



Python 101/201

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Agenda

- Introduction to the Jupyter Notebook
- Welcome to Python
- Using Numpy
- Matplotlib



https://jupyter.tacc.cloud



What are Jupyter Notebooks?

A web-based, interactive computing tool for capturing the whole computation process: developing, documenting, and executing code, as well as communicating the results.



How do Jupyter Notebooks Work?

An open notebook has exactly one interactive session connected to a kernel which will execute code sent by the user and communicate back results. This kernel remains active if the web browser window is closed, and reopening the same notebook from the dashboard will reconnect the web application to the same kernel.

What's this mean?

Notebooks are an interface to kernel, the kernel executes your code and outputs back to you through the notebook. The kernel is essentially our programming language we wish to interface with.



Jupyter Notebooks, Structure

Code Cells
 Code cells allow you to enter and run code
 Run a code cell using Shift-Enter

Markdown Cells

Text can be added to Jupyter Notebooks using Markdown cells. Markdown is a popular markup language that is a superset of HTML.



Jupyter Notebooks, Structure

Markdown Cells

You can add headings:

```
# Heading 1
# Heading 2
## Heading 2.1
## Heading 2.2
```

You can add lists

- 1. First ordered list item
- 2. Another item
- · · * Unordered sub-list.
- 1. Actual numbers don't matter, just that it's a number
- · · 1. Ordered sub-list
- 4. And another item.



Jupyter Notebooks, Structure

Markdown Cells

Jupyter Notebooks, Workflow

Typically, you will work on a computational problem in pieces, organizing related ideas into cells and moving forward once previous parts work correctly. This is much more convenient for interactive exploration than breaking up a computation into scripts that must be executed together, as was previously necessary, especially if parts of them take a long time to run.



Jupyter Notebooks, Workflow

Let a traditional paper lab notebook be your guide:

Each notebook keeps a historical (and dated) record of the analysis as it's being explored.

The notebook is not meant to be anything other than a place for experimentation and development.

Notebooks can be split when they get too long.

Notebooks can be split by topic, if it makes sense.



Jupyter Notebooks, Shortcuts

- Shift-Enter: run cell
 - Execute the current cell, show output (if any), and jump to the next cell below. If Shift-Enter is invoked on the last cell, a new code cell will also be created. Note that in the notebook, typing Enter on its own never forces execution, but rather just inserts a new line in the current cell. Shift-Enter is equivalent to clicking the Cell
 Run menu item.

Jupyter Notebooks, Shortcuts

- Ctrl-Enter: run cell in-place
 - Execute the current cell as if it were in "terminal mode", where any output is shown, but the cursor remains in the current cell. The cell's entire contents are selected after execution, so you can just start typing and only the new input will be in the cell. This is convenient for doing quick experiments in place, or for querying things like filesystem content, without needing to create additional cells that you may not want to be saved in the notebook.



Jupyter Notebooks, Shortcuts

- Alt-Enter: run cell, insert below
 - Executes the current cell, shows the output, and inserts a new cell between the current cell and the cell below (if one exists). (shortcut for the sequence Shift-Enter,Ctrl-m a. (Ctrl-m a adds a new cell above the current one.))
- Esc and Enter: Command mode and edit mode
 - In command mode, you can easily navigate around the notebook using keyboard shortcuts. In edit mode, you can edit text in cells.



Introduction to Python

Hello World!
Data types
Variables
Arithmetic operations
Relational operations
Input/Output
Control Flow

Do not forget:

Indentation matters!



Python

print("Hello World!")

Let's type that line of code into a Code Cell, and hit Shift-Enter:

Hello World!



Python

```
print(5)
print(1+1)
```

Let's add the above into another Code Cell, and hit Shift-Enter

5

2



Python - Variables

You will need to store data into variables
You can use those variables later on
You can perform operations with those variables
Variables are declared with a **name**, followed by '=' and a **value**

An integer, string,...
When declaring a variable, **capitalization** is important: 'A' <> 'a'



Python - Variables

in a code cell:

```
five = 5
one = 1
twodot = 2.0
print (five)
print (one + one)
message = "This is a string"
print (message)
```

Notice: We're not "typing" our variables, we're just setting them and allowing Python to type them for us.



