

# Scientific Programming in Python crash course

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## Objectives

1. Introduce scientific programming problems
2. Efficient matrix computations in Python
3. Visualize data in Python

## Bibliography

Jake VanderPlas. Python Data Science Handbook. Chapter 1. O'Reilly. (Link).

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# The data scientist toolkit

## Motivation

Data science is about manipulating data

- Need of specialized tools
- Two main languages: 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

# The data scientist toolkit

## Overview

Tool	Type	Description
conda	Software	Python environments and package management
iPython	Software	Advanced Python interpreter
Jupyter	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

# The data scientist toolkit

## Anaconda

Most of those tools are packaged in *Anaconda*

- Python distribution for Data Science
- Environment management for Python
- Package management system

Anaconda provides *conda*

- Packages management tool
- Environment management for Python

In addition, Anaconda provides *Spyder*

- Python IDE designed for Data Science



# The data scientist toolkit

## Conda crash introduction

### Conda environment for Data Science

1. `conda create --name ml seaborn=0.9.0`
2. `source activate ml`
3. `conda install ipython`
4. `conda install nb_conda`
5. `conda install scikit-learn`

List environments:

```
conda info --envs
```

Activate environment:

```
source activate <env>
```

Install package:

```
conda install <package>
```

List packages:

```
conda list
```

Exit environment:

```
conda deactivate
```

# NumPy

## Understanding data types in Python (I)

### Static typing

```
/* C code */  
int result = 0;  
for(int i=0; i<100; i++){  
    result += i;  
}
```

- Data types must be declared
- Data types cannot change
- Error detection in compilation
- Variables names are, basically, labels

### Dynamic typing

```
# Python code  
result = 0  
for i in range(100):  
    result += i
```

- Data types are not declared
- Data types can change
- Error detection in run-time
- Variables are complex data structures (even for simple types)



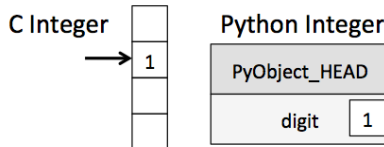
# NumPy

## Understanding data types in Python (II)

Dynamic typing must be implemented somewhere ...

Python 3.4 source code

```
struct _longobject {  
    long ob_refcnt;  
    PyTypeObject *ob_type;  
    size_t ob_size;  
    long ob_digit[1];  
};
```



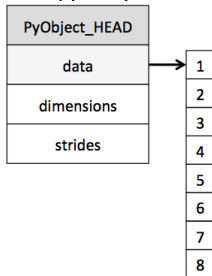
# NumPy

## Understanding data types in Python (III)

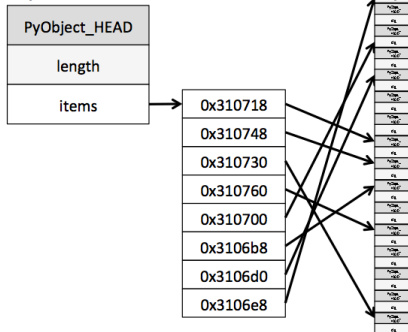
A Python list may contain different types

```
In [1]: L3 = [True, "2", 3.0, 4]
...: [type(item) for item in L3]
Out[1]: [bool, str, float, int]
```

NumPy Array



Python List



# NumPy

## Understanding data types in Python (IV)

Standard Python data types are powerful and flexible

- Flexibility has a price: Reduced performance
- Not an big issue in generic programming
- A big issue in scientific programming
- We require efficient data manipulation mechanisms: NumPy

NumPy: Python package for numeric computation

- Efficient array implementation
- Fast mathematical functions
- Random numbers generation
- Static data types: Less flexibility

Most Python modules for AI/ML depend on NumPy, in particular

- Pandas (dataframes), Scikit-learn (ML), Seaborn (data visualization)

# NumPy

## Introduction

NumPy must be imported in order to be available

- You can use `np?` or `np.<TAB>`

The main component of NumPy is `ndarray`

- Python object
- Efficient matrix representation
- Homogeneous elements

### Convention

```
import numpy as np
```

```
In [1]: array = np.array  
        ([1, 2, 3])  
In [2]: array  
Out [1]: array([1, 2, 3])  
In [3]: array = np.array  
        ([[1, 2], [3, 4]])
```

# NumPy

## NumPy array attributes

Ndarray objects expose several attributes

- **ndim**: Dimensions
- **shape**: Size of each dimension
- **size**: Number of elements
- **dtype**: Data type
- **itemsize**: Size of each element (in bytes)
- **nbytes**: Size of the array (in bytes)

```
x = np.random.randint(10, size=(3, 4))
print("x ndim: ", x.ndim)
print("x shape:", x.shape)
print("x size: ", x.size)
print("dtype:", x.dtype)
print("itemsize:", x.itemsize)
print("nbytes:", x.nbytes)
```

