Introduction to Python

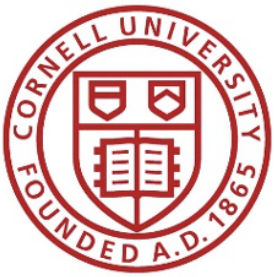
1 Introduction to Python

Chris Myers

Cornell University Center for Advanced Computing (CAC)
and
Cornell Department of Physics / Laboratory of Atomic & Solid State Physics (LASSP)

https://cac.cornell.edu/myers

c.myers@cornell.edu



Center for Advanced Computing

Python is at least 3 things:

- **A programming language**
  - Syntax, keywords, data types, objects, operators, variables, etc.
- **A software ecosystem**
  - Python Standard Library + many thousands of third-party packages for different tasks
- **A program that runs code written in the Python language**
  - An interpreter

2 Outline

- python as a program
- Python as a programming language
- *Python* as a software ecosystem

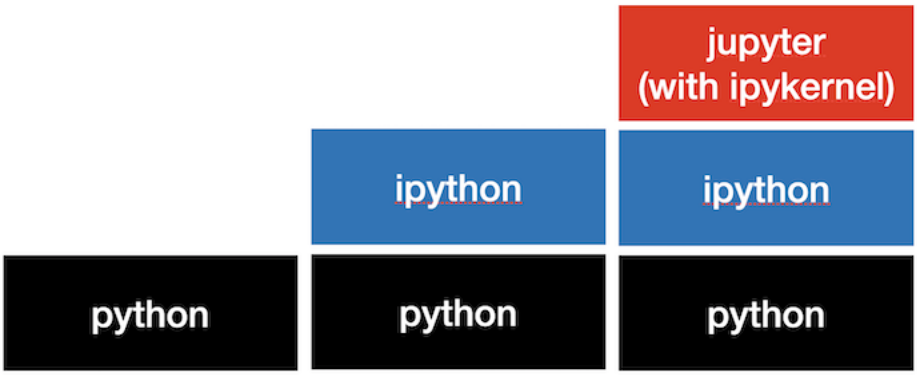
3 python as a program

3.1 Compiled vs. Interpreted Languages

- *Compiled* languages (e.g., C/C++, Fortran, Java, ...): processed by a compiler to produce an *executable* or standalone application that can be run
- *Interpreted* languages (e.g., Python, R, MATLAB, Perl, ...): processed by another program — an interpreter — that runs and executes program statements

3.2 Python interpreters

- python: the default/reference Python interpreter — formally known as CPython, and sometimes installed as python3
- ipython: an interpreter sitting on top of python (and written in Python), providing additional functionality for interactive work
- jupyter: a notebook-based software system that can process Python code by leveraging the ipython kernel (as well as kernels for other languages, such as R and Julia)
- various integrated development environments (IDEs) bundling code editors, ipython consoles, etc.
- other non-CPython-based interpreters that are not widely used: IronPython, PyPy, etc.



3.3 Python interpreters in action

- `python my_program.py`: especially useful for running in background or in batch submission systems
- `ipython`: an enhanced console with additional "magic" functionality to support interactive access
- `jupyter lab` and `jupyter notebook`: web-based environments merging code, documentation, graphics, and results

[1]:
```
2 + 2
```

[1]: 4

[2]:
```
'abc' + 'def'
```

[2]: 'abcdef'

[3]:
```
# A nice trick I learned from Chris Cameron's last seminar on JupyterLab

from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = "all"

# I will also turn off pretty-printing

%pprint
```

```
Pretty printing has been turned OFF
```

3.3.1 Installing Python and associated packages

- Your machine might already have a version of Python installed — best to leave that one alone (probably being used for sysadmin)
- Anaconda Python Distribution: installs a large collection of packages by default
- Alternatively, install a minimal distribution and create customized environments for different projects
- Miniconda
  - conda create -n my_env python numpy pandas jupyter ; conda activate my_env
- Python Virtual Environment
  - python -m venv my_env ; source my_env/bin/activate ; pip install numpy pandas jupyter

4 Python as a programming language

- General-purpose
- Object-oriented
- Dynamically typed
- Interpreted
- Extensible

4.1 A little bit of history

- Python was created by Guido van Rossum in the very late 1980s and early 1990s
- The language is named after the comedy group Monty Python, not the big snake
- The scientific computing community was an early adopter of Python
  - *abstractions and objects* for complex scientific/numerical concepts
  - *interfacing* to existing code written other languages
  - *scripting* and *steering* complex computations and workflows
  - *gluing* together different sorts of analyses
- In addition to being a very popular programming language, Python has inspired some important software memes and themes

  - "If Guido was hit by a bus?" — led to the creation of processes and standards for Python's evolution
  - "Benevolent Dictator for Life" (BDFL) — Guido's role as final arbiter of language decisions

4.2 Python as a general-purpose language

- Not constructed to support a specific problem domain
  - R: built to support statistical analysis
  - MATLAB ("Matrix Laboratory"): built to support linear algebra and matrix operations
  - Mathematica: built to support symbolic mathematics
- Much useful functionality for specific application areas is available through third-party packages
- The Python language is the substrate for tying all these pieces together
- Python is well-designed, intuitive, readable, practical, expressive, elegant, free, and open-source

