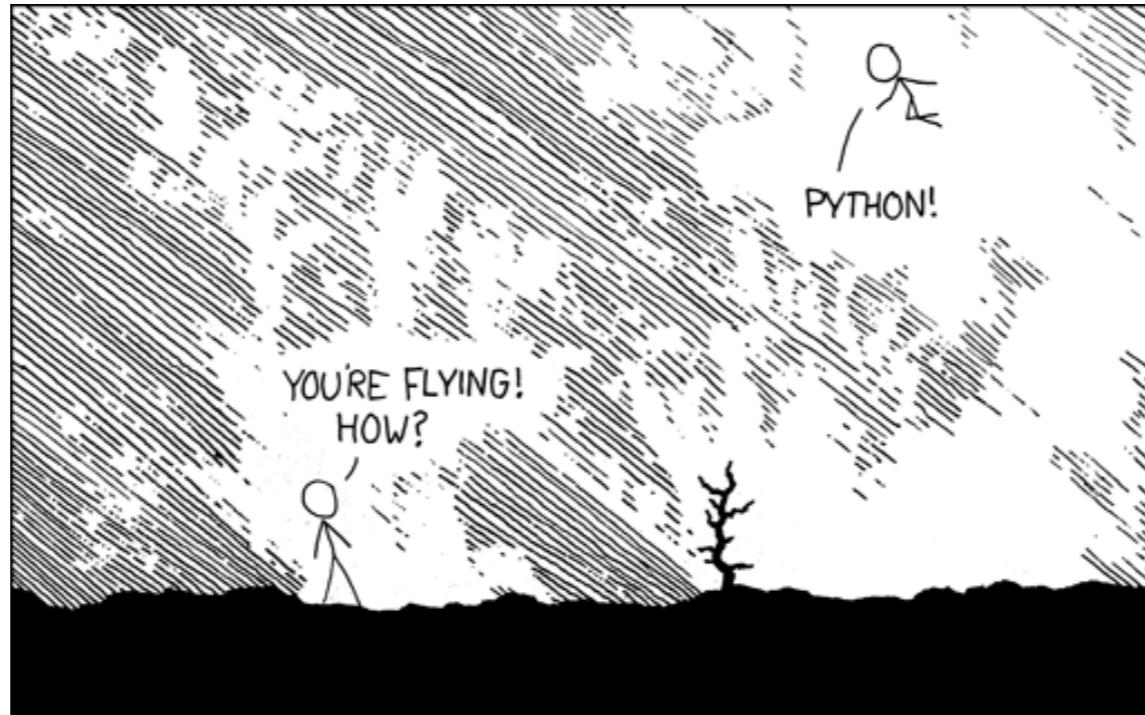
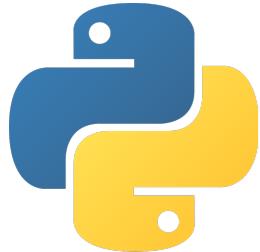


Getting Started running Python

Virtual environments, installing packages, and running code



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



Talley Lambert



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:

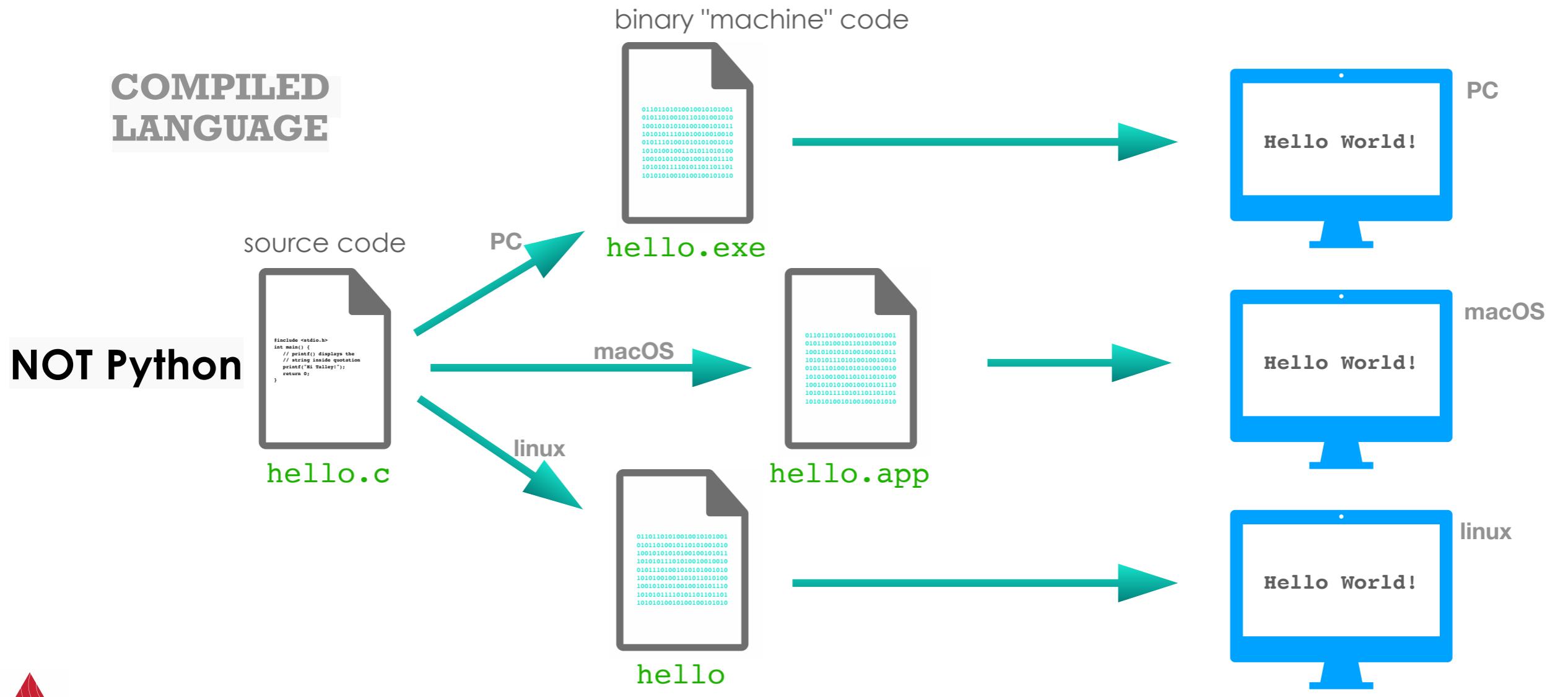
With Python, you share and run "regular" text files.
Python does all the OS-specific magic at "runtime".





What is Python?

interpreted

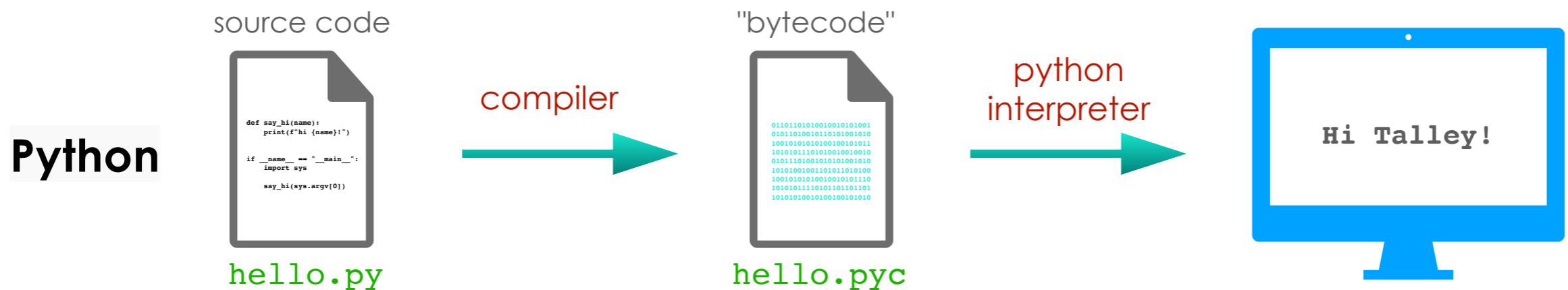




What is Python?

interpreted

INTERPRETED LANGUAGE



- 👍 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

classes



```
class Dog:
```

```
    def __init__(self, name):  
        self.name = name
```

attributes

methods



```
    def speak(self):  
        print("woof!")
```

```
fido = Dog("fido")
```

instances
("objects")





What is Python?

high-level

"high-level" ≈

- 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...)

