

Intro to scientific Python programming

Hans Petter Langtangen^{1,2}

Simula Research Laboratory¹

University of Oslo²

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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

1 Variables, loops, lists, and arrays

2 Functions and branching

3 Files

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:

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

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

```
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; 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
```

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*
(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 $t \leq 2$. 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
```

(Visualize execution)

Oops, 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 '%.16E, %.16E' % (da, a), a <= 1.2
```

(Visualize execution)

Small	round-off	error	in	da	makes
a = 1.2000000000000002					

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

```
a = 1.2
b = 0.4 + 0.4 + 0.4
boolean_condition1 = a == b           # may be False

# This is the way to do it
tol = 1E-14
boolean_condition2 = abs(a - b) < tol # True
```


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
```

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

```
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 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 :

```
>>> c = numpy.log(a)
>>> print c
[ 0.          1.38629436  2.30258509]
```

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

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

Create array of length n filled with zeros:

```
t = numpy.zeros(n)
s = numpy.zeros_like(t)  # zeros with t's size and data type
```

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)
```

Plotting

Plotting is done with matplotlib:

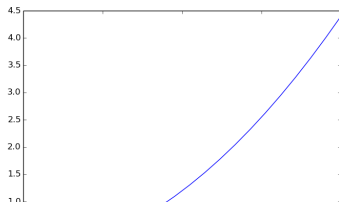
```
import numpy as np
import matplotlib.pyplot as plt

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



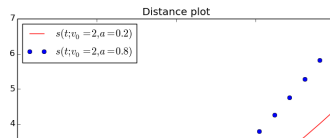
Plotting of multiple curves

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

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

t = np.linspace(0, 2, n+1)
a = 2
s0 = v0*t + 0.5*a*t**2
a = 3
s1 = v0*t + 0.5*a*t**2

plt.plot(t, s0, 'r-', # Plot s0 curve with red line
         t, s1, 'bo') # Plot s1 curve with blue circles
plt.xlabel('t')
plt.ylabel('s')
plt.title('Distance plot')
plt.legend([' $s(t; v_0=2, a=0.2)$ ', ' $s(t; v_0=2, a=0.8)$ '],
          loc='upper left')
plt.savefig('myplot.png')
plt.show()
```

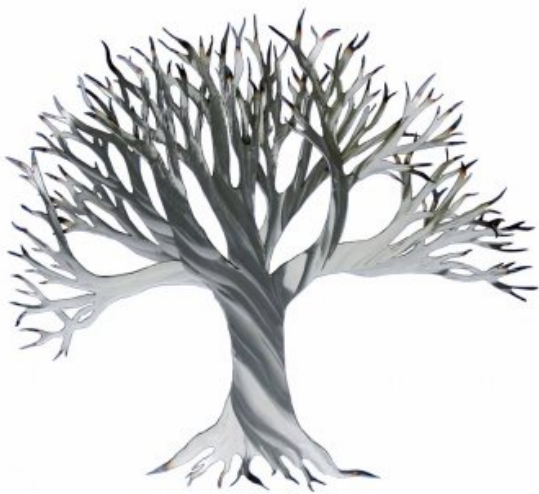


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Functions and branching



Functions

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

v_0 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):

```
>>> 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 (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 $t > t_1$:

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

Need *if test* to implement this!

Basic if-else tests

An if test has the structure

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

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

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

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]
```

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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/trailing 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!

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`

- 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`

```
import numpy as np
# Make two-dimensional array of [t, s(t)] values in each row
data = np.array([t_values, s_values]).transpose()

# Write data array to file in table format
np.savetxt('table2.dat', data, fmt=['%.2f', '%.4f'],
           header='t    s(t)', comments='# ')
```

table2.dat:

```
# t    s(t)
0.00 0.0000
0.10 0.2010
0.20 0.4040
0.30 0.6090
0.40 0.8160
0.50 1.0250
0.60 1.2360
...
1.90 4.1610
2.00 4.4000
```

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

```
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