

PATTERN RECOGNITION AND MACHINE LEARNING

Slide Set 1: Introduction and the Basics of Python

January 2017

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Course Organization

- Organized on 3rd period; January February 2017.
- Lectures every Tuesday 14-16 (TB111) and Friday 14-16 (TB111).
- 9 groups of exercises between Tuesday and Friday (sign up at POP).
- More details: http://www.cs.tut.fi/courses/SGN-41007/

Course Requirements

- 1 60% of exercise assignments solved. For 70 %, you get 1 point added to exam score; for 80 % two points and for 90% three points.
- Project assignment, which is organized in the form of a pattern recognition competition. The competition is done in groups.
 https://inclass.kaggle.com/c/gene-expression-prediction
- 3 Written exam. Max. number of points for the exam is 30 with the following scoring.

Points	<15	<18	<21	<24	<27	≥27
Grade	0	1	2	3	4	5

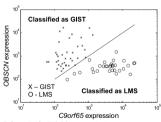
Course Contents

- 1 Python: Rapidly becoming the default platform for practical machine learning
- 2 Estimation of Signal Parameters: What are the phase, amplitude and frequency of this noisy sinusoid
- 3 **Detection Theory:** Detect whether there is a specific signal present or not
- 4 Performance evaluation: Cross-Validation, Bootstrapping, Receiver Operating Characteristics, other Error Metrics
- Machine Learning Models: Logistic Regression, Support Vector Machine, Random Forests, Deep Learning
- 6 Avoid Overlearning and Solve III-Posed Problems: Regularization Techniques

Introduction

- Machine learning has become an important tool for multitude of scientific disciplines.
- Training based approaches are rapidly substituting traditional manually engineered pipelines.
- Training based = we show examples of what is interesting and hope the machine learns to do it for us
- Model based = we have derived a model of the data and wish to learn the unknown parameters
- A few modern research topics:
 - Image recognition (what is in this image and where?)
 - Speech recognition (what do I say?)
 - Medicine (data-driven diagnosis)





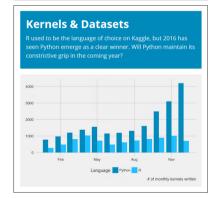
Price et al., "Highly accurate two-gene classifier for differentiating gastrointestinal stromal tumors and leiomyosarcomas," *PNAS* 2007.



Why Python?

- Python is becoming increasingly central tool for data science.
- This was not always the case: 10 years ago everyone was using Matlab.
- However, due to licensing issues and heavy development of Python, scientific Python started to gain its user base.
- Python's strength is in its variability and huge community.
- There are 2 versions: Python 2.7 and 3.6. We'll use the former one as it's better supported by most packages interesting to us.

All Python releases are Open Source (see http://www.opensource.org for the Open Source Definition).
Historically, most, but not all, Python releases have also been GPL-compatible;





Source: Kaggle.com newsletter, Dec. 2016

Alternatives to Python in Science

Python vs. Matlab

Python vs. R

- Matlab is #1 workhorse for linear algebra.
- Matlab is professionally maintained product.
- Some Matlab's toolboxes are great (Image Processing tb). Some are obsolete (Neural Network tb).
- New versions twice a year. Amount of novelty varies.
- Matlab is expensive for non-educational users.

- R has been #1 workhorse for statistics and data analysis. ^a
- R is great for specific data analysis and visualization needs.
- Lots of statistics community code in R.
- Python interfaces with other domains ranging from deep neural networks (Caffe, Theano) and image analysis (OpenCV) to even a fullblown webserver (Django/Flask)

ahttp://tinyurl.com/jynezuq

 "Matlab is made for mathematicians, R for statisticians and Python for programmers."



Essential Modules

- numpy: The matrix / numerical analysis layer at the bottom
- scipy: Scientific computing utilities (linalg, FFT, signal/image processing...)
- scikit-learn: Machine learning (our focus here)
- matplotlib: Plotting and visualization
- opencv: Computer vision
- pandas: Data analysis
- statsmodels: Statistics in Python
- caffe, theano, tensorflow, keras: Deep neural networks (we are using keras later in the course)
- **spyder**: The front end (Scientific PYthon Development EnviRonment)

Where to get Python?

