Chapter 2

Python Programming for Physicists

Soon-Hyung Yook

March 31, 2017

Table of Contents I

1. Getting Started
2. Basic Programming
   - Variables and Assignments
   - Variable Types
   - Output and Input Statements
   - Arithmetic
   - Functions, Packages, and Modules
   - Built-in Functions
   - Comment Statements
3. Controlling Programs with "if" and "while"
   - The "if" statement
   - The "while" statement
   - Break and Continue
4. Lists and Arrays
   - Lists
   - Arrays
   - Reading an Array from a File

Table of Contents II

- Arithmetic with Arrays
- Slicing

5 User-Defined Function

Why Python?

- easy to learn
- simple to use
- enormously powerful

We will only focus on the core structure of the language for computational physics. More details are easily found from on-line documents or many text book for python.

- e.g. www.python.org

Getting Started

Code

A python program consists of a list of instructions, resembling a mixture of English words and mathematics. The *list of instructions* are collectively referred to as code.

Development Environment

When you are programming, you typically work in a window or windows on your computer screen that show the program you are working on and allow you to enter or edit lines of code. Such window or windows are usually called as *development environment*. One popular development environment for python is IDLE.(But I will not use it in this class.)

Python Version

Check the python version by typing:

```
python --version
```

Python Shell

Just type

```
python3
```

then it will show some text like:

```
Python 3.5.2 (default, Sep 14 2016, 11:28:32)
[GCC 6.2.1 20160901 (Red Hat 6.2.1-1)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

The symbol “>>>” is a prompt.

First Program

- Open any text editor and type the following two-line program into the editor:

```
x=1
print(x)
```

- Save the python program as "example.py" (The name of python program must end with ".py".)
- Run the following command:

```
python3 example.py
```

- Also you can do the same thing in python shell.
- There are some other ways to do the same thing.

What is the program?

- instruction $\Longleftrightarrow$ statement
- A program is a list of statements, which the computer usually executes in the order they appear in the program.

Variables and Assignments

- Quantities on interest in a program are represented by variables.
- Variables can be numbers, sets of numbers, etc.
- Variables roughly do the same role as in ordinary algebra.
- Our first example

  `x=1`

  is an assignment statement.
- In normal algebra the variable names are usually just a single letter like x.
- In many programming languages, the variable names can have two, three, or more letters.

  `Physics_101, energy, x, y, z, t`

  are examples of allowed variables.

  `4Scores&7Years`

  is an example, which is NOT allowed as a variable name, because of &.
- In python, variable name is case sensitive.
- Naming the variable is very important!

Variable Types

- Integer
- Float
- Complex: `1.2+0.6j` Note that we use `j` for imaginary number!
- String

The type of a variable is set by the value that we give it.

How to change the variable type

```
x=1
type(x)
x=1.5
type(x)
```

- Changing the variable type in a single program is not recommended.
- Good programming style: use a variable to store only one type of quantity in a given problem

see also "`x=float(1)`"(assign a floating point value to `x`), "`x=complex(1.5)`".

Variable Types

String

```
x="This is a string"
x="1.234"
```

How to change a string into a number?

```
x="1.234"
y=float(x)
```

Location of the space: "`x = 1`" is the same with "`x=1`".
Space at the beginning of the line: function, loop

Output Statement

"print" statement

```
x=1
print(x)
```

Another example:

```
x=1
y=2
print(x,y)
```

One can also use like this:

```
x=1
y=2
print("This value of x is",x,"and the value of y is",y)
```

With different types of variables and with option "sep":

```
x=1
z=1+3j
print(x,z,sep="...")
```

Input Statement

"input" statement

```
x=input("Enter the value of x: ")
```

When the computer executes the statement it does three things:

1. It prints out the quantity, if any, inside the parentheses.
2. It waits for the user to type a value on the keyboard.
3. Then the value that the user types is assigned to the variable "x".

Example

```
x=input("Enter the value of x:")
print("The value of x is",x)
type(x)
```

Note that "x" is a string.

Input Statement

Change the string into integer, float, or complex.

```
temp=input("Enter the value of x:")
x=float(temp)
print("The value of x is",x)
type(x)
```

or more concisely:

```
x=float(input("Enter the value of x:"))
print("The value of x is",x)
type(x)
```

Try also this:

```
Enter the value of x: Hello
ValueError: invalid literal for float(): Hello
```

Arithmetic: Operators

Important Operators for Numerical Calculations

```
x=y     assgin y to x
x+y     addition
x-y     subtraction
x*y     multiplication
x/y     division
x**y    rasing x to the power of y
```

Additional Operators for Numerical Calculations

```
x//y    the integer part of x divided by y (rounded down)
x%y     modulo (can be used for float, but not for complex numbers)
```

Another Expressions for Operators

