

Virtual environments

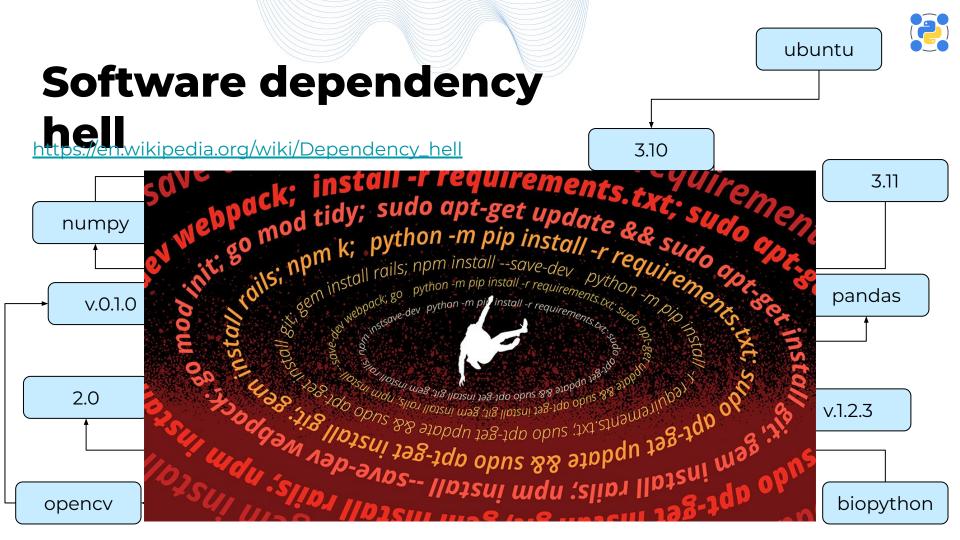
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18.10.2025



Why do we need virtual environments?







Why do we need virtual environments?

Avoiding software dependency hell

Isolation of external code from the PC

Easy to install/move/remove





Which virtual environments do we have?

venv

virtualenv

+ virtualenvwrapper

conda/mamba

renv





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Creating virtual environment

— Hands on your keyboard —

python3 -m venv my_venv

ls -al

ls -al my_venv

What do you see?





Using virtual environment

—— Hands on your keyboard ——

We can activate it and deactivate

which python

source my_venv/bin/activate

which python

deactivate

which python





Using virtual environment

—— Hands on your keyboard ——

Let's install some library!

source my_venv/bin/activate

ls my_venv/lib/python3.11/site-packages

pip install cowsay

my_venv/bin/cowsay -t hello





Using virtual environment

—— Hands on your keyboard ——

Let's install some library!

pip install biopython

numpy installed as well!

python3

from Bio.Seq import Seq
my_dna = Seq('AGTACACTGGT')
print(my_dna.complement())
 quit() / Ctrl + D





—— Hands on your keyboard ——

pip freeze

deactivate

pip freeze

source my_venv/bin/activate

pip freeze ...

