An Introduction to Programming with Python

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BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

Class Survey

- How many of you have learned any computer programming language?
  - C?
  - C++?
  - Java?
  - Fortran?
  - Python?
- How many of you have used programming in your coursework/projects?
  - What course?
  - What projects?

Who am I?

- I am a *computational scientist* at the BNL Computational Science Initiative (CSI). www.bnl.gov/compsci

- I am also a physicist performing theoretical research in particle physics. But really I am doing a lot of computer simulations.
- Columbia -> MIT -> Yale -> BU -> ANL -> BNL

What Do I Do?

- **Physics**: Study the fundamental interactions between the sub-atomic particles called quarks and gluons.
  - Empty Space is NOT Empty.
  - https://www.youtube.com/watch?v=J3xLuZNKhlY
- **Computing:** Program and run on some of the most powerful supercomputers in the world

- **Data Analysis:** Turn the data into meaningful physical results.

What is Programming?

- Here programming is short for “computer programming”, aka “coding”.
- Coding is writing a set of instructions for the computers.
  - For most of us, this means writing a human-readable program which is then transformed to machine codes that the computer can understand and execute.

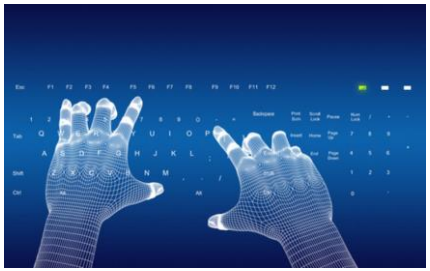


Image source: http://aquinashub.co.uk/

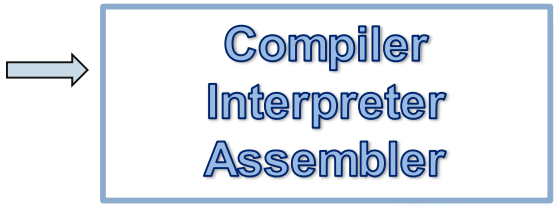


Image Source: http://ipoint-tech.com/

- But programming goes beyond simply coding, as it also involves analyzing the problem, coming up with a suitable algorithm and designing the implementation strategies etc.

What is a programming language?

- Just as we have different human languages, there are a lot of different computer programming languages, such as FORTRAN, C, C++, Python, Java, Perl, etc.
  - When I was in high school, I learned BASIC!
- A programming language defines a set of rules to write a computer program.
- Just like a human language, a programming language has a certain “vocabulary” and “grammar”.

Why do we need to know about programming?

- Programming is embedded in every aspect of modern life.
- Computers.
- Playstation, XBOX, ...
- Smart phones/TVs/watches/refrigerators/...
  - How are they smart? Computer programs!
  - Smart houses? (Eureka, anyone?)

In the Context of Science and Engineering…

- Numerical simulations and big data analytics play a significant role in the advancement of science and engineering.

- Programming is essential…
  - Aircraft simulation
  - Genome sequencing
  - Drug discovery
  - Supernova simulation
  - The origin of mass and the evolution of the universe!
  - And much more…

Introduction to Python

What is Python?

- Python is a popular computer programming language with many applications.
- It is a high-level language that is meant to be very readable, flexible and portable across different platforms (Mac OS, Windows, Linux, …).
- It is an interpreted language, meaning, the program statements are checked statement by statement.
- Needs the **python** interpreter.
- No need to compile and link the program, unlike C/C++.

Lesson Plan

- Python Basics with Demonstration [45 minutes]
  - We'll use Canopy for demonstration in class.
  - More experienced users feel free to use your own installation of python.

- Hands-On Exercises [75 minutes]
  - Generate random numbers
  - Calculate average and standard deviation
  - Monte Carlo methods

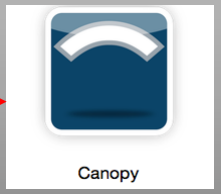
My Goals for this course

- Introduce you to the world of programming
- Give you a taste of flavors of Python
- Hopefully can motivate you to learn more about python and computer programming in general.

Starting up Canopy

- If you have Canopy installed on your own laptop, double click the launcher.

Something like this →

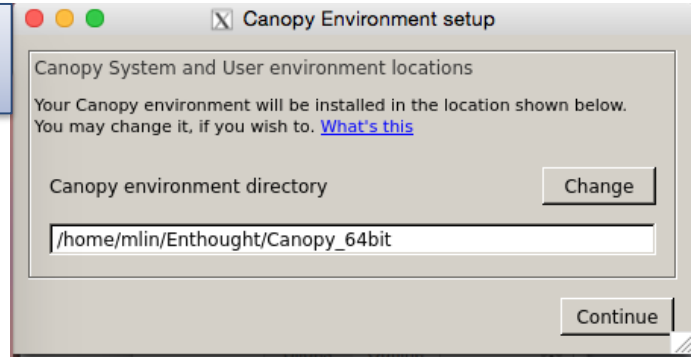


You will be asked to do some setup the first time you run Canopy. For most of you, choosing the default should suffice.