# NumPy

## NumPy data types

Python is implemented in C

- Data types in NumPy are based on those in C

Two styles to declare types

- String:  
`np.zeros(10,  
dtype='int16')`
- NumPy object:  
`np.zeros(10,  
dtype=np.int16)`

DATA TYPE	DESCRIPTION
<code>bool_</code>	Boolean (True or False) stored as a byte
<code>int_</code>	Default integer type
<code>intc</code>	Identical to C
<code>intp</code>	Integer used for indexing
<code>int8</code>	Byte
<code>int16</code>	Integer
<code>int32</code>	Integer
<code>int64</code>	Integer
<code>uint8</code>	Unsigned integer
<code>uint16</code>	Unsigned integer
<code>uint32</code>	Unsigned integer
<code>uint64</code>	Unsigned integer
<code>float_</code>	Shorthand for float64
<code>float16</code>	Half precision float
<code>float32</code>	Single precision float
<code>float64</code>	Double precision float
<code>complex_</code>	Shorthand for complex128
<code>complex64</code>	Complex number
<code>complex128</code>	Complex number

# NumPy

## NumPy notebook

### NumPy notebook

([Link to notebook](#))

# Pandas

## Introduction

A DS/ML workflow needs more features

- Missing data
- Data input
- Operations on groups
- Label columns and rows

Pandas provides all those features, and more

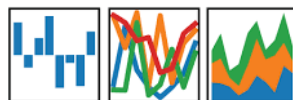
- Pandas = **PAN**el **DA**ta **S**ystem
- Built on NumPy's ndarray
- Provides **dataframes**

Pandas provides two main objects

- **Series** and **DataFrame**

# pandas

$$y_i t = \beta' x_{it} + \mu_i + \epsilon_{it}$$



### Convention

```
import numpy as np
import pandas as pd
```



# Pandas

## The Pandas Series object (I)

A **Series** is a one-dimensional array of indexed data

- NumPy arrays indices are implicit (i.e. its position)
- Series indices are explicit, and can be any type

INDEX	VALUES
'a'	0.25
'b'	0.5
'c'	0.75
'd'	0.99

Two attributes

- **values**: ndarray
- **index**: `pd.Index` object

Two indices

- Implicit: Regular index
- Explicit: Custom index

```
data = pd.Series([0.25,
                  0.5, 0.75, 1.0])
data.values
data.index
data[1:3]
```

# Pandas

## The Pandas Series object (II)

### Custom indices

```
In [1] : data = pd.Series([0.25, 0.5, 0.75, 1.0],  
                           index=['a', 'b', 'c', 'd'])
```

```
In [2]: data
```

```
Out [1]:
```

```
a      0.25  
b      0.50  
c      0.75  
d      1.00  
dtype: float64
```

```
In [3]: data['a']
```

```
Out [2]: 0.25
```

```
In [4]: data[0]
```

```
Out [3]: 0.25
```

# Pandas

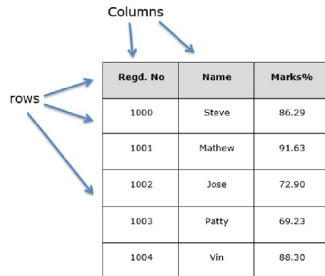
## The Pandas DataFrame object (I)

A DataFrame is a 2-D tabular data structure

- Similar to a spreadsheet
- Homogeneous columns
- Heterogeneous rows

Two read-only attributes, both `pd.Index`

- `index`: Rows
- `columns`: Columns



The diagram shows a table representing a DataFrame. The table has three columns: 'Regd. No', 'Name', and 'Marks%'. It has five rows, with the first row being the header. Arrows point from the labels 'Columns' and 'rows' to their respective parts of the table. 'Columns' has two arrows pointing to the header row, and 'rows' has three arrows pointing to the data rows.

Regd. No	Name	Marks%
1000	Steve	86.29
1001	Mathew	91.63
1002	Jose	72.90
1003	Patty	69.23
1004	Vin	88.30

(Source)

# Pandas

## The Pandas DataFrame object (II)

### DataFrame example

```
In [1]: import seaborn as sns
```

```
In [2]: iris = sns.load_dataset('iris')
```

```
In [3]: iris.head()
```

```
Out [1]:
```

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa

```
In [246]: iris.columns
```

```
Out [246]:
```

```
Index(['sepal_length', 'sepal_width', 'petal_length',  
      'petal_width', 'species'], dtype='object')
```

# Pandas

## The Pandas DataFrame object (III)

Read from a file

- Excel:  
`pd.read_excel('filename.xlsx', sheetname='mysheet')`
- CSV (very common!!!): `pd.read_csv('filename.csv')`

### CSV example

```
# This CSV file contains data about weights and heights
"id", "weight", "height", "sex", "race"
1, 143.5, 81.6, "Female", "White"
2, 109.1, 83.7, "Female", "Black"
4, 104.8, 54.6, "Female", "Hisp"
7, 130.2, 81.7, "Male", "White"
```

