Modeling and Simulation

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Lecture 2:

Introduction to Programming with Python 3 for Scientific Computing

Introduction to Programming with Python 3 for Scientific Computing Introduction to high performance computing for modeling

Why do we need programming in this course?

- We want to represent systems through modeling techniques such as mathematical models.
- These models are too complex to be solved analytically.
- Either they do not possess analytical solutions or it would take too long to compute it.
- Numerical methods exist to approximate the mathematical models used to represent systems.
- Computers are very efficient in doing large amount of computations.
- We need an efficient way to make the computer use the numerical methods.

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Computers are fast but... we always want more

For a computer model to be satisfying it must...

- Represent with good accuracy the process it is supposed to model.
- Give a solution in a reasonable amount of time.

For a program to be faster one can...

- Wait for the hardware to become faster.
- Optimize the algorithm (e.g.: quick sort).
- Optimize the way algorithm is implemented.

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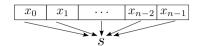
Concepts of code optimization

Example: Sum of the numbers stored in an array.

Mathematical representation

$$A = \{x_i\}_{i=0}^{n-1}, x_i \in \mathbb{N}, \quad s = \sum_{i=0}^{n-1} x_i.$$

Graphical representation



This can be Performed in 3 different ways:

The array is read linearly x_0



The array is read randomly



The sum is performed with sum

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Benchmark: Sum of $n = 10^6$ integers

Efficiency depends on the algorithm.

	Linear	Random	Sum	
Time(s)	0.0594	0.270	0.00654	
t/t_{sum}	9.08	41.3	1.0	

Efficiency depends on the programming language

	Python 3 (sum)	Numpy	C++ (linear)
Time(s)	0.00654	0.000634	0.000478
t/t_{C++}	t/t_{C++} 13.7		1.0

By coding naively, **C++** is 100 times faster than **Python** but with **NumPy** the performance is almost equivalent.

Why Python?

- Python is a modern, general-purpose, object-oriented, high-level programming language.
- **clean and simple language:** Easy-to-read and intuitive code, easy-to-learn minimalistic syntax, maintainability scales well with size of project.
- expressive language: Fewer lines of code, fewer bugs, easier to maintain
- Extensive ecosystem: many scientific libraries and environments could enhance its capability (e.g.: Numpy, Scipy, matplotlib)
- **Great performance** due to close integration with time-tested and highly optimized codes written in C.

Literature on Python 3

- Python 3 documentation : https://docs.python.org/3/
- Dive into Python 3: http://www.diveintopython3.net/
- numpy: http://numpy.scipy.org Numerical Python.
- scipy: http://www.scipy.org Scientific Python.
- matplotlib: http://www.matplotlib.org graphics library



Part I Generalities on Python 3

Variables

Container to store values that can accessed and changed. In Python (not the case in C/C++, Java for example):

- No need to declare the data type of a variable.
- Variables can change data type

Example a = 10 print(a) a = a+1 print(a) 10 a = a+1 print(a) 11 a = "Hello World!" print(a) Hello World!

Discussion

- 1: The value 10 is stored in a (a is the identifier).
- 4: a is taking a new value which is a+1.
- 7: The string "Hello World!" is stored in a.

Variables: identifiers

Rules for variable identifiers:

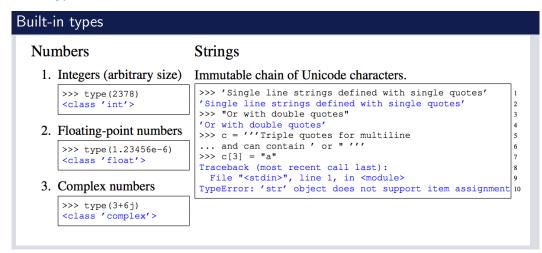
- 1. The first character can be ANY Unicode letter or the underscore.
- 2. The other characters can be ANY Unicode letter or digit or the underscore.
- 3. All the Python keywords are forbidden.
- 4. Identifiers are case sensitive.

