Python

A quickstart into the very basics

Get to know your user environment

Thank You

- https://github.com/gjbex/training-material/tree/master/Python
- *Whirlwind Tour of Python* by Jake VanderPlas (O'Reilly). Copyright 2016 O'Reilly Media, Inc., 978-1-491-96465-1. https://www.oreilly.com/programming/free/files/a-whirlwind-tour-of-python.pdf
- University of Virginia, Advanced Research Computing Services, Python Quickstart https://arcs.virginia.edu/python-quickstart
- http://www.cs.cornell.edu/courses/cs1110/2018sp/
- https://fabienmaussion.info/scientific_programming/html/00-Introduction.html
- https://justinbois.github.io/bootcamp/

See also

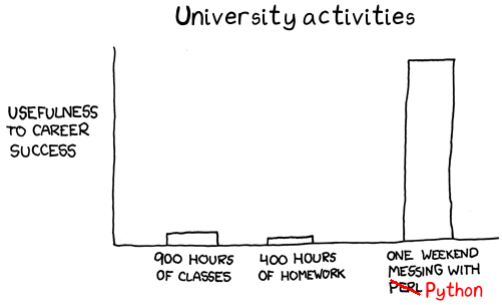
- https://www.southampton.ac.uk/~fangohr/teaching/python/book.html
- https://www.math.ubc.ca/~pwalls/math-python/
- http://troll.cs.ua.edu/ACP-PY/index.html
- https://data-flair.training/blogs/python-lambda-expressions/
- http://pages.physics.cornell.edu/~myers/teaching/ComputationalMethods/GettingStarted.html
- https://anh.cs.luc.edu/python/hands-on/3.1/handsonHtml/index.html
- https://www2.cs.duke.edu/courses/spring18/compsci101/index.php
- https://github.com/parrt/msan501
- https://docs.python-guide.org/intro/learning/

Tutorials

- https://www.python.org/about/gettingstarted/
- https://realpython.com/
- https://www.learnpython.org/

- Cheat sheets
- https://www.datacamp.com/community/data-science-cheatsheets

Why Programming



https://fabienmaussion.info/scientific_programming/img/00_messing_python.png

Why programming?

- Programming is an integral part of research
- Programming occurs on different levels:
  - Write small scripts,
  - Write complete projects,
  - Or need a good understanding of what a software packages does
- All programming languages offer to a certain extend the same building blocks
  - Understand the basic building blocks
  - Decompose your problem to fit those blocks

Programming?

- It may be (almost) impossible to solve a problem by executing commands at the command prompt.
- What is needed? A **sequence** of **precise instructions** that, once performed, will complete a **specific task**.
- Computer programs can’t do that many things, they can:
  - Assign values to variables (memory locations).
  - Make decisions based on comparisons.
  - Repeat a sequence of instructions over and over.
  - Call subprograms.

Programming language

- There are many programming languages, with changing popularity
- Check the Tiobe Index: https://www.tiobe.com/tiobe-index/
- Consider:
  - it is suited to the problem at hand?
  - is there an active community?
  - is it any good for the job market?

Key concepts in programming

- Check Isaac Computer Science: https://isaaccomputerscience.org/topics/programming_concepts?examBoard=all&stage=all
- Instructions / Basic Syntax
- Data Types
  - Classification of the type of data being stored or manipulated within a program.
  - Data types are important because they determine the operations that can be performed on the data.
- Variables
  - Named container, held by the computer in a memory location.
  - Has a unique identifier (name) that refers to a value.
- Input / Output

Key concepts in programming

- Operators
  - Arithmetic
  - Comparison
  - Logical
- Sequence:
  statements are written one after another, will be executed one statement at a time in the order that the statements are written in.
- Selection:
  execute lines of code only if a certain condition is met.
- Iteration (loop):
  repeat a group of statements .
- Subprogram (function):
  is a named sequence of statements, can be repeatedly “called” from different places in the program

And there will be errors…

- Syntax error
  - A mistake against the language rules
  - Program will not run and will return an error message
- Runtime error
  - Usually due to some missing variables, modules,…
- Semantic error
  - A mistake in the reasoning
  - Program is not executing as intended / expected

Python: setting the scene

get comfortable within the Python universe

What is the playfield?