- On the Amazon Cloud Remote Desktop, simply click the "Enthought Canopy" icon on the desktop.

Setting up Canopy

1



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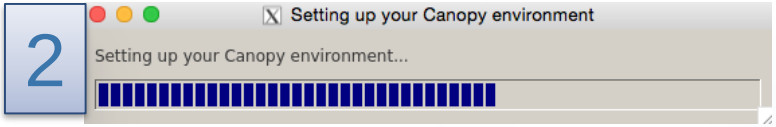

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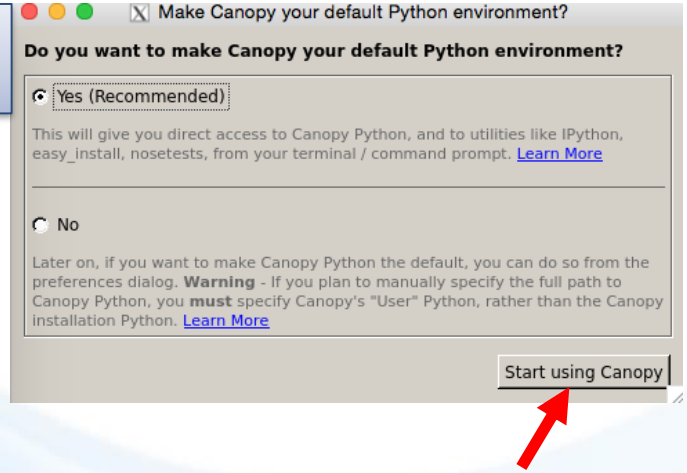