Examples

```
1 >>> àél3_aerkcàéal = 10
2 >>> 2àél3_aerkcàéal = 10
3 File "<stdin>", line 1
4 2él3_aerkcàéal = 10
5
6 SyntaxError: invalid syntax
```

```
1 >>> True = 10
2 File "<stdin>", line 1
3 SyntaxError: can't assign to keyword
4 >>> a,A = 10,20
5 >>> print(a,A)
6 10 20
```

Data types



Data types (continued)

Built-in types Other types Examples 1. Boolean type 1 >>> type (True) 2 <class 'bool'> >>> print(type(True), type(False)) 3 >>> bool("") <class 'bool' > <class 'bool' > False >>> bool("hi") 2. None Type 6 True >>> bool (0) >>> type (None) 8 False <class 'NoneType'> 9 >>> bool (10) 10 True 11 >>> print (True+True, True+False) 12 2 1

Data types (continued)

Built-in types Examples Sequence Types $|1\rangle >>> a = [1,7,29,1,39]; a[2]$ 1. list: mutable sequence. 2 29 3 >>> a[3] = "a"; print(a) >>> type([1,'is an int',2.0,'is a float']) 4 [1, 7, 29, 'a', 39] <class 'list'> 5 >>> b=('njd',[1,1],1.0) 6 >>> b[0] = 12. tuple: immutable sequence. 7 Traceback (most recent call last): File "<stdin>", line 1, in <module> >>> type((1,'is an int',2.0,'is a float')) 9 TypeError: 'tuple' object does not <class 'tuple'> 10 support item assignment |11| >>> b[1][0] = 43. range: immutable number sequence. 12 >>> print (b) 13 ('njd', [4, 1], 1.0) >>> type(range(10)) 14 >>> print(list(range(4))) <class 'range'> 15 [0, 1, 2, 3]

Operators: on numeric types

Operators (numeric type)

- Addition +, Subtraction -, Multiplication
 *.
- Real division /,Integer division //, Modulo %.
- Exponentiation ** .
- Unary +, -.

```
Examples
 1 >>> 12+15-37
 2 | -10
 3 >>> 12*15*37
 4 6660
 5 >>> 10/3
 6 3.3333333333333333
 7 >>> 10//3
 9 >>> 10%3
10
11 >>> 2.0**10
12 1024.0
13 >>> +2, -2
|14|(2, -2)
```

Operators: on sequence types

Operators: (sequence types)

- Concatenation + .
- Copies of a sequence * .
- Access to element [].
- Slice:.

[9, 2, 3, 4, 'b', 9, 2, 3, 4, 'b']

>>> a[1:4]

12 >>> a[0:4:2]
13 [9, 3]
14 >>> a[2:]
15 [3, 4, 'b']
16 >>> a[:2]
17 [9, 2]

11 [2, 3, 4]

Operators: Boolean operations and comparisons

Operators:

- <, <=, >, >=, ==, ! =.
- or, and, not.
- in or not in a sequence.

Remark:

 or and and always return one of their operands.

```
Examples
                                      1 >>> 2 or 3
 1 >>> 2<1
 2 False
 3 >>> a,b = 1,2
                                      3 >>> 2 \text{ and } 3
 4 >>> a == b
                                      5 >>> "a" == "a"
 5 False
 6 >>> 1 != 2
                                      6 True
 7 True
                                      7 >>> "a" > "b"
 |8| >>> 1 != 2 and 1 == 1
                                      8 False
 9 True
                                      9 >>> "a" and "b"
|10| >>> 1 != 2 and not 1 == 1
                                      10 'b'
11 False
                                      |11| >>> a = [1, 2, 3, 4, "b"]
                                      12 >>> "b" in a
                                      13 True
```

Control structures: conditional statements

The if statement: if condition_1: statements 1 [elif condition 2: statements 2 elif condition n: statements nl <else: statements> a = x if condition else y

