Intro to scientific Python programming

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This is a very quick intro to Python programming

- variables for numbers, lists, and arrays
- while loops and for loops
- functions
- if tests
- plotting

Method: show program code through math examples

Variables, loops, lists, and arrays

Do you have access to Python?

Many methods:

- Mac and Windows: Anaconda
- Ubuntu: `sudo apt-get install`
- Web browser (Wakari or SageMathCloud)

See How to access Python for doing scientific computing for more details!

Mathematical example

Most examples will involve this formula:

$$s = v_0 t + \frac{1}{2} a t^2 \tag{1}$$

We may view s as a function of t: $s(t)$, and also include the parameters in the notation: $s(t; v_0, a)$.

A program for evaluating a formula

Task

Compute s for $t = 0.5$, $v_0 = 2$, and $a = 0.2$.

Code

```
t = 0.5
v0 = 2
a = 0.2
s = v0*t + 0.5*a*t**2
print s
```

Execution

```
Terminal> python distance.py
1.025
```

Assignment statements assign a name to an object

```
t = 0.5                  # real number makes float object
v0 = 2                   # integer makes int object
a = 0.2                  # float object
s = v0*t + 0.5*a*t**2    # float object
```

Rule: evaluate right-hand side object, left-hand side is a name for that object

Formatted output with text and numbers

- Task: write out s=1.025
- Method: printf syntax

```
print 's=%g' % s      # g: compact notation
print 's=%.2f' % s    # f: decimal notation, .2f: 2 decimals
```

Modern alternative: format string syntax

```
print 's={s:.2f}'.format(s=s)
```

Programming with a while loop

- Task: write out a table of t and $s(t)$ values (two columns), for $t \in [0, 2]$ in steps of 0.1
- Method: while loop

```
v0 = 2
a = 0.2
dt = 0.1   # Increment
t = 0      # Start value
while t <= 2:
    s = v0*t + 0.5*a*t**2
    print t, s
    t = t + dt
```

Output of the previous program

```
Terminal> python while.py
0 0.0
0.1 0.201
0.2 0.404
0.3 0.609
0.4 0.816
0.5 1.025
0.6 1.236
0.7 1.449
0.8 1.664
0.9 1.881
1.0 2.1
1.1 2.321
1.2 2.544
1.3 2.769
1.4 2.996
1.5 3.225
1.6 3.456
1.7 3.689
1.8 3.924
1.9 4.161
```

Structure of a while loop

```
while condition:
    <intented statement>
    <intented statement>
    <intented statement>
```

Note:

- the colon in the first line
- all statements in the loop must be indented
- `condition` is a boolean expression (e.g., `t <= 2`)

The Python Online Tutor can help you understand the program flow

Python Online Tutor lets you step through the program and examine variables.

```
a = 1
da = 0.5
while a <= 3:
    print a
    a = a + da
```

(Visualize execution)

Lists

A list collects several variables (objects) in a given sequence:

```
L = [-1, 1, 8.0]
```

A list can contain any type of objects, e.g.,

```
L = ['mydata.txt', 3.14, 10]
```

Some basic list operations:

```
>>> L = ['mydata.txt', 3.14, 10]
>>> print L[0]
mydata.txt
>>> print L[1]
3.14
>>> del L[0]  # delete the first element
>>> print L
[3.14, 10]
>>> print len(L)  # length of L
2
>>> L.append(-1)  # add -1 at the end of the list
>>> print L
[3.14, 10, -1]
```

For loops

A for loop is used for visiting elements in a list, one by one:

```
>>> L = [1, 4, 8, 9]
>>> for e in L:
...     print e
...
1
4
8
9
```

Demo in the Python Online Tutor:

```
list1 = [0, 0.1, 0.2]
list2 = []
for element in list1:
    p = element + 2
    list2.append(p)
print list2
```

(Visualize execution)

For loops used traditionally an integer counter over list/array indices

```
for i in range(len(somelist)):
    # Work with somelist[i]
```

Note:

- `range` returns a list of integers
- `range(a, b, s)` returns the integers `a, a+s, a+2*s, ...` up to *but not including* (!!) `b`
- `range(b)` implies a=0 and s=1
- `range(len(somelist))` returns `[0, 1, 2]`

Let's replace our while loop by a for loop

```
v0 = 2
a = 0.2
dt = 0.1  # Increment
t_values = []
s_values = []
n = int(round(2/dt)) + 1  # No of t values
for i in range(n):
    t = i*dt
    s = v0*t + 0.5*a*t**2
    t_values.append(t)
    s_values.append(s)
print s_values  # Just take a look at a created list

# Make nicely formatted table
for t, s in zip(t_values, s_values):
    print '%.2f  %.4f' % (t, s)

# Alternative
for i in range(len(t_values)):
    print '%.2f  %.4f' % (t_values[i], s_values[i])
```

Traversal of multiple lists at the same time with `zip`

```
for e1, e2, e3, ... in zip(list1, list2, list3, ...):
```

Alternative: loop over a common index for the lists

```
for i in range(len(list1)):
    e1 = list1[i]
    e2 = list2[i]
    ...
```

Arrays

- List: collect a set of numbers or other objects in a single variable
- Lists are very flexible (can grow, can contain "anything")
- Array: computationally efficient and convenient list
- Arrays must have fixed length and can only contain numbers of the same type (integers, real numbers, complex numbers)
- Arrays require the `numpy` module

```
>>> import numpy
>>> L = [1, 4, 10.0]     # List of numbers
>>> a = numpy.array(L)   # Make corresponding array
>>> print a
[  1.   4.  10.]
>>> print a[1]
4.0
>>> print a.dtype        # Data type of an element
float64
>>> b = 2*a + 1
>>> print b
[  3.   9.  21.]
```

numpy functions creates entire arrays at once

```
>>> c = numpy.log(a)   # Take ln of all elements in a
>>> print c
[ 0.          1.38629436  2.30258509]
```

Create $n+1$ uniformly distributed coordinates in $[a, b]$:

```
t = numpy.linspace(a, b, n+1)
```

Let's use arrays in our previous program

```
import numpy
v0 = 2
a = 0.2
dt = 0.1  # Increment
n = int(round(2/dt)) + 1  # No of t values

t_values = numpy.linspace(0, 2, n+1)
s_values = v0*t + 0.5*a*t**2

# Make nicely formatted table
for t, s in zip(t_values, s_values):
    print '%.2f  %.4f' % (t, s)
```

Standard mathematical functions are found in the math module

```
>>> import math
>>> print math.sin(math.pi)
1.2246467991473532e-16          # Note: only approximate value
```

Get rid of the `math` prefix:

```
from math import sin, pi
print sin(pi)

# Or import everything from math
from math import *
print sin(pi), log(e), tanh(0.5)
```

Use the numpy module for standard mathematical functions applied to arrays

Matlab users can do

```
from numpy import *
```

The Python community likes

```
import numpy as np
print np.sin(np.pi)
```

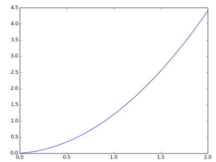
Our convention: use `np` prefix, but not in formulas involving math functions

```
import numpy as np
from numpy import sin, exp
t = np.linspace(0, 4, 1001)
p = exp(-t)*sin(2*t)
```

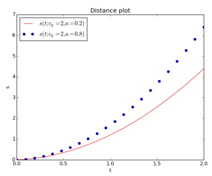
Plotting

Plotting is done with `matplotlib`:

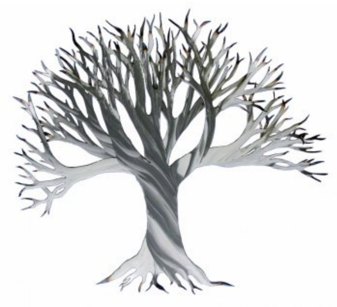
The plotfile `myplot.png` looks like



Plotting of multiple curves



Functions and branching



Functions

- $s(t) = v_0 t + \frac{1}{2}at^2$ is a mathematical function
- Can implement $s(t)$ as a Python function s(t)

```
def s(t):
    return v0*t + 0.5*a*t**2

v0 = 0.2
a = 4
value = s(3)    # Call the function
```