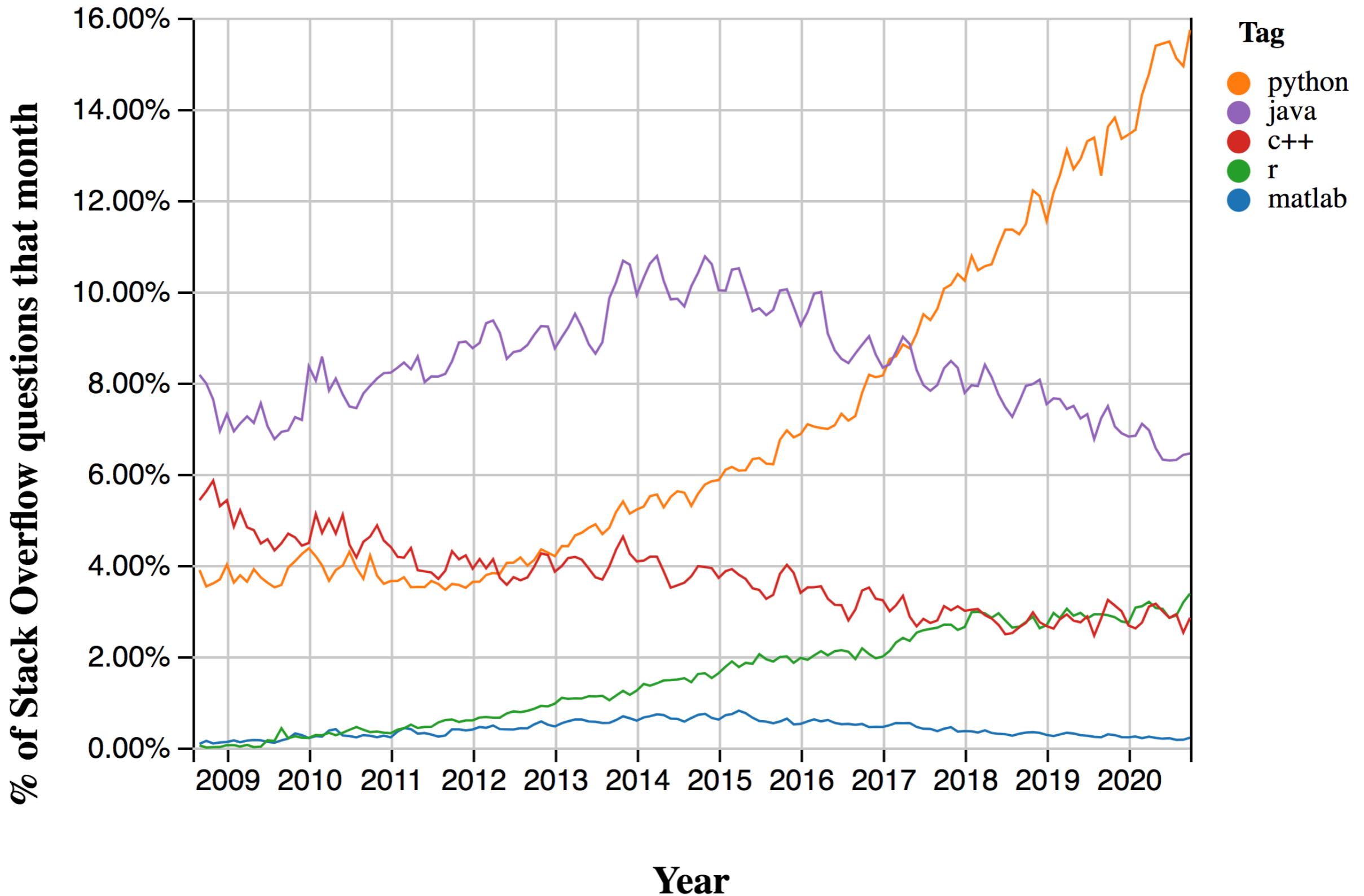
Decreased memory efficiency

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

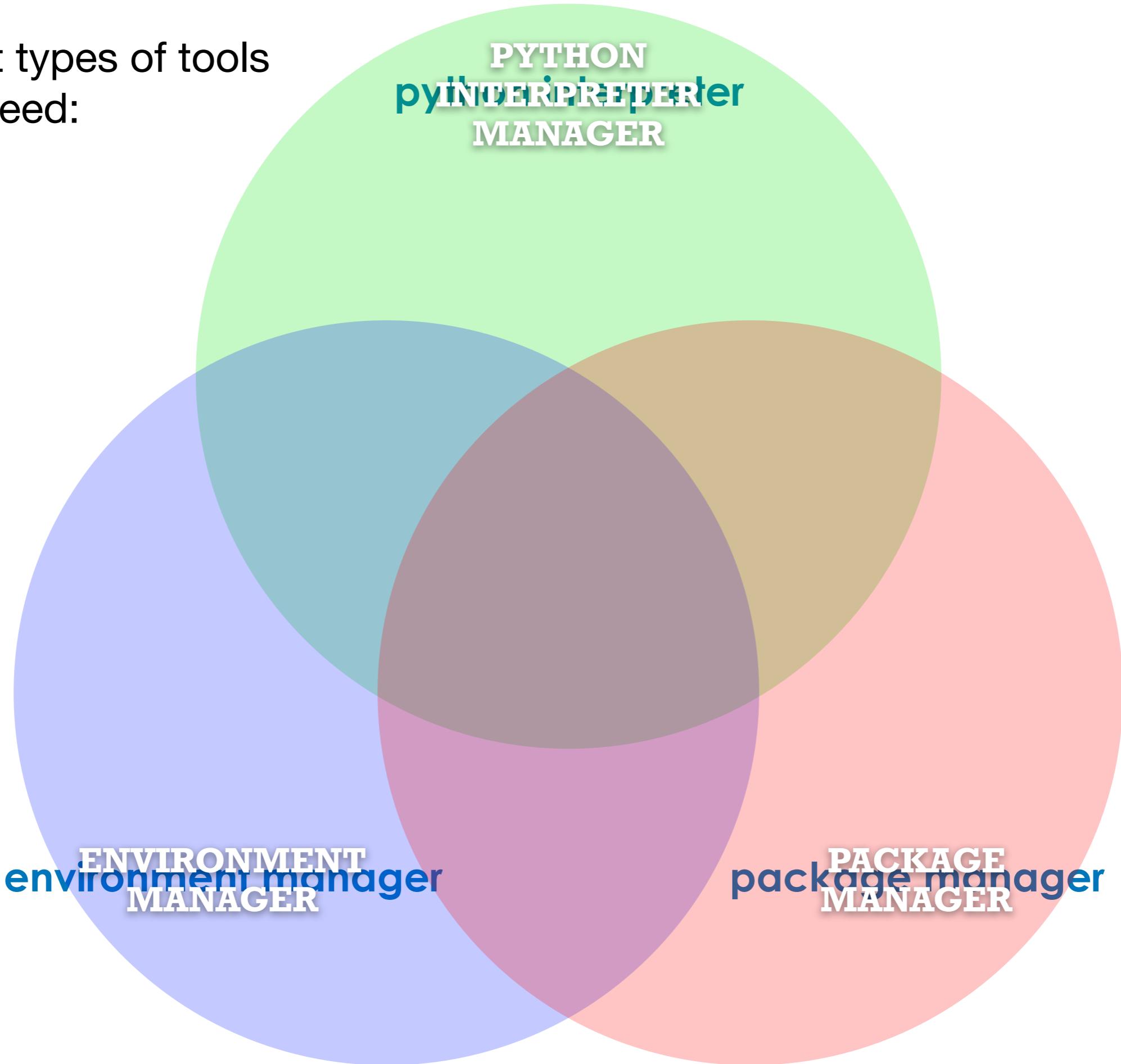
environment manager

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