- *The best way to learn a language is to "get your hands dirty"*

1
- Get data (simulation, experiment, etc.)

2
- Manipulate and process data

3
- Visualize results
  - quickly to understand,
  - high quality figures, for reports or publications

What is Python?

- From www.python.org: "Python is an interpreted, object-oriented, high-level programming language with dynamic semantics. Its high-level built in data structures, combined with dynamic typing and dynamic binding, make it very attractive for Rapid Application Development, as well as for use as a scripting or glue language to connect existing components together. Python's simple, easy to learn syntax emphasizes readability and therefore reduces the cost of program maintenance."
- Python is a general purpose programming language used for a huge variety of purposes. It's user community is growing rapidly! (https://stackoverflow.blog/2017/09/06/incredible-growth-python/)

What is Python?

- a **general purpose interpreted** programming language.
- a language that supports multiple approaches to software design, principally **structured** and **object-oriented** programming.
- provides **automatic memory management** and **garbage collection**
- **dynamically** typed.

Why Python?

- Python is quick to program in (*explorative programming*)
- Python is popular in research, and has lots of libraries for science
  Widely used – extensive capabilities, documentation, and support
- Python interfaces well with faster languages
- Python is free
- Cross-platform (Windows, Mac, Linux)
- Access to advanced math, statistics, and database functions
- *Why write programs for research?*
  - Scripted research can be tested and reproduced
  - Programs are a rigorous way of describing data analysis for other researchers, as well as for computers. By sharing codes, which are much more easy for a non-author to understand than spreadsheets

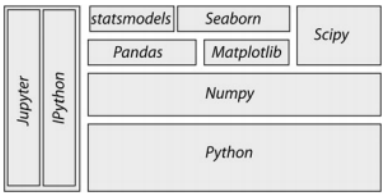
http://github-pages.ucl.ac.uk/rsd-engineeringcourse/ch00python/00pythons.html

Popular Python?

- Popular programming languages?
- https://www.tiobe.com/tiobe-index/
- What is Python used for?
- https://www.jetbrains.com/research/devecosystem-2018/python/

Python ecosystem

- Large and active ecosystem
- Core Python
  - Standard libraries
  - third-party packages:
    - *NumPy* for manipulation of homogeneous array-based data,
    - *Pandas* for manipulation of heterogeneous and labeled data,
    - *SciPy* for common scientific computing tasks,
    - *Matplotlib* for publication-quality visualizations,
    - *IPython* for interactive execution and sharing of code, etc. *Python versions*



Python versions

- Current 3.x
  - More clean than 2.x
  - Python 3.x introduced some backwards-incompatible changes to the language, so code written for 2.7 may not work under 3.x and vice versa.
  - Almost all Python libraries supported
- Version 2.7.x
  - Last of the 2.x releases
  - Many Python 3.x features have been retrofitted
  - All libraries support it

Note: in-application scripting may be stuck at Python 2.7!

Python 2 countdown: https://pythonclock.org/

- *Taken from GJ Bex*

User Environment

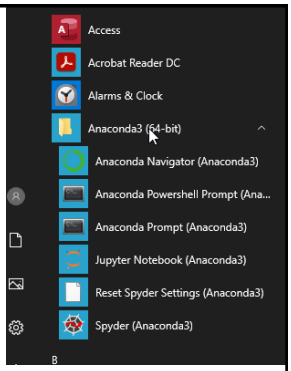
Running Python Code

- https://docs.anaconda.com/anaconda/user-guide/getting-started/
- https://realpython.com/run-python-scripts/
- https://plot.ly/python/ipython-vs-python/
- https://yihui.name/en/2018/09/notebook-war/
- https://www.theatlantic.com/science/archive/2018/04/the-scientific-paper-is-obsolete/556676/
- https://fangohr.github.io/blog/installation-of-python-spyder-numpy-sympy-scipy-pytest-matplotlib-via-anaconda.html