Python - Data Types

in a code cell:

```
integer_variable = 100
floating_point_variable = 100.0
string_variable = "Name"
```

Notice: We're not "typing" our variables, we're just setting them and allowing Python to type them for us.



Python - Data Types

Variables have a type

```
You can check the type of a variable by using the type() function: print (type(integer_variable))
```

It is also possible to change the type of some basic types:

```
str(int/float): converts an integer/float to a string
int(str): converts a string to an integer
float(str): converts a string to a float
```

Be careful: you can only convert data that actually makes sense to be transformed



Python - Arithmetic Operations

```
Addition
                              1 + 1 = 2
+
          Subtraction
                              5 - 3 = 2
                             4/2 = 2
          Division
%
          Modulo
                              5 % 2 = 1
*
                              5 * 2 = 10
         Multiplication
                              5 // 2 = 2
          Floor division
**
                              2 ** 3 = 8
          To the power of
```

Python - Arithmetic Operations

Some experiments:

```
print (5/2)
print (5.0/2)
print ("hello" + "world")
print ("some" + 1)
print ("number" * 5)
print (3+5*2)
```

Python - Arithmetic Operations

Some more experiments:

```
number1 = 5.0/2
number2 = 5/2

what type() are they?
type(number1)
type(number2)

now, convert number2 to an integer:
int(number2)
```



Python – Reading from the Keyboard

Let put the following into a new Code Cell:

```
numIn = input("Please enter a number: ")
```

Let's run this cell!



Python – Reading from the Keyboard

Let put the following into a new Code Cell:

Let's run this cell!

put the word **Hello** as your input.

What happened?



Python – Making the output prettier

Let put the following into a new Code Cell:

```
print ("The number that you wrote was : ", numIn)
print ("The number that you wrote was : %d" % numIn)
print ("the string you entered was: ", stringIn)
print ("the string you entered was: %s" % stringIn)
 Want to make it prettier?
     \n for a new line
     \t to insert a tab
print (" your string: %s\n your number: %d", %(numIn, stringIn))
```

TACC

for floating points, use %f

Python – Writing to a File

Let put the following into a new Code Cell:

```
my file = open("output file.txt",'w')
var1 = "This is a string\n"
my file.write(vars)
var2 = 10
my file.write("\n")
my file.write(str(var2))
var3 = 20.0
my_file.write("\n")
my file.write(str(var3))
my_file.close()
```

When opening a file, you need to decide "how" you want to open it: Just read?

Are you going to write to the file?

If the file already exists, what do you want to do with it?

- r read only (default)
- w write mode: file will be overwritten if it already exists
- a append mode: data will be appended to the existing file



Let's read from the file we created in the previous cell.

```
my_file = open("output_file.txt",'r')
content = my_file.read()
print(content)
my_file.close()
```

Let's read it line by line

```
my file = open("output file.txt",'r')
var1 = my file.readline()
var2 = my file.readline()
var3 = my file.readline()
var4 = my file.readline()
print("String: ", var1)
print("Blank: ", var2)
print("Integer: ", var3)
print("Float: ", var4)
my file.close()
```



```
Tweak it a bit to make the code easier to read... introducing 'with'!
'with' will very nicely close your file for you
(Note the indentation!!)
with open("output file.txt", 'r') as f:
     var5 = f.readline()
     var6 = f.readline()
     var7 = f.readline()
    var 8 = f.readline()
     print("String: ", var5)
     print("Blank: ", var6)
     print("Integer: ", var7)
     print("Float: ", var8)
```

Python - Control Flow

So far we have been writing instruction after instruction where every instruction is executed

What happens if we want to have instructions that are only executed if a given condition is true?