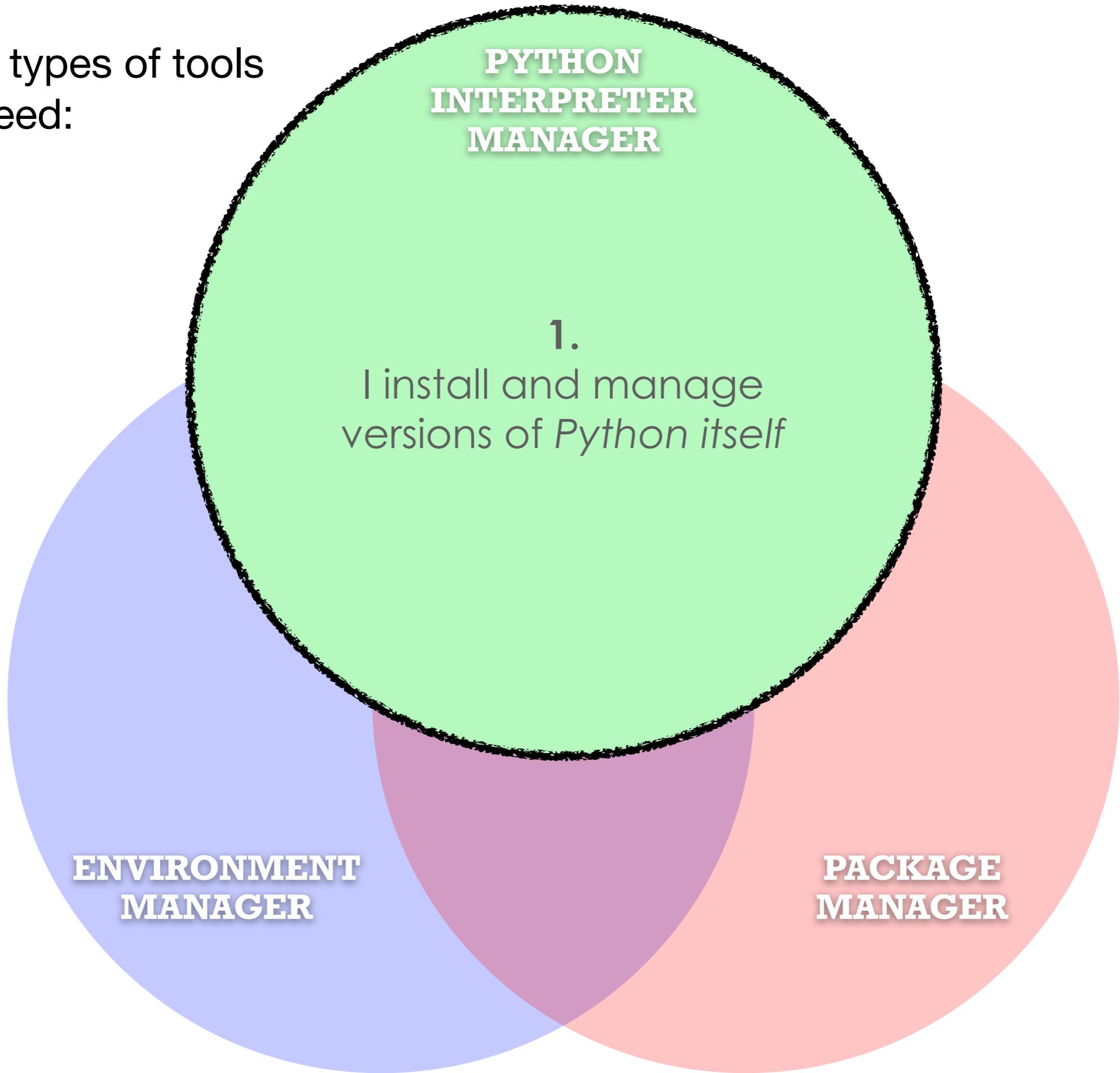


The three
important types of tools
you will need:



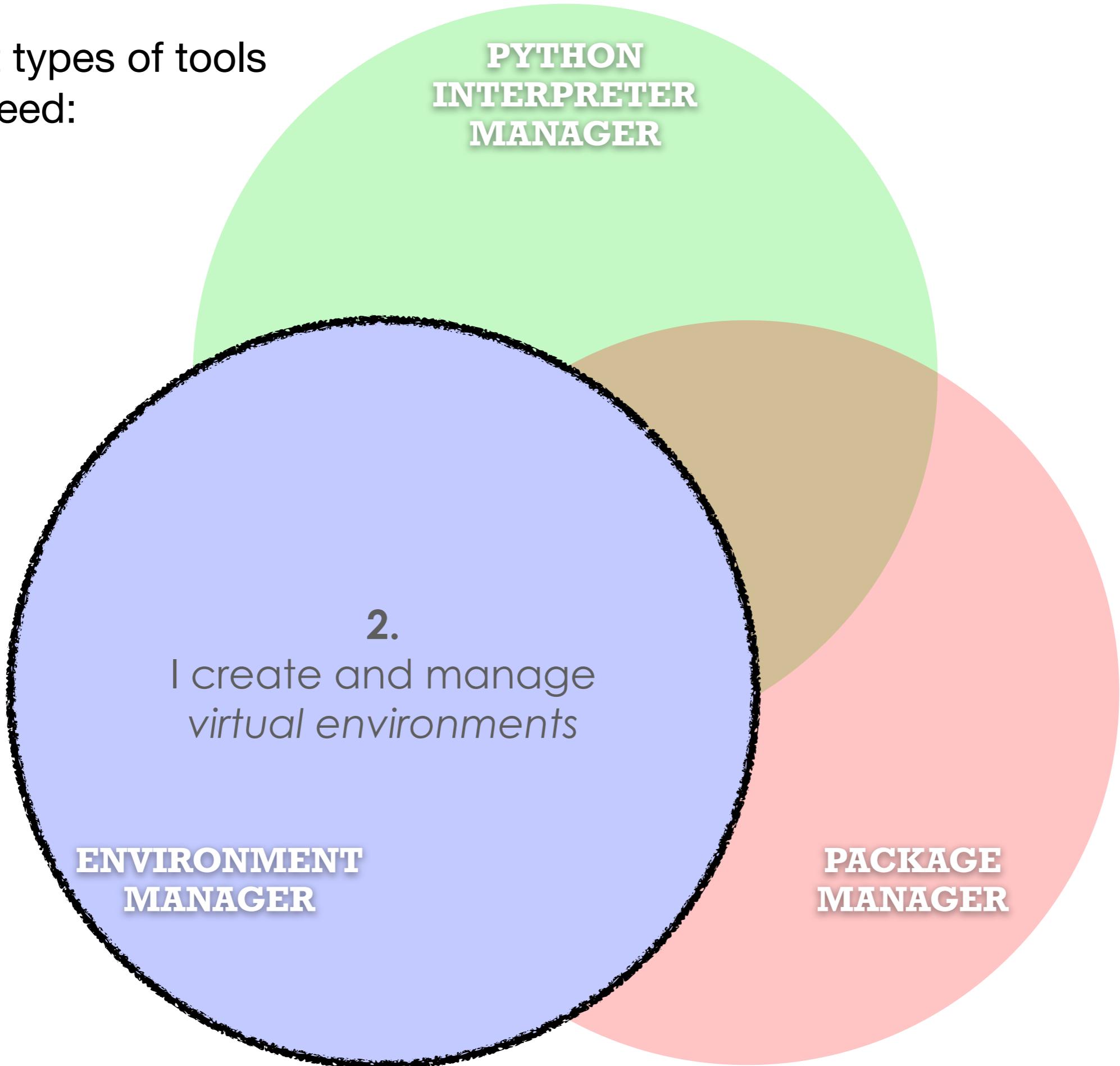


The three
important types of tools
you will need:



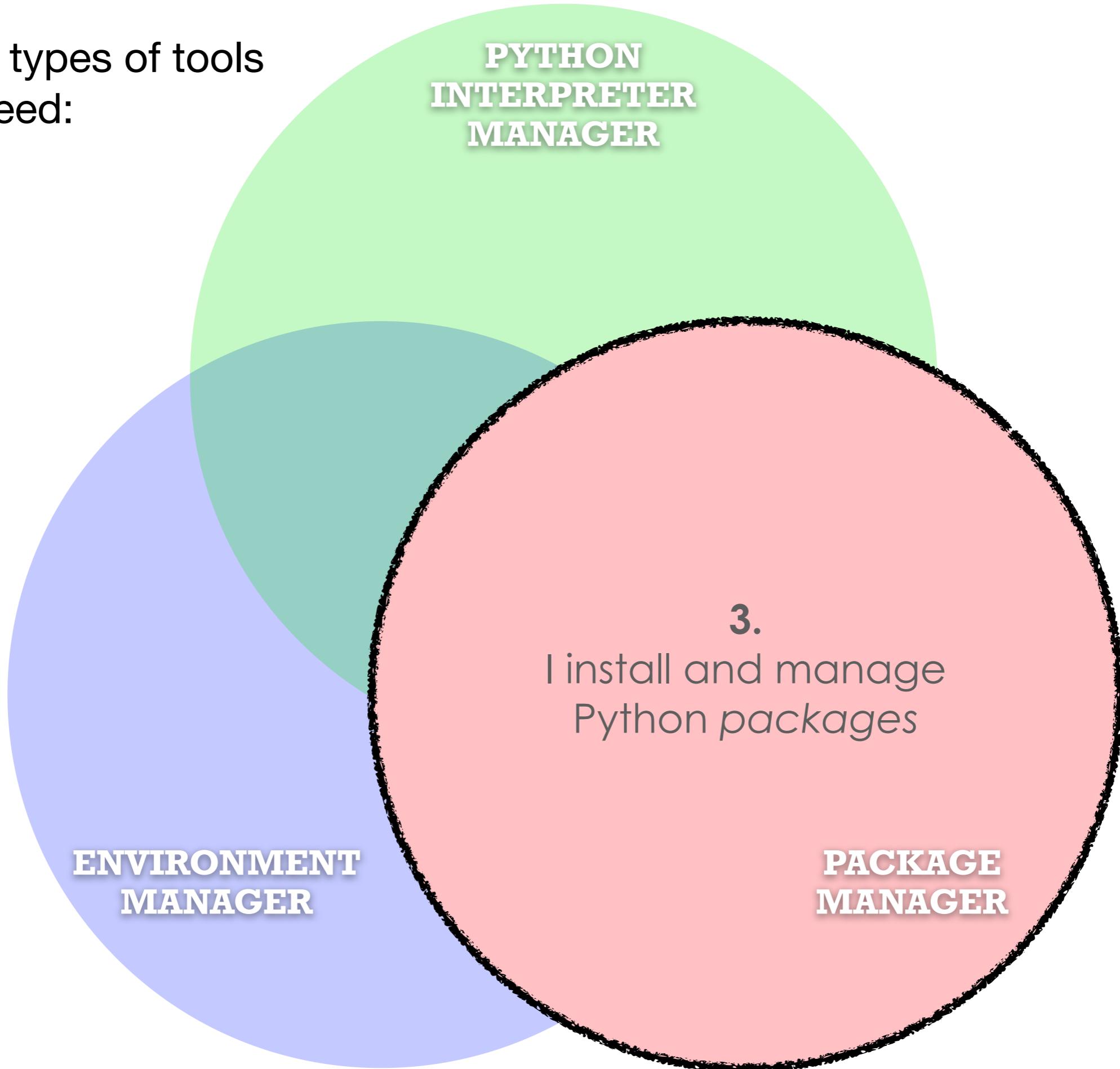


The three
important types of tools
you will need:





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
```

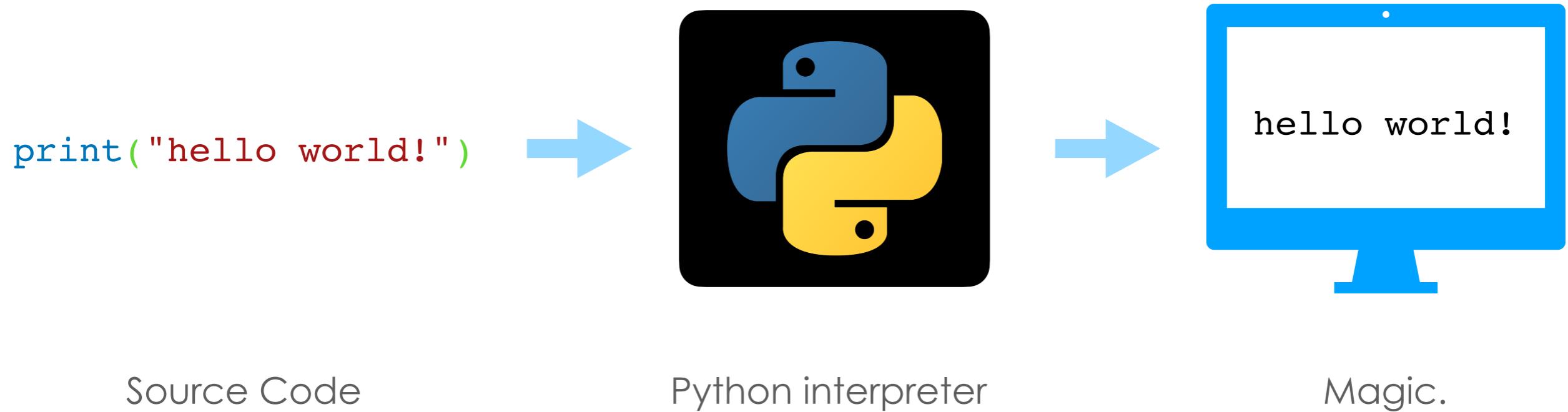




What is the Python interpreter?