CVS can be exported from MS Excel or programmatically

# Pandas

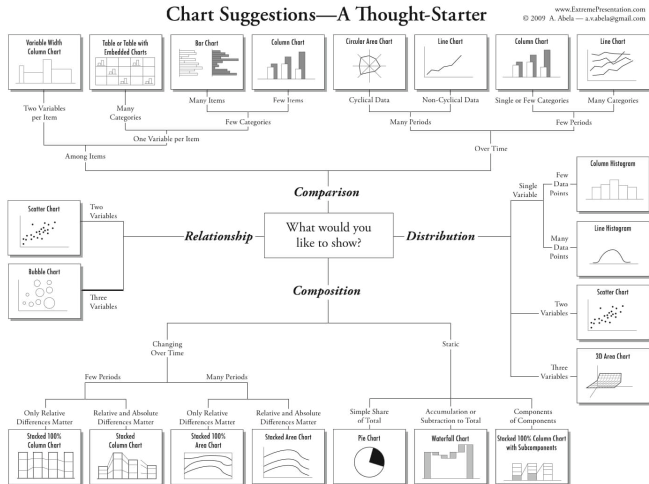
## Pandas notebook

NumPy notebook

[\(Link to notebook\)](#)

# Data visualization

## Motivation



(Source)  
(Alternative resource)

# Data visualization

## Matplotlib (I)

Matplotlib is a Python package

- Based on NumPy
- Imitates Matlab

Three operation modes

- Scripts.  
Must use `plt.show()` to enter event loop. Use it once!
- IPython shell.  
Must use `%matplotlib`
- IPython notebook. Two modes
  - `%matplotlib inline`
  - `%matplotlib notebook`

### Convention

```
import matplotlib as mpl
import matplotlib.pyplot as plt
```

### myplot.py

```
import matplotlib.pyplot as plt
import numpy as np

x = np.linspace(0, 10, 100)

plt.plot(x, np.sin(x))
plt.plot(x, np.cos(x))

plt.show()
```



# Data visualization

## Matplotlib (II)

Matplotlib comes with two interfaces

- Matlab-like. Old-fashioned function-oriented API.
- Object-oriented. Object-oriented and more powerful API.

### Matlab API

```

^^ Iplt.figure() # create a plot

^^ I# create the first of two
    panels and set current axis
^^ Iplt.subplot(2, 1, 1) # (rows,
    columns, panel number)
^^ Iplt.plot(x, np.sin(x))

^^ I# create the second panel and
    set current axis
^^ Iplt.subplot(2, 1, 2)
^^ Iplt.plot(x, np.cos(x));
^^ I

```

### OO API

```

^^ Iplt.figure() # create a plot

^^ I# create the first of two
    panels and set current axis
^^ Iplt.subplot(2, 1, 1) # (rows,
    columns, panel number)
^^ Iplt.plot(x, np.sin(x))

^^ I# create the second panel and
    set current axis
^^ Iplt.subplot(2, 1, 2)
^^ Iplt.plot(x, np.cos(x));
^^ I

```

# Pandas

## Matplotlib notebook

Matplotlib notebook

([Link to notebook](#))

# Data visualization

## Seaborn (I)

Seaborn is a modern data-visualization Python package

- Based on matplotlib
- ... it uses matplotlib indeed
- Pandas-aware
- High level
- Advanced visualizations
- Easy to use

Still under development! (v. 0.9)

### Convention

```
import seaborn as sns
```

This documentation is for Seaborn  
0.9 or newer

# Data visualization

## Seaborn (II)

### Display initialization

- `plt.show()`
- `%matplotlib`

### Style initialization

- Default Seaborn style `sns.set()`
- By default, same style than `matplotlib`

### Several functions ...

- ... similar parameters

### Parameters

- `x`: Data axis x
- `y`: Data axis Y
- `data`: Dataframe name
- `hue`: Color
- `style`: Style
- `sizes`: Size
- `kind`: Alternate representation

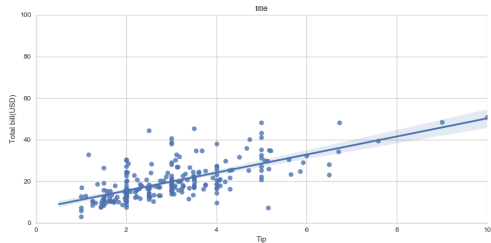
# Data visualization

## Seaborn (III)

### Typical Seaborn usage

1. Prepare data
2. Set up aesthetics
3. Plot
4. Customize the plot

```
import matplotlib.pyplot as plt
import seaborn as sns
# Prepare data
tips = sns.load_dataset("tips")
# Set up aesthetics
sns.set_style("whitegrid")
# Plot
g = sns.lmplot(x="tip", y="total_bill", data=tips, aspect=2)
# Plot customization
g = (g.set_axis_labels("Tip", "Total bill (USD)").set(xlim=(0, 10), ylim=(0, 100)))
plt.title("title")
plt.show(g)
```



# Seaborn

## Seaborn notebook

Seaborn notebook

([Link to notebook](#))