Let's look at some example of booleans. type the following into a code cell

```
a = 2
b = 5

print (a>b)
print (a<b)
print (a == b)
print (a != b)
print (b>a or a==b)
print (b<a and a==b)</pre>
```

The if/else construction allows you to define conditions in your program

```
(Don't forget your indentation!!)

if conditionA:
    statementA
  elif conditionB:
    statementB
  else:
    statementD
  this line will always be executed (after the if/else)
```



statementD

(Indentation is IMPORTANT!)

The if/else construction allows you to define conditions in your program

if conditionA:
 statementA
elif conditionB:
 statementB
else:

conditions are a datatype known as booleans, they can only be true or false

this line will always be executed (after the if/else)



A simple example

```
simple_input = input("Please enter a number: ")
if (int(simple_input)>10):
    print ("You entered a number greater than 10")
else:
    print ("you entered a number less than 10")
```



Python - if/else/elif

You can also nest if statements together:

```
if (condition1):
    statement1
    if (condition2):
        statement2
    else:
        if (condition3):
            statement3 # when is this statement executed?
else: # which 'if' does this 'else' belong to?
    statement4 # when is this statement executed?
```



enter a number from the keyboard into a variable.

using type casting and if statements, determine if the number is even or odd



Python - For Loops

When we need to iterate, execute the same set of instructions over and over again... we need to loop! and introducing range()

```
(Indentation is IMPORTANT!)
for x in range(0, 3):
    print ("Let's go %d" % x)
```

Python – For Loops, nested loops

When we need to iterate, execute the same set of instructions over and over again... we need to loop! and introducing range()

```
for x in range(0, 3):
    for y in range(0,5):
        print ("Let's go %d %d" % (x,y))
```

using nested for-loops and nested if statements, write a program that loops from 3 to 1000 and print out the number if it is a prime number.



using a for loop, find the triples that satisfies:

$$a*a + b*b = c*c$$

where

Python - While Loops

Sometimes we need to loop while a condition is true...

(remember to indent!)

```
i = 0  # Initialization
while (i < 10):  # Condition
    print (i)  # do_something
    i = i + 1  # Why do we need this?</pre>
```

using a while loop, find the prime numbers less than 1000



A list is a sequence, where each element is assigned a position (index) First position is 0. You can access each position using [] Elements in the list can be of different type

```
mylist1 = ["first item", "second item"]
mylist2 = [1, 2, 3, 4]
mylist3 = ["first", "second", 3]
print(mylist1[0], mylist1[1])
print(mylist2[0])
print(mylist3)
print(mylist3[0], mylist3[1], mylist3[2])
print(mylist2[0] + mylist3[2])
```

```
It's possible to use slicing:
    print(mylist3[0:3])
    print(mylist3)

To change the value of an element in a list, simply assign it a new value:
    mylist3[0] = 10
    print(mylist3)
```

There's a function that returns the number of elements in a list len(mylist2)

Check if a value exists in a list:

```
1 in mylist2
```

Delete an element

```
len(mylist2)
del mylist2[0]
print(mylist2)
```

Iterate over the elements of a list:

```
for x in mylist2:
    print(x)
```

```
There are more functions
  max(mylist), min(mylist)
```

It's possible to add new elements to a list:

```
my_list.append(new_item)
```

We know how to find if an element exists, there's a way to return the position of that element:

```
my_list.index(item)
```

Or how many times a given item appears in the list:

```
my list.count(item)
```



create a 3 lists:

one list, x, holding numbers going from 0 to 100 one list, y1, holding x*x one list, y2, holding x*x*x

write these out to a file with the format:

x, y1, y2

Python – user defined functions

User-defined functions are reusable code blocks; they only need to be written once, then they can be used multiple times. They can even be used in other applications, too.

These functions are very useful, from writing common utilities to specific business logic. These functions can also be modified per requirement. The code is usually well organized, easy to maintain, and developer-friendly.

As user-defined functions can be written independently, the tasks of a project can be distributed for rapid application development.

A well-defined and thoughtfully written user-defined function can ease the application development process.



Python – user defined functions

Step 1: Declare the function with the keyword def followed by the function name.

Step 2: Write the arguments inside the opening and closing parentheses of the function, and end the declaration with a colon.

Step 3: Add the program statements to be executed.

Step 4: End the function with/without return statement.