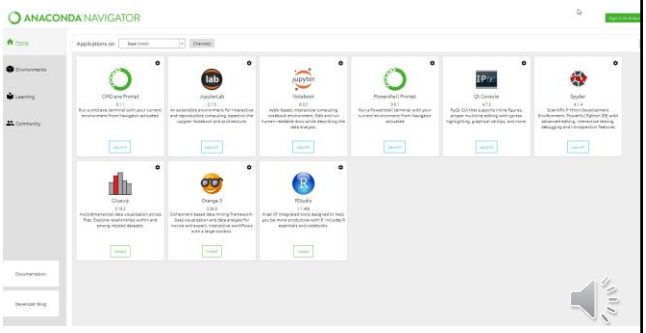
Making it work

- Write the code
  - choose a good editor (or integrated development environment - IDE)
    - featuring color coding, syntax checks, ...
  - code is just a text file
- Convert to machine code
  - make sure that you have the right interpreter (or compiler) available
- Run the code
  - run on the command line
  - run in a script mode (Python)
  - run in IDE or in Jupyter notebooks

Where to start?



- 2 elements needed for programming in Python:
  - writing and editing Python code
  - running that code in an interpreter
- Choose a platform - primary ways to run Python code:
  1. Terminal
     1. Python interpreter
     2. IPython interpreter
     3. Running scripts
  2. IDE
     - Spyder
  3. Jupyter notebook.



How do I get Python?

- core Python package
  - https://www.python.org/downloads/
  - easy to install but probably *not* the way to go.
- Using a distribution simplifies the process of setting up your python environment, includes core Python, necessary data packages, and integrates useful tools (IDE's, notebooks, etc)
  Python Distributions:
  - Anaconda distribution
    - https://www.anaconda.com/
    - Download: https://www.anaconda.com/distribution/
  - WinPython (https://winpython.github.io/)
    - Windows specific data science distribution

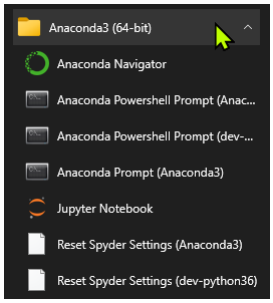
Anaconda installation

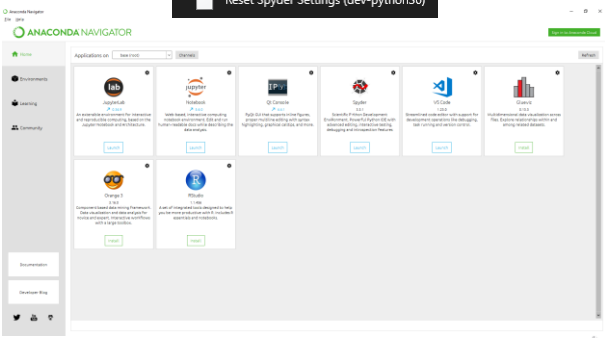
- Installation documentation:
  https://docs.anaconda.com/anaconda/install/
- Downloading and installing Anaconda is simple.
- Download the installer – follow the wizard

- Anaconda installation – managed PC - Windows
- Install as Admin under C:\Workdir\MyApps\Anaconda3

