Scientific Programming in Python

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster Universitario en Ingeniería Industrial

Departamento de Automática

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ISG

Objectives

1. Motivate the need of efficient matrix representations.
2. Introduce some Python scientific tools.
3. Handle data representations in Python.
4. Basic data visualization with Python.
5. Provide a background for scientific programming.

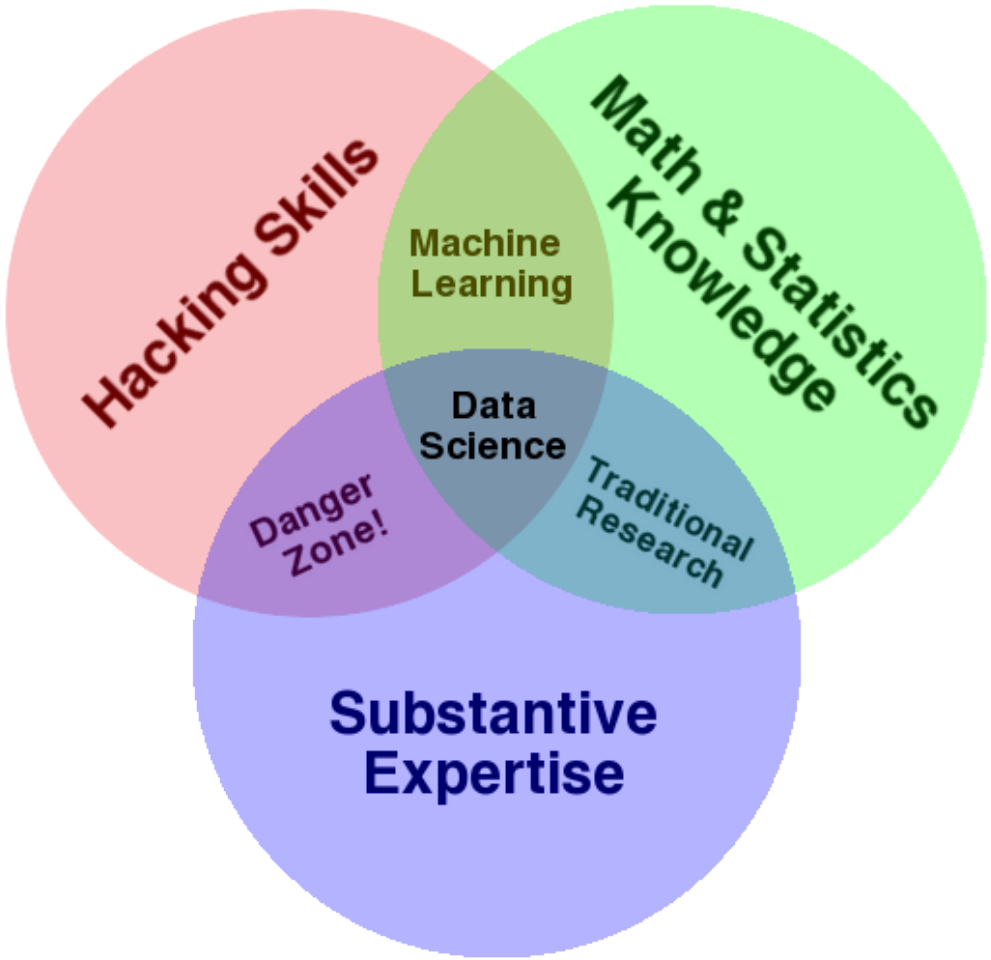
Bibliography

Jake VanderPlas. *Python Data Science Handbook*. Chapters 1, 2, 3 and 4. O'Reilly. (Link).

