



Power Python 101

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Agenda

- Introduction to the Jupyter Notebook
- Numpy Array vs Standard List
- Threads and Processors
- Vectorization
- Using Numpy with Threads
- Pandas
- Data Science



https://designsafe-ci.org



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.



Python - Variables, Refresh

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, refresh

```
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



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)
```



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))
```



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

Numpy gives us the array

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



NumPy, First Steps

And gives us an easier way to perform some simple math on them

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

VS.

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

```
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:



indexing:



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:])
```



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

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```
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
```

Threads, Multithreading, Processes in a Nutshell

What is a thread?

A thread is a path of execution within a process.

A process can contain multiple threads.

What is a process?

a process is the instance of a computer program that is being executed by one or many threads.



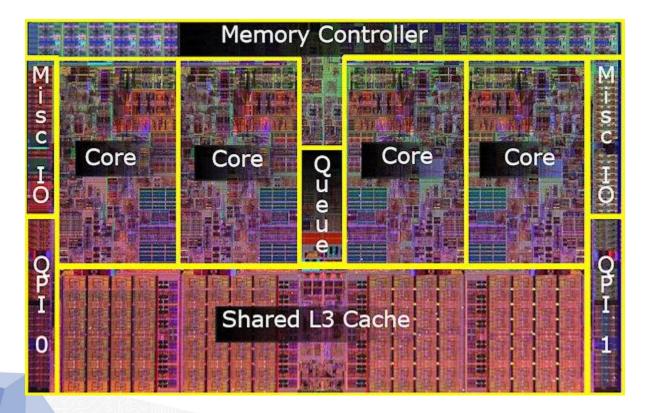
Threads, Multithreading, Processes in a Nutshell

Multithreading?

A thread is also known as lightweight process. The idea is to achieve parallelism by dividing a process into multiple threads.



The big picture





Advantages of Multithreading

- 1. **Responsiveness**: If the process is divided into multiple threads, if one thread completes its execution, then its output can be immediately returned.
- 2. **Faster context switch:** Context switch time between threads is lower compared to process context switch. Process context switching requires more overhead from the CPU.
- 3. *Effective utilization of multiprocessor system*: If we have multiple threads in a single process, then we can schedule multiple threads on multiple processor. This will make process execution faster.



Advantages of Multithreading

4. **Resource sharing**: Resources like code, data, and files can be shared among all threads within a process.

Note: stack and registers can't be shared among the threads. Each thread has its own stack and registers.

- 5. **Communication**: Communication between multiple threads is easier, as the threads shares common address space. while in process we have to follow some specific communication technique for communication between two process.
- 6. **Enhanced throughput of the system**: If a process is divided into multiple threads, and each thread function is considered as one job, then the number of jobs completed per unit of time

Parallel Programming in a Nutshell

doing multiple things at the same time

- running code simultaneously on different CPUs
- running code on the same CPU using multiple threads and achieving speedups by taking advantage of "wasted" CPU cycles

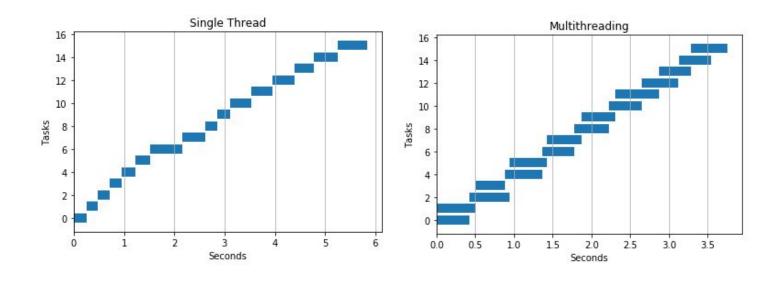


A note about parallelism in Python

the **global interpreter lock** is a mutex - concurrency control, which is instituted for the purpose of preventing race conditions - that protects access to Python objects...



Parallel Programming in a Nutshell





Vectorization

not vectorized

b

1 * 6

а

2 | * | 7

3 | * | 8

4 * 9

5 | * | 10

vectorized

a

b

1

6

2

3

4

L

*

8

9

5

*

10

5 operations

2 operations



NumPy, Vectorization

```
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)
```



Pandas, What is it?