Examples

```
x = int(input("Enter your velocity : "))

if x >= 120:
    y = x-120
    x = 120
    print("Going too fast. Velocity reduced by ", y)
elif x <= 80:
    y = 80-x
    x = 80
    print("Going too slow. Velocity increased by ", y)
else:
    print("Everything is fine.")</pre>
```

```
1 x = int(input("Input an integer: "))
2 a = "even" if x%2 == 0 else "odd"
3 print(x, " is an ", a, " number.")
```

Control structures: loops

The for statement: for variable in sequence: statements_1 [else: statements_2]

```
Examples

animals = ["cat", "dog", "cow", "bird"]
for x in animals:
    if x=="cow":
        break
    print(x)
else:
    print("no cow in my list")

cat
dog
1

1

1

2

2

6

8

6

9

10
```

Control structures: loops

The while statement:

```
while condition:
    statements_1
[else:
    statements_2]
```

Examples

```
1  x = int(input("Enter a number : "))
2  ary = list(range(x))
3  tot = 0
4  i = 0
5  while i < len(ary):
6   tot += ary[i]
7   i += 1
8  else:
9   print("Total ended normally.")
10
11  print("The sum is: ",tot)</pre>
```

Functions

Syntax:

```
def function_name(parameter_list):
    [""" comments (doc) """]
    statements
    [return]
```

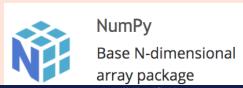
Remarks

- Functions Provided some input parameters compute one or more results (e.g.: f:x → √x).
- The *return* and *comments* statements are optional.
- The return statement ends the function and returns.
- Functions always return *None* by default.

Functions

Example: Code Result def isPrime (number): isPrime (number) """Check if number is prime""" Check if number is prime if number <= 1: return False is not a prime number is not a prime number for i in range (2, number): is a prime number if number % i == 0: is a prime number is not a prime number return False Q return True 5 is a prime number is not a prime number 10 help(isPrime) is a prime number is not a prime number for j in range (0,13): if (isPrime(j)): is not a prime number print(j, " is a prime number") is not a prime number 14 is a prime number 15 else: 11 print(j, " is not a prime number") is not a prime number 16

Part II Introduction to Numpy





NumPy

- Extension package to Python for multi-dimensional arrays.
- Build around high-performance multi-dimensional array data structures.
- Closer to hardware (efficiency).
- Designed for scientific computation (convenience).
- Also known as array oriented computing.

Efficiency vs python array

```
In [1]: L = range(1000)
In [2]: %timeit [i**2 for i in L]
1000 loops, best of 3: 403 us per loop
In [3]: a = np.arange(1000)
In [4]: %timeit a**2
100000 loops, best of 3: 12.7 us per loop
```

An array could represent:

- Values of an experiment/simulation at discrete time steps
- Signal recorded by a measurement device, e.g. sound wave
- Pixels of an image, grey-level or colour
- 3-D data measured at different X-Y-Z positions, e.g. MRI scan
- . . .

```
\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}
```



colour image as $N \times M \times 3$ -array

Numpy: The basics

```
Import conventions:

import numpy as np
```

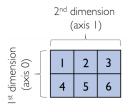
Example of arrays:

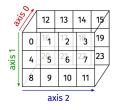
```
• 1-D:
```

```
a = np.array([0,1,2,3])
```

• 2-D, 3-D, ...:

```
# 2 x 3 array
b = np.array([[1,2,3],
[4,5,6]])
```





Numpy: Array Construction Routines

```
Homogeneous data
 Zeros:
    a=np.zeros((3, 3))
 Ones:
       b=np.ones((3, 3))
 • diag:
       c=np.diag(np.array([1, 2, 3]))
 • eye:
       d=np.eye(3)
```

	а	
0	0	0
0	0	0
0	0	0
	b	
1	1	1
1	1	1
1	1	1
	С	
1	0	0
0	2	0
0	0	3

Numpy: Array Construction Routines

```
Numerical ranges
 Evenly spaced:
         a=np.arange(4) #0 ... n-1 (!)
         b=np.arange(3,7) #start, end-1
 • By number of points:
       #start, end, num, endpoint
       c=np.linspace(0, 1, 6)
       d=np.linspace(0, 1, 6, endpoint=False)
```

```
a
0 | 1 | 2 | 3

b
3 | 4 | 5 | 6

c
0. | 0.2 | 0.4 | 0.6 | 0.8 | 1.

d
0. | 0.2 | 0.4 | 0.6 | 0.8
```