Table of Contents

Overview

Data Science



Data Science

The data scientist tookit (I)

Data science is about manipulating data

- Need of specialized tools
- Two main languajes: R and Python

Python is a general purpose programming language

- Easy integration
- Huge ecosystem of packages and tools

Need of data-oriented tools

- Features provided by third-party tools

Data Science

The data scientist tookit (II)

Tool	Type	Description
`iPython`	Software	Advaced Python interpreter
`Jupiter`	Software	Python notebooks (Python interpreter)
`Numpy`	Package	Efficient array operations
`Pandas`	Package	Dataframe support
`Matplotlib`	Package	Data visualization
`Seaborn`	Package	Data visualization with dataframes
`Scikit-learn`	Package	AI/ML package for Python

Data Science

Anaconda

All those tools are packaged in `Anaconda`

- Python distribution for Data Science

Anaconda provides `Spyder`

- Python IDE designed for Data Science

Other tools provided by Anaconda

- Conda: Packages management tool
- TensorFlow: Deep Learning
- Many others

Data Science

Python IDEs for Data Science (I)

iPython

iPython = Interactive Python

- Extended funcionality
- Enhanced UI
- External editor

Running iPython:

```
$ ipython
```

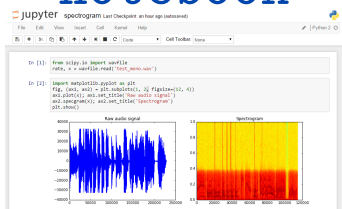
Jupyter

Python notebooks

- Web-based IDE
- Documentation
- Integration with GitHub
- Uses iPython

Running Jupyter:

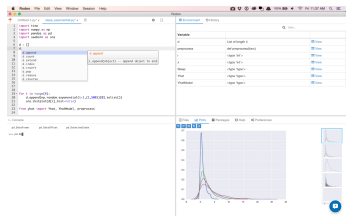
```
$ jupyter notebook
```



Rodeo

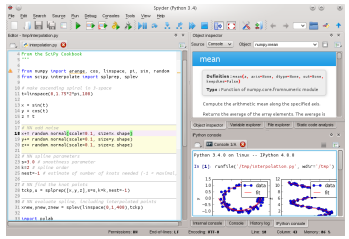
Python version of RStudio

- Good for R developers
- Not included in Anaconda
- Uses iPython



Spyder

Matlab-like IDE



Data Science

Python IDEs for Data Science (II)

Exercises

Write a Python script that shows the multiplication table of the number 5. Write the script using each one of the following environments:

1. iPython + text editor of your choice.
2. Jupiter.
   - Bonus track: Publish the notebook in GitHub.
3. Spyder.
4. Rodeo.

iPython

Basics (I)

In regular Python ...

- most objects come with a docstring attribute
- docstring accesible thorugh `help()`

iPython provides `?', a shortcut to `help()`

- `len?`, `list?`, `list.append?`
- Try to type just `?'

Easy access to source code with `??'

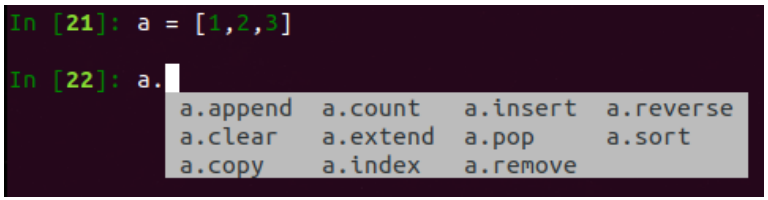
- Does not work with most buildin functions!

iPython

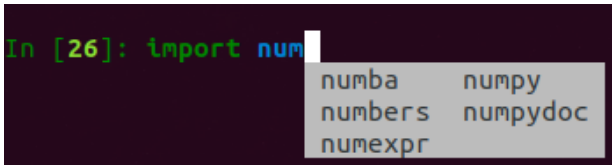
Basics (II)

Press `<tab>` to complete almost everything

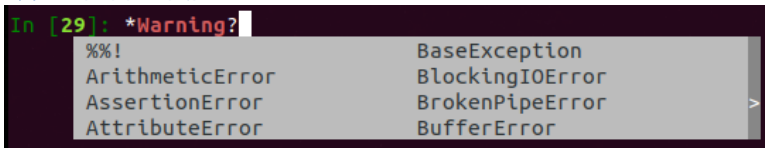
- Object contents



- Packages



- Wildcards



iPython

Basics (III): Keyboard shortcuts

Navigation

Keystroke	Action
`Ctrl-a`	Move cursor to the beginning of the line
`Ctrl-e`	Move cursor to the end of the line
`Ctrl-b`	Move cursor back one character
`Ctrl-f`	Move cursor forward one character