```
$ 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

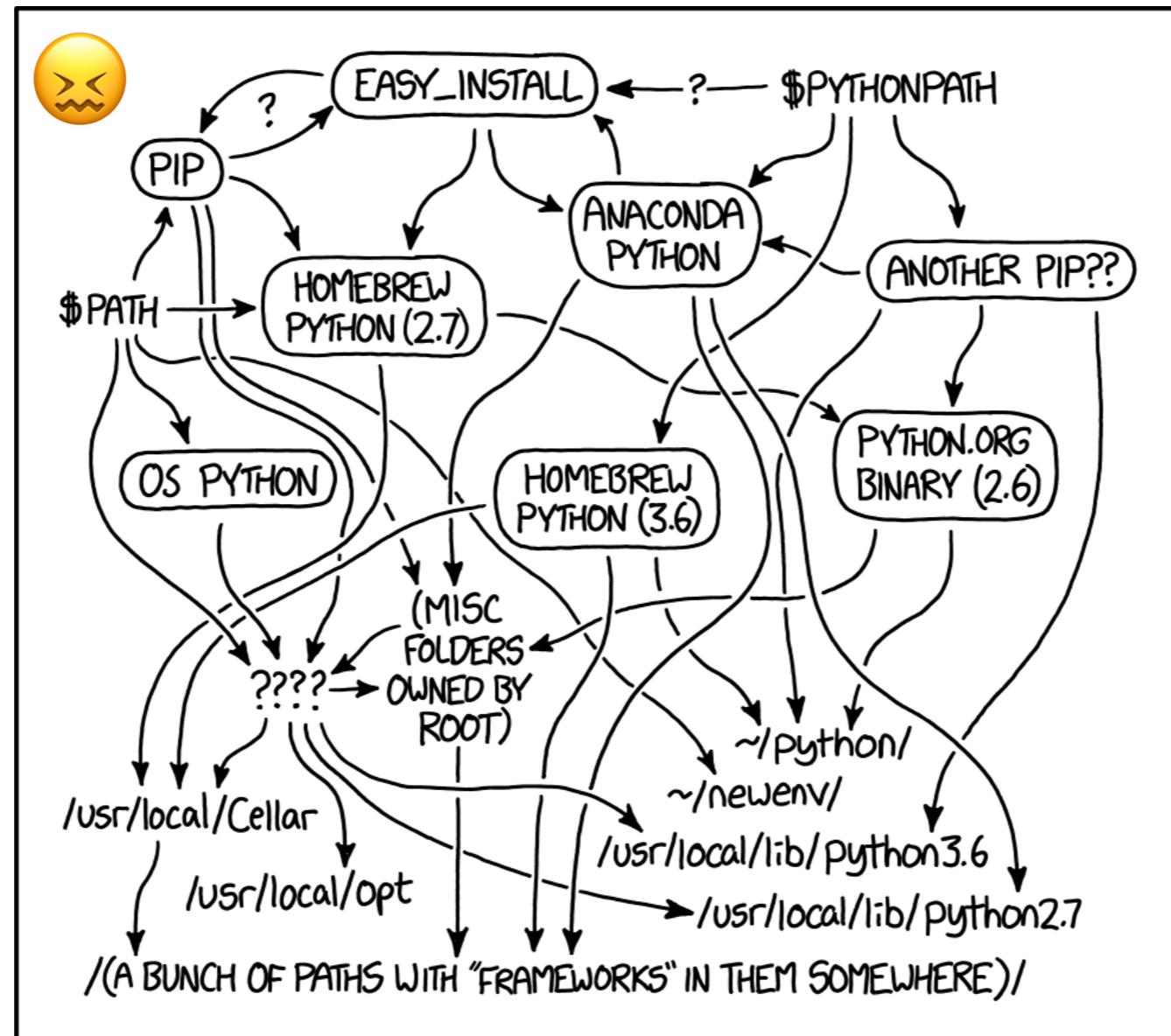


For this and many other reasons... don't use your system python (if you have one)!





OK, then how should I get Python?



Tl;dr: install uv

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





PYTHON INTERPRETER MANAGER

pyenv

brew

winget

conda/
mamba

uv

ENVIRONMENT MANAGER

PACKAGE MANAGER





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.

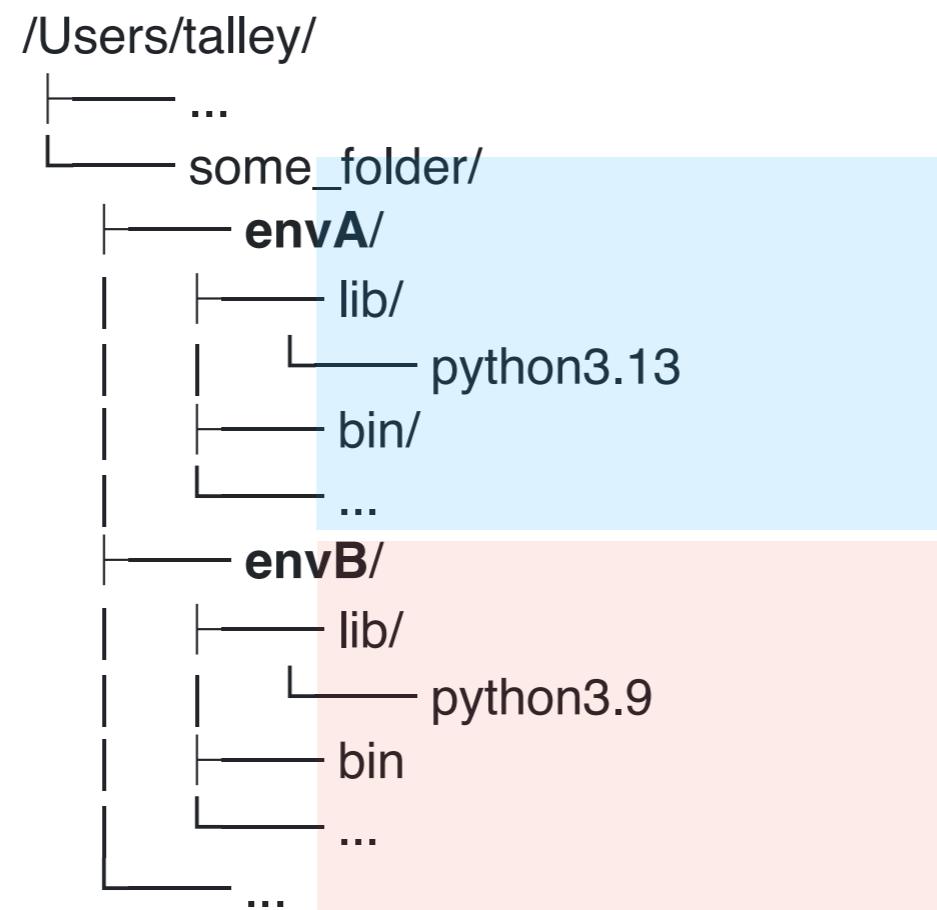




What is a python virtual environment?

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

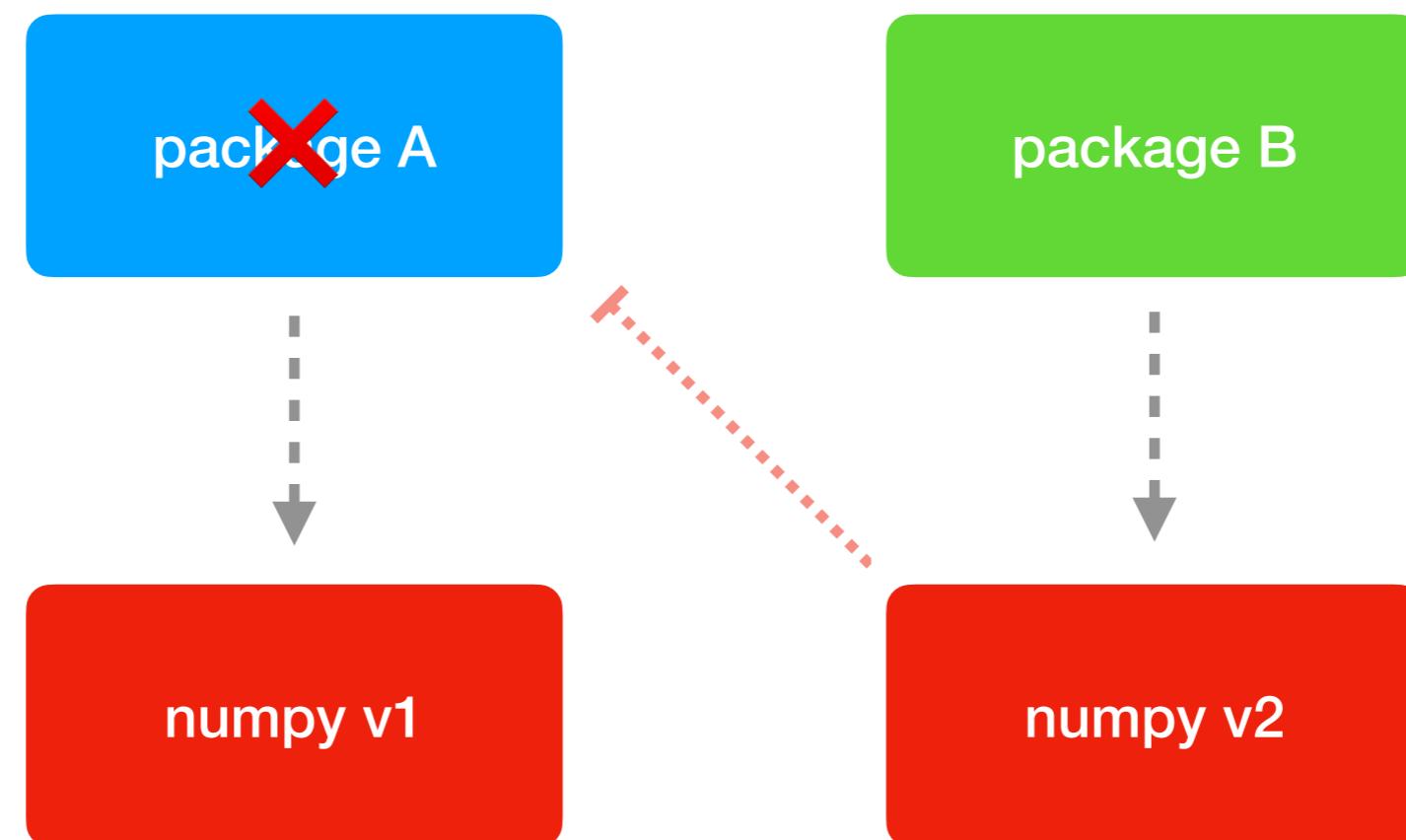
... (It's usually a literal folder somewhere on your computer...)