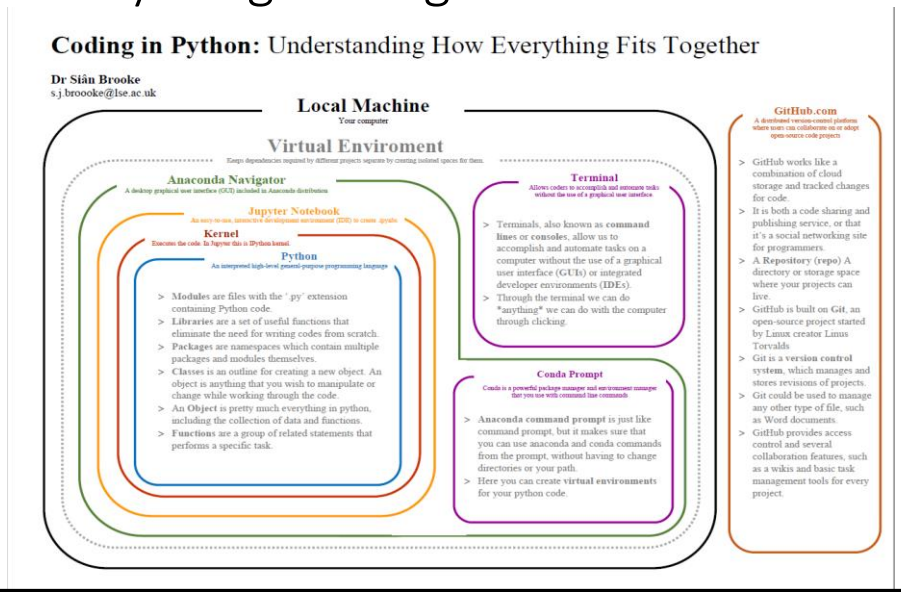
Anaconda Navigator

- https://docs.anaconda.com/navigator/index.html
- The Navigator is a main landing page for working with your python environment.
- Launch editors (spyder, jupyter notebook, etc.) to develop python code
- Manage (install packages, etc.) the python environment





How everything fits together



https://www.sianbrooke.co.uk/dr-brookes-blog/coding-in-python-understanding-how-everything-fits-together

Check this out

- https://www.sianbrooke.co.uk/dr-brookes-blog/coding-in-python-managing-packages-with-conda-and-pip
- https://www.earthdatascience.org/courses/intro-to-earth-data-science/python-code-fundamentals/use-python-packages/introduction-to-python-conda-environments/
- Quick intro into
  - Packages, modules
  - Why working with environments: keep dependencies
  - Installing with conda, pip

Why Environments?

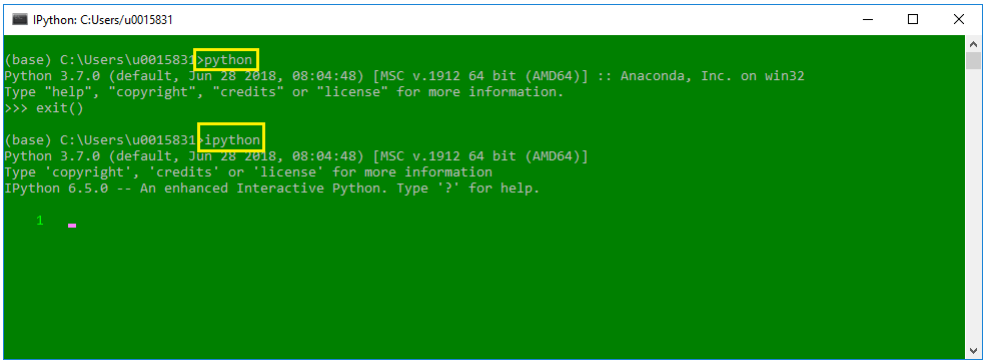
- A major barrier to reproducibility in the world of computational science is package dependencies.
- When sharing code, we want to be able to setup a computer ecosystem that is exactly the same as when we were developing the code. This is where environments come in.

Python interpreter

https://realpython.com/run-python-scripts/

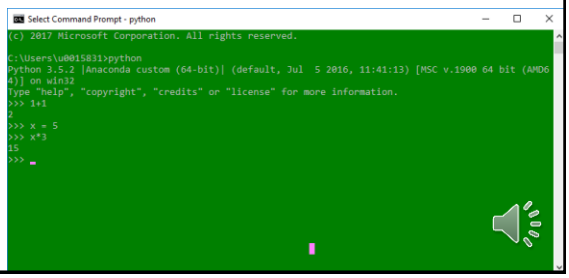
Python interpreter

- The interpreter is able to run Python code in two different ways:
  - As a piece of code typed into an interactive session
  - As a script or module