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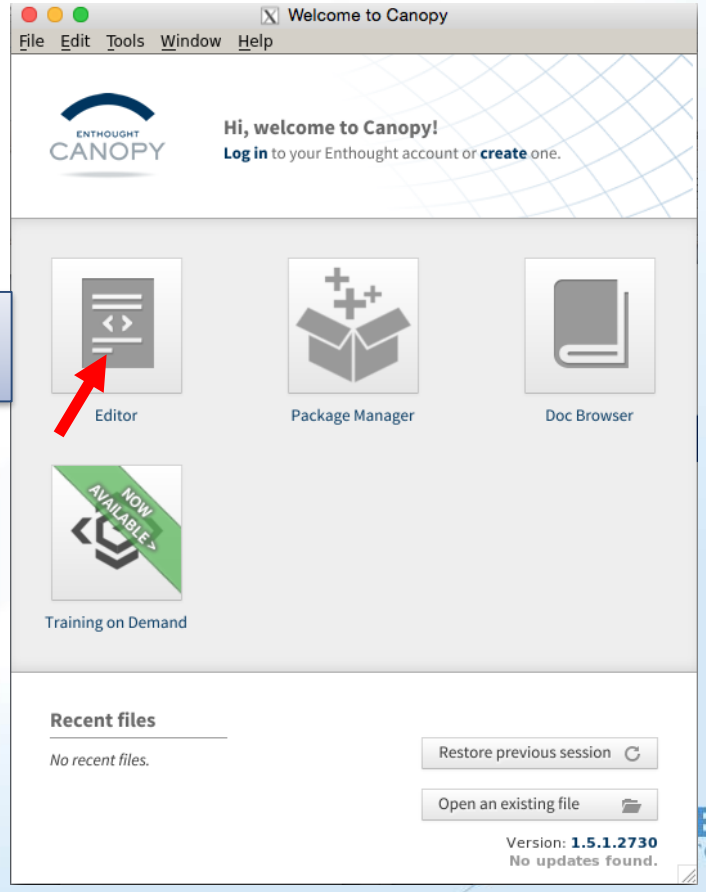
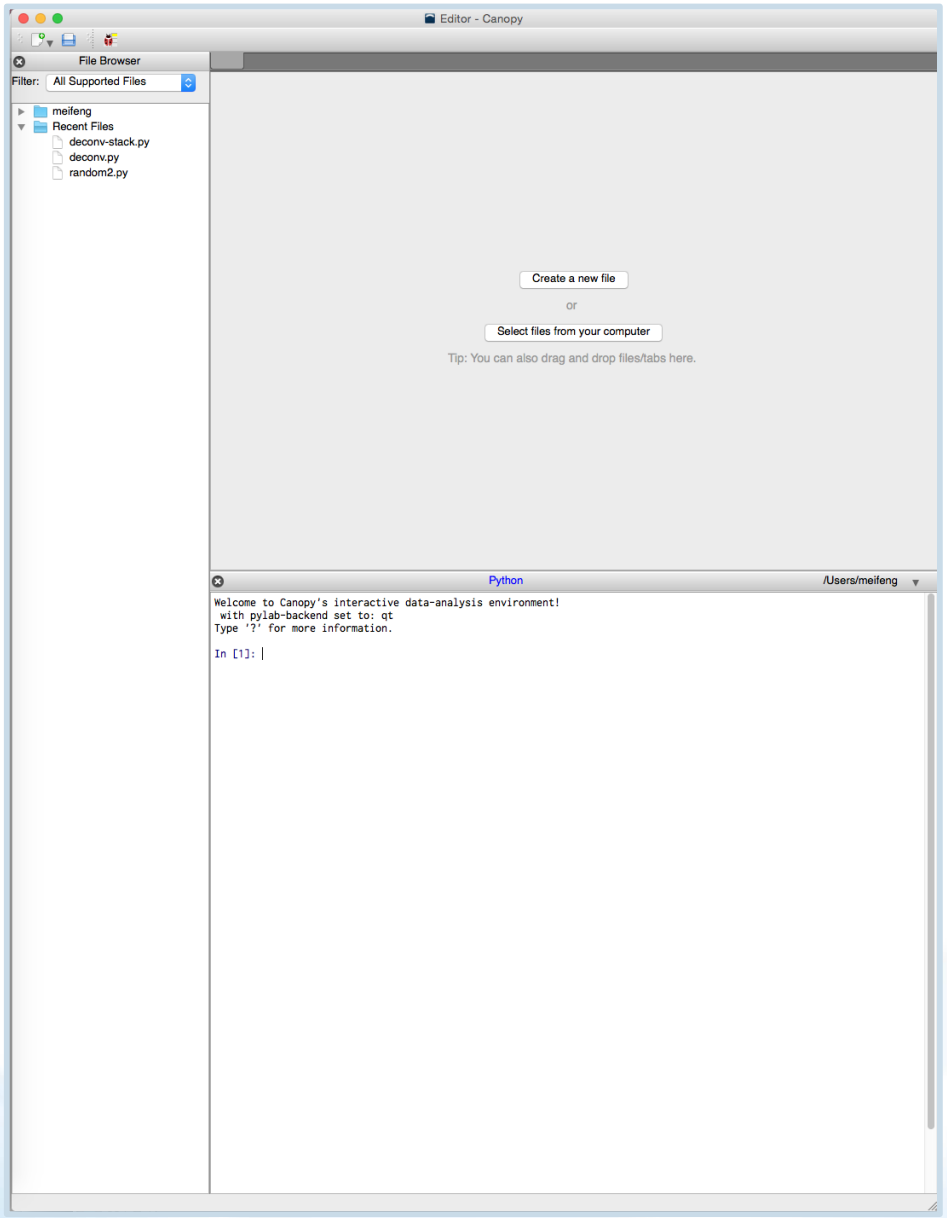




text editor

the IPython shell

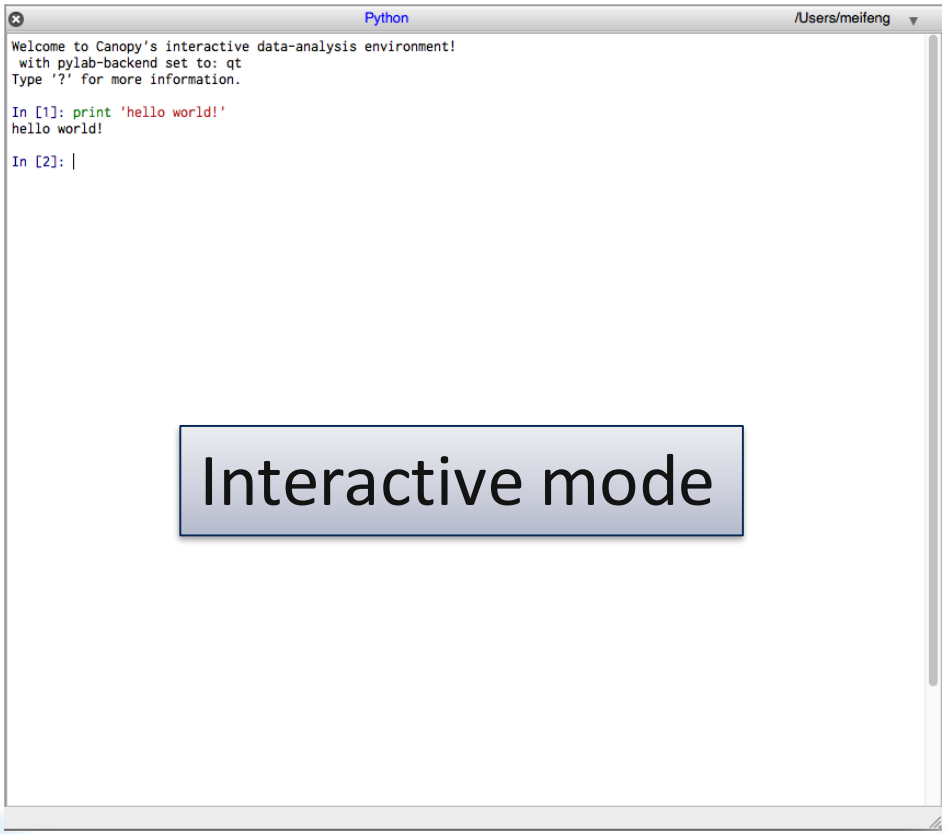
An enhanced interactive python shell.