- It is possible to construct your custom Python environment by installing individual modules (base from python.org and libraries from, e.g., http://www.lfd.uci.edu/~gohlke/pythonlibs/).
- Alternatively, one may install a full distribution, such as
 - Anaconda https://www.continuum.io/downloads ← my favorite
 - Enthought Canopy http://www.enthought.com/
- ...or in linux:

```
# apt-get install python
# apt-get install python-numpy
# apt-get install python-sklearn
# apt-get install python-matplotlib
# apt-get install spyder
```

The Language

- Python was designed to be a highly readable language.
- Python uses whitespace to delimit program blocks.
 First you hate it, later you love it.
- All used modules are imported using an import declaration.
- The members of a module are referred using the dot: np.cos([1,2,3])
- Interpreted language. Also interactive with IPython extensions.

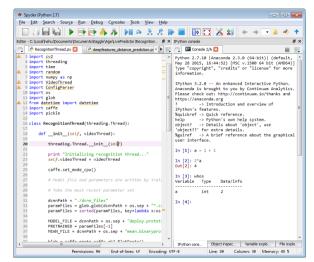
```
8 import matplotlib.pyplot as plt
 9 import numpy as np
10 from sklearn.linear model import Ridge
11 from sklearn.linear model import Lasso
13 def get obs matrix(x, order = 5):
14
      Return the observation matrix
16
      constructed from powers of vector x.
17
18
19
      H = [1]
      for k in range(order):
           H.append(x**k)
23
24
      H = np.arrav(H).T
26
      return H
28 if
     name == " main ":
30
      # generate a noisy sinusoid
31
32
      np.random.seed(2015)
33
34
35
      x = np.arange(0.1.01.0.08)
      y = np.cos(2 * 2*pi*x) \setminus
           + 0.35*np.random.randn(x.shape[0])
37
      v2 = np.cos(1 * 2*pi*x) 
           + 0.35*np.random.randn(x.shape[0])
      x = np.arange(0.1.01.0.04)
```

Things to Come

- Following slides will introduce the basic Python usage within scientific computing.
 - The editor and the environment
 - · Matlab slightly better than Python
 - Linear algebra
 - Matlab better than Python
 - Programming constructs (loops, classes, etc.)
 - Python better than Matlab
 - Machine learning
 - Python a lot better than Matlab

Spyder Editor

- In this course we use the Spyder editor.
- The editor window contains two panes: editor on the left and console on the right.
- F5: Run code; F9: Run selected region.
- Alternatively, you can use whatever editor you like, and run everything on the command line.



```
Terminal -- + ×
hehu@hehu-vm - $ echo "print 'hello world'" > hello.py
hehu@hehu-vm - $ python hello.py
hello world
hehu@hehu-vm - $ |
```

Python Basics

- Python code can be executed either from a script file (*.py) or in the interactive mode (just like Matlab).
- For the interactive mode; just execute python from the command line.
- Alternatively, ipython (if installed) starts Python in a more user-friendly mode:
 - Tab-completion works
 - Many utility functions (e.g., ls, pwd, cd)
 - Magic functions (e.g., %run, %timeit, %edit, %pastebin)

```
ehu@hehu-vm ~ $ ipvthon
Python 2.7.6 (default, Jun 22 2015, 17:58:13)
Type "copyright", "credits" or "license" for more information.
IPvthon 1.2.1 -- An enhanced Interactive Pvthon.
          -> Introduction and overview of iPython's features.
equickref -> Quick reference.
          -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
            builtin function or method
            <built-in function range>
            Python builtin
range(stop) -> list of integers
range(start, stop[, step]) -> list of integers
Return a list containing an arithmetic progression of integers.
range(i, j) returns [i, i+1, i+2, ..., j-1]; start (!) defaults to \theta.
When step is given, it specifies the increment (or decrement).
For example, range(4) returns [0, 1, 2, 3]. The end point is omitted!
These are exactly the valid indices for a list of 4 elements.
   2]: range(1, 7, 2)
        [1, 3, 5]
```

Command range creates a list of integers. Compare to Matlab's syntax 1:2:6.