4.3 Python as an object-oriented language

- Object-oriented means:
  - support for bundling together data and functions into complex data "objects"
  - support for defining new data types (classes) representing different abstractions useful for different problem domains
    - arrays, dataframes, networks, models, estimators, figures, etc.
- Python is practical and not strict — also supports procedural and functional programming
- Everything in Python is an object
  - a *type*
  - a *value*
  - some *attributes* (data defined in association with objects)
  - some *methods* (functions defined in association with objects)
  - a *namespace* that organizes attributes and methods

4.3.1 Everything in Python is an object

- `2+2 -> (2).__add__(2)` # where the `+` operator results in a call to the method `int.__add__`
- `'abc' + 'def'` produces the string 'abcdef', where the `+` operator calls the method `str.__add__`
- the dot operator accesses elements in an object's namespace

[4]:
```
# the built-in function dir() returns a list of names in a namespace

dir(2)
```

[4]:
```
['__abs__', '__add__', '__and__', '__bool__', '__ceil__', '__class__',
'__delattr__', '__dir__', '__divmod__', '__doc__', '__eq__', '__float__',
'__floor__', '__floordiv__', '__format__', '__ge__', '__getattribute__',
'__getnewargs__', '__gt__', '__hash__', '__index__', '__init__',
'__init_subclass__', '__int__', '__invert__', '__le__', '__lshift__', '__lt__',
'__mod__', '__mul__', '__ne__', '__neg__', '__new__', '__or__', '__pos__',
```

```
'__pow__', '__radd__', '__rand__', '__rdivmod__', '__reduce__', '__reduce_ex__',
'__repr__', '__rfloordiv__', '__rlshift__', '__rmod__', '__rmul__', '__ror__',
'__round__', '__rpow__', '__rrshift__', '__rshift__', '__rsub__',
'__rtruediv__', '__rxor__', '__setattr__', '__sizeof__', '__str__', '__sub__',
'__subclasshook__', '__truediv__', '__trunc__', '__xor__', 'as_integer_ratio',
'bit_length', 'conjugate', 'denominator', 'from_bytes', 'imag', 'numerator',
'real', 'to_bytes']
```

4.4 Python as a dynamically typed language

- variables acquire the type of whatever is assigned to them
  - `x = 3` # x is an integer (int)
  - `x = 3.14` # x is a floating-point number (float)
  - `x = "Hello, world"` # x is a string
- as compared to *statically typed languages*, where the types of variables are declared, and errors are reported if data of a different type are assigned to a variable
- dynamic typing is often used in interpreted languages
- static typing is often used in compiled languages

4.5 Python as an interpreted language

- processed by an interpreter
  - the python interpreter (CPython) does on-the-fly compilation to intermediate bytecodes
- each statement executed sequentially
- very useful for interactive analysis, development, and prototyping
- programs are typically slower than for compiled languages
  - trading off development time vs. execution time

4.6 Python as an extensible language

- The Python language defines a C/Python Application Programming Interface (API)
- C/Python API enables the CPython interpreter to process compiled code written in C and other languages and to make the associated data and functions accessible in a Python program
- Many programs *written in the Python language* are actually calling compiled functions written in other languages, resulting in much higher computational performance than for pure Python code alone
- Many tools exist for generating interfaces to compiled code, compiling bits of Python code to "extension modules", etc.
- See our Cornell Virtual Workshop (CVW) topic on Python for High Performance at https://cvw.cac.cornell.edu/python

4.7 Built-in data types in Python

- numeric types: int, float, complex, bool
- string data types
- containers: lists, dictionaries, sets, tuples
- functions
- classes

- modules
- etc.

4.8 Built-in container types in Python

- **lists**: ordered, mutable sequences of objects, indexed by their integer position (starting at 0)
- **dictionaries**: mappings from a set of keys to associated values (akin to maps, hashes, associative arrays, etc.)
- **sets**: unordered collections of unique elements with support for set algebra (unions, intersections, differences, etc.)
- **tuples**: ordered, immutable sequences of objects, useful for bundling together related items
- **strings**: ordered, immutable sequences of characters, supporting many string-processing operations

Along with many other non-built-in container types defined in external packages, such as:

- arrays (of any dimensionality) — defined in numpy
- series and dataframes — defined in pandas

4.9 Python as a calculator

- addition + ; subtraction - ; multiplication * ; division /
- power ** ; modulo % ; floor division //

[5]:
```
(19 + (2*3 - 4*7) / (8 % 3))**3
```

[5]:
```
512.0
```

[6]:
```
x = 3
y = 14

z = (x * y) - (x + y)

z
```

[6]:
```
25
```

4.10 Code blocks and indentation

The readability of Python code is a key goal of its design. Using indentation to identify code blocks is central to that goal. Using a code editor that understands Python syntax and indentation helps a lot.

Python:

C/C++:

4.11 Code blocks and indentation (continued)

Python:

MATLAB:

4.12 Control flow

- Looping: for, while, continue, break
- Branching: if-elif-else
- Exception handling: try-except

4.13 Iteration and iterables

[7]:
```
for c in ['A', 'B', 'C', 'D', 'E']:
    print(c)
```

```
A
B
C
D
E
```

[8]:
```
for i in range(10):
    print(i)
```

```
0
1
2
3
4
5
6
7
8
9
```

[9]:
```
print(range(10))
```

```
range(0, 10)
```

[10]:
```
range?
```

[11]:
```
for i in range(4, 17, 3):
    print(i)
```

```
4
7
10
13
16
```

[12]:
```
list(range(10))
```

[12]:
```
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

[13]:
```
sum(range(10))
```

[13]:
```
45
```

4.14 Iterating over other iterables

[14]:
```
a_dictionary = {'A': 1, 'B': 2, 'C': 3}

for key,value in a_dictionary.items():
    print(key, value)
```

```
A 1
B 2
C 3
```

4.15 Comprehensions

[15]:
```
# List comprehensions

squares = [n*n for n in range(10)]

squares
```

[15]:
```
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

[16]:
```
# Dictionary comprehensions

import string
mapping = {c:i for i,c in enumerate(string.ascii_letters)}

mapping
```

