ML Basics

Python Setup

Learning goals

- Understand the different package management systems
- Be comfortable in settig up a python environment
- Know how to make your work reproducible with Python

0. INSTALLATION OF PYTHON

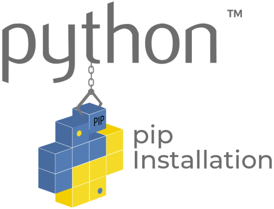
Python can be installed in many ways, e.g. by

- .. directly downloading it from `python.org`: `https://www.python.org/downloads/`
- .. downloading Miniconda: `https://docs.conda.io/en/latest/miniconda.html`
- .. installing Python via the Anaconda distribution: `https://docs.anaconda.com/anaconda/install/`

0. PACKAGE MANAGEMENT IN PYTHON

Unlike in R/RStudio (which you might be used to), package management in Python is a little more of a mess: There are *two* (concurring) package management systems:

- `pip` (+ PyPi)
- `conda` (+ Anaconda repository)



0. PACKAGE MANAGEMENT IN PYTHON

Key facts (`pip`)

- Installs packages from the Python Package Index (PyPi)
- Pip packages are source distributions (compiler needed) or wheels[1]
- Installs dependencies in a recursive, serial loop
- Limited to Python software
- No built-in support for **virtual environments** (but possible)
- $>$ 150k packages available on PyPi

[1] tl;dr: wheels are smaller + install faster than a source distribution and do not require a compiler

0. PACKAGE MANAGEMENT IN PYTHON

Key facts (`conda`)

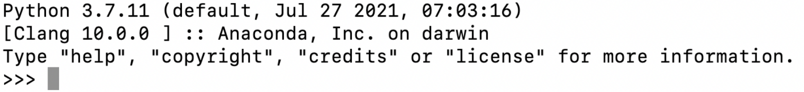
- Installs packages from the Anaconda repository
- Conda packages are binaries, no need for compilers
- SAT solver to verify requirements of all packages
- Not limited to Python software
- Easier to create/manage **virtual environments**
- $\sim$ 1.5k packages available in the Anaconda repository

1. PYTHON VIA THE CONSOLE

Start Python in Terminal / Console / Command Line

```
python
```

Approximate result:



```
Python 3.7.11 (default, Jul 27 2021, 07:03:16)
[Clang 10.0.0 ] :: Anaconda, Inc. on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> 
```

Similar to R console:

```
1+1
```

Exit with Ctrl-D or

```
exit()
```

2. ANACONDA

Anaconda is a widely used open-source distribution of Python:
`https://www.anaconda.com`

3. MINICONDA

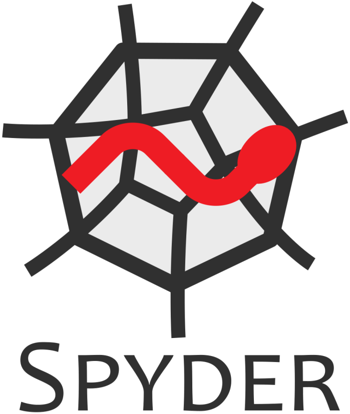
We recommend downloading and installing *Miniconda*, since it

- .. directly brings `conda` (as well as `pip`)
- .. is a minimal installer (only the core parts, unlike Anaconda)

Source: `https://www.mrdbourke.com/get-your-computer-ready-for-machine-learning-using-anaconda-miniconda-and-conda/`

4. SPYDER

Spyder is a complete IDE for Python (very similar to RStudio)



- It directly comes with the Anaconda distribution
- It can also be installed from `https://www.spyder-ide.org/`

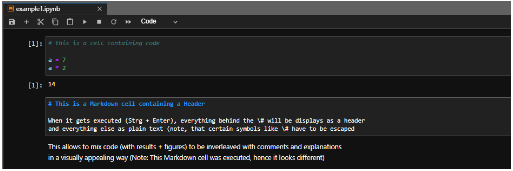
5. JUPYTER NOTEBOOKS/LAB

A Jupyter Notebook is a slightly different way of writing and presenting Python codes. It is a web application that lets you develop Python code in your browser.
Useful for explorative analyses and for beginning stages of a project, where you need frequent feedback.

```
conda install jupyterlab
```

5. JUPYTER NOTEBOOKS/LAB

Code cells vs. Markdown cells

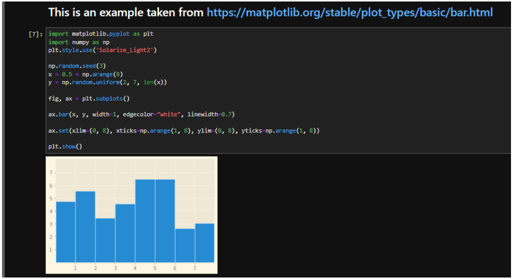


```
[1]: # this is a cell containing code

     a = 7
     a * 2

[1]: 14
```

```
# This is a Markdown cell containing a Header

When it gets executed (Strg + Enter), everything behind the \# will be displays as a header
and everything else as plain text (note, that certain symbols like \# have to be escaped
```