Python – user defined functions

```
def userDefFunction (arg1, arg2, arg3
...):
  program statement1
  program statement3
  program statement3
  return;
```

write a user defined function that accepts an integer as an argument then prints out that many number of prime numbers



write a user defined function that accepts an integer as a parameter then returns the next prime number.



A prime gap is the difference between two successive prime numbers. The n-th prime gap, denoted gn or g(pn) is the difference between the (n + 1)-th and the n-th prime numbers

Write a program that uses your prime number generator functions and print out the first set of prime numbers where the prime gap is greater than 13



Python – Anonymous Functions

type the following into a cell:

```
x = lamda a: a * 10
print (x(10))
```

Python - Anonymous Functions

try the following definition:

```
def myfunc(x):
    return lambda a: a*x

y = myfunc(10)
print (y(5))
z = myfunc(100)
print (z(5))
```



Questions? Comments?



Monte Carlo Pi

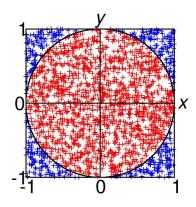
Sequential Algorithm

A Monte Carlo algorithm for approximating π uniformly generates the points in the square [-1, 1] \times [-1, 1]. Then it counts the points which lie in the inside of the unit circle.



Sequential Algorithm

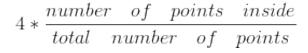
A Monte Carlo algorithm for approximating π uniformly generates the points in the square [-1, 1] x [-1, 1]. Then it counts the points which lie in the inside of the unit circle.

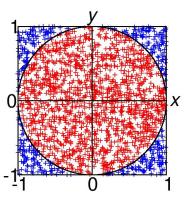




Sequential Algorithm

An approximation of π is then computed by the following formula:







Algorithm

```
double approximatePi(int numSamples)
{
  float x, y;
  int counter = 0;
  for (int s = 0; s != numSamples; s++)
  {
     x = random number between -1, 1;
     y = random number between -1, 1;
}

if (x * x + y * y < 1)
  {
     counter++;
     }
}

return 4.0 * counter / numSamples;
}</pre>
```

Let's code this in Python, Google to see what command in Python produces a random number



Python - NumPy

"Numerical Python"

open source extension module for Python provides fast precompiled functions for mathematical and numerical routines adds powerful data structures for efficient computation of multi-dimensional arrays and matrices.



NumPy, First Steps

Let build a simple list, turn it into a numpy array and perform some simple math.

```
import numpy as np
cvalues = [25.3, 24.8, 26.9, 23.9]
C = np.array(cvalues)
print(C)
```

NumPy, First Steps

Let build a simple list, turn it into a numpy array and perform some simple math.

```
print(C * 9 / 5 + 32)
VS.
```

```
fvalues = [ x*9/5 + 32 for x in cvalues]
print(fvalues)
```

NumPy, Cooler things

```
import time
size_of_vec = 1000
def pure_python_version():
    t1 = time.time()
   X = range(size_of_vec)
   Y = range(size_of_vec)
    Z = []
    for i in range(len(X)):
        Z.append(X[i] + Y[i])
    return time.time() - t1
def numpy_version():
    t1 = time.time()
   X = np.arange(size_of_vec)
    Y = np.arange(size_of_vec)
    Z = X + Y
    return time.time() - t1
```



NumPy, Cooler things

Let's see which is faster.

```
t1 = pure_python_version()
t2 = numpy_version()
print(t1, t2)
```



```
A = np.array([ [3.4, 8.7, 9.9],
               [1.1, -7.8, -0.7],
               [4.1, 12.3, 4.8]]
print(A)
print(A.ndim)
B = np.array([[[111, 112], [121, 122]],
               [[211, 212], [221, 222]],
               [[311, 312], [321, 322]] ])
print(B)
print(B.ndim)
```

The shape function:

The shape function can also *change* the shape:

```
x.shape = (3, 6)
print(x)

x.shape = (2, 9)
print(x)
```



A couple more examples of shape:



NumPy, Multi-Dimension Arrays

indexing:

NumPy, Multi-Dimension Arrays

slicing:

```
A = np.array([
[11,12,13,14,15],
[21,22,23,24,25],
[31,32,33,34,35],
[41,42,43,44,45],
[51,52,53,54,55]])
print(A[:3,2:])
print(A[:3,2:])
```

NumPy, Multi-Dimension Arrays

function to create an identity array

```
np.identity(4)
```



NumPy, By Example

The example we will consider is a very simple (read, trivial) case of solving the 2D Laplace equation using an iterative finite difference scheme (four point averaging, Gauss-Seidel or Gauss-Jordan). The formal specification of the problem is as follows. We are required to solve for some unknown function u(x,y) such that $\nabla 2u = 0$ with a boundary condition specified. For convenience the domain of interest is considered to be a rectangle and the boundary values at the sides of this rectangle are given.

```
def TimeStep(self, dt=0.0):
     """Takes a time step using straight forward Python loops."""
     g = self.grid
    nx, ny = g.u.shape
    dx2, dy2 = g.dx**2, g.dy**2
    dnr inv = 0.5/(dx2 + dy2)
    u = g.u
    err = 0.0
    for i in range(1, nx-1):
         for j in range(1, ny-1):
             tmp = u[i,j]
             u[i,j] = ((u[i-1, j] + u[i+1, j])*dy2 +
                      (u[i, j-1] + u[i, j+1])*dx2)*dnr inv
             diff = u[i,j] - tmp
             err += diff*diff
     return numpy.sqrt(err)
```

NumPy, By Example

The example we will consider is a very simple (read, trivial) case of solving the 2D Laplace equation using an iterative finite difference scheme (four point averaging, Gauss-Seidel or Gauss-Jordan). The formal specification of the problem is as follows. We are required to solve for some unknown function u(x,y) such that $\nabla 2u = 0$ with a boundary condition specified. For convenience the domain of interest is considered to be a rectangle and the boundary values at the sides of this rectangle are given.

```
def numericTimeStep(self, dt=0.0):
    """Takes a time step using a NumPy expression."""
   g = self.grid
   dx2, dy2 = g.dx**2, g.dy**2
   dnr_inv = 0.5/(dx^2 + dy^2)
   u = g.u
   g.old u = u.copy() # needed to compute the error.
   # The actual iteration
    u[1:-1, 1:-1] = ((u[0:-2, 1:-1] + u[2:, 1:-1])*dy2 +
                     (u[1:-1,0:-2] + u[1:-1, 2:])*dx2)*dnr inv
    return_g.computeError()
```

NumPy, Exercise

Jacobi

```
Algorithm.
* Find D, the Diagonal of of A : diag(A)
* Find R, the Remainder of A - D : A - diagflat(A)
* Choose your initial guess, x[0]
    * Start iterating, k=0
        * While not converged do
           * Start your i-loop (for i = 1 to n)
               * sigma = 0
                * Start your j-loop (for j = 1 to n)
                   * If j not equal to i
                       * sigma = sigma + a[i][j] * x[j][k]
                 * End j-loop
               * x[i]k = (b[i] - sigma)/a[i][i] : x = (b - dot(R,x)) / D
           * End i-loop
        * Check for convergence
    * Iterate k, ie. k = k+1
```

Matplotlib, What is it?

It's a graphing library for Python. It has a nice collection of tools that you can use to create anything from simple graphs, to scatter plots, to 3D graphs. It is used heavily in the scientific Python community for data visualisation.



Jupyter

https://jupyter.tacc.cloud



Matplotlib, First Steps

Let's plot a simple sin wave from 0 to 2 pi.

First let's, get our code started by importing the necessary modules.

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



Matplotlib, First Steps

Let's add the following lines, we're setting up x as an array of 50 elements going from 0 to 2*pi

```
x = np.linspace(0, 2 * np.pi, 50)
plt.plot(x, np.sin(x))
plt.show() # Show the graph.
```

Let's run our cell!



Let's plot another curve on the axis

```
plt.plot(x, np.sin(x),
          x, np.sin(2 * x))
plt.show()
```

Let's run our cell!



