Introduction to Scientific Python programming - Adapted to TKT4140 Numerical Methods with Computer Laboratory

Hans Petter Langtangen^{1,2} (hpl@simula.no)

Leif Rune Hellevik^{3,1} (leif.r.hellevik@ntnu.no)

¹Center for Biomedical Computing, Simula Research Laboratory

²Department of Informatics, University of Oslo

³Biomechanichs Group, Department of Structural Engineering NTNU

Dec 11, 2015

Contents

Index 24

This is a very quick intro to Python programming

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

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:

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

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.

Python 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

Rule:

- evaluate right-hand side; it results in an object
- left-hand side is a name for that object

Formatted output with text and numbers

- Task: write out text with a number (3 decimals): 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</pre>
```

Output of the previous program

```
Terminal> python while.py
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

Note:

- the colon in the first line
- all statements in the loop must be indented (no braces as in C, C++, Java, ...)
- condition is a boolean expression (e.g., t <= 2)

Let's take a closer look at the output of our program

```
Terminal> python while.py
0 0.0
0.1 0.201
0.2 0.404
...
1.8 3.924
1.9 4.161
```

The last line contains 1.9, but the while loop should run also when t=2 since the test is $t \le 2$. Why is this test False?

Let's examine the program in the Python Online Tutor

Python Online Tutor: step through the program and examine variables

```
a = 0
da = 0.4
while a <= 1.2:
    print a
    a = a + da</pre>
```

(Visualize execution)

Ooops, why is a <= 1.2 when a is 1.2? Round-off errors!

```
a = 0
da = 0.4
while a <= 1.2:
    print a
    a = a + da
    # Inspect all decimals in da and a
    print 'da=%.16E\na=%.16E' % (da, a)
    print 'a <= 1.2: %g' % (a <= 1.2)</pre>
```

(Visualize execution)

Rule: never a == b for real a and b! Always use a tolerance!

```
\begin{array}{l} a = 1.2 \\ b = 0.4 + 0.4 + 0.4 \\ boolean\_condition1 = a == b \\ \# \ \textit{This is the way to do it} \\ tol = 1E-14 \\ boolean\_condition2 = abs(a - b) < tol \\ \# \ \textit{True} \end{array}
```

A list collects several objects in a given sequence

A list of numbers:

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

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

```
L = ['mydata.txt', 3.14, 10] # string, float, int
```

Some basic list operations:

```
>>> L = ['mydata.txt', 3.14, 10]
>>> print L[0]  # print first element (index 0)
mydata.txt
>>> print L[1]  # print second element (index 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]
```

Store our table in two lists, one for each column

```
v0 = 2
a = 0.2
dt = 0.1  # Increment
t = 0
t_values = []
s_values = []
while t <= 2:
    s = v0*t + 0.5*a*t**2
    t_values.append(t)
    s_values.append(s)
    t = t + dt
print s_values  # Just take a look at a created list

# Print a nicely formatted table
i = 0
while i <= len(t_values)-1:
    print '%.2f %.4f' % (t_values[i], s_values[i])
    i += 1  # Same as i = i + 1</pre>
```

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)

Traditional for loop: integer counter over list/array indices

```
somelist = ['file1.dat', 22, -1.5]
for i in range(len(somelist)):
```

```
# access list element through index
print 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

```
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 implementation
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]
    e3 = list3[i]
    ...
```

Arrays are computationally efficient lists of numbers

- Lists collect a set of 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

Examples on using arrays

```
>>> import numpy
>>> L = [1, 4, 10.0]
                        # List of numbers
>>> a = numpy.array(L) # Convert to array
>>> print a [ 1. 4. 10.]
>>> print a[1]
                        # Access element through indexing
4.0
>>> print a[0:2]
                        # Extract slice (index 2 not included!)
[ 1. 4.]
>>> print a.dtype
                        # Data type of an element
float64
>>> b = 2*a + 1
                        # Can do arithmetics on arrays
>>> print b
[ 3. 9. 21.]
```

numpy functions creates entire arrays at once

Apply ln to all elements in array a:

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)
```

Note: no explicit loop for computing s_values!

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 *
  x = linspace(0, 1, 101)
  y = exp(-x)*sin(pi*x)

The Python community likes
  import numpy as np
  x = np.linspace(0, 1, 101)
  y = np.exp(-x)*np.sin(np.pi*x)

Our convention: use np prefix, but not in formulas involving math functions
  import numpy as np
  x = np.linspace(0, 1, 101)

from numpy import sin, exp, pi
  y = exp(-x)*sin(pi*x)
```

Array assignment gives view (no copy!) of array data

Consider array assignment b=a:

```
a = np.linspace(1, 5, 5)
b = a
```

Here, b is a just *view* or a pointer to the data of a - no copying of data! See the following example how changes in b inflict changes in a

```
>>> a
array([ 1., 2., 3., 4., 5.])
>>> b[0] = 5
>>> a
array([ 5., 2., 3., 4., 5.])
>>> a[1] = 9
>>> b
array([ 5., 9., 3., 4., 5.])
```

Copying array data requires special action via the copy method

```
>>> c = a.copy()  # copy all elements to new array c

>>> c[0] = 6  # a is not changed

>>> a

array([ 1., 2., 3., 4., 5.])

>>> c

array([ 6., 2., 3., 4., 5.])

