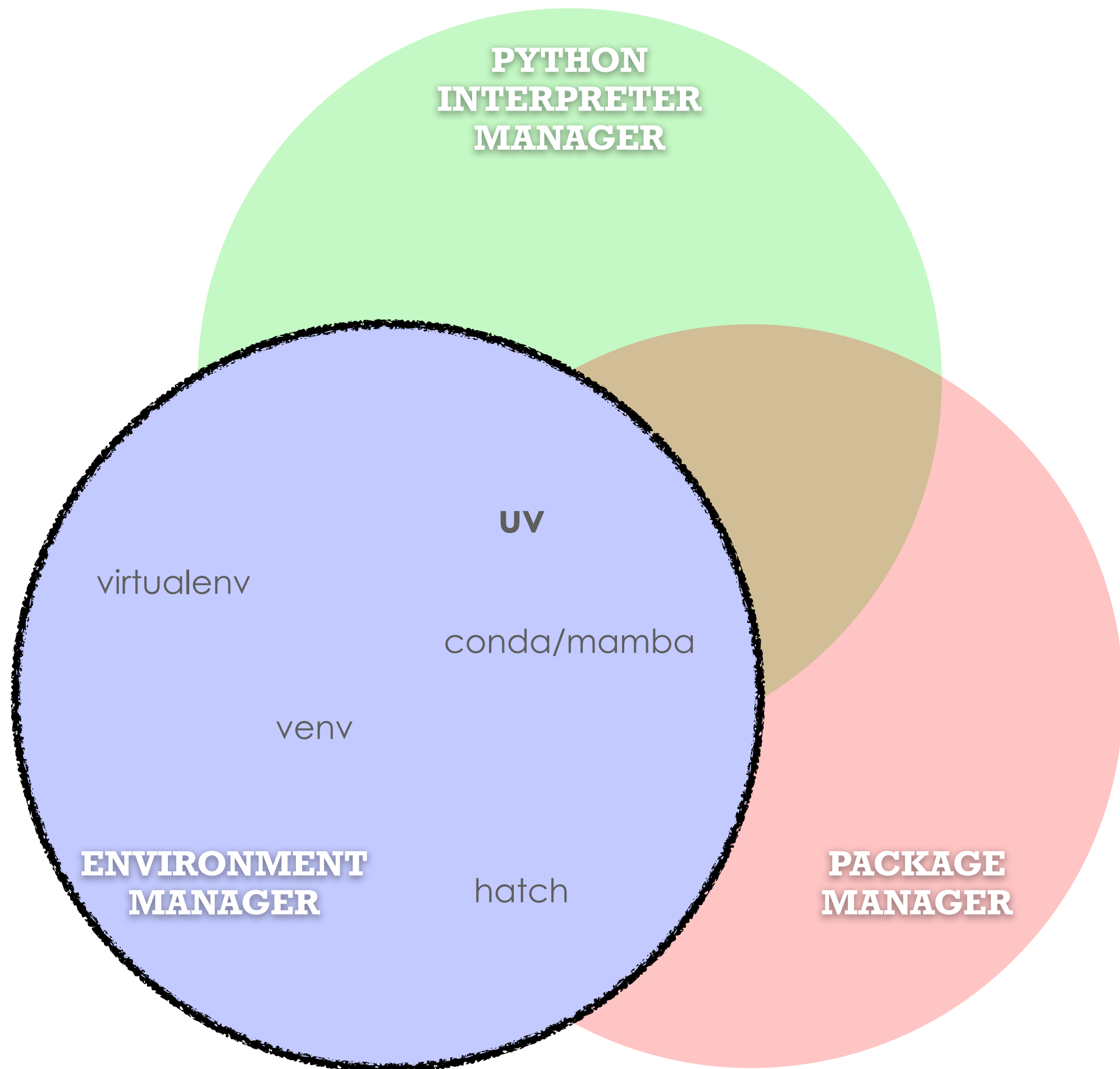
How do I create a virtual environment?

You need... **an environment manager**

Examples:

- venv
- virtualenv
- conda/mamba
- pipenv
- poetry
- uv







How do I create a virtual environment?

```
uv venv [ENV_NAME]
```

(defaults to ".venv")

```
~/Desktop/project
```

```
→
```

```
I
```





How do I create a virtual environment?

```
uv venv [ENV_NAME]
```

(defaults to ".venv")

TIP: Specify Python version with `--python/-p`

```
uv venv -p 3.10
```

```
uv venv -p 3.13
```





You need to "activate" it first...

```
source .venv/bin/activate
```

```
.venv\Scripts\activate
```

This sets up your terminal environment to know where to find things...