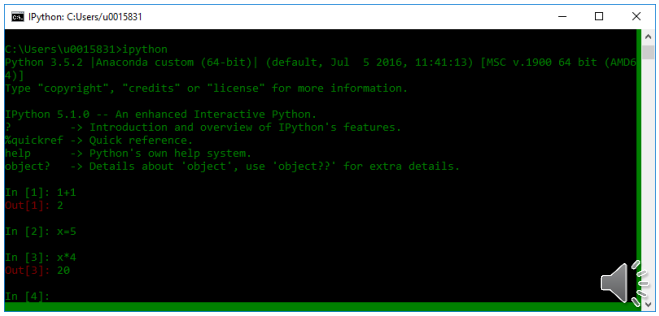
Python interpreter

- The most basic way to execute Python code is line by line within the Python interpreter (interactive session).
- The Python interpreter can be started by typing: `python`
  - Terminal on Mac OS X and Unix/Linux systems,
  - (anaconda)Command Prompt application in Windows
  - >>> by default
  - help() starts the helper environment



IPython interpreter

- Enhanced Interactive shell
- Enhancements to the basic Python interpreter: `ipython`
- https://stackoverflow.com/questions/12370457/what-is-the-difference-between-python-and-ipython



IPython interpreter

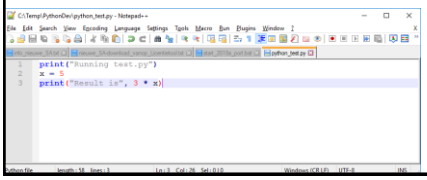
- IPython is an enhanced version of python that makes interactive python more productive.
  - Tab autocompletion (on class names, functions, methods, variables)
  - More explicit and color-highlighted error messages
  - Better history management
  - Basic UNIX shell integration (run simple shell commands such as cp, ls, rm, cp, etc. directly from the IPython command line)
  - Nice integration with many common GUI modules (PyQt, PyGTK, and tkinter)
  - https://www.quora.com/What-is-the-difference-between-IPython-and-Python-Why-would-I-use-IPython-instead-of-just-writing-and-running-scripts

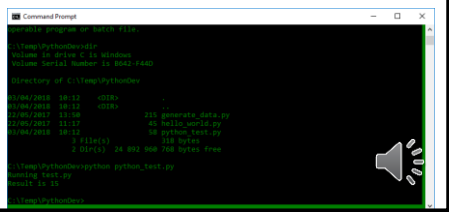
Magic commands

- https://ipython.readthedocs.io/en/stable/interactive/magics.html
- An enhancement in IPython known as magic commands
- Know more: `magic` command.
  Information of a specific magic function is obtained by `%magicfunction?`
- Designed to solve various common problems in standard data analysis. There are two types of magic commands –
- 2 types
  - Line magics
    - They are similar to command line calls. They start with % character. Rest of the line is its argument passed without parentheses or quotes.
  - Cell magics
    - They have %% character prefix. Unlike line magic functions, they can operate on multiple lines below their call.

Python scripts

- Programs: save code to file, and execute it all at once.
  - Script: A plain text file containing Python code that is intended to be directly executed by the user
  - By convention, Python scripts are saved in files with a `.py` extension.





Run Python script

Linux

- Write script in editor
- Run script using Python interpreter
  `python hello_world.py`
- Make script executable
- `chmod u+x hello_world.py`
- Run script directly
  `./hello_world.py`

Windows

- Write script in editor
- Run script using Python interpreter
  `python hello_world.py`
- Run script directly
  `hello_world.py`

Python scripts

- Linux

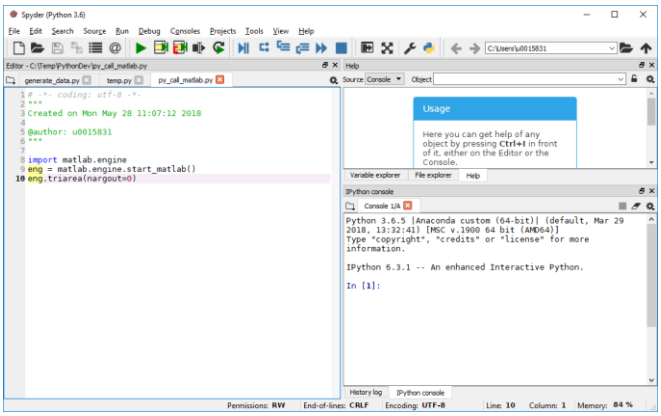
`#!/usr/bin/env python`

  - determines the script's ability to be executed like a standalone executable without typing `python` in the terminal
  - double clicking it in a file manager (when configured properly).