Standard Python Shell vs. IPython

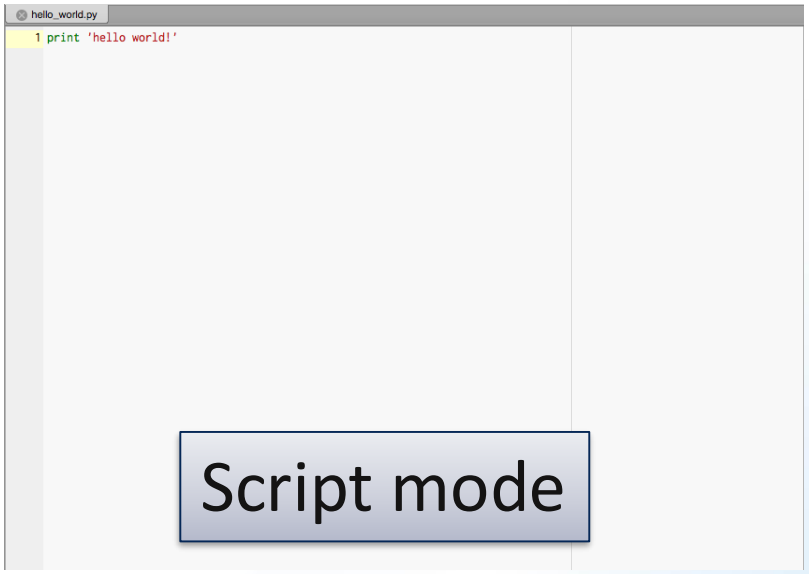
- The standard python shell
  - Barebones interpreter
  - This is what you get with the standard Python distribution.

- IPython -- An advanced python shell
  - Tab completion of variable names
  - Supports some Unix/Windows commands
  - Inline documentation
  - Syntax highlighting
  - Good for beginners

Two Ways to Use Python

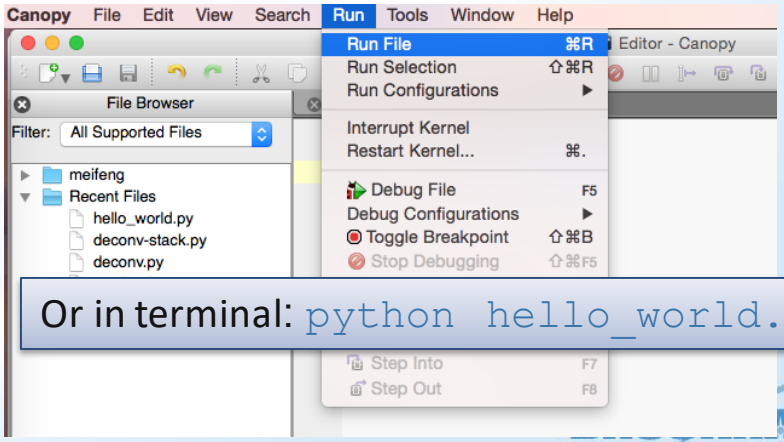


Interactive mode



Script mode

Good for prototyping code segments or as a calculator.



Or in terminal: `python hello_world.py`

Good to know

- There are two major releases of Python: Python 2.x and Python 3.x

- Python 3.x is not backward compatible. So make sure you know which version you are using.
  - If you are using a terminal, you can check by running:
    - `python --version`
  - In the interactive mode, you can check with
    - `print sys.version`
  - On the Amazon RD, it should return:
    - `Python 2.7.11 --  64-bit`

- We will be using Python 2.x.