Now that we've got an environment set up...

let's install some packages!





"Packages" bring in additional functionality

Packages may sometimes be referred to as "libraries"

super awesome
"scientific python ecosystem"



Just think of each of these
as a **folder** of **.py** files





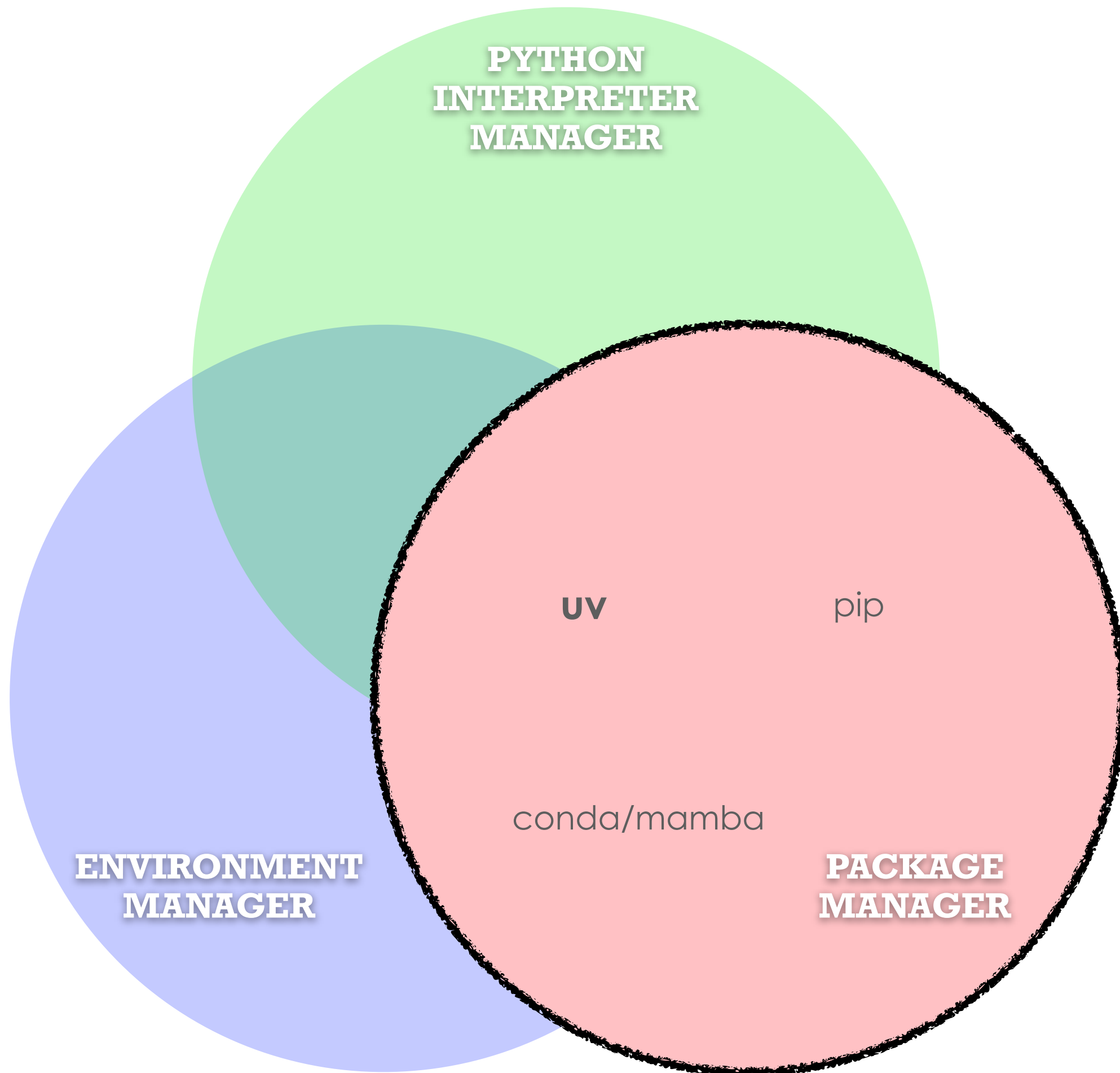
How do I get Python packages?