This allows to mix code (with results + figures) to be inverleaved with comments and explanations
in a visually appealing way (Note: This Markdown cell was executed, hence it looks different)

Creating e.g. figures



This is an example taken from https://matplotlib.org/stable/plot_types/basic/bar.html

```
[7]: import matplotlib.pyplot as plt
     import numpy as np
     plt.style.use('Solarize_Light2')

     np.random.seed(3)
     x = 0.5 + np.arange(8)
     y = np.random.uniform(2, 7, len(x))

     fig, ax = plt.subplots()

     ax.bar(x, y, width=1, edgecolor="white", linewidth=0.7)

     ax.set(xlim=(0, 8), xticks=np.arange(1, 8), ylim=(0, 8), yticks=np.arange(1, 8))

     plt.show()
```

5. JUPYTER NOTEBOOKS/LAB

- When you click into a cell and you see your cursor, then you are in **Edit Mode**
- Write your Code/Explanations and execute with `Ctrl+Enter`
- Hit `Esc`: Cursor disappears, cell is still selected
  (you are in **Command mode** now)
- Now there are, among others, certain shortcuts available:
  - `A` will insert a new cell *above* the current one
  - `B` will insert one *below*
  - `C` copies the selected cell
  - `X` cuts the selected cell
  - `V` pastes copied/cut cell below
  - `M` switches the cell mode to *Markdown*
  - `Y` switches it to *Code*
  - `Up` selects cell above
  - `Down` selects cell below

6. R-STUDIO

It is (meanwhile) also possible to use good old RStudio as an IDE for writing Python code:

- Install the `reticulate` packages in R
- Select the desired Python interpreter at `Tools > Global Options > Python`
- `New File > Python Script`

6. R-STUDIO

You can also use Python in conjunction with R Markdown
(as you will observe quite often in our slides)

```python
import pandas as pd

x = pd.DataFrame({"a": [1,2,3,4],
                  "b": ["c", "d", "e", "f"]})
x
```

7. VIRTUAL ENVIRONMENTS

Assume the following scenario:

- We have two ongoing projects, `Project A` and `Project B`
- Both projects need some package `pkg_xy`
- `Project A` needs `v1.2.0` while `Project B` requires `v2.1.3`
- What can we do about this???

Solution: **Work with virtual environments**

- You can also tell RStudio to activate environments automatically by ticking the box at:
- □ `Automatically activate project-local Python environments`

7. VIRTUAL ENVIRONMENTS

Virtual Environments allow you to

- .. have different entire version of Python running on your machine (`Python 2`, `Python 3.x`, `Python 3.y`, ..)
- .. maintain different versions of packages for your projects

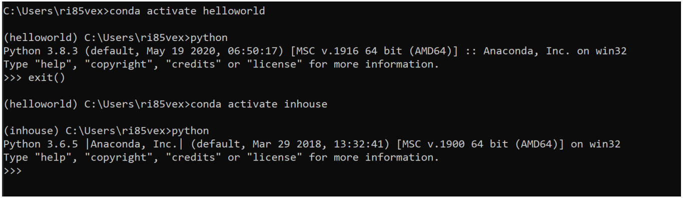
They can be created/activated/deactivated via

```
conda create --name some_name python=3.9
conda activate some_name
conda deactivate some_name
```

Useful commands: Conda Cheat Sheet

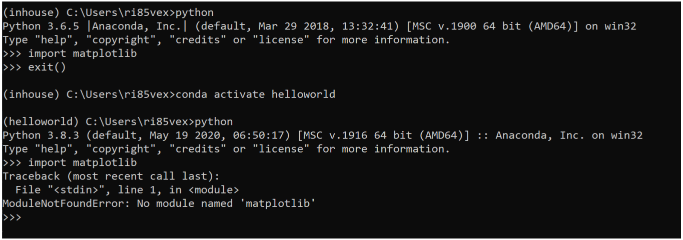
7. VIRTUAL ENVIRONMENTS

Different versions of Python



```
C:\Users\ri85vex>conda activate helloworld

(helloworld) C:\Users\ri85vex>python
Python 3.8.3 (default, May 19 2020, 06:50:17) [MSC v.1916 64 bit (AMD64)] :: Anaconda, Inc. on win32
Type "help", "copyright", "credits" or "license" for more information.
>>> exit()

(helloworld) C:\Users\ri85vex>conda activate inhouse

(inhouse) C:\Users\ri85vex>python
Python 3.6.5 |Anaconda, Inc.| (default, Mar 29 2018, 13:32:41) [MSC v.1900 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Different (versions of) packages



```
(inhouse) C:\Users\ri85vex>python
Python 3.6.5 |Anaconda, Inc.| (default, Mar 29 2018, 13:32:41) [MSC v.1900 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license" for more information.
>>> import matplotlib
>>> exit()

(inhouse) C:\Users\ri85vex>conda activate helloworld

(helloworld) C:\Users\ri85vex>python
Python 3.8.3 (default, May 19 2020, 06:50:17) [MSC v.1916 64 bit (AMD64)] :: Anaconda, Inc. on win32
Type "help", "copyright", "credits" or "license" for more information.
>>> import matplotlib
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'matplotlib'
>>>
```

8. MANAGING PACKAGES

Via `conda`:

```
conda install pandas
conda install pandas==1.3.5
conda update pandas
conda remove pandas
conda list
```

Via `pip`:

```
pip install pandas
pip install pandas==1.3.5
pip install pandas --upgrade
pip uninstall pandas
pip freeze
```

8. MANAGING PACKAGES

Instruct `conda` which version you want to have installed:

- Exact (1.3.5)

```
conda install pandas==1.3.5
```

- Fuzzy (1.3.0, 1.3.1, etc.)

