1. Python and Python packages

## Outline

#### Python

NumPy, JAX & PyTorch

 $(ML \cup MD) \cap Biophysics$ 

## Python

- ▶ a high-level, interpreted programming language
- known for its simplicity and readability
- widely used in scientific computing, data analysis, and ML
- ▶ a glue language for integrating different libraries and tools
- many numerical and scientific libraries available as Python packages
- has a large and active community

an extremely fast Python package and project manager

- https://docs.astral.sh/uv
- can install Python and Python packages and manage projects
- install uv on macOS or Linux
  \$ curl -LsSf https://astral.sh/uv/install.sh | sh
- install uv on Windows:
   powershell -c "irm https://astral.sh/uv/install.ps1
   iex"
- after installation, run uv in the terminal to see the help message

#### Project management with uv

- \$ uv init myproject
- \$ cd myproject
- \$ uv run python
- \$ uv add --dev notebook
- \$ uv run ipython
- \$ uv add numpy

#### **Interactive Python**

\$ uv run python

```
$ uv run ipython
Python 3.12.5 (main, Aug 14 2024, 04:32:18) [Clang 18.1.8 ]
Type 'copyright', 'credits' or 'license' for more information
IPython 8.31.0 -- An enhanced Interactive Python. Type '?' for help.
In [1]: 2 + 3
Out[1]: 5
In [2]: 3 * (9 - 8) / 4
Out[2]: 0.75
```

In [3]:

\$ uv run jupyter notebook

#### Python scripts

- create and edit a Python script file (e.g., myscript.py) with a text editor
- recommend using the Visual Studio Code editor
- run the script with \$ uv run python myscript.py
- or run the script in an interactive IPython session, i.e.
   \$ uv run ipython
   Python 3.12.5 (main, Aug 14 2024, 04:32:18) [Clang 18.1.8 ]
   Type 'copyright', 'credits' or 'license' for more information
   IPython 8.31.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]: %run myscript.py

## **Python basics**

variables and data types

control flow

functions

classes and objects

modules and packages

#### tutorials

## Outline

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## NumPy

- a Python package for numerical computing
- array as the fundamental data structure
- vectors and matrices are 1D and 2D arrays, respectively
- arrays can have any number of dimensions
- array manipulations and linear algebra operations
- vectorized operations for efficiency
- Numpy quickstart
- Numpy for absolute beginners

- similar to NumPy but with additional features
- automatic differentiation
- automatic vectorization
- ▶ just-in-time (JIT) compilation
- ► can run on CPU, GPU, and TPUs

# **PyTorch**

- ► a popular deep learning library
- tensor as the fundamental data structure, similar to NumPy arrays
- implements various neural network layers
- automatic differentiation
- support for vectorization and parallelization
- ► GPU acceleration

## NumPy, JAX, and PyTorch

- > all are widely used in scientific computing and machine learning
- this course will mostly use NumPy and JAX
- but learn all three if you can
- all have good documentation and tutorials online