You need... **a package manager**

Examples:

- pip
- conda/mamba
- uv pip







How do I get Python packages?

```
uv pip install <package>
```

```
~/Desktop/project via my_env  
→ uv pip install 'cellpose[gui]'
```





Tip: show installed packages with

`uv pip list`

```
→ uv pip list
Package                Version
-----
cellpose                4.0.6
fastremap               1.17.1
filelock                3.18.0
fill-voids              2.1.0
fsspec                  2025.5.1
imagecodecs              2025.3.30
jinja2                  3.1.6
markupsafe               3.0.2
mpmath                   1.3.0
natsort                  8.4.0
networkx                 3.5
numpy                    2.3.1
opencv-python-headless  4.11.0.86
pillow                   11.3.0
roifile                  2025.5.10
scipy                    1.16.0
segment-anything         1.0
setuptools               80.9.0
sympy                    1.14.0
tifffile                 2025.6.11
torch                    2.7.1
torchvision              0.22.1
tqdm                     4.67.1
typing-extensions        4.14.1
```





Where did it install?? How does Python find code?

```
import os
import sys

import matplotlib
import numpy as np

import my_module
```

From where??





How does Python find code?

`sys`

is a module
in the "standard library"

`sys.path`

`path`

is a variable
in the `sys` module

```
>>> import sys

>>> print(sys.path)
# on mac/linux
[
  '.../.venv/lib/python3.X',
  '.../.venv/lib/python3.X/lib-dynload',
  '',
  '.../.venv/lib/python3.X/site-packages',
]
```





How does Python find code?

`sys.path`

```
>>> import sys
```

```
>>> print(sys.path)
```

```
# on mac/linux
```

```
[  
    '.../.venv/lib/python3.X',  
    '.../.venv/lib/python3.X/lib-dynload',  
    '',  
    '.../.venv/lib/python3.X/site-packages',  
]
```

```
>>> import sys
```

```
>>> print(sys.path)
```

```
# on Windows:
```

```
[  
    '...\.venv\Lib',  
    '...\.venv\DLLs',  
    '',  
    '...\.venv\Lib\site-packages',  
]
```

For more:

<https://docs.python.org/3/library/sys.html#sys.path>

<https://leemendelowitz.github.io/blog/how-does-python-find-packages.html>





How does Python find code?

"standard library" modules

```
import os
import sys
```

mac/linux:

<env>/lib/pythonX.Y

windows:

<env>\Lib

installed third-party packages

```
import matplotlib
import numpy as np
```

mac/linux:

<env>/lib/pythonX.Y/site-packages

windows:

<env>\Lib\site-packages

your own local stuff...

```
import my_module
```

"" # meaning "current directory"

sys.path

```
[
    './.venv/lib/python3.X',
    './.venv/lib/python3.X/lib-dynload',
    '',
    './.venv/lib/python3.X/site-packages',
]
```

+ anything else you add to
sys.path!

That's where pip installs!

```
# tip; find the file:
import numpy
print(numpy.__file__)
```