[16]:
```
{'a': 0, 'b': 1, 'c': 2, 'd': 3, 'e': 4, 'f': 5, 'g': 6, 'h': 7, 'i': 8, 'j': 9,
'k': 10, 'l': 11, 'm': 12, 'n': 13, 'o': 14, 'p': 15, 'q': 16, 'r': 17, 's': 18,
't': 19, 'u': 20, 'v': 21, 'w': 22, 'x': 23, 'y': 24, 'z': 25, 'A': 26, 'B': 27,
'C': 28, 'D': 29, 'E': 30, 'F': 31, 'G': 32, 'H': 33, 'I': 34, 'J': 35, 'K': 36,
'L': 37, 'M': 38, 'N': 39, 'O': 40, 'P': 41, 'Q': 42, 'R': 43, 'S': 44, 'T': 45,
'U': 46, 'V': 47, 'W': 48, 'X': 49, 'Y': 50, 'Z': 51}
```

4.16 Exceptions and error handling

[17]:
```
for denominator in [5,4,3,2,1,0]:
    print(1 / denominator)
```

```
0.2
0.25
0.3333333333333333
0.5
1.0
```

```
---------------------------------------------------------------------------
ZeroDivisionError                         Traceback (most recent call last)
Input In [17], in <cell line: 1>()
      1 for denominator in [5,4,3,2,1,0]:
----> 2     print(1 / denominator)

ZeroDivisionError: division by zero
```

[18]:
```
for denominator in [5,4,3,2,1,0]:
    try:
        print(1 / denominator)
    except ZeroDivisionError:
        print("Cannot divide by 0")
```

```
0.2
0.25
0.3333333333333333
0.5
1.0
Cannot divide by 0
```

4.17 Exceptions and error handling (continued)

[ ]:
```
#filename = 'a_file_that_does_not_exist.txt'
#inputfile = open(filename, 'r')
#lines = inputfile.readlines()
#inputfile.close()
```

[19]:
```
filename = 'a_file_that_does_not_exist.txt'
try:
    inputfile = open(filename, 'r')
    lines = inputfile.readlines()
    inputfile.close()
except FileNotFoundError:
    print(f'{filename} does not exist')
```

```
a_file_that_does_not_exist.txt does not exist
```

4.18 Defining functions

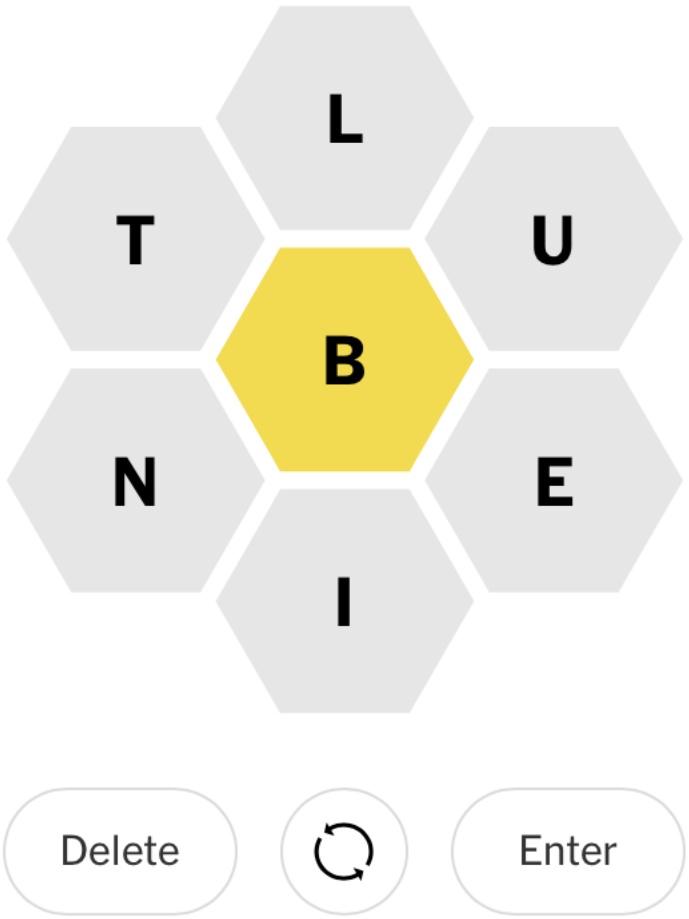
[20]:
```
# def is keyword to define a new function; return is keyword to return a value␣
↪from a function

def concatenate(string1, string2, separator=' '):
    return string1 + separator + string2

concatenate('abc', 'def')   # uses default argument for separator

concatenate('abc', 'def', '..')   # overrides default argument

concatenate(separator='--', string2='DEF', string1='ABC')   # uses keyword␣
↪arguments
```