Numpy: Array Construction Routines

```
Basic data types
         a=np.array([1, 2, 3])
         a.dtype
 dtype('int64')
        b=np.array([1., 2., 3.])
        b.dtype
 dtype('float64')
        c=np.array([1, 2, 3], dtype=float)
        c.dtype
 dtype('float64')
```

There are also other types:

- Complex.
- Bool.
- Strings.
- int32.
- uint32.
- uint64.

Indexing and slicing

Basics

- Indexing starts at 0.
- Negative indices count from the end of the list to the beginning



- Basic slices syntax: [start:stop:step]
- if values are omitted:
 - start: starting from 1st element.
 - stop: until (and including) the last element.
 - step: all elements between start and stop-1.

```
>>> a[0, 3:5]
array([3, 4])
>>> a[4:, 4:]
                                   10
                                                  13
                                        11
                                                       14
                                                            15
array([[44, 55],
        [54, 5511)
                                  20
                                        21
                                                  23
                                                      24
                                                            25
>>> a[:, 2]
                                   30
                                        31
                                                  33
                                                       34
                                                            35
a([2, 12, 22, 32, 42, 52])
                                  40
                                        41
>>> a[2::2, ::2]
array([[20, 22, 24],
                                        51
        [40, 42, 4411)
>>> a[(0.1.2.3.4), (1.2.3.4.5)]
array([1, 12, 23, 34, 45])
>>> a[3:, [0,2,5]]
array([[30, 32, 35],
                                           20
      [40, 42, 45].
      [50, 52, 5511)
>>  mask = np.array([1,0,1,0,0,1], dtype=bool)
>>> a[mask, 21
array([2, 22, 52])
```

Numerical operations on arrays

Elementwise operations

• With scalars:

```
a=np.array([1, 2, 3, 4])
a=a + 1
a=2**a
```

• Arithmetic operates elementwise:

```
b=np.ones(4) + 1
b=a - b
b=a * b
```

Warning: * NOT matrix multiplication!

```
c = np.ones((3, 3))
c=c*c #NOT matrix multiplication!
```

а			
1	2	3	4
a			
2	3	4	5
а			
4	9	16	25



Numerical operations on arrays

```
Dot Product
 ndarray:
       x=np.array([1,2,3])
       y=np.array([-7,8,9])
       dot=np.dot(x,y)#dot=36
 matrix Class:
       x=np.matrix([[2, 3], [3, 5]])
       y=np.matrix([[2, 2], [5, -1]])
       z = x * y
```

		_			
-	1	2	· 	-	2
			_	_	
		У	_		_
-	7	8	3	(9
					_
		Х			
	2				
	3	4	-3 -5	_	
	3		5		
У					
	2	Τ	2		
	5	\top	_1		



Numerical operations on arrays

Universal functions (ufuncs)

Trigonometric functions

sin, cos, tan, arcsin, arccos, arctan, hypot, arctan2, degrees, radians, unwrap, deg2rad, rad2deg

Hyperbolic functions

sinh, cosh, tanh, arcsinh, arccosh, arctanh

Rounding

around, round_, rint, fix, floor, ceil, trunc

Sums, products, differences

prod, sum, nansum, cumprod, cumsum, diff, ediff1d, gradient, cross, trapz

Exponents and logarithms

exp, expm1, exp2, log, log10, log2, log1p, logaddexp, logaddexp2

Other special functions

i0, sinc

Floating point routines

signbit, copysign, frexp, ldexp

Arithmetic operations

add, reciprocal, negative, multiply, divide, power, subtract, true_divide, floor_divide, fmod, mod, modf, remainder