Good to know

- Code blocks are organized by indentation
- Single-line comments start with #
- Multiline comments start and end with matching ``` (three single quotation marks) or """ (three double quotation marks)
- Comments are ignored by the interpreter, except when the first line begins with `#!`
  - `#!/usr/bin/python`
  - It tells the Operating System (OS) that the program is to be processed by /usr/bin/python.
- Demo: `hello_world.py`

Python Basic Building Blocks

1. Data Types: `int, float, str, long, bool,…`
2. Variables: `variable_name = value`
3. Collection Data Types: tuples, lists, sets, dictionaries
4. Logical Operators: `==, >, <, and, or, not, in`
5. Arithmetic Operators: `+, -, /, *, **, %, …`
6. Input / Output: `input/raw_input, print, open, close`
7. Control Flow Statements: `if/elif/else,while,for`
8. Creating and Using Functions: `def, import`

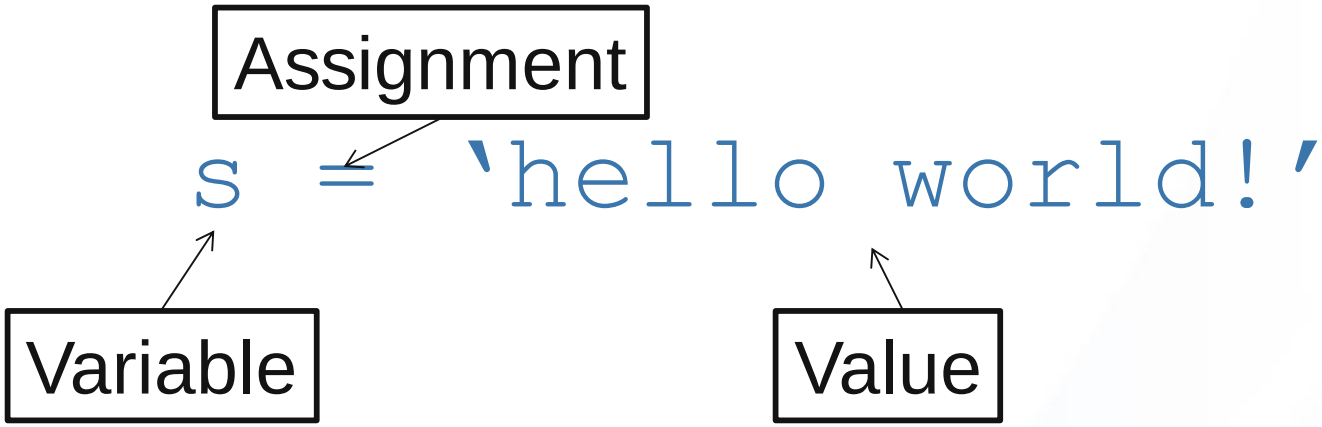
- Other programming languages have more or less the same components, with different syntaxes.

Data Types

- Built-in data types:
  - `int` positive or negative whole numbers, e.g. 5, 100, -2
  - `float` decimal numbers, 1.2, 3.14159, -10.0
  - `str` 'hello', "This is a string"
  - `bool` Only two values of this type: `True` or `False`
- Useful Utilities
  - `type(some_value or variable)`
  - `sys.float_info`
  - `sys.maxint`
- Type conversion:
  - `float(2) -> 2.0,int(1.1) -> 1`
  - Be careful: `2/3` -> 0. Make sure one of them is a float.

Note: You can also have user-defined data types: classes, which we are not going to cover.

Variables and Assignment



- Variables have to be in one word. Can't start with a number, but otherwise can be any combinations of numbers, letters and some special characters: _ and -.
  - `my_variable, var1, var2, ...`
- Can't be any of the Python reserved words, such as `if, else, True, False, class`, etc.
- Assignments can also be
  - `a, b = 1.0, 2.2 -> a = 1.0, b = 2.2`

Collection Data Types: Represent a group of values

- List
  - `name = ['Alice', 'Bob', 'Charlie', 'David'],`
  - `age = [20, 22, 23, 21]`
  - List is mutable (append, remove, insert, …)
  - indexing, slicing
  - `len(a), range([start,]stop[,step])`
- Dictionaries: associative `key:value` pairs
  - `age={'Alice':20, 'Bob':22, 'Charlie':23, 'David':21}`
  - Indexing: `age['Alice']`
  - Insertion: `age['Edward'] = 19`
  - In random order by default. Try: `print age`
- Tuples
  - `Results = (1.1, 2.0)`
  - Not mutable. Can have mixed data types, nested tuples.
- Sets:
  - `set1={1,2,3,4}, set2={2,3,4,5}`
  - `set1&set2 -> {2,3,4}`

Logical Operation

- Returns `True` or `False`
- Demo
  - `==`
  - `<, >`
  - `and`
  - `or`
  - `not`