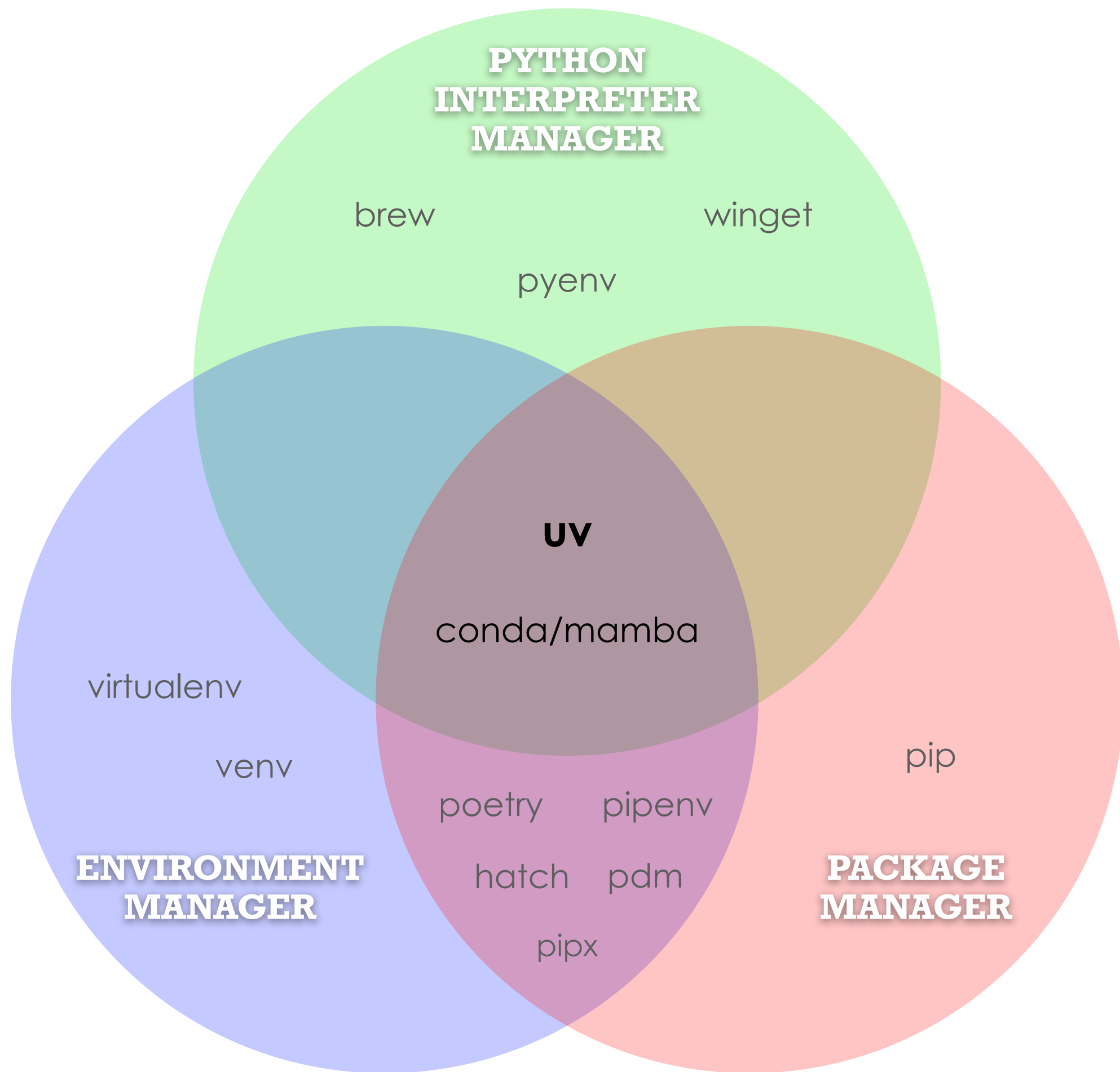


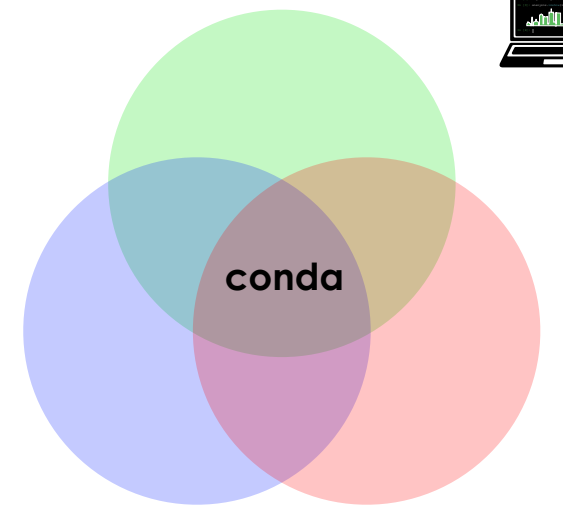


Now you know...

- ☒ What **Python** is
- ☒ Where it "lives" on your computer and **where it finds code** to run
- ☒ What **virtual environments** are, and how they help us isolate installed packages.
- ☒ What **packages** are, and how they bring in additional functionality.







<https://github.com/conda/conda>

Conda is an open-source, cross-platform, language-agnostic
package management system
and **environment management** system

There are many "flavors" ... I recommend using **micromamba**:

<https://mamba.readthedocs.io/en/latest/installation/micromamba-installation.html>

For our purposes ... the most important difference between
uv and **conda** will be where they download packages from





uv pip vs. conda



<https://pypi.org>

`pip/uv pip`
installs **Python** packages
from **PyPI**
into **any environment**



<https://anaconda.org/>

`conda`
installs **any kind of** package
from **Anaconda**
into a **conda environment**





uv pip vs. conda

There *may* be cases where you *must* install a package via conda,
e.g. for certain performance GPU computing tasks

... otherwise, stick with `uv venv` and `uv pip`





(Re)creating environments with dependency files

pip / uv-pip

requirements.txt

```
numpy>=1.14.1
scipy>=1.0.1
matplotlib>=2.0.0,!3.0.0
networkx>=2.0
pillow>=4.3.0
imageio>=2.3.0
```

Create env and install

```
uv venv
```

```
uv pip install -r requirements.txt
```

https://pip.pypa.io/en/stable/user_guide/#requirements-files

conda

environment.yml

```
name: myenv
channels:
  - conda-forge
  - defaults
dependencies:
  - python=3.7
  - pip
  - numpy>=1.14.1
  - scipy
  - pip:
    - tifffile
```

Create env and install

```
conda env create -f environment.yml
```

<https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html>





Listing dependencies within a script

my_file.py

```
# /// script
# requires-python = ">=3.13"
# dependencies = [
#     "numpy",
# ]
# ///

from numpy import add

print(add(1, 2))
```

This is a great (newer) convention in the Python world.