History

Keystroke	Action
`Ctrl-p` (↑)	Previous command
`Ctrl-n` (↓)	Next command
`Ctrl-r`	Reverse-search

Text entry

Keystroke	Action
`Ctrl-d`	Delete next character in line
`Ctrl-k`	Cut text from cursor to end of line
`Ctrl-u`	Cut text from beginning of line to cursor
`Ctrl-y`	Yank (paste) previously cut text

iPython

iPython magic commands

Magic commands: iPython extension of Python syntax

- Not valid in regular Python
- Provides handly features
- Widely used in DS and ML

Two flavours

- % prefix: Line magics - single line
- % % prefix: Cell magics - several lines

Help available

- `%magic`: Magic commands
- `%lsmagic`: List of magic commands

iPython

Pasting code blocks: %paste and %cpaste

Pasting code in Python is troublesome

- %paste: Paste one time
- %%cpaste: Paste several times

```
def donothing(x):
    return x
```

%paste

```
In [20]: %paste
   def donothing(x):
    return x

## -- End pasted text --
```

%cpaste

```
In [25]: %cpaste
Pasting code; enter '--' alone on the line
to stop or use Ctrl-D.
:       def donothing(x):
            return x:
:--
```

iPython

Running external code: %run and %timeit

%run: Execute script

- Many optional arguments
- Checkout %run?

```
In [40]: %run donothing.py

In [41]: donothing(10)
Out[41]: 10
```

%timeit: Computes execution time

- Executes a single line
- Automatic adjustment of runs
- Shows basic statistics

```
In [33]: %timeit [n ** 2 for n in range(200)]
71.6 µs ± 1.84 µs per loop
(mean ± std. dev. of 7 runs, 10000 loops each)

In [34]: %timeit [n ** 2 for n in range(2000)]
753 µs ± 16.2 µs per loop
(mean ± std. dev. of 7 runs, 1000 loops each)
```

%%timeit: Several lines

iPython

Input and output history (I)

iPython stores its history as objects

- `In`: Input commands
  - List storing commands
- `Out`: Commands output
  - Dictionary storing outputs
  - Not all commands have outputs

```
In [1]: import math
In [2]: math.sin(2)
Out[2]: 0.9092974268256817
In [3]: math.cos(2)
Out[3]: -0.4161468365471424
In [4]: Out[2] ** 2 + Out[3] ** 2
Out[4]: 1.0
```

iPython

Input and output history (II)

Fast access to history: Underscore (_)

- Variable containing the last output
- Example: `print(_)`

Double and triple underscores

- Example: `print(__)`
- Example: `print(___)`

Trick: Shortcut to access (_n)

- Out[n] = _n, with n=number
- Example: `print(_2)`

Magic command to show history

- `%history`

Supressing command output (;)

- Example: `4 * 2;`

iPython

iPython shell commands

iPython provides easy interaction with the shell

- Execution of shell commands from iPython
- Use prefix `!'
- Example: `!ls`, `!pwd`

Save shell output in Python variables

- Example: `files = !ls`

Use Python variables in shell

- Example: `!echo {files}`

iPython

Automagic

Problems with some shell commands

```
In [23]: !pwd
/repositorios/pythonCourse
In [24]: !cd ..
In [25]: !pwd
/repositorios/pythonCourse
```

Some magic commands here to help

- `%cd`, `%ls`, `%mkdir`, `%pwd`, ...

Those magics are regularly used ...

- ... so common that % is no longer required (automagic)
- Working with iPython is almost like working with a Unix-like shell

Automagic commands

`cat`, `cp`, `env`, `ls`, `man`, `mkdir`, `more`, `mb`, `pwd`, `rm` and `rmdir`