```
conda install pandas==1.3
```

- Greater or equal (1.3.5 or higher)

```
conda install "pandas>=1.3.5"
```

- OR (1.3.4 or 1.3.5)

```
conda install "pandas==1.3.4|1.3.5"
```

- AND (1.3.3, 1.3.4, but not 1.4)

```
conda install "pandas>=1.3.3,<1.4"
```

Creating isolated environments and running different versions of Python as well as different packages (or versions) of them works perfectly fine *(for us)*.

What if we want to share our code with others? Make it publicly available? Across platforms?

There needs to be some standardized way to do so, right?[2]

- `environment.yml` (conda)
- `requirements.txt` (pip)

[2] Rhetorical question ;-)

9. REPRODUCIBILITY

- Create an environment:[3]
  (with specific Python version and some packages)

```
conda create -n my_env python=3.7 pandas numpy scikit-learn
```

- Activate the conda environment:

```
conda activate my_env
```

- Export the specifications of your conda environment:

```
conda env export > environment.yml
```

[3] Note, that `-n` is the short version of the `--name` flag

9. REPRODUCIBILITY

Result (abbreviated to fit on the slide):

```
name: my_env
channels:
  - defaults
dependencies:
  - blas=1.0=mkl
  - bottleneck=1.3.2=py37h2a96729_1
  - ...
  - numpy=1.21.2=py37hfca59bb_0
  - numpy-base=1.21.2=py37h0829f74_0
  - openssl=1.1.1l=h2bbff1b_0
  - packaging=21.3=pyhd3eb1b0_0
  - pandas=1.3.4=py37h6214cd6_0
  - pip=21.2.4=py37haa95532_0
  - pyparsing=3.0.4=pyhd3eb1b0_0
  - python=3.7.11=h6244533_0
  - python-dateutil=2.8.2=pyhd3eb1b0_0
  - pytz=2021.3=pyhd3eb1b0_0
  - scikit-learn=1.0.1=py37hf11a4ad_0
  - scipy=1.7.1=py37hbe87c03_2
  - ...
prefix: C:\Users\ri85vex\Miniconda3\envs\my_env
```

9. REPRODUCIBILITY

- *Note 1:* As you can see, this also includes all sorts of packages that are automatically installed when creating an environment
- *Note 2:* We observe some cryptic stuff after the version of each package
- *Note 3:* Those packages installed via pip are **also handled by this file** (see next slide)
- *Note 4:* The `prefix` is ignored when using the `.yml`-file for creation. So you can simply delete it after the export.

9. REPRODUCIBILITY

- Install some package via `pip`:

```
pip install matplotlib
```

- Result (abbreviated to fit on the slide):

```
name: my_env
channels:
  - defaults
dependencies:
  - blas=1.0=mkl
  - bottleneck=1.3.2=py37h2a96729_1
  - ca-certificates=2021.10.26=haa95532_2
  - certifi=2021.10.8=py37haa95532_0
  - icc_rt=2019.0.0=h0cc432a_1
  - intel-openmp=2021.4.0=haa95532_3556
  - ...
  - pip:
    - cycler==0.11.0
    - fonttools==4.28.5
    - kiwisolver==1.3.2
    - matplotlib==3.5.1
    - pillow==9.0.0
prefix: C:\Users\ri85vex\Miniconda3\envs\my_env
```

9. REPRODUCIBILITY

- Using the “–from-history“ flag

```
conda env export --from-history > environment.yml

```

- .. allows you to create a reduced version of the `.yml`-file containing only the packages (+ version) you explicitly installed (**via conda**):

```
name: my_env
channels:
  - defaults
dependencies:
  - scikit-learn
  - numpy
  - python=3.7
  - pandas
prefix: C:\Users\ri85vex\Miniconda3\envs\my_env

```

9. REPRODUCIBILITY

- Export specifications of the `pip` packages:

```
pip freeze > requirements.txt

```

- Can be installed in a conda environment via:

```
pip install -r requirements.txt

```

- **But**: Requiring others to execute these two steps is cumbersome!

9. REPRODUCIBILITY

- Best practice: Create `.yml`-file manually

```
name: my_env
channels:
  - defaults
dependencies:
  - python=3.7.11
  - numpy=1.21.2
  - pandas=1.3.4
  - scikit-learn=1.0.1
  - pip=21.2.4
  - pip:
    # works for regular pip packages
    - matplotlib==2.0.0
    # also works for whole requirements-files:
    - -r requirements.txt

```

- Finally: Create environment from `.yml`-file:

```
conda env create -f environment.yml

```