It is supported by uv.

```
uv run my_file.py
```





One more cool trick...

Run a command provided by *any* Python package

`uvx [COMMAND]`

- Creates a Python environment
- Installs package with the same name as `[COMMAND]`
- Runs that `[COMMAND]`
- If the package and command don't have the same name:

`uvx --from [PACKAGE] [COMMAND]`

```
→ uvx cowsay -t 'hello world!'

-----
| hello world! |
=====
      \
       ^ ^
      (oo)\_____)
      (__)\/       )\/\
           ||----w |
           ||     ||
```





IP[y]: IPython

Interactive Computing

<https://ipython.readthedocs.io>

- Souped up interactive console (use `ipython` instead of `python`)
- Tab autocompletion

```
In [1]: import math
```

```
In [2]: math.| <press tab>
```

<code>acos()</code>	<code>cos()</code>	<code>factorial()</code>	<code>isfinite()</code>	<code>modf()</code>	<code>sqrt()</code>
<code>acosh()</code>	<code>cosh()</code>	<code>floor()</code>	<code>isinf()</code>	<code>nan</code>	<code>tan()</code>
<code>asin()</code>	<code>degrees()</code>	<code>fmod()</code>	<code>isnan()</code>	<code>perm()</code>	<code>tanh()</code>
<code>asinh()</code>	<code>dist()</code>	<code>frexp()</code>	<code>isqrt()</code>	<code>pi</code>	<code>tau</code>
<code>atan()</code>	<code>e</code>	<code>fsum()</code>	<code>ldexp()</code>	<code>pow()</code>	<code>trunc()</code>
<code>atan2()</code>	<code>erf()</code>	<code>gamma()</code>	<code>lgamma()</code>	<code>prod()</code>	
<code>atanh()</code>	<code>erfc()</code>	<code>gcd()</code>	<code>log()</code>	<code>radians()</code>	
<code>ceil()</code>	<code>exp()</code>	<code>hypot()</code>	<code>log10()</code>	<code>remainder()</code>	
<code>comb()</code>	<code>expm1()</code>	<code>inf</code>	<code>log1p()</code>	<code>sin()</code>	
<code>copysign()</code>	<code>fabs()</code>	<code>isclose()</code>	<code>log2()</code>	<code>sinh()</code>	





IP[y]: IPython

Interactive Computing

<https://ipython.readthedocs.io>

- Souped up interactive console (use `ipython` instead of `python`)
- Tab autocompletion
- Easy help/documentation (`?` and `??`)

```
In [5]: math.isclose?
```

```
Signature: math.isclose(a, b, *, rel_tol=1e-09, abs_tol=0.0)
```

```
Docstring:
```

```
Determine whether two floating point numbers are close in value.
```

```
    rel_tol
```

```
        maximum difference for being considered "close", relative to the  
        magnitude of the input values
```

```
    abs_tol
```

```
        maximum difference for being considered "close", regardless of the  
        magnitude of the input values
```

```
Return True if a is close in value to b, and False otherwise.
```

```
For the values to be considered close, the difference between them  
must be smaller than at least one of the tolerances.
```





IP[y]: IPython

Interactive Computing

<https://ipython.readthedocs.io>

- Souped up interactive console (use `ipython` instead of `python`)
- Tab autocompletion
- Easy help/documentation (`?` and `??`)
- "magics" (e.g. `%run`, `%debug`, ...)

<https://ipython.readthedocs.io/en/stable/interactive/magics.html>

```
In [1]: %run some_script.py
```

... then resume interactive usage with all of the variables from `some_script.py` available





IP[y]: IPython

Interactive Computing

<https://ipython.readthedocs.io>

- Souped up interactive console (use `ipython` instead of `python`)
- Tab autocompletion
- Easy help/documentation (`?` and `??`)
- "magics" (e.g. `%run`, `%debug`, ...)
<https://ipython.readthedocs.io/en/stable/interactive/magics.html>
- Command history (press up/down to navigate previous commands)





<https://jupyter.org/>

JupyterLab

<https://jupyterlab.readthedocs.io/>

Jupyter Notebooks offer inline figures and integrated (markdown) documentation. ... right next to your interactive code.