[20]:
```
'abc def'
```

[20]:
```
'abc..def'
```

[20]:
```
'ABC--DEF'
```

4.19 Putting the pieces together: Spelling Bee




```
# spellingbee.py

import itertools

available = 'BEILNTU'
center = available[0]

start = 'BL'
length = 5
exclude = {'II', 'UU', 'BBB', 'TTT', 'NNN', 'LLL', 'EEE'}

def words(available, start, length):
    num_unknown = length - len(start)
    iterator = itertools.product(available, repeat=num_unknown)
    return [start + ''.join(letters) for letters in iterator]

allwords = words(available, start, length)

for w in allwords:
    not_excluded = True
    for ex in exclude:
        if ex in w:
            not_excluded = False
    if not_excluded and center in w:
        print(w)
```

Import the itertools module, rather than figuring out the combinatorics for myself

Assign some variables to store data

Use built-in Python set object to hold exclusions

Define a function (note the indented code block)

Call a function from the itertools module

Use a list comprehension to create a list of all possible words

Call our function to generate all possible words

Loop over all words (note the nested indented code blocks)

Check if the word contains an excluded substring

Print the word if it is not excluded and it contains the center letter

[21]:
```python
# spellingbee.py

import itertools

available  = 'BEILNTU'
center = available[0]

start  = 'BL'
length = 5
exclude = {'II', 'UU', 'BBB', 'TTT', 'NNN', 'LLL', 'EEE'}

def words(available, start, length):
    num_unknown = length - len(start)
    iterator = itertools.product(available, repeat=num_unknown)
    return [start + ''.join(letters) for letters in iterator]


allwords = words(available, start, length)

for w in allwords:
    not_excluded = True
    for ex in exclude:
        if ex in w:
            not_excluded = False
    if not_excluded and center in w:
        print(w)
```

```
BLBBE
BLBBI
BLBBL
BLBBN
BLBBT
BLBBU
BLBEB
BLBEE
BLBEI
BLBEL
BLBEN
BLBET
BLBEU
BLBIB
BLBIE
BLBIL
BLBIN
BLBIT
BLBIU
BLBLB
```

BLBLE
BLBLI
BLBLL
BLBLN
BLBLT
BLBLU
BLBNB
BLBNE
BLBNI
BLBNL
BLBNN
BLBNT
BLBNU
BLBTB
BLBTE
BLBTI
BLBTL
BLBTN
BLBTT
BLBTU
BLBUB
BLBUE
BLBUI
BLBUL
BLBUN
BLBUT
BLEBB
BLEBE
BLEBI
BLEBL
BLEBN
BLEBT
BLEBU
BLEEB
BLEEI
BLEEL
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BLEET
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BLNTU
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BLULU
BLUNB
BLUNE
BLUNI
BLUNL
BLUNN
BLUNT
BLUNU
BLUTB
BLUTE
BLUTI
BLUTL
BLUTN
BLUTT
BLUTU

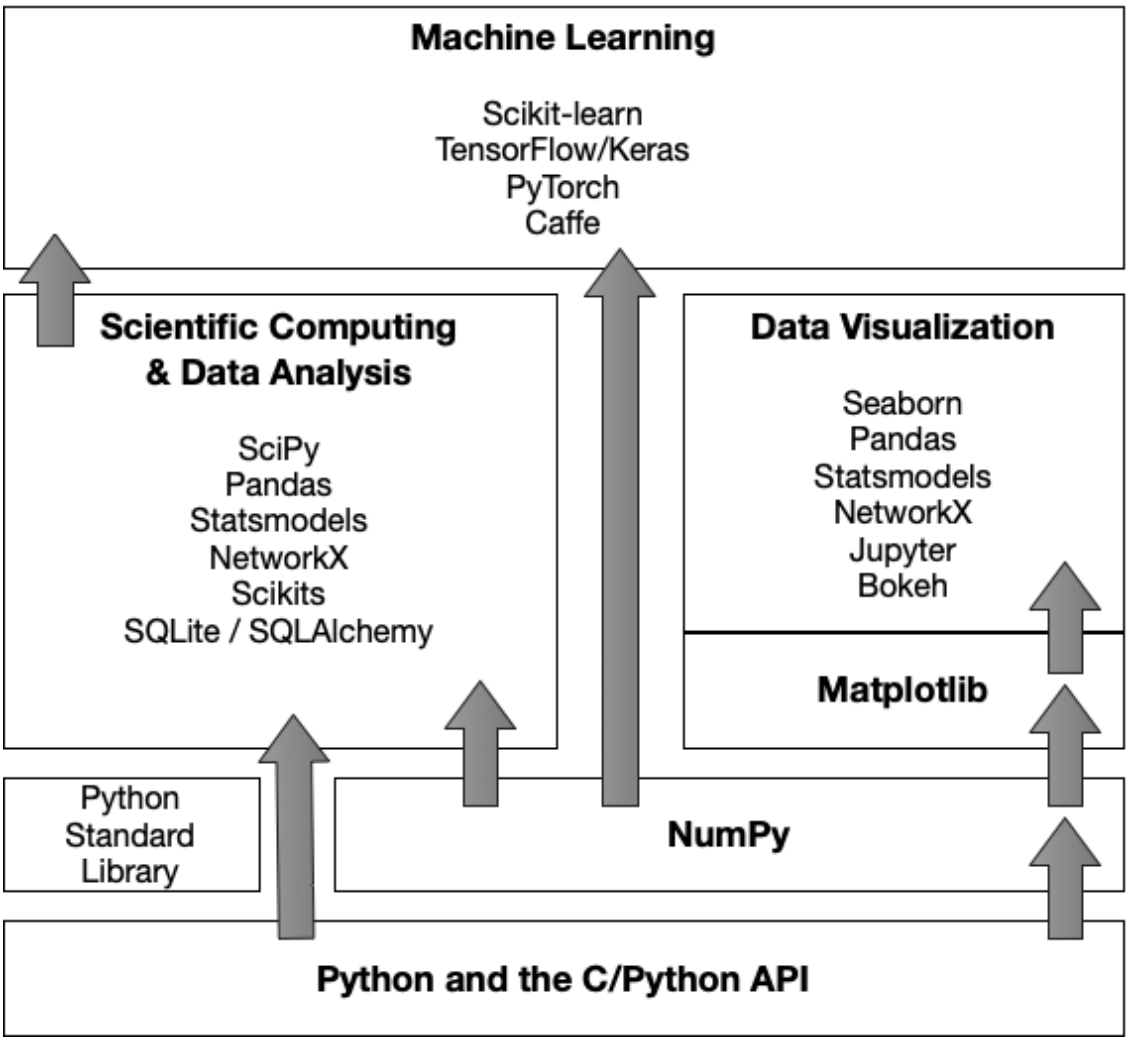
[22]:
```
%whos
```

```
Variable           Type             Data/Info
-------------------------------------------
InteractiveShell   MetaHasTraits    <class
'IPython.core.inte<...>eshell.InteractiveShell'>
a_dictionary       dict             n=3
allwords           list             n=343
available          str              BEILNTU
c                  str              E
center             str              B
concatenate        function         <function concatenate at 0x10749dee0>
denominator        int              0
ex                 str              LLL
exclude            set              {'II', 'BBB', 'UU', 'NNN', 'EEE', 'TTT',
'LLL'}
filename           str              a_file_that_does_not_exist.txt
i                  int              16
itertools          module           <module 'itertools' (built-in)>
key                str              C
length             int              5
mapping            dict             n=52
not_excluded       bool             False
squares            list             n=10
start              str              BL
string             module           <module 'string' from
'/U<...>lib/python3.9/string.py'>
value              int              3
w                  str              BLUUU
words              function         <function words at 0x10749de50>
x                  int              3
y                  int              14
z                  int              25
```