Note:

- functions start with the keyword def
- statements belonging to the function must be indented
- function input is represented by arguments (separated by comma if more than one)
- function output is returned to the calling code
- v0 and a are *global variables*
- v0 and a must be initialized before s is called

Functions can have multiple arguments

v0 and a as function arguments instead of global variables:

```
def s(t, v0, a):
    return v0*t + 0.5*a*t**2

value = s(3, 0.2, 4)    # Call the function

# More readable call
value = s(t=3, v0=0.2, a=4)
```

Keyword arguments are arguments with default values

```
def s(t, v0=1, a=1):
    return v0*t + 0.5*a*t**2

value = s(3, 0.2, 4)          # specify new v0 and a
value = s(3)                  # rely on v0=1 and a=1
value = s(3, a=2)             # rely on v0=1
value = s(3, v0=2)            # rely on a=1
value = s(t=3, v0=2, a=2)     # specify everything
value = s(a=2, t=3, v0=2)     # any sequence allowed
```

- Arguments without the argument name are called *positional arguments*
- Positional arguments must always be listed before the keyword arguments in the function and in any call
- The sequence of the keyword arguments can be arbitrary

Vectorization speeds up the code

Scalar code (work with one number at a time):

```
def s(t, v0, a):
    return v0*t + 0.5*a*t**2

for i in range(len(t)):
    s_values[i] = s(t_values[i], v0, a)
```

Vectorized code: apply s to the entire array

```
s_values = s(t_values, v0, a)
```

How can this work?

- Array: t
- Expression: v0*t + 0.5*a*t**2
- r1 = v0*t (scalar times array)
- r2 = t**2 (square each element)
- r3 = 0.5*a*r2 (scalar times array)
- r1 + r3 (add each element)

Python functions written for scalars normally work for arrays too!

True if computations involve arithmetic operations and math functions:

```
from math import exp, sin

def f(x):
    return 2*x + x**2*exp(-x)*sin(x)

v = f(4)   # f(x) works with scalar x

# Redefine exp and sin with their vectorized versions
from numpy import exp, sin, linspace
x = linspace(0, 4, 100001)
v = f(x)   # f(x) works with array x
```

However, if tests are not allowed:

```
def f(x):
    return -1 if x < 0 else x**4*exp(-x)*sin(x)

x = linspace(0, 4, 100001)
v = f(x)   # will not work
```

Python functions can return multiple values

Return $s(t) = v_0 t + \frac{1}{2}at^2$ and $s'(t) = v_0 + at$:

```
def movement(t, v0, a):
    s = v0*t + 0.5*a*t**2
    v = v0 + a*t
    return s, v

s_value, v_value = movement(t=0.2, v0=2, a=4)
```

`return s, v` means that we return a *tuple* ($\approx$ list):

```
>>> def f(x):
...     return x+1, x+2, x+3
...
>>> r = f(3)     # Store all three return values in one object r
>>> print r
(4, 5, 6)
>>> type(r)      # What type of object is r?
<type 'tuple'>
>>> print r[1]
5
```

Tuples are constant lists (cannot be changed)

A more general mathematical formula

Equations from basic kinematics:

$$v = \frac{ds}{dt}, \quad s(0) = s_0$$
$$a = \frac{dv}{dt}, \quad v(0) = v_0$$

Integrate to find $v(t)$:

$$\int_0^t a(t)dt = \int_0^t \frac{dv}{dt}dt$$

which gives

$$v(t) = v_0 + \int_0^t a(t)dt$$

Integrate again over $[0, t]$ to find $s(t)$:

Basic if-else tests

An if test has the structure

```
if condition:
    <statements when condition is True>
else:
    <statements when condition is False>
```

Here,

- `condition` is a boolean expression with value `True` or `False`.

```
if t <= t1:
    s = v0*t + 0.5*a0*t**2
else:
    s = v0*t + 0.5*a0*t1**2 + a0*t1*(t-t1)
```

