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 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

The data scientist toolkit

Overview

Tool	Type	Description
`conda`	Software	Python environments and package management
`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

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 crush 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 (Linux):

```
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, basicly, 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)

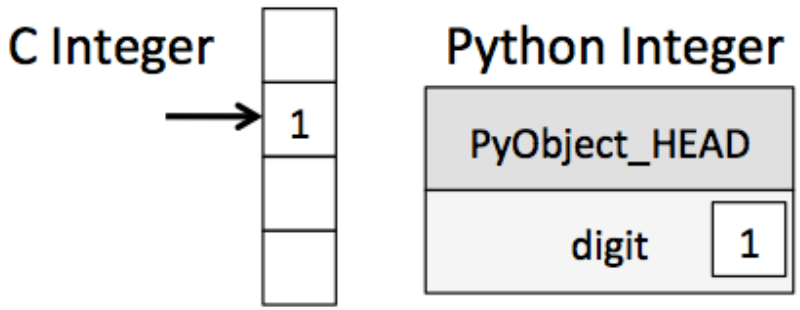
NumPy

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];
};
```

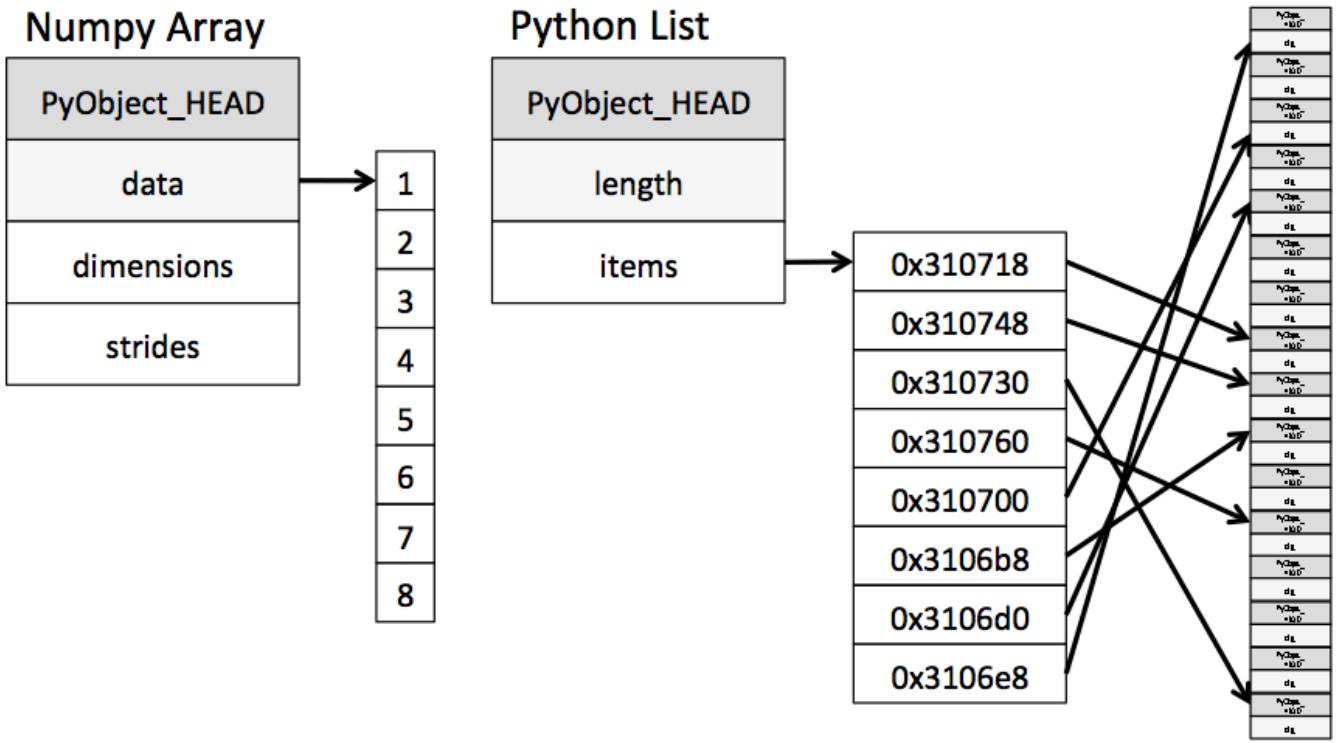


NumPy

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

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

NumPy

NumPy notebook

NumPy notebook

(Link to notebook)