It's a nice format for exploration, communication & teaching.

The screenshot displays the JupyterLab interface with several open notebooks and a file browser on the left. The file browser shows a directory structure with files like 'Altair.ipynb', 'Data.ipynb', 'Fasta.ipynb', 'Julia.ipynb', 'Lorenz.ipynb', and 'R.ipynb'. The main workspace contains several notebooks:

- In Depth: Linear Regression**: A notebook with text and code. The code includes a plot of 'Maximum Daily Temperature (C)' vs 'Date' for Seattle weather from 2012-2015, and a bar chart showing the number of records for different weather types (drizzle, fog, rain, snow, sun).
- Simple**: A notebook with a 'Slide Type' dropdown and 'Raw NBConvert Format' dropdown. It also has a 'Cell Metadata' section and 'Notebook Metadata' section.
- Julia**: A notebook showing a plot of 'Sepal.Length' vs 'Sepal.Width' for the 'Iris' dataset, and a console output showing eigenvalues and eigenvectors.
- python notebook**: A notebook showing a plot of 'Sepal.Length' vs 'Sepal.Width' for the 'Iris' dataset, and a console output showing the Lorenz system of differential equations.
- R**: A notebook showing a scatter plot of 'Sepal.Length' vs 'Sepal.Width' for the 'Iris' dataset, and a console output showing the head of the 'iris' dataset.

The interface also includes a 'Launcher' panel with icons for Python 3, C++11, C++14, C++17, Julia 1.1.0, phylogenetics (Python 3.7), and R. The bottom status bar shows 'Mode: Command', 'Ln 1, Col 1', and 'Lorenz.ipynb'.





Running notebooks with uv via juv



<https://github.com/manzt/juv>

```
uvx juv init notebook.ipynb
```

```
uvx juv run notebook.ipynb
```

- Ensures a Python environment with Jupyter installed
- Starts a Jupyter server
- Installs any dependencies listed inline at the top of the notebook





Jupyter (notebook/lab) is great
particularly for sharing code with figures & teaching ...

but

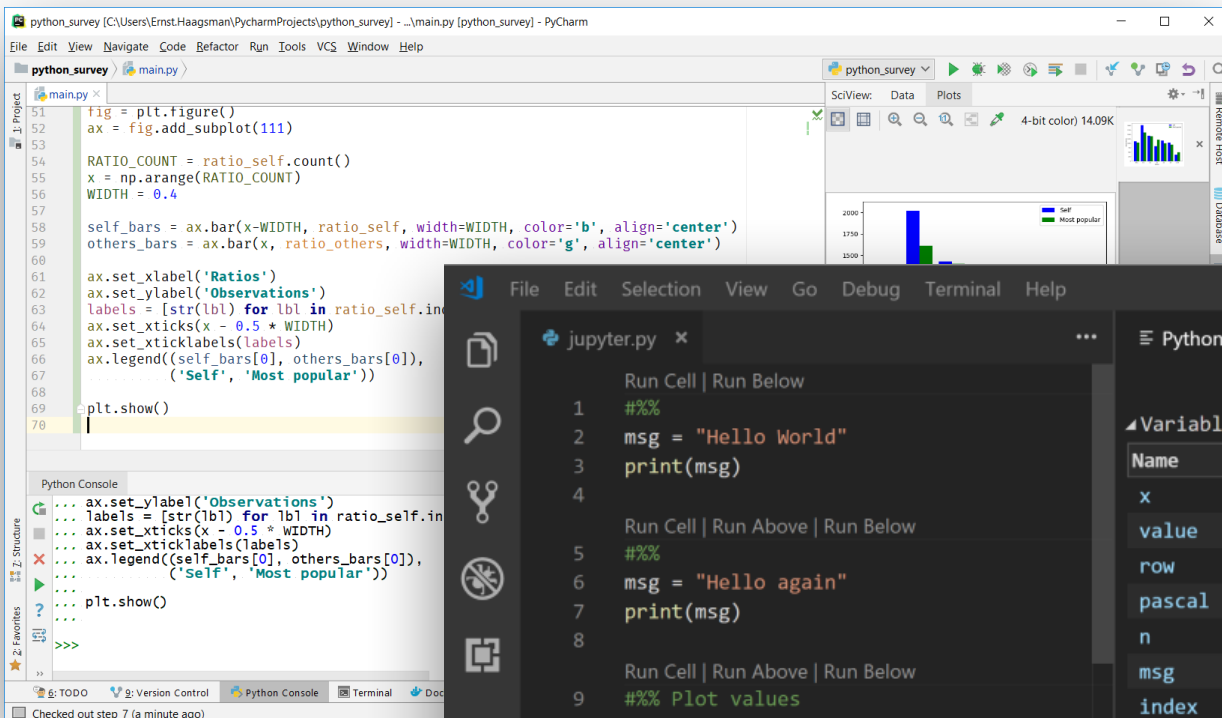
being comfortable using Python/IPython *without* a notebook
is critical