5 *Python* as a software ecosystem

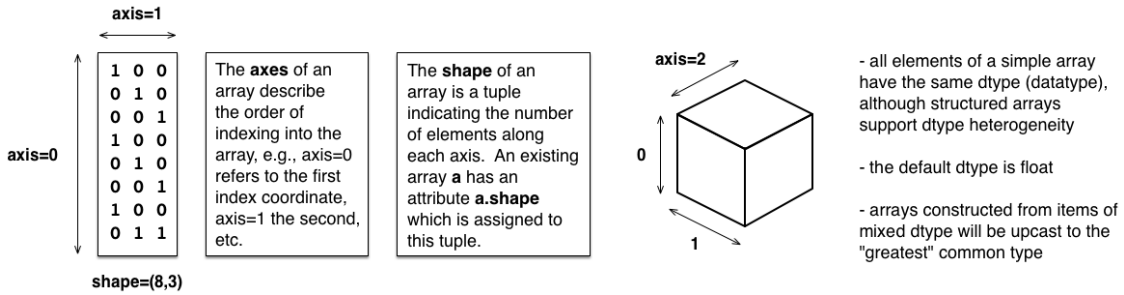
- The core Python language provides a substrate
  - for using programming constructs to define functions, classes, and control flows
  - for importing and using functions and classes defined in external packages
- Actually, Python consists of multiple ecosystems used for different tasks
  - a scripting environment used in operating systems and for systems administration tasks
  - a set of tools for web programming and website development
  - a set of packages for generation of graphical user interfaces (GUIs)
  - an environment for scientific computing, data science, and machine learning
- Python Standard Library: https://docs.python.org/3/library/index.html

5.1 Python for Scientific Computing, Data Science, and Machine Learning



5.1.1 NumPy (Numerical Python)

- multidimensional arrays (ndarray = "N-dimensional array")
- "array syntax" enabling compact expressions and efficient computations
- access to functionality for linear algebra and random numbers
- a substrate for array-based computations throughout the Python ecosystem
- similar in spirit to the role that arrays/matrices play in MATLAB
  - see https://numpy.org/doc/stable/user/numpy-for-matlab-users.html



5.1.2 Numpy

[23]:
```
import numpy as np

x = np.array([[1,2,3], [4,5,9], [7,8,9]])
y = np.random.random((3,3))

w = 3*x + 4*y

x
y
w

x.sum(axis=0)
```

[23]:
```
array([[1, 2, 3],
       [4, 5, 9],
       [7, 8, 9]])
```

[23]:
```
array([[0.61288401, 0.91090789, 0.56815764],
       [0.30120234, 0.9396962 , 0.06910196],
       [0.91803854, 0.85746682, 0.06649826]])
```

[23]:
```
array([[ 5.45153604,  9.64363156, 11.27263056],
       [13.20480935, 18.7587848 , 27.27640783],
       [24.67215416, 27.42986727, 27.26599303]])
```