Spyder

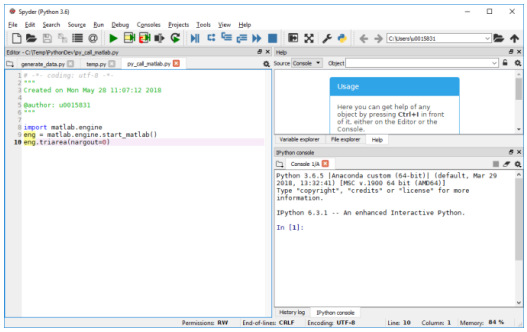
IDE: Spyder

- Integrate different aspects of programming and running code.
- SPyDER: "*Scientific Python Development EnviRonment*" https://www.spyder-ide.org/
- Several tools in one integrated environment (cfr MATLAB desktop)
  - a code editor
  - IPython interpreter / console
  - variable inspector
  - control icons
- Documentation: https://docs.spyder-ide.org/current/index.html



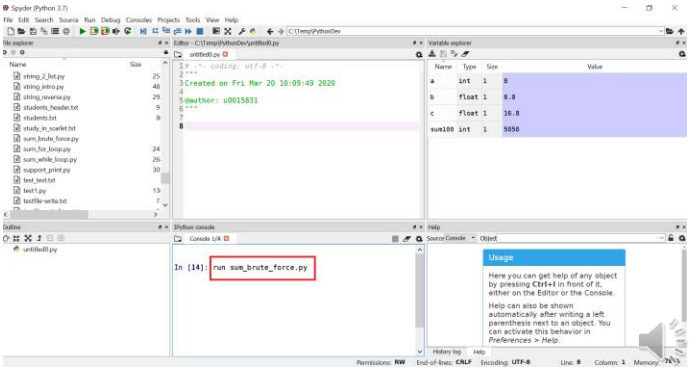
IDE: Spyder

- Spyder for code development.
  - Start from Anaconda Navigator
  - Command window: `spyder`
- Magic commands apply
  - Clear Console:
    - `%cls`
  - Clear all variables from Variable Explorer (reset the namespace):
    - `%reset`
  - With `automagic on`, % prefix not needed



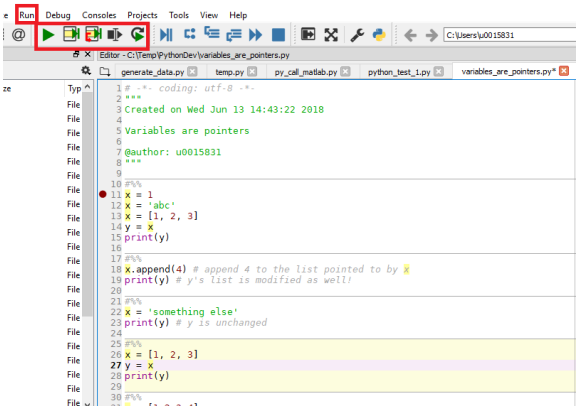
Running scripts in Spyder console

- Run a .py file from the console
  - `run script.py`
- Tab autocompletion works!



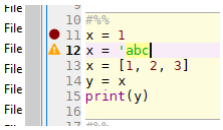
Running scripts in Spyder

- Run scripts either with the green arrow icons or through the Run menu. *Run/green arrow* runs the entire script.
- *Run selection or current line* will run a highlighted portion of the script.
- Create **cells** by enclosing chunks of code with lines consisting of
  #%%
  Run cell/green arrow with a box runs the cell.
- *File: first_prog_1.py*



Running scripts in Spyder

- A yellow triangle beside a line indicates a syntax error or potential problem.
- Tab completion for names familiar to it. It can show a list of members of a package for your selection, and when you have chosen a function it can show you a list of its arguments.