Pandas

Introduction

A DS/ML workflow needs more features

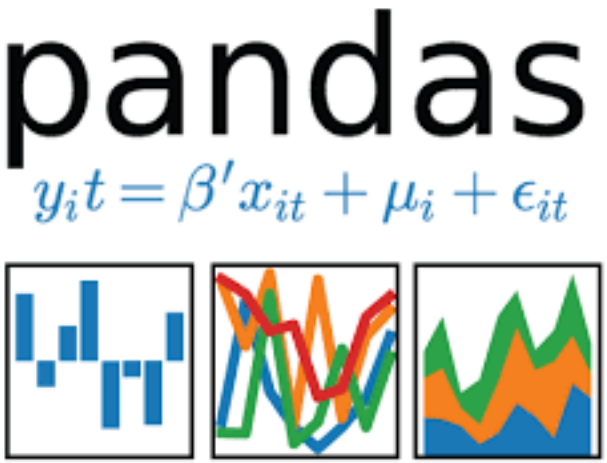
- Missing data
- Data input
- Operations on groups
- Label columns and rows

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`



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

Two attributes

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

Two indices

- Implicit: Regular index
- Explicit: Custom index

Index	Values
'a'	0.25
'b'	0.5
'c'	0.75
'd'	0.99

```
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

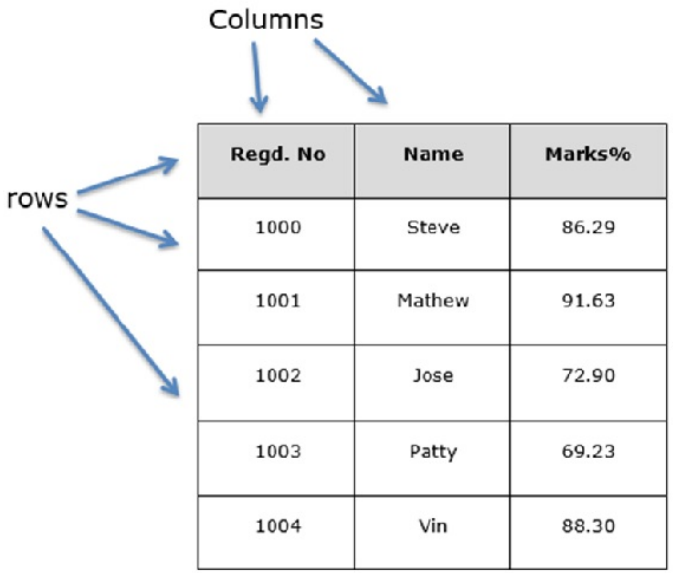
The Pandas `DataFrame` object (I)

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



(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 programatically

Pandas

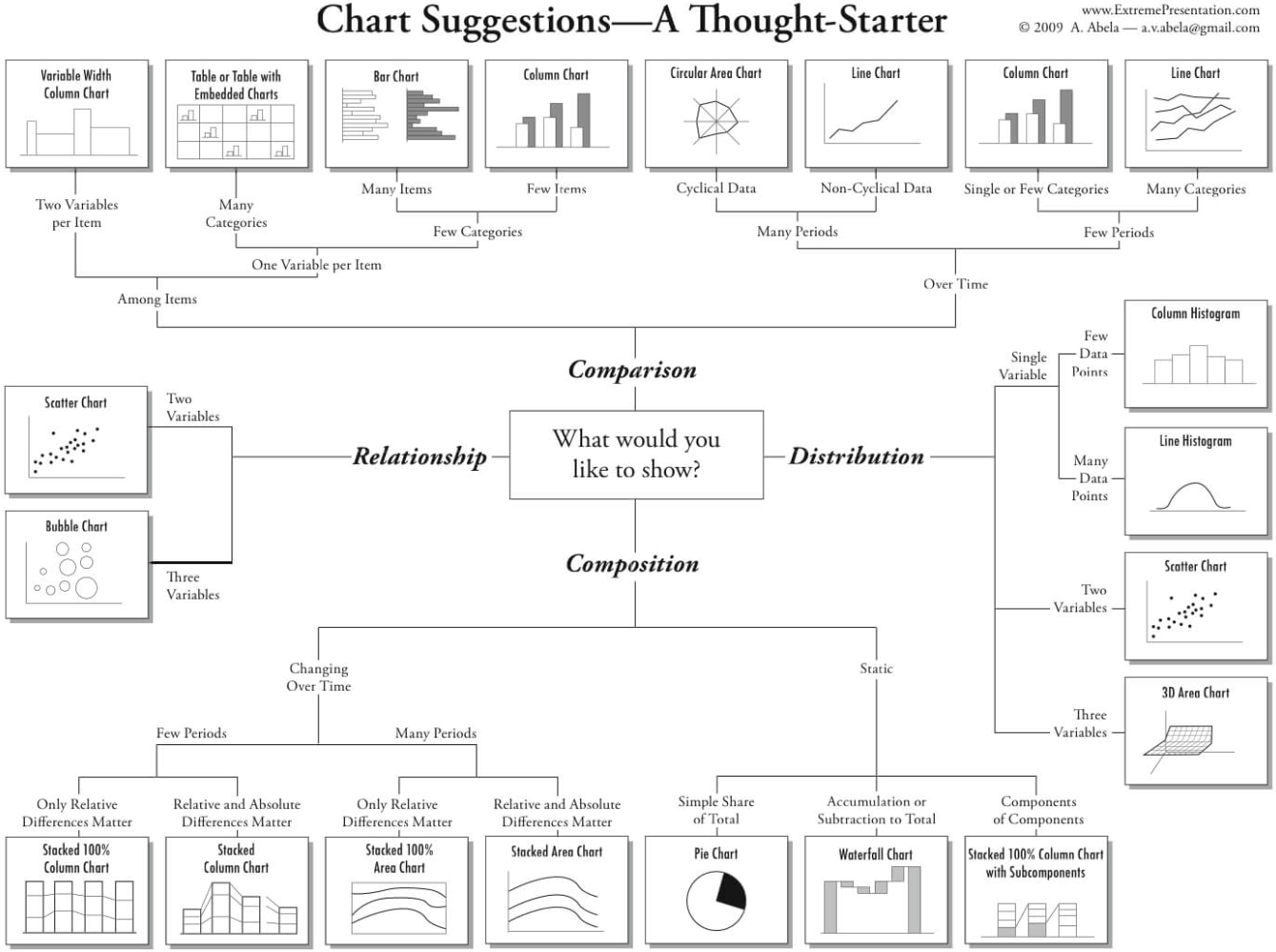
Pandas notebook

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 powerfull 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

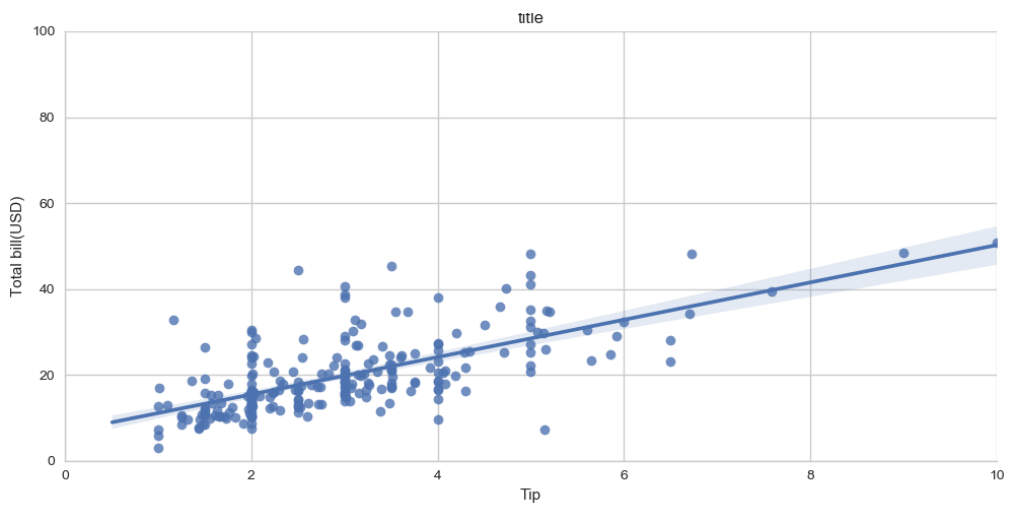
Data visualization

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)