[23]:
```
array([12, 15, 21])
```

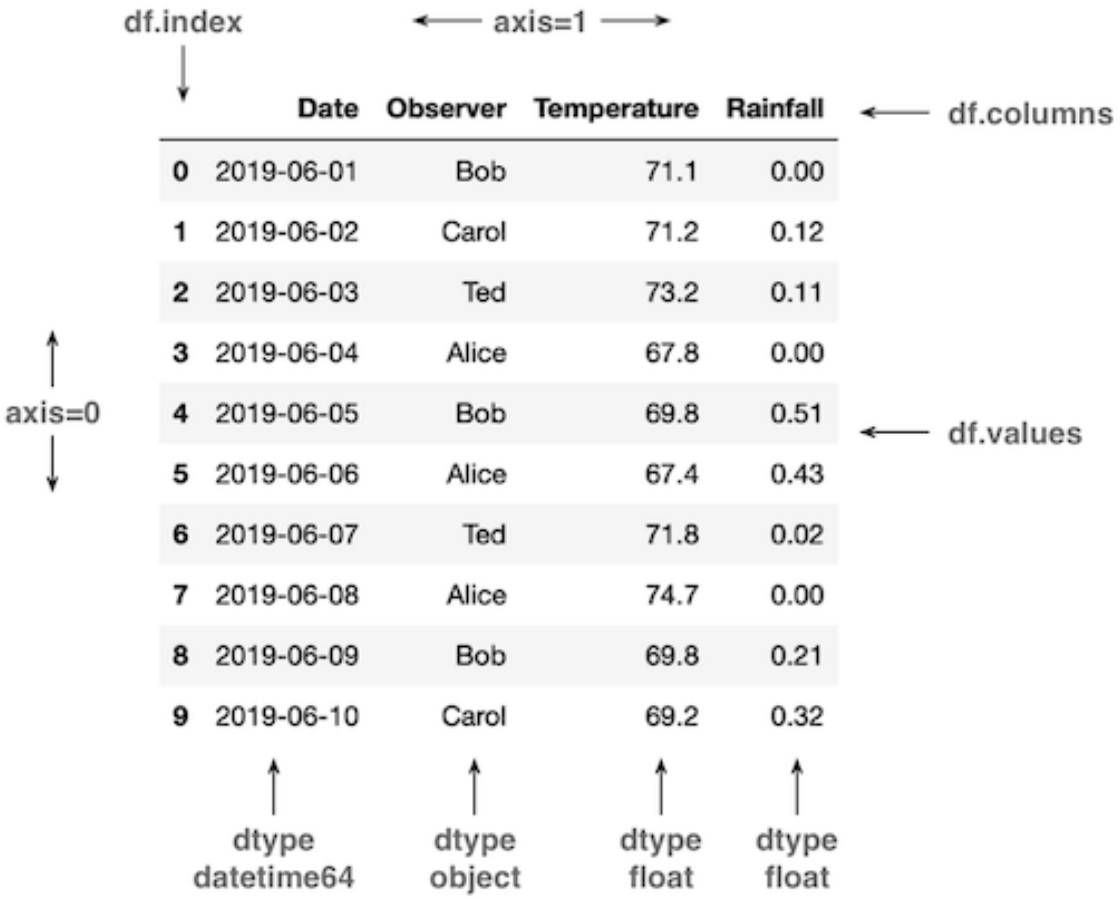
5.1.3 SciPy (Scientific Python)

- Special functions (scipy.special)
- Integration (scipy.integrate)
- Optimization (scipy.optimize)
- Interpolation (scipy.interpolate)
- Fourier Transforms (scipy.fft)
- Signal Processing (scipy.signal)
- Linear Algebra (scipy.linalg)
- Sparse eigenvalue problems with ARPACK
- Compressed Sparse Graph Routines (scipy.sparse.csgraph)
- Spatial data structures and algorithms (scipy.spatial)
- Statistics (scipy.stats)
- Multidimensional image processing (scipy.ndimage)
- File IO (scipy.io)

5.1.4 Pandas

- DataFrames and Series for dealing with tabular data (e.g., spreadsheets)

  - uses NumPy underneath for much of the data processing
- Support for:
  - reading from csv/excel files and SQL databases (and dealing with missing data)
  - adding new columns derived from existing columns
  - groupby functions that perform aggegrate computations over subsets of data
  - lots more



	Date	Observer	Temperature	Rainfall
0	2019-06-01	Bob	71.1	0.00
1	2019-06-02	Carol	71.2	0.12
2	2019-06-03	Ted	73.2	0.11
3	2019-06-04	Alice	67.8	0.00
4	2019-06-05	Bob	69.8	0.51
5	2019-06-06	Alice	67.4	0.43
6	2019-06-07	Ted	71.8	0.02
7	2019-06-08	Alice	74.7	0.00
8	2019-06-09	Bob	69.8	0.21
9	2019-06-10	Carol	69.2	0.32

See our Cornell Virtual Workshop (CVW) topic on Python for Data Science:

- Data Processing and Visualization: https://cvw.cac.cornell.edu/pydatasci1
- Data Modeling and Machine Learning: https://cvw.cac.cornell.edu/pydatasci2

5.2 Python for Data Visualization

- Tools for generating figures and images
  - Matplotlib: the cornerstone and workhorse of the Python data visualization universe
    - Pandas: uses Matplotlib for visualizing data from DataFrames
    - Seaborn: uses Matplotlib with a focus on statistical distributions and multivariate relationships
    - Statsmodels: uses Matplotlib for plotting results of statistical modeling (e.g., regressions)
  - Plotnine: a Python implementation of the "grammar of graphics" (R/gpplot2)
- Tools for generating interactive data visualizations

