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UNIVERSITÀ
DEGLI STUDI
DI PADOVA

Introduction to Python and Scikit-Learn

Machine Learning 2022-23

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Python

- Interpreted high-level general-purpose programming language
- It is open source !
- Object Oriented programming model
- Current version is 3.9
  - There are relevant changes from Python 2.x to 3.x
  - For this course we'll use Python 3.x

Resources:

- Website: http://www.python.org
- Documentation: http://www.python.org/doc/

Modules: SciPy ecosystem

SciPy (pronounced "Sigh Pie") is a Python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, these are some of the core packages:

NumPy
Base N-dimensional array package

SciPy library
Fundamental library for scientific computing

Matplotlib
Comprehensive 2D Plotting

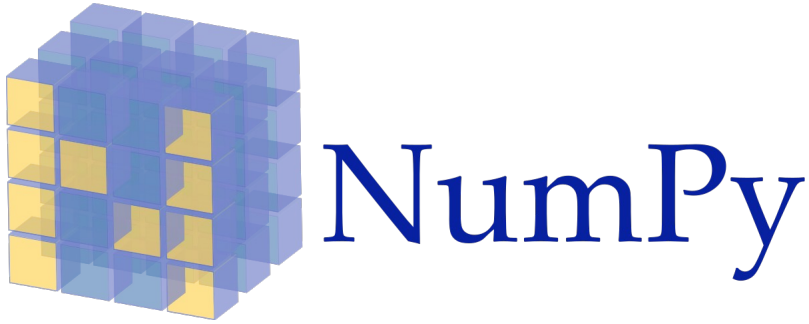
IP[y]:
IPython

IPython
Enhanced Interactive Console

Sympy
Symbolic mathematics

pandas
Data structures & analysis

Modules: NumPy



- Scientific computation capabilities within Python
  - Similar to Matlab functionalities
- Fast array operations
- 2D arrays, multi-D arrays, linear algebra, etc…

Resources:

- Downloads: http://numpy.scipy.org/
- Tutorial: http://www.scipy.org/

Modules: scikit-learn

- Machine Learning library in Python
- Simple and efficient tools for data mining and data analysis
- Based on numpy and scipy
- Open source
- We'll use this library for the labs !!
- Documentation: http://scikit-learn.org/stable/documentation.html
- Reference Manual: http://scikit-learn.org/stable/modules/classes.html

scikit-learn: What's inside

1. Supervised learning
   - 1.1. Generalized Linear Models
   - 1.2. Linear and Quadratic Discriminant Analysis
   - 1.3. Kernel ridge regression
   - 1.4. Support Vector Machines
   - 1.5. Stochastic Gradient Descent
   - 1.6. Nearest Neighbors
   - 1.7. Gaussian Processes
   - 1.8. Cross decomposition
   - 1.9. Naive Bayes
   - 1.10. Decision Trees
   - 1.11. Ensemble methods
   - 1.12. Multiclass and multilabel algorithms
   - 1.13. Feature selection
   - 1.14. Semi-Supervised
   - 1.15. Isotonic regression
   - 1.16. Probability calibration
   - 1.17. Neural network models (supervised)

2. Unsupervised learning
   - 2.1. Gaussian mixture models
   - 2.2. Manifold learning
   - 2.3. Clustering
   - 2.4. Biclustering
   - 2.5. Decomposing signals in components
   - 2.6. Covariance estimation
   - 2.7. Novelty and Outlier Detection
   - 2.8. Density Estimation
   - 2.9. Neural network models (unsupervised)

3. Model selection and evaluation
4. Dataset transformations
5. Dataset loading utilities
6. Computing with scikit-learn

Setup: Your Home PC or Laptop

For your PC:

- ❑ Install ***Anaconda*** (with Python 3)
- ❑ Install ***scikit-learn*** (if not already installed by Anaconda)
  - Install scikit-learn with anaconda: `conda install scikit-learn`
    - or install with pip: `pip install -U scikit-learn`
  - It requires: Python (>= 3.4), NumPy (>= 1.8.2), SciPy (>= 0.13.3)
  - If required install the dependencies with pip or conda
- ❑ Install ***jupyter notebook***
  - ❑ With anaconda it is installed by default
  - ❑ Can be launched with : `jupyter notebook` or `jupyter-lab`

Setup Labs PCs

- Start the computer under linux
- To login you can use your DEI account
- Setup Anaconda 3 environment with Python 3:

```
source /nfsd/opt/anaconda352/anaconda352.sh
```

- Launch jupyter notebook or lab

```
jupyter notebook  or  jupyter-lab
```

Tutorials

Useful resources to learn the basics of Python programming:

- See the provided *python_intro_labs* script
- Look at http://cs231n.github.io/python-numpy-tutorial/
- You can find a Jupyter notebook version of the tutorial at:
  https://github.com/kuleshov/cs228-material/blob/master/tutorials/python/cs228-python-tutorial.ipynb

How to use: 1. Python Interpreter

- Interactive interface to Python (similar to matlab command window)
- Launch with the python command from the bash/command prompt