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



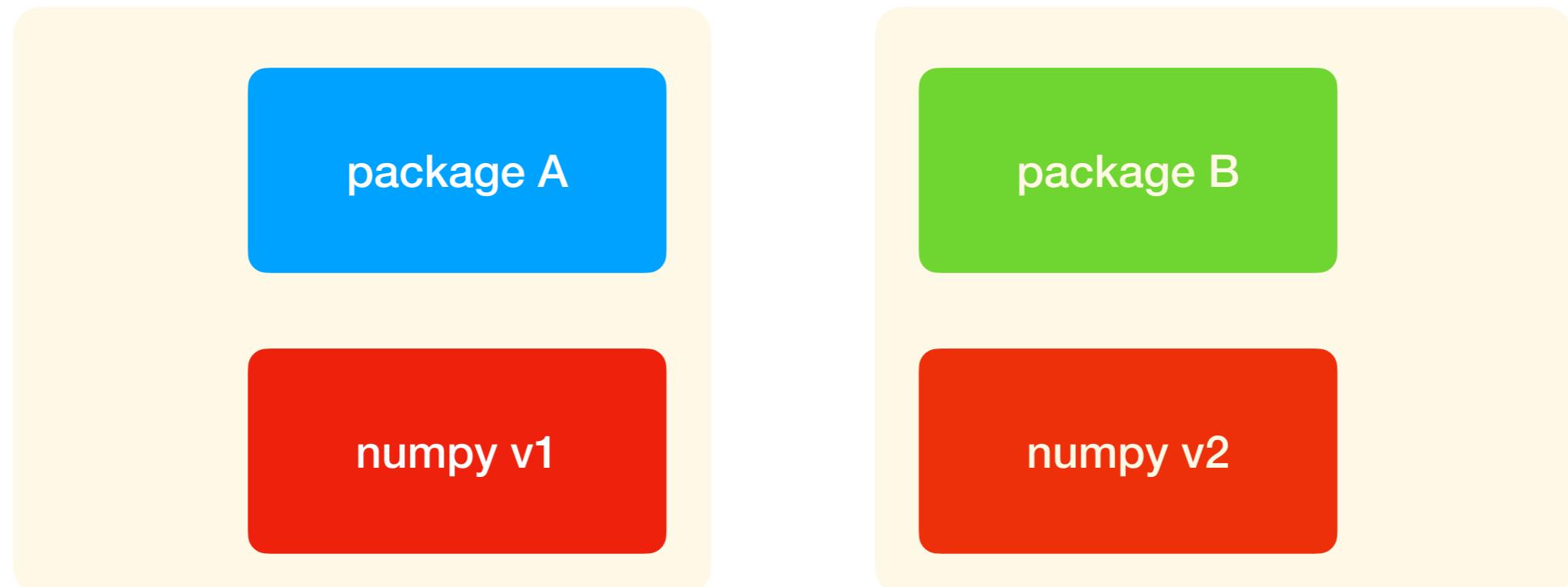


Why would I need more than 1 environment?

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**

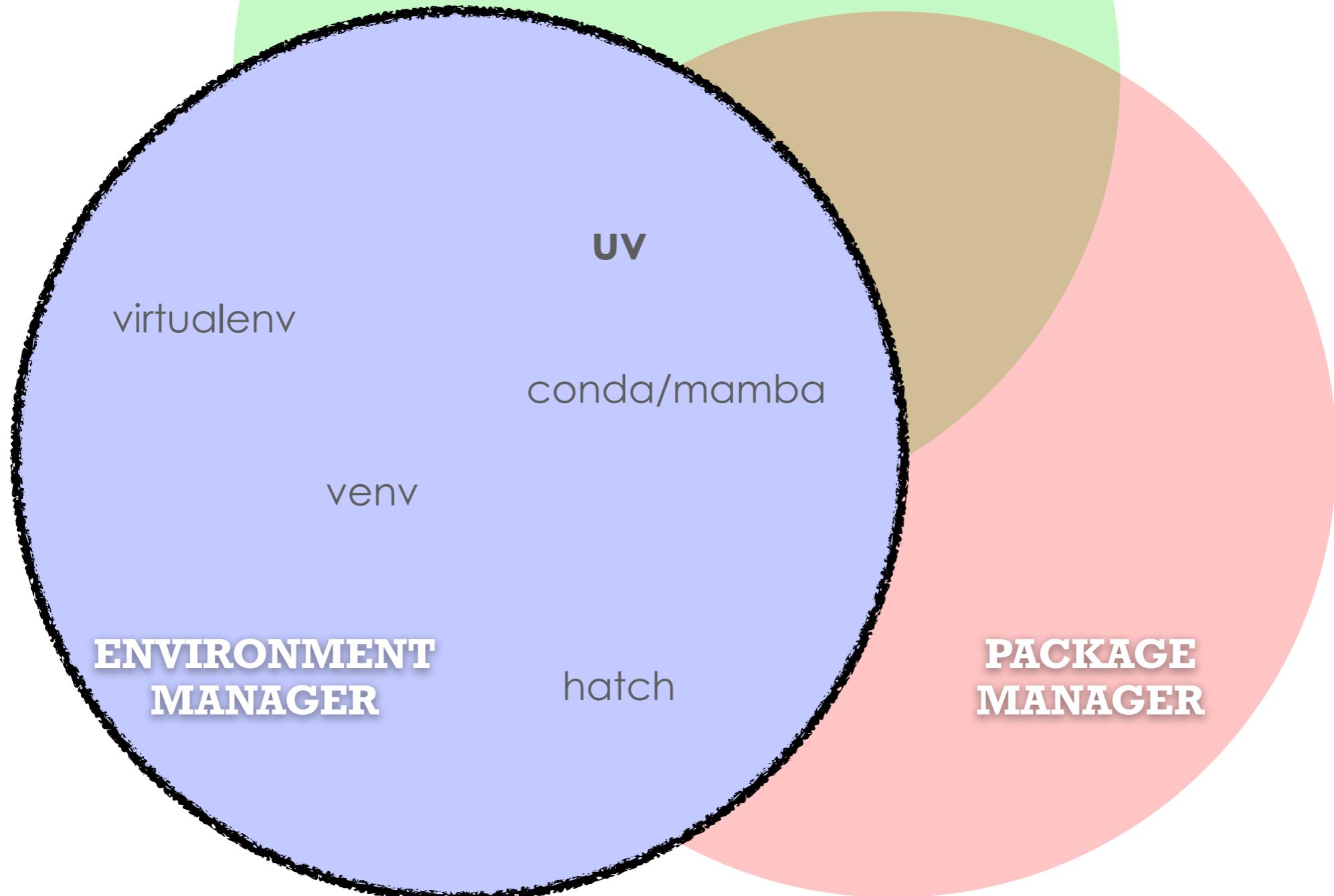
Examples:

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





PYTHON INTERPRETER MANAGER





How do I create a virtual environment?