  - Bokeh, Plotly, Altair
- Tools for 3D visualization of 3D objects
  - VTK, Paraview, Mayavi

5.2.1 Plotting with matplotlib

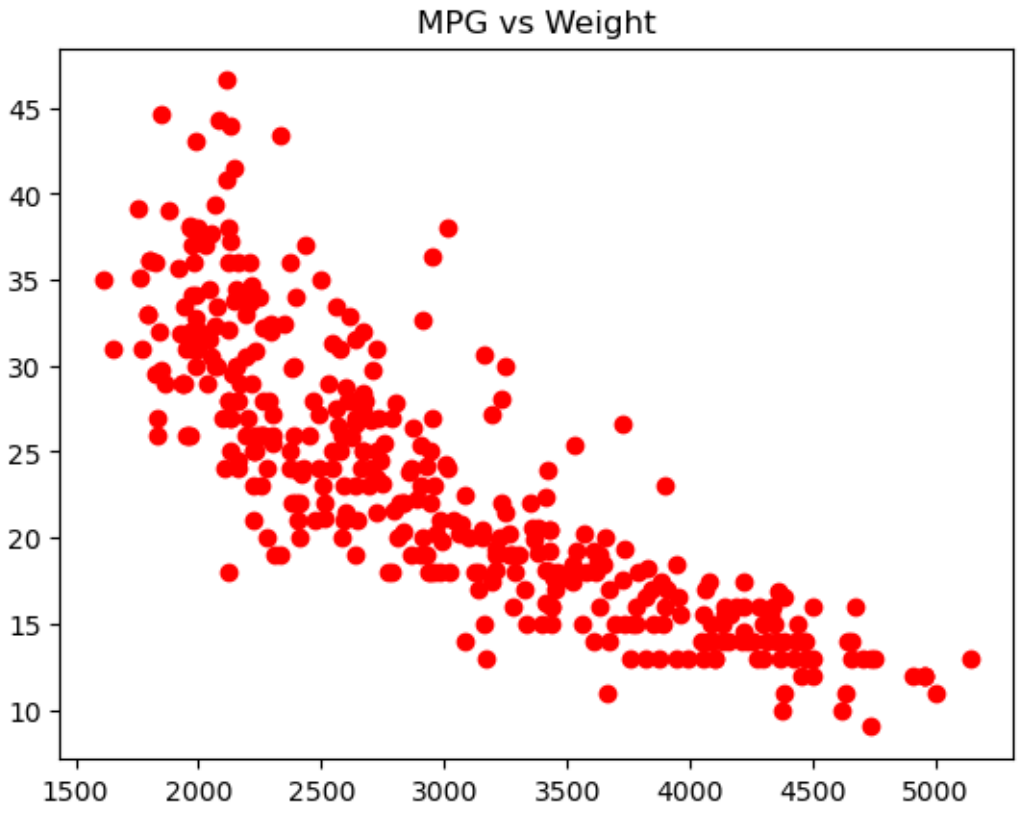
[24]:
```
import pandas as pd
from bokeh.sampledata.autompg import autompg_clean as df

df.head()
```

[24]:

	mpg	cyl	displ	hp	weight	accel	yr	origin	\
0	18.0	8	307.0	130	3504	12.0	70	North America	
1	15.0	8	350.0	165	3693	11.5	70	North America	
2	18.0	8	318.0	150	3436	11.0	70	North America	
3	16.0	8	304.0	150	3433	12.0	70	North America	
4	17.0	8	302.0	140	3449	10.5	70	North America	

	name	mfr
0	chevrolet chevelle malibu	chevrolet
1	buick skylark 320	buick
2	plymouth satellite	plymouth
3	amc rebel sst	amc
4	ford torino	ford

[25]:
```
import matplotlib.pyplot as plt

plt.scatter(df.weight, df.mpg, color='red')
plt.title('MPG vs Weight');
```