A software library written for the Python for data manipulation and analysis. In particular, it offers data structures and operations for manipulating numerical tables and time series



Pandas, The DataFrame

The primary pandas data structure.

Two-dimensional size-mutable, heterogeneous tabular data structure with labeled axes (rows and columns). Arithmetic operations align on both row and column labels. Can be thought of as a dict-like container for Series objects.



```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```



```
s = pd.Series([1,3,5,np.nan,6,8])
s
```



```
dates = pd.date_range('20180101', periods=6)
dates
```



```
df = pd.DataFrame(np.random.randn(6,4),
  index=dates, columns=list('ABCD'))
df
```



```
df2 = pd.DataFrame({ 'A' : 1.,'B' :
    pd.Timestamp('20130102'),'C' :
    pd.Series(1,index=list(range(4)),dtype='float32'),'D' :
    np.array([3] * 4,dtype='int32'),'E' :
    pd.Categorical(["test","train","test","train"]),'F' :
    'foo' })
df2
```

Pandas, Viewing Data

Some common/useful functions

```
df.head()
df.tail(3)
df.index
df.columns
df.values
df.describe()
df.T
df.sort index(axis=1, ascending=False)
df.sort values(by='B')
```



Pandas, Selecting Data by Label

Some common/useful functions

```
df['A']
df[0:3]
df['20130102':'20130104']
df.loc[dates[0]]
df.loc[:,['A','B']]
df.loc['20130102':'20130104',['A','B']]
df.loc['20130102',['A','B']]
df.loc[dates[0],'A']
```



Pandas, Selecting Data by Position

Some common/useful functions

```
df.iloc[3]
df.iloc[3:5,0:2]
df.iloc[[1,2,4],[0,2]]
df.iloc[1:3,:]
df.iloc[:,1:3]
df.iloc[1,1]
df.iloc[1,1]
```



Pandas, CSV Files

manipulating CSV files.

```
ts = pd.Series(np.random.randn(1000), index=pd.date range('1/1/2000',
 periods=1000))
ts = ts.cumsum() ## cumulative sum
df = pd.DataFrame(np.random.randn(1000, 4), index=ts.index,columns=['A',
 'B', 'C', 'D'])
df = df.cumsum()
df.to csv('foo.csv')
pd.read csv('foo.csv')
```



Pandas, CSV Files

filtering data made easy... return of lambda

```
df = pd.DataFrame(np.random.randn(1000, 4), index=ts.index,columns=['A',
'B', 'C', 'D'])
  = df.cumsum()
df.loc[lambda df: df.B > 10] ## What do you think this does?
```



Dataset 1



Dataset 2

Dataset 3



Joining along rows

```
df_new = pd.concat([df_a, df_b])
df_new
```



Joining along columns

```
d.concat([df_a, df_b], axis=1)
```



Merging

```
pd.merge(df_new, df_n, on='subject_id')
```

Merging, Outer Join

```
pd.merge(df_a, df_b, on='subject_id', how='outer')
```



Merging, Inner Join

```
pd.merge(df_a, df_b, on='subject_id', how='inner')
```



Merging, Right Join