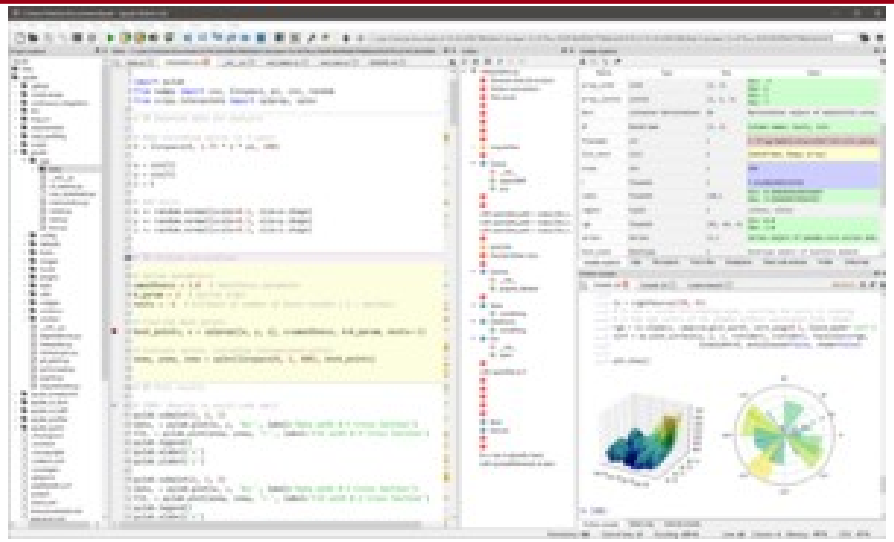
```
[python36] C:\Users\root>python
          Python 3.6.2 |Anaconda custom (64-bit)| (default, Jul 20 2017, 12:30:02)        [MSC
v.1900 64 bit (AMD64)] on win32
          Type "help", "copyright", "credits" or "license" for more information.
          >>>
```

- Python interpreter evaluates inputs:

```
>>> 3*(7+2)
27
```

- Python prompts with '>>>'.
- To exit Python: `exit()`

How to use: 2. Write Source and Run



- Write your source code and save in a .py file
- You can use any editor or IDE of your choice
  - e.g., PyCharm or Visual Studio Code
- Anaconda also provides the spyder environment that has some debugging tools
- Run the file:

```
python filename.py
```

How to use: 3. Jupyter notebook / lab

- Run with : `jupyter notebook` or `jupyter-lab`
  - Jupyter lab has some extra features
- Interactive environment inside the web browser
- You can run each block of code and see the output
- Can combine code and text (comments / description)
- ***We'll use jupyter notebooks for the lab deliveries***

Basics: Operators and Variables

- Assignment uses = and comparison uses ==

- For numbers: + - * / % are as expected
  - Special use of + for string concatenation
  - Special use of % for string formatting (as with *printf* in C)
  - Logical operators are words (and, or, not) *not* symbols

- The basic printing command is print

- The first assignment to a variable creates it
- Variable types don't need to be declared
- Python figures out the variable types on its own

Basic Datatypes

Integers

x = 3 (x is an int)

z = 5 / 2 # Answer is 2.5 in Python 3 and 2 in Python 2 !!

Floats

x = 3.456 (x is a float)

Strings

Can use " " or ' ' to specify : "abc" 'abc' are the same thing

Whitespaces

- Whitespace is meaningful in Python
  - especially indentation and placement of newlines
- Use a newline to end a line of code
- No braces { } to mark blocks of code in Python
  - … use consistent indentation instead !
  - The first line with more indentation starts a nested block
  - The first line with less indentation is outside of the block
- Often a colon (:) appears at the start of a new block
  - E.g., for function and class definitions
- Start comments with # – the rest of line is ignored

Assignments

- Binding a variable in Python means setting a name to hold a reference to some object
- Assignment creates references, not copies
- Names in Python do not have an intrinsic type
  - Objects have types !
  - Python determines the type of the reference automatically based on the data object assigned to it
- You create a name the first time it appears on the left side of an assignment expression: (e.g., x = 3)
- A reference is deleted via garbage collection after any names bound to it have passed out of scope

Arrays

- Handled through the numpy library
- A numpy array is a grid of values, all of the same type
- It is indexed by a tuple of non-negative integers
- The *shape* of an array is a tuple of integers giving the size of the array along each dimension

Examples:

```
import numpy as np
a = np.array([1, 2, 3])   # Create a rank 1 array
print(type(a))            # Prints "<class 'numpy.ndarray'>"
print(a.shape)            # Prints "(3,)"
print(a[0], a[1], a[2])   # Prints "1 2 3"
a[0] = 5                  # Change an element of the array
print(a)                  # Prints "[5, 2, 3]"

b = np.array([[1,2,3],[4,5,6]])    # Create a rank 2 array
print(b.shape)                     # Prints "(2, 3)"
print(b[0, 0], b[0, 1], b[1, 0])   # Prints "1 2 4"
```