PyCharm

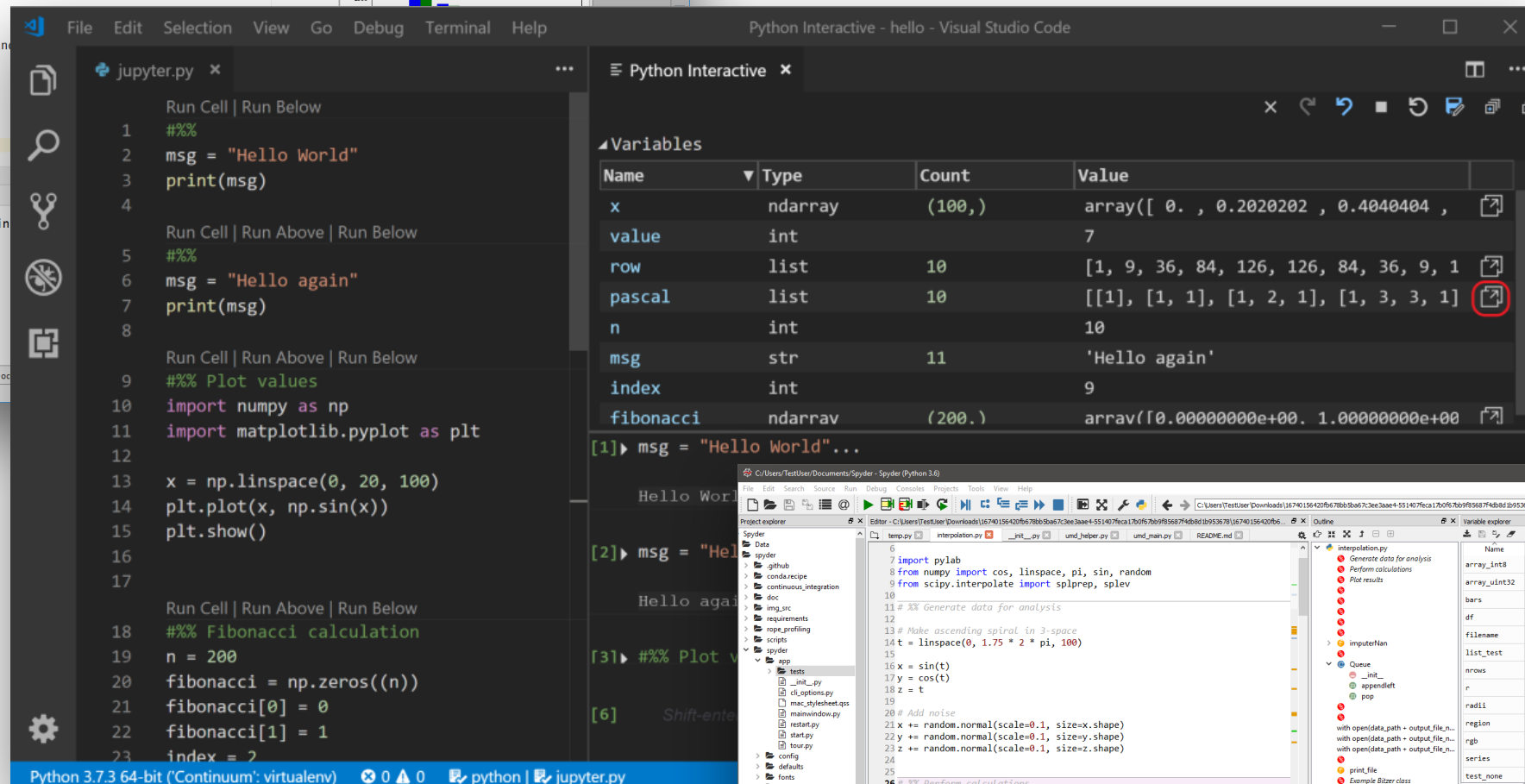
<https://www.jetbrains.com/pycharm/>



Integrated Development Environments ("IDE")