Arithmetic Operators

- Demo: +, -, *, /, **, %
  - **: power
  - %: modulo
- Order of executions
  - When in doubt, use parentheses

Input and Output (I/O)

- Standard I/O (Prints to screen, or takes input from keyboard)
  - `print`
  - `input` – automatically detects the type based on the input
  - `raw_input –` everything is considered a string.
  - Hint: check using `type(arg)`

- File I/O (demo in examples)
  - `open` (returns a file handle)
    - `Infile = open('mydata.dat','r')`
    - `Outfile = open('output.dat','w')`
  - `read, readlines, readline, for line in f:`
  - `write`
  - `close`

Control Flow Statements

- Conditional: `if/elif/else`
  - Only execute if the statement is True
  - Can have nested conditionals

```
print "Type a number:"
n = input()

if type(n) == int:
    if n%2 == 0:
        print n, "is an even number"
    else:
        print n, "is an odd number"
else:
    print n, "is not an integer"
```

- Looping: `for, while`

```
print "for loop:"
for n in range(10):
    if n%2 == 0:
        print n, "is an even number"
    else:
        print n, "is an odd number"

print "while loop:"
x = 11
while x < 20:
    if x%2 == 0:
        print x, "is an even number"
    else:
        print x, "is an odd number"
    x=x+1
```

Functions

- Functions have the form `func([argument list])`
  - Examples: `sqrt(2), sin(pi), range(1,100,2),` etc.

- In addition to the built-in functions, we can also define our own

```
def my_func(arg1, arg2):
    do something
    return results
```

- For example:

```
def square(x):
    return x*x
print square(2)
```

Classes, Modules and Libraries

- The true power of Python lies in the vast collection of open-source modules and libraries that are freely available.
- Python comes with limited built-in functions. To use the external modules and functions, we have to let python know beforehand.
- Ways to access external functions
  - `import module_name`
    - For C programmers, this is much like `#include<header.h>`
  - `from module_name import func`
  - Example:

```
import math
math.sqrt(2)

from math import sqrt
sqrt(2)
```

An Example – Random Numbers

- Task 1
  - Generate *N* normally/Gaussian distributed random numbers with an average of μ (mu) and standard deviation σ (sigma)
  - Write them to disk
- Task 2
  - Read them back in
  - Compute the average and standard deviation
  - Display the results on terminal
- Task 3 (Time permitting)
  - Compute and display the histogram of the numbers
  - Do a curve fit

Normal/Gaussian Distribution

From Wikipedia:

A normal distribution is:

$$f(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

The parameter μ in this definition is the mean or expectation of the distribution (and also its median and mode). The parameter σ is its standard deviation; its variance is therefore σ^2. A random variable with a Gaussian distribution is said to be normally distributed and is called a normal deviate.

If μ= 0 and σ = 1, the distribution is called the standard normal distribution or the unit normal distribution