Help

For each command, help is there to refresh your memory:

```
>>> help("".strip) # strip is a member of the string class
Help on built-in function strip:
strip(...)
S.strip([chars]) -> string or unicode

Return a copy of the string S with leading and trailing
whitespace removed.
If chars is given and not None, remove characters in chars instead.
If chars is unicode, S will be converted to unicode before stripping
```

- In *ipython*, the shortcut ? is available, too (see previous slide).
- Many people prefer to Google for python strip instead; matter of taste.

Using Modules

- Python libraries are called modules.
- Each module needs to be imported before use.
- Three common alternatives:
 - 1 Import the full module: import numpy
 - 2 Import selected functions from the module: from numpy import array, sin, cos
 - Import all functions from the module:
 from numpy import *

```
>>> sin(pi)
NameError: name 'sin' is not defined
>>> from numpy import sin, pi
>>> sin(pi)
1.2246467991473532e-16
```

```
>>> import numpy as np
>>> np.sin(np.pi)
1.2246467991473532e-16
```

```
>>> from numpy import *
>>> sin(pi)
1.2246467991473532e-16
```

Using Modules

A few things to note:

- All methods support shortcuts; e.g., import numpy as np.
- Sometimes import <module> fails, if the module is in fact a collection of modules.
 For example, import scipy. Instead, use import scipy.signal
- Importing all functions from the module is not recommended, because different modules may contain functions with the same name.

```
>>> import scipy
>>> matfile = scipy.io.loadmat("myfile.mat")
AttributeError: 'module' object has no attribute 'io'
```

```
>>> import scipy.io as sio
>>> matfile = sio.loadmat("myfile.mat") # Works OK
```

```
>>> from scipy.io import loadmat
>>> matfile = loadmat("myfile.mat") # Works OK
```

NumPy

- Practically all scientific computing in Python is based on numpy and scipy modules.
- NumPy provides a numerical array as an alternative to Python list.
- The list type is very generic and accepts any mixture of data types.
- Although practical for generic manipulation, it is becomes inefficient in computing.
- Instead, the NumPy array is more limited and more focused on numerical computing.

```
# Python list accepts any data types
v = [1, 2, 3, "hello", None]
```

```
# We like to call numpy briefly "np"
>>> import numpy as np

# Define a numpy array (vector):
>>> v = np.array([1, 2, 3, 4])

# Note: the above actually casts a
# Python list into a numpy array.

# Resize into 2x2 matrix
>>> V = np.resize(v, (2, 2))

# Invert:
>>> np.linalg.inv(V)
array([[2., 1.],
[[1.5, -0.5]])
```

More on Vectors

np.arange creates a range array (like 1:0.5:10 in Matlab)

```
>>> np.arange(1, 10, 0.5) # Arguments: (start, end, step)
array([ 1. , 1.5, 2. , 2.5, 3. , 3.5, 4. , 4.5, 5. , 5.5, 6. ,
6.5, 7. , 7.5, 8. , 8.5, 9. , 9.5])

# Note that the endpoint is not included (unlike Matlab).
```

Most vector/matrix functions are similar to Matlab:

Matrices

 A matrix is defined similarly; either by specifying the values manually, or using special functions.

```
# A matrix is simply an array of arrays
# May seem complicated at first, but is in fact
# nice for N-D arrays.

>>> np.array([[1, 2], [3, 4]])
array([[1, 2], [3, 4]])

>>> from scipy.linalg import toeplitz, hilbert # You could also " ...import *"

>>> toeplitz([3, 1, -2])
array([[3, 1, -2], [1, 3, 1], [-2, 1, 3]])

>>> hilbert(3)
array([[1, 0.5, 0.3333333], [0.5], [0.3333333], [0.5], [0.3333333], [0.5], [0.5], [0.3333333], [0.5], [0.5], [0.3333333], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.5], [0.
```