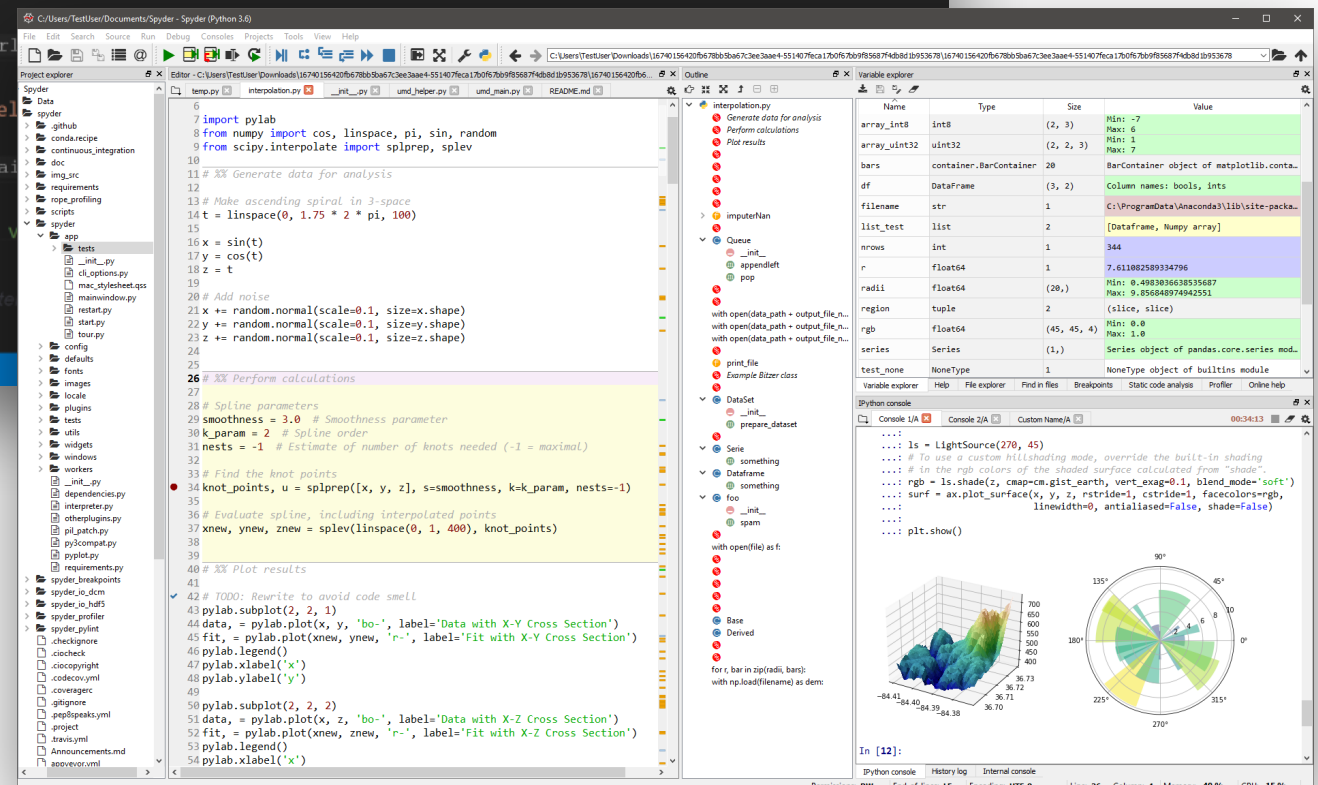
VS Code

<https://code.visualstudio.com/>



Spyder

<https://github.com/spyder-ide/spyder>





Summary

- Get Python by installing uv: <https://docs.astral.sh/uv/getting-started/installation/>
- Create new environments (often) with: `uv venv`
- Consider environments "disposable" ... don't get attached :)
Use `requirements.txt` (for pip) or `environment.yml` (for conda) files to rebuild them easily
- Use `uv pip install` to install packages.
(For some difficult binary packages, you'll need conda)
- If you're experiencing mysterious errors... make a new environment!
- `uv run <command>` to quickly execute a script/command in an environment
- `uvx <command>` to run a command from *any* package in an isolated env.
- Use Jupyter for a browser based IDE/notebook/console with rich media, widgets, markdown, etc... But know how to use Python without it!





Any questions?

lingering confusions?