Let's see if we can make the plots easier to read

```
plt.plot(x, np.sin(x), 'r-o',
        x, np.cos(x), 'g--')
plt.show()
```

Let's run this cell!



```
Colors:
Blue - 'b'
Green - 'g'
Red - 'r'
Cyan - 'c'
Magenta - 'm'
Yellow - 'v'
Black - 'k' ('b' is taken by blue so the last letter is
used)
White - 'w'
```

```
Lines:
   Solid Line - '-'
   Dashed - '-'
   Dotted - '.'
   Dash-dotted - '-:'
Often Used Markers:
   Point - '.'
   Pixel - '.'
   Circle - 'o'
   Square - 's'
   Triangle - '^'
```

Matplotlib, Subplots

Let's split the plots up into subplots

```
plt.subplot(2, 1, 1) # (row, column, active area)
plt.plot(x, np.sin(x), 'r')
plt.subplot(2, 1, 2)
plt.plot(x, np.cos(x), 'g')
plt.show()
```

using the subplot() function, we can plot two graphs at the same time within the same "canvas". Think of the subplots as "tables", each subplot is set with the number of rows, the number of columns, and the active area, the active areas are numbered left to right, then up to down.



Matplotlib, Scatter Plots

Let's take our sin curve, and make it a scatter plot

```
y = np.sin(x)
plt.scatter(x,y)
plt.show()
```

call the scatter() function and pass it two arrays of x and y coordinates.



Matplotlib, add a touch of color

Let's mix things up, using random numbers and add a colormap to a scatter plot

```
x = np.random.rand(1000)
y = np.random.rand(1000)
size = np.random.rand(1000) * 50
color = np.random.rand(1000)
plt.scatter(x, y, size, color)
plt.colorbar()
plt.show()
```



Matplotlib, add a touch of color

Let's see what we added, and where that takes us

```
plt.scatter(x, y, size, color)
plt.colorbar()
...
```

We brought in two new parameters, size and color, which will vary the diameter and the color of our points. Then adding the colorbar() gives us a nice color legend to the side.



Matplotlib, Histograms

A histogram is one of the simplest types of graphs to plot in Matplotlib. All you need to do is pass the hist() function an array of data. The second argument specifies the amount of bins to use. Bins are intervals of values that our data will fall into. The more bins, the more bars.

```
plt.hist(x, 50)
plt.show()
```

Matplotlib, Adding Labels and Legends

Let's go back to our sin/cos curve example, and add a bit of clarification to our plots

```
x = np.linspace(0, 2 * np.pi, 50)
plt.plot(x, np.sin(x), 'r-x', label='Sin(x)')
plt.plot(x, np.cos(x), 'g-^', label='Cos(x)')
plt.legend() # Display the legend.
plt.xlabel('Rads') # Add a label to the x-axis.
plt.ylabel('Amplitude') # Add a label to the y-axis.
plt.title('Sin and Cos Waves') # Add a graph title.
plt.show()
```

Let's go back to our dataframe, and graph out x*x+y*y as a mesh

```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import
Axes3D
```



Let's create our function and our empty array and look at the contour

```
z1 = np.empty([2001,2001])
im = plt.imshow(z1, cmap='hot')
fig = plt.colorbar(im,
orientation='horizontal')
plt.show(fig)
```

Filling out an array manually...

```
z = np.empty([2001, 2001])
for x in np.arange(-10,10,.01):
    i = i + 1
    for y in np.arange(-10,10,.01):
        j = j + 1
        z[i][j] = x*x + y*y
```

Here we can simplify it!

```
def f1(x,y):
    return (x*x+y*y)

x = np.linspace(-10, 10, 2000)
y = np.linspace(-10, 10, 2000)

X, Y = np.meshgrid(x, y)
Z = f1(X, Y)
```

And now plot it out

```
fig1 = plt.figure()
ax = plt.axes(projection='3d')
ax.contour3D(X, Y, Z, 50, cmap='hot')
ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('z');
ax.view_init(45, 0)
```



Questions? Comments?