5.2.2 Interative plotting with bokeh

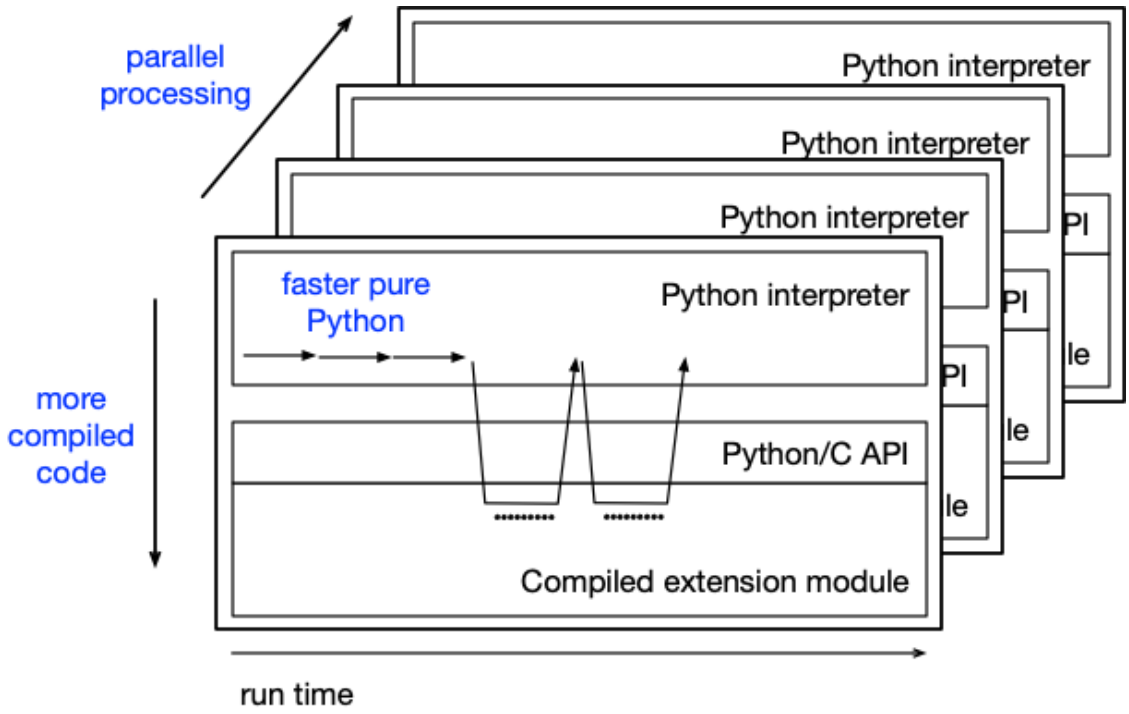
[26]:
```
from bokeh.plotting import figure, show
from bokeh.models import ColumnDataSource
from bokeh.io import output_notebook
output_notebook()

p = figure()

source = ColumnDataSource(df)
hover_tips = [(c, "@"+c) for c in source.column_names]

p = figure(tools='pan,box_zoom,hover,reset', tooltips = hover_tips, width=400,␣
 ↪height=400)

p.circle(x='weight', y='mpg', source=source, size=10, color='green', alpha=0.5)
p.xaxis.axis_label = 'weight'
p.yaxis.axis_label = 'mpg'

show(p)
```

[26]:
```
GlyphRenderer(id='1066', ...)
```

5.3 Python for Machine Learning and Deep Learning

- Scikit-learn (sklearn)
  - a large variety of algorithms and lots of documentation about different ML methods
  - classification, regression, clustering, dimensionality reduction, model selection, etc.
  - estimators, pre-processors, transformers, pipelines
- Deep Learning with Neural Networks
  - TensorFlow / Keras ; PyTorch ; Caffe
  - widely used for a broad array of tasks, such as image classification, speech recognition, text generation, protein structure prediction, etc.
  - packages extend numpy-like arrays with the power of *automatic differentation* to support gradient computations and backpropagation for use in training neural networks

5.4 Accelerating Python Code (Python and Performance)



5.4.1 Array operations with NumPy

[ ]:
```
import numpy as np
a = np.random.random((1000,1000))
b = np.random.random((1000,1000))

c = a + b    # throws ValueError if a and b not the same shape
```

[ ]:
```
%%timeit

c = a + b
```

[ ]:
```
%%timeit

assert(a.shape == b.shape) # throws AssertionError if a and b not the same shape
c = np.zeros_like(a) # prefills a zero array of the correct shape

for i in range(a.shape[0]):
    for j in range(a.shape[1]):
        c[i,j] = a[i,j] + b[i,j]
```

[ ]:
```
# Speedup?
```

5.5 An Introduction to Python and an overview of possible future topics

- ~~Introduction to Python~~
- Python for Scientific Computing and Data Science
- Python for Data Visualization
- Python for Machine Learning and Deep Learning
- Accelerating Python Code

6 Python as a language and an ecosystem

- An expressive programming language for crafting custom analyses and workflows
- A rich set of interoperating packages and libraries for processing data and investigating complex systems

6.1 Any Questions?

[ ]:
```

```

7 Supplemental material

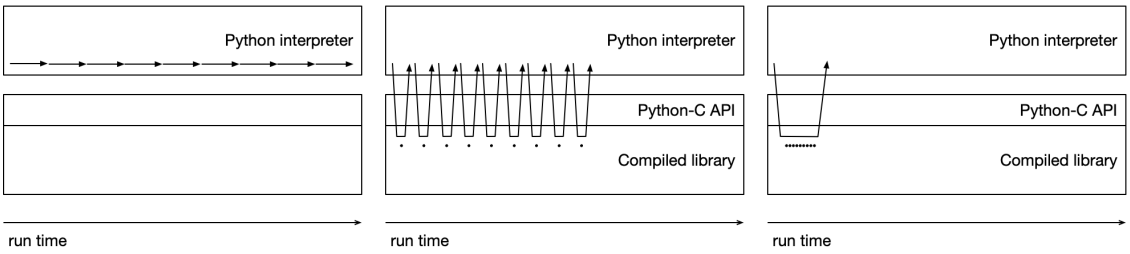
7.1 Putting the pieces together: Ciphers

[ ]:
```
letters = "ABCDEFGHIJKLMNOPQRSTUVWXYZabcdefghijklmnopqrstuvwxyz"
cipher = {letters[i]: letters[(i-3) % len(letters)] for i in range(len(letters))}

cipher
```

[ ]:
```
def transform_message(message, cipher):
    tmsg = ''
    for c in message:
        tmsg = tmsg + cipher.get(c, c)
```

```
    return tmsg

test = "I come to bury Caesar, not to praise him."

transform_message(test, cipher)

decoder = {v:k for k,v in cipher.items()}

transform_message(transform_message(test, cipher), decoder)
```

7.2 Compiled extension modules



7.2.1 Plotting with pandas (and tweaking with matplotlib)

[ ]:
```
df.plot.scatter(x="weight", y="mpg", color='blue')
plt.title('MPG vs Weight');
```