Normal/Gaussian Distribution

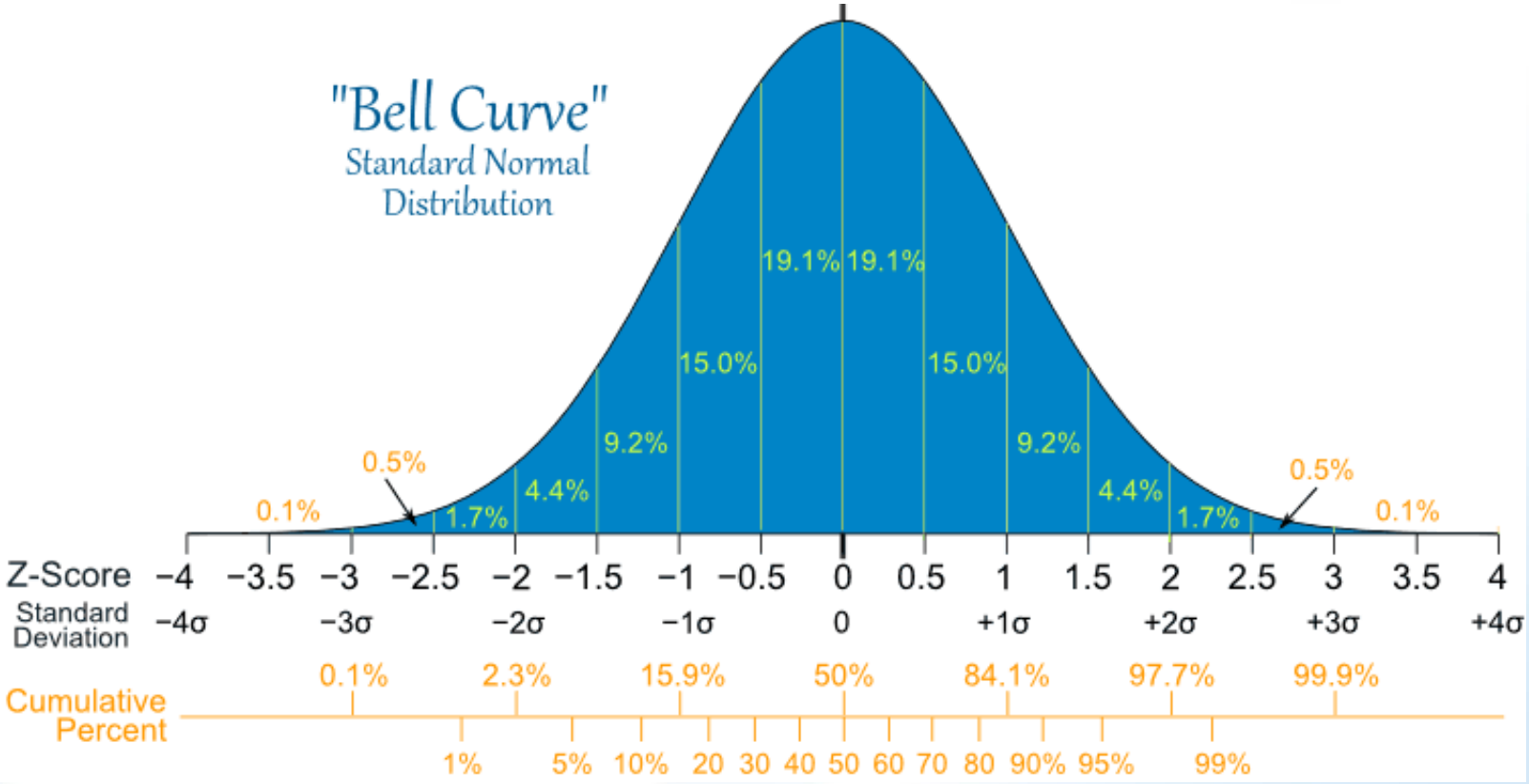


Image source: http://www.mathsisfun.com

Task1: Generate and save the random numbers

- Code demo: generate.py

- Features demonstrated:
  - Import external functions
  - Assignments
  - List operation
  - For loop
  - File output

```
import os
import random

# change the current directory to my workshop directory
workshop_dir = '/Users/meifeng/Dropbox/BNL/CSC/Mini-Semester-Jan2015/examples/'
os.chdir(workshop_dir)

# set the number of random numbers we want
N = 10000

# mean
mu = 0.0

# standard deviation
sigma = 1.0

# create an empty list
data = []

# append each random number to the list
for i in range(N):
    data.append(random.gauss(0,1.0))

# open the output file to write
outfile = open('ran_data.dat','w')

# write the data to disk
for i in range(N):
    outfile.write("%d %e\n" %(i, data[i]))

outfile.close()
```

Statistical Analysis of Data

- We can calculate the mean and standard deviation of the random numbers we just generated, and compare them to the input values: μ = 0, σ = 1.0
- Mean:

$$\mu = \frac{1}{N}\sum_{i=0}^{N-1} x_i = \frac{1}{N}(x_0 + x_1 + ... + x_{N-1})$$

- Standard deviation:

$$\sigma = \sqrt{\frac{\sum_{i=0}^{N-1}(x_i - \mu)^2}{N}}$$

Task2: Calculate the mean and standard deviation

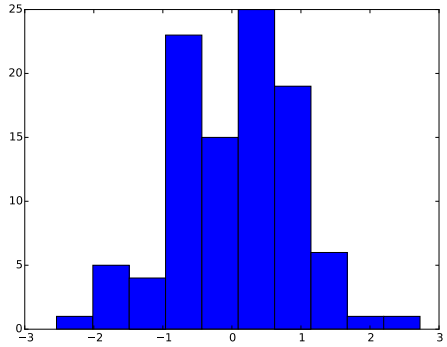
- Code demo: analyze.py

- Features demonstrated:
  - File input
  - User-defined functions
  - Type conversion

```
import os
from math import sqrt

# create a function to calculate the mean and standard deviation
# of an input list
def stat(data):
    tot = 0.0
    N = len(data)
    for i in range(N):
        tot += data[i]
    avg = tot/N

    for i in range(N):
        tot += (data[i] - avg)**2
    var = tot/N
    return avg, sqrt(var)

# change the current directory to my workshop directory
workshop_dir = '/Users/meifeng/Dropbox/BNL/CSC/Mini-Semester-Jan2015/examples/'
os.chdir(workshop_dir)

data = []

infile = open('ran_data.dat','r')
for line in infile: # line is a string
    _, val = line.split() # _ is a dummy variable
    data.append(float(val)) # needs to convert string to float

infile.close()

print 'average, standard deviation = ', stat(data)
```

Histogram

- A histogram is a graphical representation of the distribution of data.