Multi-branch if tests

```
if condition1:
    <statements when condition1 is True>
elif condition2:
    <statements when condition1 is False and condition2 is True>
elif condition3:
    <statements when condition1 and conditon 2 are False
     and condition3 is True>
else:
    <statements when condition1/2/3 all are False>
```

Just if, no else:

```
if condition:
    <statements when condition is True>
```

Implementation of a piecewisely defined function with if

A Python function implementing the mathematical function

$$s(t) = \begin{cases} s_0 + v_0 t + \frac{1}{2}a_0 t^2, & t \le t_1 \\ s_0 + v_0 t_1 + \frac{1}{2}a_0 t_1^2 + a_0 t_1 (t - t_1), & t > t_1 \end{cases}$$

reads

```
def s_func(t, v0, a0, t1):
    if t <= t1:
        s = v0*t + 0.5*a0*t**2
    else:
        s = v0*t + 0.5*a0*t1**2 + a0*t1*(t-t1)
    return s
```

Python functions containing if will not accept array arguments

```
>>> def f(x): return x if x < 1 else 2*x
...
>>> import numpy as np
>>> x = np.linspace(0, 2, 5)
>>> f(x)
Traceback (most recent call last):
...
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

Problem: `x < 1` evaluates to a boolean array, not just a boolean

Remedy 1: Call the function with scalar arguments

```
n = 201  # No of t values for plotting
t1 = 1.5

t = np.linspace(0, 2, n+1)
s = np.zeros(n+1)
for i in range(len(t)):
    s[i] = s_func(t=t[i], v0=0.2, a0=20, t1=t1)
```

Can now easily plot:

```
plt.plot(t, s, 'b-')
plt.plot([t1, t1], [0, s_func(t=t1, v0=0.2, a0=20, t1=t1)], 'r--')
plt.xlabel('t')
plt.ylabel('s')
plt.savefig('myplot.png')
plt.show()
```

Remedy 2: Vectorize the if test with `where`

Functions with if tests require a complete rewrite to work with arrays.

```
s = np.where(condition, s1, s2)
```

Explanation:

- `condition`: array of boolean values
- `s[i] = s1[i]` if `condition[i]` is `True`
- `s[i] = s2[i]` if `condition[i]` is `False`

Our example then becomes

```
s = np.where(t <= t1,
             v0*t + 0.5*a0*t**2,
             v0*t + 0.5*a0*t1**2 + a0*t1*(t-t1))
```

Note that `t <= t1` with array `t` and scalar `t1` results in a boolean array `b` where `b[i] = t[i] <= t1`.

Remedy 3: Vectorize the if test with array indexing

- Let `b` be a boolean array (e.g., `b = t <= t1`)
- `s[b]` selects all elements `s[i]` where `b[i]` is `True`
- Can assign some array expression `expr` of length `len(s[b])` to `s[b]`: `s[b] = (expr)[b]`

Our example can utilize this technique with `b` as `t <= t1` and `t > t1`:

```
s = np.zeros_like(t)  # Make s as zeros, same size & type as t
s[t <= t1] = (v0*t + 0.5*a0*t**2)[t <= t1]
s[t > t1]  = (v0*t + 0.5*a0*t1**2 + a0*t1*(t-t1))[t > t1]
```

Files

File reading

Put input data in a text file:

```
v0 = 2
a = 0.2
dt = 0.1
interval = [0, 2]
```

How can we read this file into variables `v0`, `a`, `dt`, and `interval`?

Code for reading files with lines `variable = value`

```
infile = open('.input.dat', 'r')
for line in infile:
    # Typical line: variable = value
    variable, value = line.split('=')
    variable = variable.strip()  # remove leading/traling blanks
    if variable == 'v0':
        v0 = float(value)
    elif variable == 'a':
        a = float(value)
    elif variable == 'dt':
        dt = float(value)
    elif variable == 'interval':
        interval = eval(value)
infile.close()
```

Splitting lines into words is a frequent operation

