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

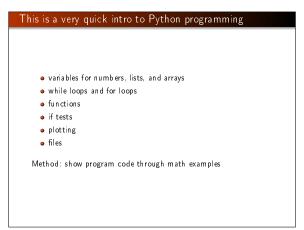
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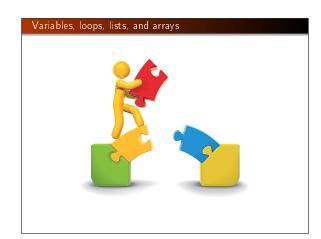
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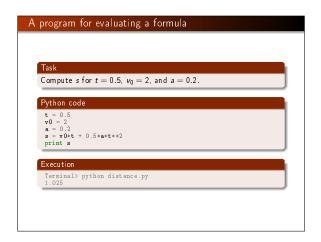
Mar 15, 2015







```
Mathematical example s=v_0t+\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).
```



Assignment statements assign a name to an object t = 0.5 v0 = 2 a = 0.2 s = v0*t + 0.5*a*t**2 Rule: e evaluate right-hand side; it results in an object eleft-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 ∈ [0,2] in steps of 0.1
• Method: while loop

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

```
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
```

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)

```
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 L[3.14, 10, -1]
```

```
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 + f</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]
```

```
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 **edt
    s = v0**t + 0.5**a****2
    t_values.append(t)
    s_values.append(s)
    print s_values # Just take a look at a created list
# Nake nicely formatted table
for t, sin zip(t_values, s_values):
    print '%.2f %.4f' % (t, s)
# Ilternative implemention
for i in range(len(t_values)):
    print '%.2f %.4f' % (t_values[i], s_values[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")

• Arrays require the numpy module

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)

```
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]
    ...
```

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 'N. 21 %.41 % (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.linepace(0, 2, n+1)
s = v0+t + 0.5*a+t**2

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

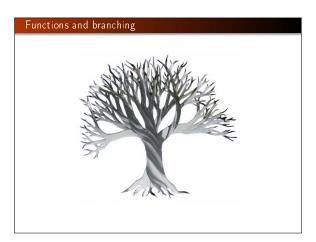
The plotfile myplot.png looks like
```

```
Copies and views of numpy arrays

• Given numpy array a=np.linspace(1,10,10)
• The assignment b=a creates a view or a pointer to the data of a
• The original array is not copied in memory

See the following example how changes in b inflict changes in a

>>> a=np.linspace(1,5,5)
>>> a array([ 1, 2, 3, 4, 5.1)
>>> b=a
>>> b[0]=5
>>> a array([ 5, 2, 3, 4, 5.1)
>>> b
array([ 5, 2, 3, 4, 5.1)
>>> can be a deep copy which also copies the data in memory use
a.copy() as in the following example
>>> a=np.linspace(1,5,5)
>>> c=a.copy()
```



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
- vO and a are global variables, which must be initialized before s(t) is called

Functions can have multiple arguments

vO 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
>>> r = f(3)

>>> print r

(4, 5, 6)

>>> type(r)

<type 'tuple'>

>>> print r[1]
                      # What type of object is r?
```

Tuples are constant lists (cannot be changed)

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!

A more general mathematical formula (part 1)

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):

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

which gives

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

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

Basic if-else tests

An if test has the structure

```
<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

```
if condition1:
<statements when condition1 is False and condition2 is True>
elif condition3:
    <statements when condition1 and condition 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

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

reads

```
def s_func(t, v0, a0, t1):
```

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 = mp.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

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

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:

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?

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()

>>> line = 'v0 = 5.3' >>> variable, value = line.split('=') >>> variable '5.3' >>> variable '5.3' >>> variable.strip() # strip away blanks 'v0' Note: must convert value to float before we can compute with the value!

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 = eval('[-1, 8, 10, 11]') >>> obj2 = eval('[-1, 8, 10, 11]') >>> obj3 = eval('[-1, 8, 10, 11]') >>> from math import sin, pi >>> x = 1 >>> obj3 = eval('sin(pi*x)') >>> obj3, type(obj3) (1.224 64 67 991 47 36 52 e-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!

```
Demo:

Terminal> python calc.py "1 + 0.5*2"
2.0
Terminal> python calc.py "sin(pi*2.5) + exp(-4)"
1.018315638887342

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', 'v')
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))
```

import numpy as np # Make two-dimensional array of [t, s(t)] values in each row data = np. array(it_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 1.0350 0.60 1.2360 0.61 1.2360 0.61 1.2360 0.61 1.2360 0.61 1.2360 0.61 1.2360 0.61 1.2360 0.62 0.236 0.360 0

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

Tridiagonal and sparse matrices

- SciPy offers a 2-D sparse matrix package for numeric data.
- The 'spdiags' function scipy.sparse.spdiags may be used to construct a sparse matrix
- Note that all the diagonals may 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

An example are given below for a tri-diagonal matrix:

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
- __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!

- self must always be the first argument
- self is never used in calls
- 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 z:

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

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(v 0=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 $f(x, y, z; p_1, p_2, ..., p_n)$

- ullet 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
```