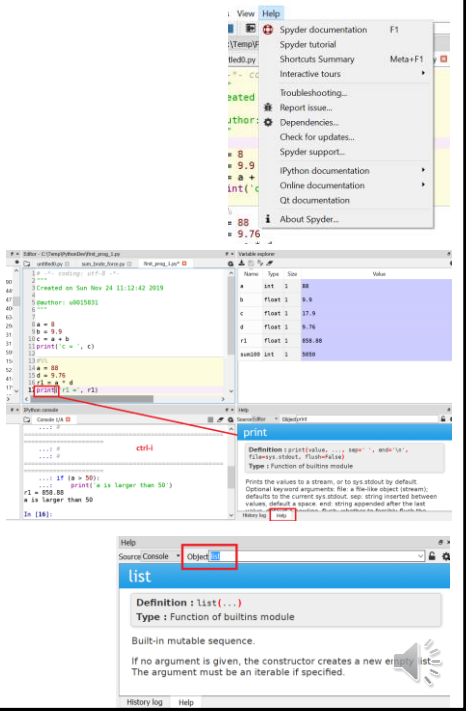
Spyder Help

- Help on Spyder from Help menu
- Help related to Python
  - Select a command and press `ctrl-I`
    - Information opens in help window
  - Enter object in help window
- help(command) in console

```
In [18]: help(print)
Help on built-in function print in module builtins:

print(...)
    print(value, ..., sep=' ', end='\n',
file=sys.stdout, flush=False)

    Prints the values to a stream, or to sys.stdout by
default.
    Optional keyword arguments:
```



Jupyter

getting_started_jupyter.ipynb

Jupyter notebook

- A nice idea popularized by Mathematica is a “notebook” interface, where you can run and re-run commands
- In the notebook, you can easily mix code with comments, and mix code with the results of that code; including graphics, …
- https://realpython.com/jupyter-notebook-introduction/
- https://docs.anaconda.com/ae-notebooks/4.2.2/user-guide/basic-tasks/apps/jupyter/
- https://towardsdatascience.com/5-reasons-why-jupyter-notebooks-suck-4dc201e27086

Jupyter notebook

- Excellent for
  - Explorative programming
  - Data exploration
  - Communication, especially across domains
- Problems
  - What was (re-)executed, what not?
  - Version control?

- https://github.com/gjbex/training-material/blob/master/Python/python_intro.pptx

Jupyter notebook vs Jupyterlab

- Basically, Jupyterlab is the new generation user interface for executing and editing notebook documents, similar to the Jupyter notebook.
- Jupyterlab is more advanced and offers more features,
- It gives a more IDE-like experience.

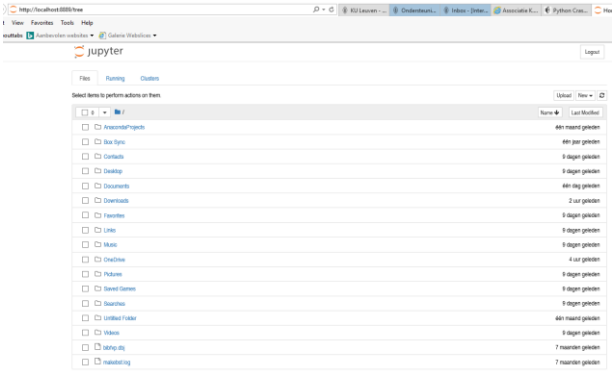
- Beginner: start with Jupyter notebook

Jupyter: how to start

- Anaconda Navigator:
  - Start menu
  - Launch jupyter
- Anaconda prompt
  - open terminal and navigate to the **directory** where you would like to save your notebook
  - `jupyter notebook`