Handling complex numbers

angle, real, imag, conj

Miscellaneous

convolve, clip, sqrt, square, absolute, fabs, sign, maximum, minimum, fmax, fmin, nan_to_num, real_if_close, interp

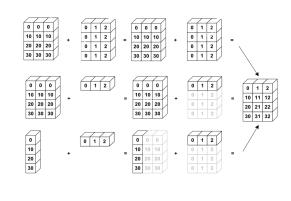
Numerical operations on arrays

Broadcasting

- Basic operations on numpy arrays (addition, etc.) are elementwise.
- This works on arrays of the same size.
- It's also possible to do operations on arrays of different sizes if NumPy can transform these arrays so that they all have the same size: this conversion is called broadcasting.
- e.g:

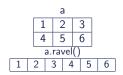
np.array([1, 2, 3]) + 1:

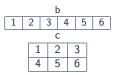
I
2
3
+
I
I
I
I
$$\rightarrow$$
2
3
4



Numerical operations on arrays

Array shape manipulation • Flattening: 1 a = np. array([[1,2,3],[4,5,6]]) 2 a.ravel() • Reshaping: The inverse operation to flattening 1 b = a.ravel() 2 c = b.reshape((2, 3))





Summary

Tips

What do you need to know to get started?:

- Know how to create arrays : array, arange, ones, zeros.
- Know the shape of the array with array.shape, then use slicing to obtain different views of the array: array[::2], etc. Adjust the shape of the array using reshape or flatten it with ravel.
- Obtain a subset of the elements of an array and/or modify their values.
- Know miscellaneous operations on arrays, such as finding the mean or max (array.max(), array. mean()). No need to retain everything, but have the reflex to search in the documentation (online docs, help(), lookfor())!!
- For advanced use: master the indexing with arrays of integers, as well as broadcasting. Know more NumPy functions to handle various array operations.

Part III Introduction to SciPy



SciPy

- Extension package contains various toolboxes dedicated to common issues in scientific computing.
- Built on numpy. All functionality from numpy seems to be available in scipy as well.
- Composed of task-specific sub-modules such as interpolation, integration, optimization, image processing, statistics, special functions, etc...

SciPy sub-modules:

scipy.cluster	Vector quantization / Kmeans
scipy.constants	Physical and mathematical constants
scipy.fftpack	Fourier transform
scipy.integrate	Integration routines
scipy.interpolate	Interpolation
scipy.io	Data input and output
scipy.linalg	Linear algebra routines
scipy.ndimage	n-dimensional image package
scipy.odr	Orthogonal distance regression
scipy.optimize	Optimization
scipy.signal	Signal processing
scipy.sparse	Sparse matrices
scipy.spatial	Spatial data structures and algorithms
scipy.special	Any special mathematical functions
scipy.stats	Statistics

Numerical integration: scipy.integrate

```
Function integrals

The most generic integration routine is scipy.integrate.quad(). For example, to compute \int_0^{\pi/2} \sin(t) dt:

from scipy.integrate import quad
res, err = quad(np.sin, 0, np.pi/2)
# res is the result, is should be close to 1
np.allclose(res, 1)
# err is an estimate of the err
np.allclose(err, 1 - res)
```

Other integration schemes are available: scipy.integrate.fixed_quad(), scipy.integrate.quadrature(), scipy.integrate.romberg()...

Numerical integration: scipy.integrate

Integrating differential equations

scipy.integrate also features routines for integrating Ordinary Differential Equations (ODE). In particular, **scipy.integrate.odeint()** solves ODE of the form: dy/dt = f(y1, y2, ..., t0, ...) For example, to solve the ODE $\frac{dy}{dt} = -2*y$ between $t = 0 \dots 4$, with the initial condition y(t=0) = 1:

```
y(t = 0) = 1:
from scipy.integrate import odeint
def calc_derivative(ypos, time):
    return -2 * ypos

time = np.linspace(0, 4, 40)
y = odeint(calc_derivative, y0=1, t=time)
```

End of Lecture 2:

Introduction to Programming with Python 3 for Scientific Computing