`uv venv [ENV_NAME]`

(defaults to ".venv")

```
~/Desktop/project
→ █
```





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"



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





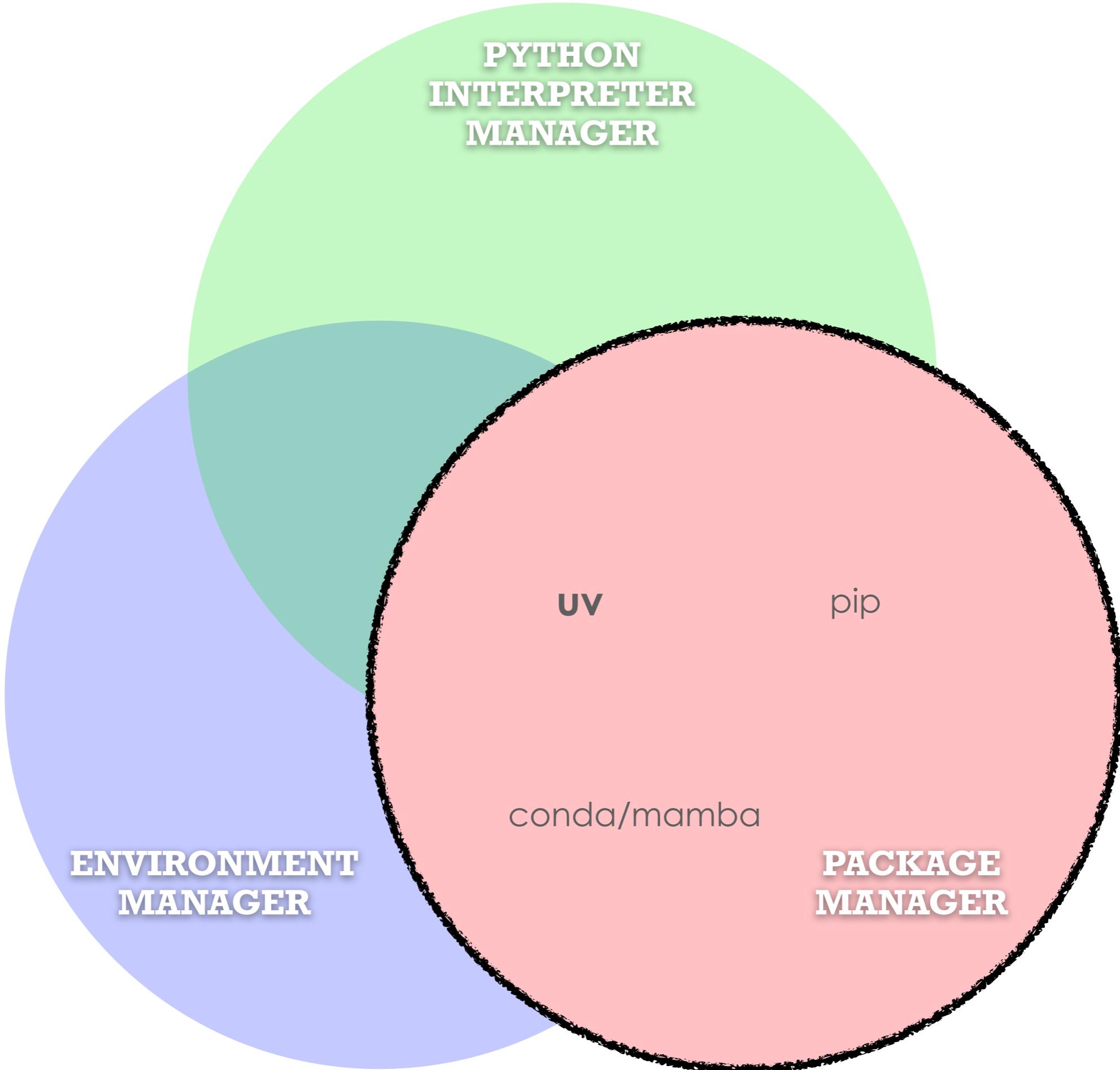
How do I get Python packages?

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
segmentAnything    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__)
```

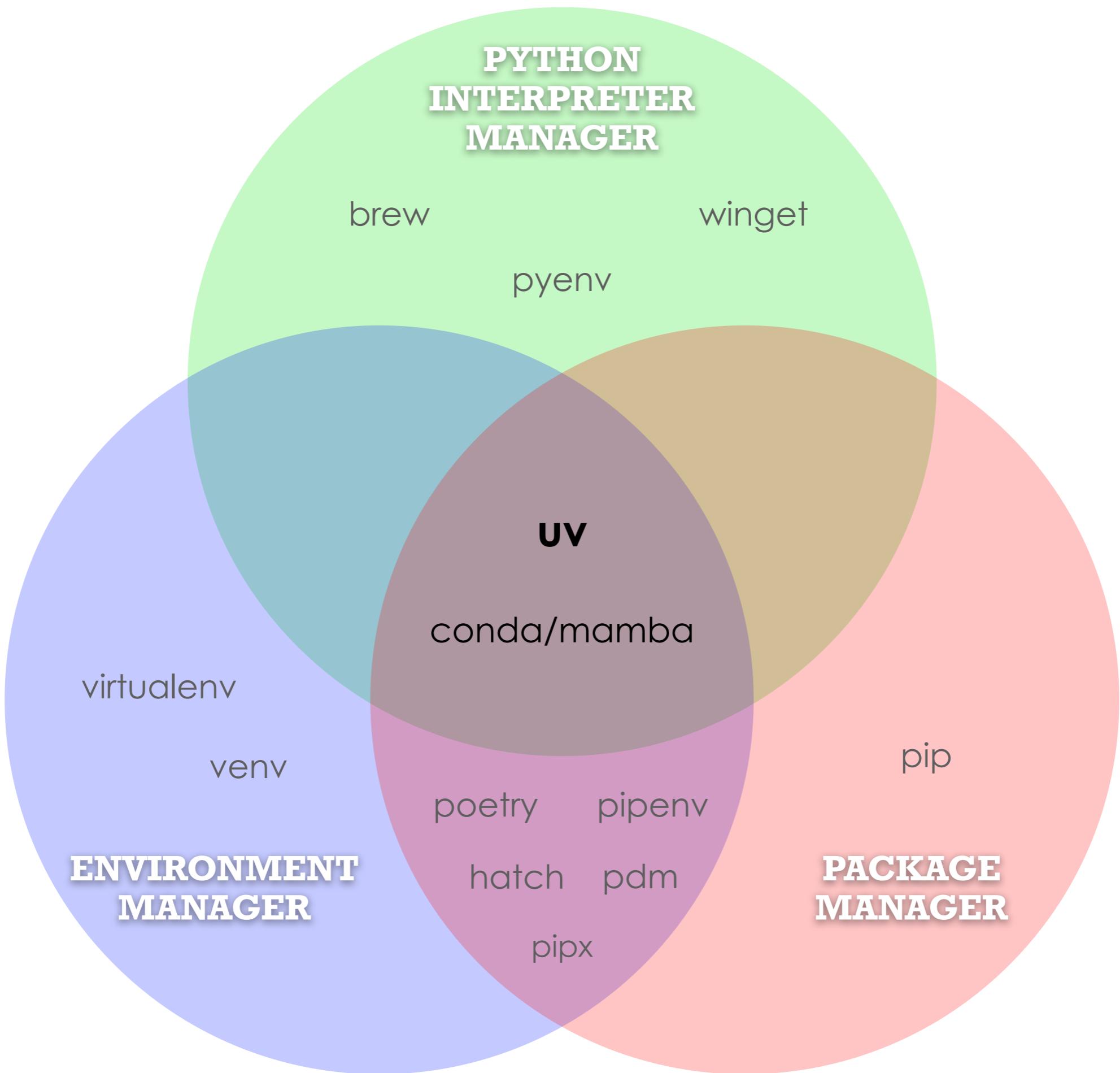


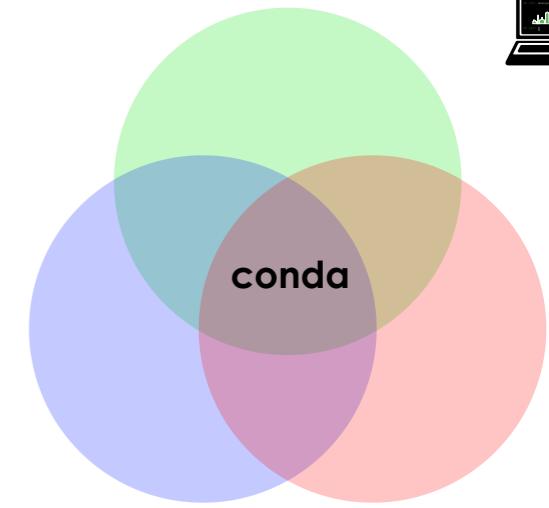


Now you know...

- 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**



see also: <https://jakevdp.github.io/blog/2016/08/25/conda-myths-and-misconceptions/>





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 autocomplete