```
>>> line = 'v0 = 5.3'
>>> variable, value = line.split('=')
>>> variable
'v0 '
>>> value
' 5.3'
>>> variable.strip()  # strip away blanks
'v0'
```

Note: must convert `value` to `float` before we can compute with the value!

Modern Python often applies the `with` statement for file handling

```
with open('.input.dat', 'r') as infile:
    for line in infile:
        ...
```

No need to close the file when using `with`

File writing

- We have t and $s(t)$ values in two lists, `t_values` and `s_values`
- Task: write these lists as a nicely formatted table in a file

Code:

```
outfile = open('table1.dat', 'w')
outfile.write('# t    s(t)\n')  # write header
for t, s in zip(t_values, s_values):
    outfile.write('%.2f  %.4f\n' % (t, s))
```

Simplified writing of tabular data to file via `numpy.savetxt`

```
import numpy as np
# Make two-dimensional array of [t, s(t)] values in each row
data = np.array([t_values, s_values]).transpose()
np.savetxt('table2.dat', data, fmt=['%.2f', '%.4f'],
           header='t    s(t)', comments='# ')
```

Simplified reading of tabular data from file via `numpy.savetxt`

```
data = np.loadtxt('table2.dat', comments='#')
```

Note:

- Lines beginning with the comment character # are skipped in the reading
- `data` is a two-dimensional array: `data[i,0]` holds the t value and `data[i,1]` the $s(t)$ value in the `i`-th row

Classes

- All objects in Python are made from a class
- You don't need to know about classes to use Python
- But class programming is powerful

- Class = functions + variables packed together
- A class is a logical unit in a program
- A large program as a combination of appropriate units

A very simple class

- One variable: a
- One function: dump for printing a

```python
class Trivial:
    def __init__(self, a):
        self.a = a

    def dump(self):
        print self.a
```

Class terminology: Functions are called *methods* and variables are called *attributes*.

How can we use this class?

First, make an *instance* (object) of the class:

```python
t = Trivial(a=4)
t.dump()
```

Note:

- The syntax `Trivial(a=4)` actually means `Trivial.__init__(t, 4)`
- `self` is an argument in `__init__` and `dump`, but not used in the calls
- `__init__` is called *constructor* and is used to construct an object (instance) if the class

The `self` argument is a difficult thing for newcomers...

It takes time and experience to understand the `self` argument in class methods!

1. `self` must always be the first argument
2. `self` is never used in calls
3. `self` is used to access attributes and methods inside methods

We refer to a more comprehensive text on classes for better explanation of `self`.

`self` is confusing in the beginning, but later it greatly helps the understanding of how classes work!

A class for representing a mathematical function

Function with one independent variable t and two parameters v_0 and a:

$$s(t; v_0, a) = v_0 t + \frac{1}{2} a t^2$$

Class representation of this function:

- v0 and a are variables (data)
- A method to evaluate $s(t)$, but just function of t

Usage:

```python
s = Distance(v0=2, a=0.5)  # create instance
v = s(t=0.2)               # compute formula
```

The class code

```python
class Distance:
    def __init__(self, v0, a):
        self.v0 = v0
        self.a = a

    def __call__(self, t):
        v0, a = self.v0, self.a  # make local variables
        return v0*t + 0.5*a*t**2

s = Distance(v0=2, a=0.5)  # create instance
v = s(t=0.2)               # actually s.__call__(t=0.2)
```

Class implementation of $f(x, y, z; p_1, p_2, \ldots, p_n)$

- The n parameters $p_1, p_2, \ldots, p_n$ are attributes
- `__call__(self, x, y, z)` is used to compute $f(x, y, z)$

```python
class F:
    def __init__(self, p1, p2, ...):
        self.p1 = p1
        self.p2 = p2
        ...

    def __call__(self, x, y, z):
        # return formula involving x, y, z and self.p1, self.p2 ...

f = F(p1=..., p2=..., ...)   # create instance with parameters
print f(1, 4, -1)            # evaluate f(x,y,z) function
```