Matrix Product

- Matrix multiplication is different from Matlab. Use np.dot or np.matmul.
- With NumPy version 1.10+ and Python 3.5+, matrix multiplication can be done with the @ operator: A @ B.

```
$ python 3.5.2 (default, Nov 17 2016, 17:05:23)
>>> import numpy as np
>>> A = np.random.rand(3,3)
>>> B = np.random.rand(3,3)
>>> A = ng.random.rand(3,3)
>>> A = ng.random.rand(3,3)
=>> A = B = np.random.rand(3,3)
=>> A = D = np.random.rand(3,3)
=>> A = D = np.random.rand(3,3)
=>> A = np.random.rand(3,3)
=> A = np.random.rand(3,3)
== np.random.r
```

- Indexing of vectors uses the colon notation, too.
- Below, we extract selected items from the vector 1...10:

```
>>> x = np.arange(1, 11)
>>> x[0:8:2] # Unlike Matlab, indexing starts from 0
array([1, 3, 5, 7])

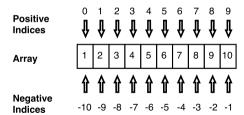
# Note: use square brackets for indexing
# Note2: colon operator has the order start:end:step;
# not start:step:end as in Matlab
```

The start and end points can be omitted:

```
>>> X[5:] # All items from the 5'th
array([ 6, 7, 8, 9, 10])
>>> X[5:] # All items until the 5'th
array([1, 2, 3, 4, 5])
>>> X[5:] # All items with step 3
array([ 1, 4, 7, 10])
```

 Negative indices are counted from the end (-1 = the last, -2 = second-to-last, etc.):

```
>>> x[-3:] # Three last items
array([ 8, 9, 10])
>>> x[:::1] # Items in inverse order
array([10, 9, 8, 7, 6, 5, 4, 3, 2, 1])
```



- Also matrices can be indexed similarly. This operation is called *slicing*, and the result is a *slice* of the matrix.
- Here we request for items on the rows 2:4 = [2,3] and columns 1,2,4 (shown in red).
- Note, that with matrices, the first index is the row; not "x-coordinate".
- This order is called "Fortran style" or "column major" while the alternative is "C style" or "row major".

- To specify only column or row indices, use ":" alone.
- Now we wish to extract two bottom rows.
- M[4:, :] reads "give me all rows after the 4th and all columns".
- In this case, alternative forms would be,
 e.g., M[-2:, :] and M[[4,5], :].

N-Dimensional arrays

- Higher-dimensional arrays are frequently encountered in machine learning.
- For example, a set of 1000 color images of size $w \times h = 128 \times 96$ is represented as a $1000 \times 3 \times 96 \times 128$ array.
- Here, dimensions are: image index, color channel, y-coordinate, x-coordinate.
- Sometimes, a shorter name is used: "(b, c, 0, 1) order".

```
# Generate a random "image" array:
>>> A = np. random. rand(1000. 3. 96. 128)
# What size is it?
>>> A. shape
(1000 . 3 . 96 . 128 )
# Access the pixel (4, 3) of 2nd color channel
# of the 2nd image
>>> A[1, 2, 3, 4]
0.36569219631994954
# Request all color channels:
>>> A[1, :, 3, 4]
array([ 0.32306666,  0.60012626,  0.3656922 ])
# Request a complete 96x128 color channel:
>>> A[1, 2, :, :]
array([[ 0.19102217 ...
0.8846471811)
# Equivalent shorter notation:
>>> A[1, 2, ...]
array([[ 0.19102217 ...
 0.8846471811)
```

Functions

- Functions are defined using the def keyword.
- Function definition can appear anywhere in the code.
- Functions can be imported to other files using import.
- Function arguments can be positional or named (see code).
- Named arguments improve readability and are handy for setting the last argument in a long list.

```
# Define our first function
def hello(target):
    print ("Hello " + target + "!")
>>> hello("world")
Hello world!
>>> hello("Finland")
Hello Finland!
# We can also define the default argument:
def hello(target = "world"):
    print ("Hello " + target + "!")
>>> hello()
Hello world!
>>> hello("Finland")
Hello Finland!
# One can also assign using the name:
>>> hello(target = "Finland")
Hello Finland!
```