```
In [1]: import math

In [2]: math.| <press tab>
      acos()      cos()      factorial()  isnan()    modf()      sqrt()
      acosh()     cosh()      floor()       isinf()    nan        tan()
      asin()      degrees()   fmod()       isnan()    perm()      tanh()
      asinh()     dist()      frexp()      isqrt()   pi         tau
      atan()       e          fsum()      ldexp()   pow()      trunc()
      atan2()     erf()      gamma()     lgamma()  prod()
      atanh()     erfc()     gcd()       log()     radians()
      ceil()      exp()      hypot()     log10()   remainder()
      comb()      expm1()    inf()       log1p()   sin()
      copysign()   fabs()     isclose()   log2()    sinh()
```





IP[y]: IPython

Interactive Computing

<https://ipython.readthedocs.io>

- Souped up interactive console (use `ipython` instead of `python`)
- Tab autocomplete
- 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 autocomplete
- 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 autocomplete
- 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 shows a Jupyter Notebook interface with several open notebooks and a central dashboard.

- File Bar:** File, Edit, View, Run, Kernel, Tabs, Settings, Help.
- Left Sidebar:** Shows a file tree with notebooks like Altair.ipynb, Cpp.ipynb, Data.ipynb, Fasta.ipynb, Julia.ipynb, and Linear Regression.ipynb.
- Central Dashboard:** Displays a "Launcher" section with icons for Python 3, C++11, C++14, C++17, Julia 1.1.0, phylogenetics (Python 3.7), and R. It also shows a "Seattle Weather: 2012-2015" plot and a "Julia" notebook.
- Open Notebooks:**
 - Linear Regression.ipynb:** A notebook titled "In Depth: Linear Regression" discussing linear regression models. It includes code to generate a scatter plot and a snippet of notebook metadata.
 - Altair.ipynb:** A notebook showing a scatter plot of Seattle weather data.
 - Lorenz.ipynb:** A notebook titled "Julia" showing a Lorenz attractor plot.
 - R.ipynb:** A notebook titled "python notebook" showing an Iris dataset plot.
 - Julia.ipynb:** A notebook titled "R" showing an Iris dataset plot.
- Bottom Status Bar:** Shows "Python 3 | Idle", "Mode: Command", "Ln 1, Col 1", and the current notebook name.



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/>

Code editor showing `main.py` with Python code for generating a bar chart. The terminal shows the output of running the script.

```

51 fig = plt.figure()
52 ax = fig.add_subplot(111)
53 RATIO_COUNT = ratio_self.count()
54 x = np.arange(RATIO_COUNT)
55 WIDTH = 0.4
56
57 self_bars = ax.bar(x-WIDTH, ratio_self, width=WIDTH, color='b', align='center')
58 others_bars = ax.bar(x, ratio_others, width=WIDTH, color='g', align='center')
59
60 ax.set_xlabel('Ratios')
61 ax.set_ylabel('Observations')
62 labels = [str(lbl) for lbl in ratio_self.index]
63 ax.set_xticks(x - 0.5 * WIDTH)
64 ax.set_xticklabels(labels)
65 ax.legend((self_bars[0], others_bars[0]), ('Self', 'Most popular'))
66
67 plt.show()

```

Python Console output:

```

ax.set_ylabel('Observations')
labels = [str(lbl) for lbl in ratio_self.index]
ax.set_xticks(x - 0.5 * WIDTH)
ax.set_xticklabels(labels)
ax.legend((self_bars[0], others_bars[0]), ('Self', 'Most popular'))
plt.show()

```

Jupyter notebook cell with "Hello World" code. Spyder's variable table shows the state of the variables.

Name	Type	Count	Value
x	ndarray	(100,)	array([0., 0.2020202, 0.4040404, ...])
value	int	7	7
row	list	10	[1, 9, 36, 84, 126, 126, 84, 36, 9, 1]
pascal	list	10	[[1], [1, 1], [1, 2, 1], [1, 3, 3, 1]]
n	int	10	10
msg	str	11	'Hello again'
index	int	9	9
fibonacci	ndarray	(200,)	array([0.0000000e+00, 1.0000000e+00, ...])

Python 3.7.3 64-bit ('Continuum': virtualenv) 0 ▲ 0 python | jupyter.py

Spyder

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

Integrated Development Environments ("IDE")

VS Code

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

Python Interactive window showing code execution and variable values. Variable Explorer shows the current state of variables.

Name	Type	Count	Value
x	ndarray	(100,)	array([0., 0.2020202, 0.4040404, ...])
value	int	7	7
row	list	10	[1, 9, 36, 84, 126, 126, 84, 36, 9, 1]
pascal	list	10	[[1], [1, 1], [1, 2, 1], [1, 3, 3, 1]]
n	int	10	10
msg	str	11	'Hello again'
index	int	9	9
fibonacci	ndarray	(200,)	array([0.0000000e+00, 1.0000000e+00, ...])

Python Interactive window showing code execution and variable values. A 3D surface plot is displayed in the terminal area.

```

6 import pylab
8 from numpy import cos, linspace, pi, sin, random
9 from scipy.interpolate import splprep, splev
10
11 # %% Generate data for analysis
12 t = linspace(0, 1.75 * 2 * pi, 100)
13
14 x = sin(t)
15 y = cos(t)
16 z = t
17
18 # Add noise
19 x += random.normal(scale=0.1, size=x.shape)
20 y += random.normal(scale=0.1, size=y.shape)
21 z += random.normal(scale=0.1, size=z.shape)
22
23 # Make ascending spiral in 3-space
24
25 # Perform calculations
26
27 # Spline parameters
28 smoothness = 3.0 # Smoothness parameter
29 k_param = 2 # Spline order
30 nests = -1 # Estimate of number of knots needed (-1 = maximal)
31
32 # Find the knot points
33 knot_points, u = splprep([x, y, z], s=smoothness, k=k_param, nests=nests)
34
35 # Evaluate spline, including interpolated points
36 xnew, ynew, znew = splev(linspace(0, 1, 400), knot_points)
37
38
39 # Plot results
40
41 # 7000: Rewrite to avoid code smell
42
43 pylab.subplot(2, 2, 1)
44 data, = pylab.plot(x, y, 'bo-', label='Data with X-Y Cross Section')
45 fit, = pylab.plot(xnew, ynew, 'r-', label='Fit with X-Y Cross Section')
46 pylab.legend()
47 pylab.xlabel('x')
48 pylab.ylabel('y')
49
50 pylab.subplot(2, 2, 2)
51 data, = pylab.plot(x, z, 'bo-', label='Data with X-Z Cross Section')
52 fit, = pylab.plot(xnew, znew, 'r-', label='Fit with X-Z Cross Section')
53 pylab.legend()
54 pylab.xlabel('x')

```





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?**