>>> b

array([ 5., 2., 3., 4., 5.])
```

Note: b has still the values from the previous example

Construction of tridiagonal and sparse matrices

- SciPy offers a sparse matrix package scipy.sparse
- The spdiags function may be used to construct a sparse matrix from diagonals
- Note that all the diagonals must have the same length as the dimension of their sparse matrix - consequently some elements of the diagonals are not used
- The first k elements are not used of the k super-diagonal
- The last k elements are not used of the -k sub-diagonal

Example on constructing a tridiagonal matrix

Example on solving a tridiagonal system

We can solve Ax = b with tridiagonal matrix A: choose some x, compute b = Ax (sparse/tridiagonal matrix product!), solve Ax = b, and check that x is the desired solution:

```
>>> x = np.linspace(-1, 1, N)  # choose solution
>>> b = A.dot(x)  # sparse matrix vector product
>>> import scipy.sparse.linalg
>>> x = scipy.sparse.linalg.spsolve(A, b)
>>> print x
[-1.  -0.6 -0.2  0.2  0.6  1. ]
```

Check against dense matrix computations:

```
>>> A_d = A.toarray()  # corresponding dense matrix
>>> b = np.dot(A_d, x)  # standard matrix vector product
>>> x = np.linalg.solve(A_d, b)  # standard Ax=b algorithm
>>> print x
[-1. -0.6 -0.2  0.2  0.6  1. ]
```

Plotting

Plotting is done with matplotlib:

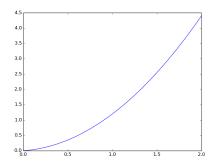
```
import numpy as np
import matplotlib.pyplot as plt

v0 = 0.2
a = 2
n = 21  # No of t values for plotting

t = np.linspace(0, 2, n+1)
s = v0*t + 0.5*a*t**2

plt.plot(t, s)
plt.savefig('myplot.png')
plt.show()
```

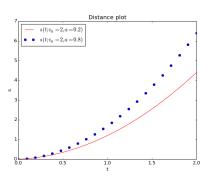
The plotfile myplot.png looks like



Plotting of multiple curves

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

v0 = 0.2
n = 21  # No of t values for plotting
```



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, which must be initialized before s(t) 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?

• Expression: v0*t + 0.5*a*t**2 with array t

• 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
```

Python functions can return multiple values

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

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):

Tuples are constant lists (cannot be changed)

A more general mathematical formula (part I)

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

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

A more general mathematical formula (part II)

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

$$s(t) = s_0 + v_0 t + \int_0^t \left(\int_0^t a(t) dt \right) dt$$

Example: $a(t) = a_0$ for $t \in [0, t_1]$, then a(t) = 0 for $t > t_1$:

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

Need if test to implement this!

Basic if-else tests

An if test has the structure

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

reads

return s

```
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</pre>
     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}
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)
```

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.xlabel('t')
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 \le t1, v0*t + 0.5*a0*t**2, v0*t + 0.5*a0*t1**2 + a0*t1*(t-t1))
```

Note that $t \le t1$ with array t and scalar t1 results in a boolean array b where $b[i] = t[i] \le t1$.

Remedy 3: Vectorize the if test with array indexing

- Let b be a boolean array (e.g., b = $t \le t1$)
- 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 \leq t1 and 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
'y0'
```

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

The magic eval function

eval(s) executes a string s as a Python expression and creates the corresponding Python object

```
>>> obj1 = eval('1+2')  # Same as obj1 = 1+2
>>> obj1, type(obj1)
(3, <type 'int'>)
>>> obj2 = eval('[-1, 8, 10, 11]')
>>> obj2, type(obj2)
([-1, 8, 10, 11], <type 'list'>)
>>> from math import sin, pi
>>> x = 1
>>> obj3 = eval('sin(pi*x)')
>>> obj3, type(obj3)
(1.2246467991473532e-16, <type 'float'>)
```

Why is this so great? We can read formulas, lists, expressions as text from file and with eval turn them into live Python objects!

Implementing a calculator in Python

Demo:

```
Terminal> python calc.py "1 + 0.5*2"
2.0
Terminal> python calc.py "sin(pi*2.5) + exp(-4)"
1.0183156388887342

Just 5 lines of code:

import sys
command_line_expression = sys.argv[1]
from math import * # Define sin, cos, exp, pi, etc.
result = eval(command_line_expression)
print result
```

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 table 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

Simplified reading of tabular data from file via numpy.loadtxt

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

Note:

- \bullet 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

```
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:

```
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
- ullet __init__ is called constructor and is used to construct an object (instance) if the class
- t.dump() actually means Trivial.dump(t) (self is t)

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 as a function of t

Usage:

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

The class code

```
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 $f(x, y, z; p_1, p_2, \dots, p_n)$

- 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)

```
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
```

Index

visualization, 11

```
array, 7
                                         while loop, 3
assignment statement, 3
                                         zip, 7
boolean expression, 4, 16
branching, 16
False, 4
float, 3
for loop, 6
format string syntax, 3
global variables, 13
graphics, 11
if test, 16
import of modules, 9
int, 3
keyword arguments, 13
linspace, 8
list, 5
math, 9
mathematical functions, 9
matplotlib, 11
multiple lists traversal with zip, 7
multiple return values, 14
numpy, 7
objects, 3
plotting, 11
print statement, 3
program file, 2
Python Online Tutor, 5
text editor, 2
True, 4
variable, 3
vectorization, 14
vectorized functions, 14
vectorizing if tests, 17
```