- The histogram of the random numbers we generated should be an approximation of the normal distribution.
- The more data we generate, the closer our histogram is to the normal distribution.

Task3: Fit the data and plot the histogram

- Code demo: fit.py

- Features demonstrated:
  - Use of external libraries: numpy, scipy and matplotlib
  - Plotting
  - Curve fitting with scipy

```
import os
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.mlab as mlab
from scipy.stats import norm

# change the current directory to my workshop directory
workshop_dir = '/Users/meifeng/Dropbox/BNL/CSC/Mini-Semester-Jan2015/examples/'
os.chdir(workshop_dir)

# input file
infile = 'ran_data.dat'

# read and unpack the data
x, y = np.loadtxt(infile, unpack=True)
nbins = 100

# fit the data to the normal distribution
# and obtain the mean and standard deviation
(mu, sigma) = norm.fit(y)

print "From Gaussian fit, mu = ", mu, "sigma = ", sigma

fig = plt.figure()

# position of the subplots. The numbers read as M x N plots, ith plot
timeseries = fig.add_subplot(211)
histogram = fig.add_subplot(223)
histogram_norm = fig.add_subplot(224)

# make the histogram plots!
histogram.hist(y, nbins, normed=False, align='mid',
    facecolor='blue', alpha=0.9)
histogram.set_xlabel('Random Number Value')
histogram.set_ylabel('Counts')
n, bins, patches = histogram_norm.hist(y, nbins, normed=True,
    align='mid',facecolor='green', alpha=0.9)

histogram_norm.set_xlabel('Random Number Value')
histogram_norm.set_ylabel('Fraction')

# plot the Gaussian fit
gauss = mlab.normpdf(bins, mu, sigma)
histogram_norm.plot(bins, gauss, 'r-', linewidth=2)

# time series plot
timeseries.plot(x,y,'r-')
timeseries.set_xlabel('Index')
timeseries.set_ylabel('Random Number Value')
fig.subplots_adjust(hspace=0.5,wspace=0.5)

# display the plot
fig.show()

# save a hard copy
fig.savefig('histogram.pdf')
```

Hands-On Exercises

Exercise #1

- Print numbers 1 to 100 to stdout
- Elements needed:
  - `print`
  - `range` function
  - `for` loop

Exercise #2

- Print 100 random numbers in the format of:
  - <index> <random number>
- New Elements needed:
  - `from random import random`
  - `random()` will generate one flat-distribution random number between [0,1]

Statistical Analysis of Data

- Mean:

$$\mu = \frac{1}{N}\sum_{i=0}^{N-1} x_i = \frac{1}{N}(x_0 + x_1 + ... + x_{N-1})$$

- Standard deviation:

$$\sigma = \sqrt{\frac{\sum_{i=0}^{N-1}(x_i - \mu)^2}{N}}$$

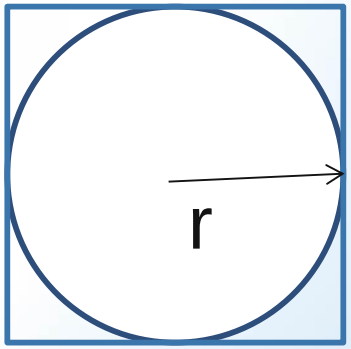
Exercise #3

- Write a function to calculate the mean and standard deviation of a list
- Calculate the mean and standard deviation of the generated random numbers

- New elements needed:
  - Store the random numbers in a list
  - Self defined function: def func()
  - The `sqrt` function from the `math` module

Exercise #4

- Monte Carlo Methods: numerical methods that use random numbers to do repeated sampling and obtain results.
- Estimate the value of π using the Monte Carlo method.



- Area of the square: $4r^2$
- Area of the circle: πr^2
- If we throw darts randomly at the square, the probability of them landing inside the circle is $\pi/4$
- Monte Carlo estimation of π:
  - Generate N points with coordinates (x, y), where x and y are random numbers between 0 and 1
  - If sqrt(x^2 + y^2) < 1, $N_{in} = N_{in} + 1$
  - $N_{in} / N = \pi / 4$ ➔ $\pi = 4\ N_{in} / N$

Closing Remarks

- Python is powerful and fun.
- It's a good first language to learn if you don't have any programming experience.

- You can find many useful resources on the internet.
  - Official Python website: www.python.org
  - Online video courses:
    - www.udacity.com
    - www.coursera.org
    - www.edx.org
  - Codecademy interactive coding tutorials:
    - http://www.codecademy.com/tracks/python

```
print "Have fun coding!"
```