Loops and Stuff

```
for lang in ['Assembler', 'Python', "Matlab", 'C++']:
   if lang in ["Assembler", "C++"]:
     print ("I am ok with %s." % (lang))
   else:
     print ("I love %s." % (lang))
```

```
I am ok with Assembler.
I love Python.
I love Matlab.
I am ok with C++.
```

```
# Read all lines of a file until the end

fp = open("myfile.txt", "r")
lines = []

while True:
    try:
        line = fp.readline()
        lines.append(line)
    except:
    # File ended
    break

fp.close()
```

- Loops and other usual programming constructs are easy to remember.
- for can loop over anything iterable, such as a list or a file.
- In Matlab, appending values to a vector in a loop is not recommended. Python lists are actual lists, so appending is fine.

Example: Reading in a Data File

 Suppose we need to read a csv file (text file with Comma Separated Values) into Python.

```
1 Sample_ID,MI;M2;M3;M4;M5;M6;M7;M8;M9;M10;M11;M12;M1
2 $0;0.063915;0.033242;0.018484;0.0086177;0.035629;0.0
3 $1;0.025409;0.051085;0.056305;0.021738;0.02741;0.01
4 $2;0.02536;0.036123;0.054195;0.009735;0.027521;0.0
5 $3;0.012817;0.029652;0.07929;0.050677;0.039737;0.05
6 $4;0.019846;-0.010577;-0.0075045;0.019042;0.068786;
```

- The file consists of 216 rows (samples) with 4000 measurements each.
- We will write file reading code from scratch.
- Alternatively, many modules contain csv-reading functions
 - numpy.loadtxt or numpy.genfromtxt
 - csv.reader
 - pandas.read_csv

Example: Reading in a Data File

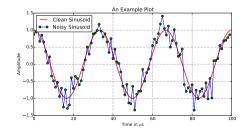
```
import numpy as np
if __name__ == "__main__":
   X = [] # Rows of the file go here
   # We use Pvthon's with statement.
   # Then we do not have to worry
    # about closing it.
   with open("ovarian.csv", "r") as fp:
       # File is iterable, so we can
       # read it directly (instead of
       # using readline).
        for line in fp:
           # Skip the first line:
           if "Sample ID" in line:
               continue
```

```
# Otherwise, split the line
        # to numbers:
       values = line.split(":")
        # Omit the first item
        # ("S1" or similar):
       values = values[1:]
        # Cast each item from
       # string to float:
       values = [float(v) for v in values]
        # Append to X
       X.append(values)
# Now. X is a list of lists. Cast to
# Numpy array:
X = np.array(X)
print ("All data read.")
print ("Result size is %s" % (str(X.shape)))
```

Visualization

```
import matplotlib.pvplot as plt
import numpy as no
N = 100
n = np.arange(N) # Vector [0,1,2,...,N-1]
x = np.cos(2 * np.pi * n * 0.03)
x \text{ noisy} = x + 0.2 * np.random.randn(N)
fig = plt.figure(figsize = [10,5])
plt.plot(n, x, 'r-',
         linewidth = 2.
         label = "Clean Sinusoid")
plt.plot(n, x_noisy, 'bo-',
         markerfacecolor = "green".
         label = "Noisy Sinusoid")
plt.grid("on")
plt.xlabel("Time in $\mu$s")
plt.vlabel("Amplitude")
plt.title("An Example Plot")
plt.legend(loc = "upper left")
plt.show()
plt.savefig("../images/sinusoid.pdf".
            bbox_inches = "tight")
```

- The matplotlib module is our plotting library.
- Function names are often similar to Matlab.
- Usually you want to "import matplotlib.pyplot".
- Alternatively, "from matplotlib.pylab import *" makes the environment very similar to Matlab.
- Code also in https://github.com/mahehu/SGN-41007





Another Example

- Even rather complicated graphics are easy to generate using Matplotlib.
- The code for the attached diagram is shown in https://github.com/ mahehu/SGN-41007.