Sequence Types

1. Tuple
- A simple immutable ordered sequence of items
- Items can be of mixed types, including collection types

2. Strings
- Immutable
- Conceptually very much like a tuple

3. List
- Mutable ordered sequence of items of mixed types

4. (*Dictionaries*)
- Store a mapping between a set of keys and a set of values

Functions

Functions:

- *def* creates a function and assigns it a name
- *return* sends a result back to the caller
- Arguments are passed by assignment
- Arguments and return types are not declared

Examples:

```
def <name>(arg1, arg2, ..., argN):
    <statements>
    return <value>

def times(x,y):
    return x*y
```

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Lab 0: Your First Program in Python

Develop a simple application in the last part of the lab:

1. Load the provided .csv file with the used car data
2. Use a linear regression to estimate the car prices from the year, kilometers or engine power
   - You can make a simple 1D regression from each one of the parameters independently
   - *(optional) If you like to experiment try a 2D or 3D regression combining multiple cues*
3. Firstly use the scipy *linregress* function
   - Alternatively you can use the sklearn.linear_model.LinearRegression class
4. Have a look at the correlation coefficient to see which of the 3 features works better
5. *(optional)* try to manually implement the least square algorithm
   - You should get exactly the same solution of *linregress* !
   - If never used least squares you can do it later after the lectures on linear models
6. Plot the data and the lines representing the output of the *linregress* and least square algorithms

Linear Regression with scikit-learn

scipy.stats.linregress

- The function calculates a linear least-squares regression for two sets of measurements
- scipy.stats.linregress(x, y=None)[source]

Parameters:

- x, y : array_like Two sets of measurements. Both arrays should have the same length. If only x is given (and y=None), then it must be a two-dimensional array where one dimension has length 2. The two sets of measurements are then found by splitting the array along the length-2 dimension

Returns:

- slope : float slope of the regression line
- intercept : float intercept of the regression line
- rvalue : *float* *correlation coefficient (see box, : total correlation, 0 no correlation)*
- pvalue : float two-sided p-value for a hypothesis test whose null hypothesis is that the slope is zero, using Wald Test with t-distribution of the test statistic
- stderr : float Standard error of the estimated gradient

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

Least Squares (optional, presented later)

- Compute gradient of MSE on training set and set to 0

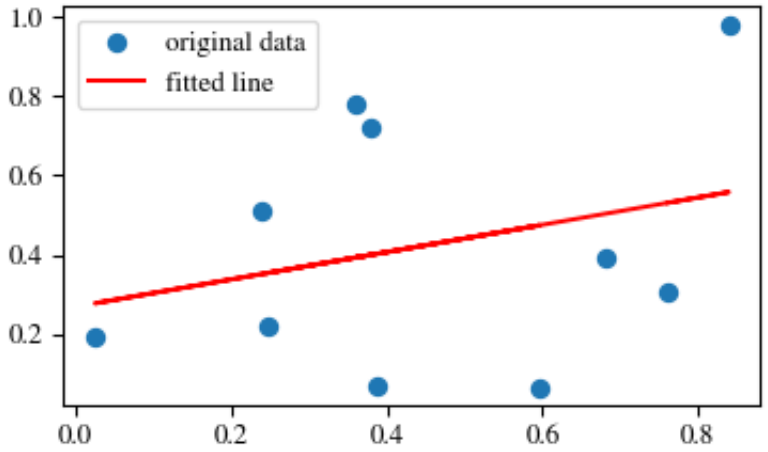
$$L_s = \frac{1}{m}\sum_{i=1}^{m}(< \boldsymbol{w}, \boldsymbol{x}_i > - y_i)^2 \rightarrow \frac{\partial L_s}{\partial \boldsymbol{w}} = \frac{2}{m}\sum_{i=1}^{m}(< \boldsymbol{w}, \boldsymbol{x}_i > - y_i)\boldsymbol{x}_i = 0$$

- Set $A = \left(\sum_{i=1}^{m} \boldsymbol{x}_i \boldsymbol{x}_i^T\right) \quad \boldsymbol{b} = \sum_{i=1}^{m} y_i \boldsymbol{x}_i$
- The solution is:

$$\boldsymbol{w} = A^{-1}\boldsymbol{b}$$

- *w[0]: intercept* *w[1]: slope*
- The computation is done using homogeneous coordinates
- Python: 1D array and *m x 1* 2D array are different objects
- Inverse of a matrix: np.linalg.inv(M)

Plot Data with matplotlib



Plot the data along with the fitted line using matplotlib

```
>>> import matplotlib.pyplot as plt
>>> plt.plot(x, y, 'o', label='original data')
>>> plt.plot(x, intercept + slope*x, 'r', label='fitted line')
>>> plt.legend()
>>> plt.show()
```

Task for Lab 0

1. Load a dataset with used car data
2. Use a linear regression to estimate the car prices from the year, kilometers or engine power
3. Understand which of the 3 features works better and visualize your results

For lab 0 there is no homework, it is just to get used with Python

For help ask to the instructor or to the TA