```
pd.merge(df_a, df_b, on='subject_id', how='right')
```



Merging, Left Join

```
pd.merge(df_a, df_b, on='subject_id', how='left')
```

Pandas, Summary of Features

Pandas allow for:

Boolean Indexing
Statistical Operations
Histogramming
Merging Data
SQL Style Joins
SQL Style Appends
SQL Style Grouping
Reshaping
Pivoting
and more!







What is Data Science

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Data Science 101

What is Data?



Data Science 101



What is Data what is data in computer what is data in statistics what is data mining what is data on a phone what is data analysis what is data in dbms what is data collection what is data roaming what is data processing what is data science Report inappropriate predictions



Data is a set of values of subjects with respect to qualitative or quantitative variables. Data and information or knowledge are often used interchangeably; however data becomes information when it is viewed in context or in post-analysis. Wikipedia



Data is everywhere!

Where is your data?



What makes data important?





Data Science is data science is different now data science is a branch of data science is the future data science is overrated data science is hard data science is a fad data science is just statistics data science is not science data science is dead data science is a team sport Report inappropriate predictions



Data science is a multi-disciplinary field that uses scientific methods, processes, algorithms and systems to extract knowledge and insights from structured and unstructured data. Wikipedia



Data Science is the ability to understand that there is a story hidden in the data.



100 Million Dollars - Southwest Airlines saved by reducing the time their airplanes sat idle on the tarmac

39 Million Gallons - the amount of fuel UPS saved by optimizing its fleet

32,000 Dollars the amount of money it costs TACC to have our machines sitting idle



Data is worth money.



BIG DATA

There isn't a readily available definition of Big Data because you can't "see it"



We are in the era of Big Data

There was a road to get to this moment with a few important stops along the way, and it's a road on which we're probably still nowhere near the end. To get to the data driven world we have today, we needed **scale**, **speed**, and **ubiquity**.

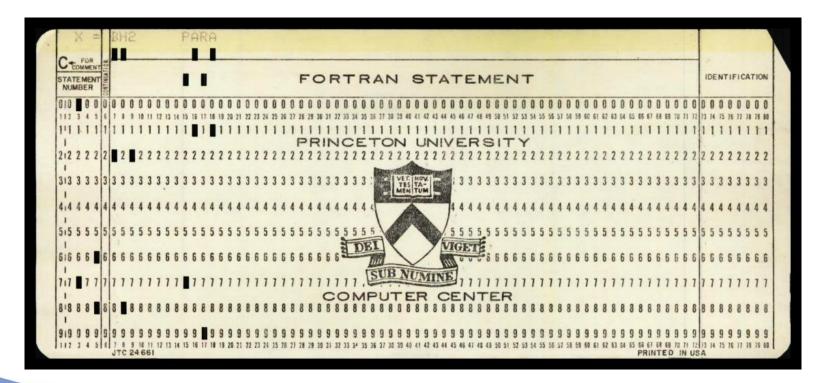


Scale

Data started with the punch card introduced by Herman Hollereith in 1890

7.34 inches wide by 3.25 inches high and approximately .07 inches thick, a punch card was a piece of paper or cardstock containing holes in specific locations that corresponded to specific meanings.







Scale

Coding up data and programs through a series of holes in a piece of paper can only *scale* so far

it was revolutionary for its day because the existence of semi autotic data tallying allowed for faster and more accurate computation.



Speed

the second prong of the big data revolution involves how fast we can move around and compute with data.



Ubiquity

Definition: the fact of appearing everywhere or of being very common.



Putting the science in data science

it's short answer to what you can do with the billions upon billions upon of data points being collected



The data is there.

It exists

There's something valuable in it.

But what does it mean? What's going on? What can you learn? How can you use it to make better science?

Data analysis is all about asking these types of questions.



Here's the catch

You have to understand how the data came to be and what the goals of the process are in order to do good analytic work.



Experimentation has been around for a long time.

People have been testing out new ideas for far longer than data science has been a thing.

Experimentation is at the heart of a lot of modern data work.



Machine Learning

Data scientists define machine learning as the process of using machines to better understand a process or system, and recreate, replicate or augment that system.



Machine Learning, Supervised Learning

Supervised learning is probably the most well known of the branches of data science.

All about predicting something you've seen before.

You try to analyze what the outcome of the process was in the past and build a system that tries to draw out what matters and build predictions for the next time it happens.



Machine Learning, Unsupervised Learning

You can do a lot of machine learning work without an observed outcome or target.

Unsupervised learning is less concerned about making predictions than understanding and identifying relationships or associations that might exist within the data.



Machine Learning, Unsupervised Learning

The K Means algorithm.

This technique, calculates the distance between different points of data and groups similar data together.

This The "suggested new friends" feature on Facebook



Machine Learning, Reinforcement Learning

Reinforcement learning requires an active feedback loop.

Reinforcement learning requires a dynamic dataset that interacts with the real world.



Artificial Intelligence

Artificial Intelligence wants some kind of human interaction and is intended to be somewhat human or "intelligent" in the way it carries out those interactions. Therefore, that interaction becomes a fundamental part of the product a person seeks to build. Data science is more about insight and building systems. It places less emphasis on human interaction and more on providing intelligence, recommendations, or insights.



In a nutshell

Data is important.

We need to understand what the data is

What the data means

To find the underlying story



Questions? Comments?