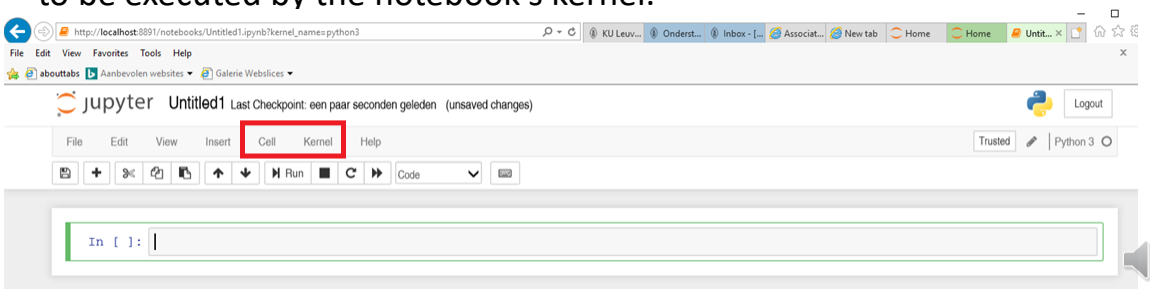
Jupyter

- Notebook Dashboard, specifically designed for managing your Jupyter Notebooks.
- Use it as the launchpad for exploring, editing and creating your notebooks.
- Start the dashboard on any system via the command prompt (or terminal on Unix systems): `jupyter notebook`
  The current working directory will be the start-up directory.



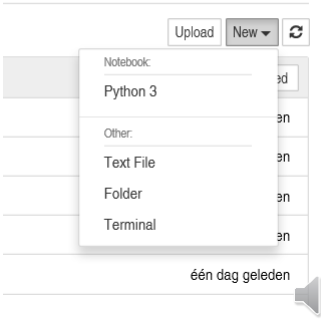
Jupyter notebook

- Jupyter is essentially an advanced word processor.
- A kernel is a "computational engine" that executes the code contained in a notebook document.
- A cell is a container for text to be displayed in the notebook or code to be executed by the notebook's kernel.



Jupyter notebook

- Browse to the folder in which you would like to create your first notebook,
- Click the "New" drop-down button in the top-right and
- Select "Python 3" (or the version of your choice).

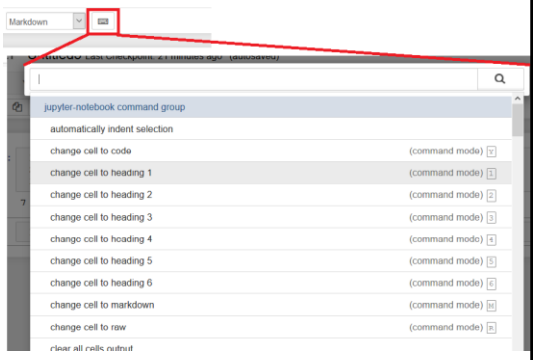


Jupyter: basics of editing

- Jupyter notebook: sequence of cells
  - Code
    - Label “In [ ]” in front of the code
    - a * will appear when executing
    - replaced by a number that always increases by one with each cell execution. This allows for keeping track of the order in which the cells in the notebook have been executed.
  - Markdown
- Important shortcut: ctrl+Enter (execute cell)
- Color code
  - Blue bar on the left: active cell in command mode
  - Click in cell, changes in edit mode – Green bar
- Jupyter will periodically autosave the notebook

Jupyter: basics of editing

- try to know the basic shortcuts
- **Command mode** shortcuts:
  - Basic navigation: enter, **shift-enter**, up/k, down/j
  - Saving the notebook: s
  - Change Cell types: y, m, 1-6, t
    - m to change the current cell to Markdown,
    - y to change it back to code
  - Cell creation: a, b
    - a to insert a new cell above the current cell,
    - b to insert a new cell below
  - Cell editing: x, c, v, d, z
    - c copy selected cells
    - x cut selected cells
    - v paste copied cells
    - d + d (press the key twice) to delete the current cell
    - z undo cell deletion



Jupyter: some tips

- Run a notebook on the command line with `ipython`
- Jupyter notebook tips https://www.dataquest.io/blog/jupyter-notebook-tips-tricks-shortcuts/
- https://www.dataquest.io/blog/jupyter-notebook-tutorial/
- https://jupyter4edu.github.io/jupyter-edu-book/
- https://reproducible-science-curriculum.github.io/workshop-RR-Jupyter/
- Change the default startup directory
  - https://stackoverflow.com/questions/35254852/how-to-change-the-jupyter-start-up-folder
- Change the default browser
  - https://support.anaconda.com/customer/en/portal/articles/2925919-change-default-browser-in-jupyter-notebook