Saving info about our venv





—— Hands on your keyboard ——

pip freeze

deactivate

pip freeze

source my_venv/bin/activate

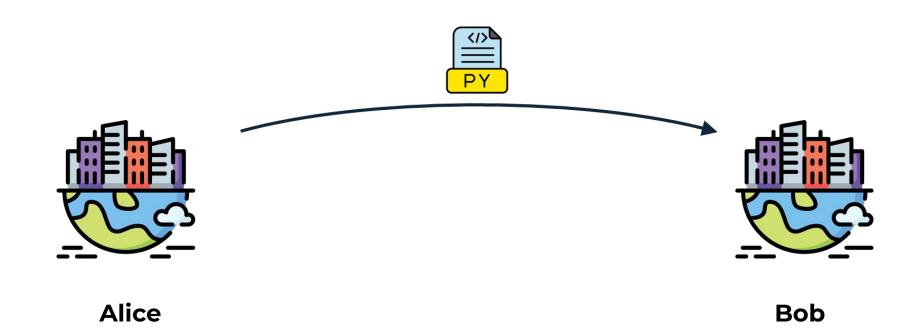
pip freeze > requirements.txt

cat requirements.txt

Saving info about our venv









—— Hands on your keyboard ——

Reproducing venv

python3 -m venv my_venv2

source my_venv2/bin/activate

ls my_venv2/lib/python3.11/site-packages

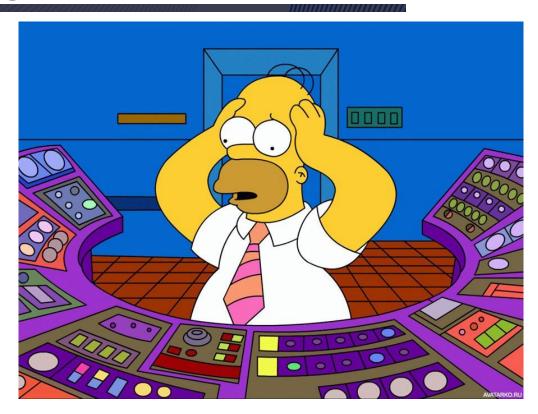
pip install -r requirements.txt

ls my_venv2/lib/python3.11/site-packages





Deleting virtual environment





Deleting virtual environment

—— Hands on your keyboard ——

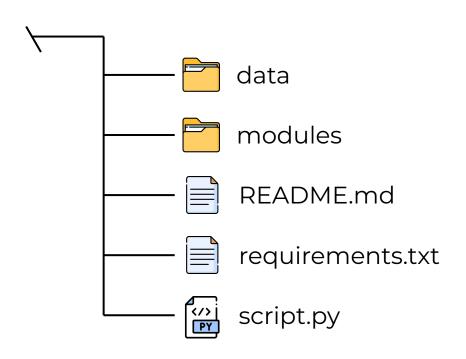
Don't forget to

deactivate

rm -r my_venv2



Example bioinformatics project







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+ virtualenvwrapper

conda / mamba

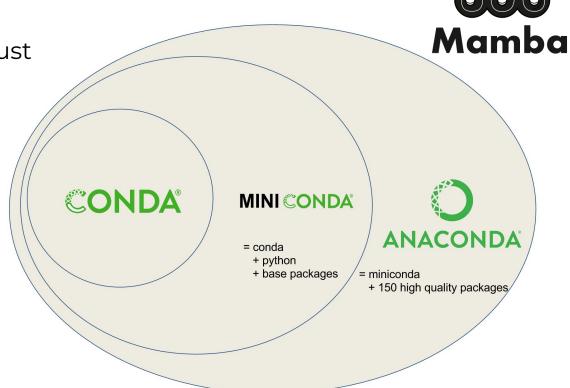
renv





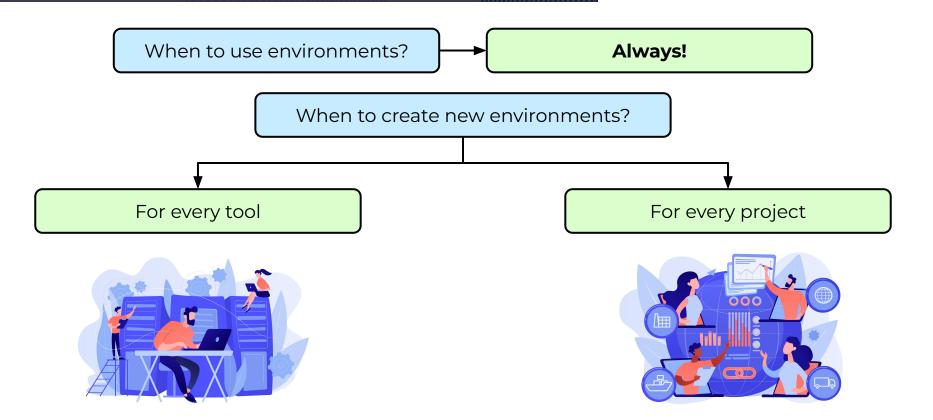
Conda environments

To manage more than just python packages





Two conda strategies





Using conda/mamba

—— Hands on your keyboard ——

Creating environments

conda create -n new_env

conda activate new_env

conda deactivate

People often make aliases ca and cda





Using conda/mamba

—— Hands on your keyboard ——

Inspecting environments

conda env list

conda list

conda info

conda env export



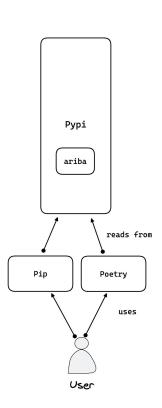


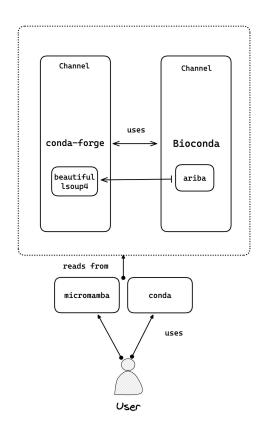
Conda channels

Conda channels are remote repositories with packages











Using conda/mamba

—— Hands on your keyboard ——

Sharing environments

conda install -c channel

conda env export > environment.yaml

conda env create -f environment.yaml

conda env export --from-history





Wrap up

Make and use virtual environments

Always make requirements or yaml