```
x+=y    same with x=x+y
x-=y    same with x=x-y
x*=y    same with x=x*y
x/=y    same with x=x/y
x//=y   same with x=x//y
```

Operators

Comparison Operators

```
x==y
x!=y
x<y
x<=y
x>y
x>=y
in...   membership
```

Logical Operators

```
x and y
x or y
x not y
```

Operators

Bitwise Operators

```
x|y    Bitwise OR
x&y    Bitwise AND
x^y    Bitwise XOR
x>>y   shift the bits of integer x rightwards y places
x<<y   shift the bits of integer x leftwards y places
```

More on the assignment operator

x,y=1, 2.5 x,y=y,x

Example and Exercises in the book!

Packages, Modules, Functions

Packages

collections of related useful things

- Each package has its own name:
  - e.g. `math` package

Modules

- Some large packages are for convenience split into smaller subpackages
- Such subpackages are usually called as modules.
- A module in a larger package is referred to as

  `packagename.modulename`

Function

- Something like a black box.
- Similar to the mathematical function.

Mathematical Functions

Example of mathematical functions

```
log()
log10()
exp()
sin(),cos(),tan()
asin(),acos(),atan()
sinh(),cosh(),tanh()
sqrt
```

Usage I

```
import math    # import the math package
y=math.sin(math.pi)
```

Usage II

```
from math import log   # import log function from the math package
y=log(28.0)
```

Mathematical Functions

Usage III

```
from math import log,pi,sin   # import log, sin,pi from the math package

from math import *    # import everything in the math package
```

Import from module

```
import numpy.linalg   # import numpy.linalg module

from numpy.linalg import inv    # import inv function in the numpy.linalg module
```

See Example 2.2

Built-in Functions

Built-in Functions

- There are some functions in python which do not come from any package.
- These functions are always available in every program.
- No need to import them.

Examples:

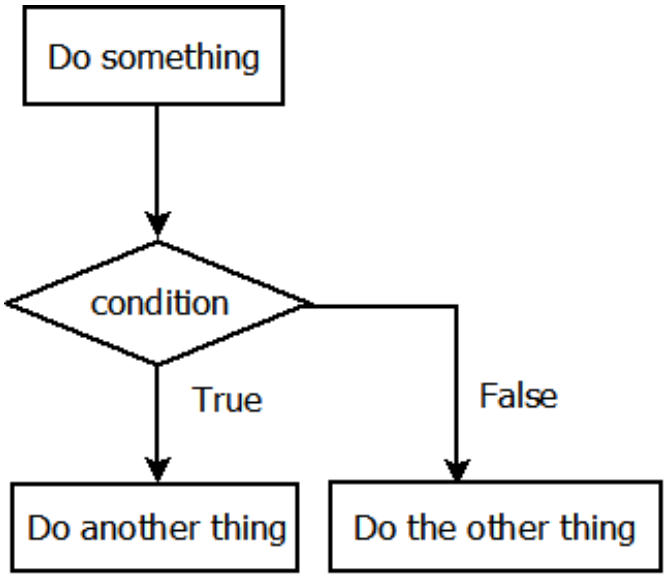
```
x=float(1)
x=input("Enter the value of x: ")
print(x)
...
```

Exercises in the textbook.

Comments

Comment starts with hash mark "#".

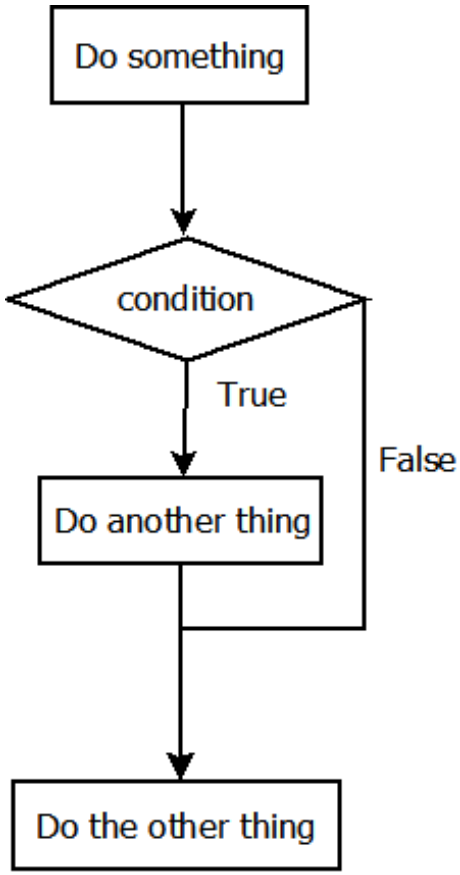
The if statement



Example:

```
x=int(input("Enter the value x= "))
if x>10:
  print("x>10")
else:
  print("x<10")
```

The if statement



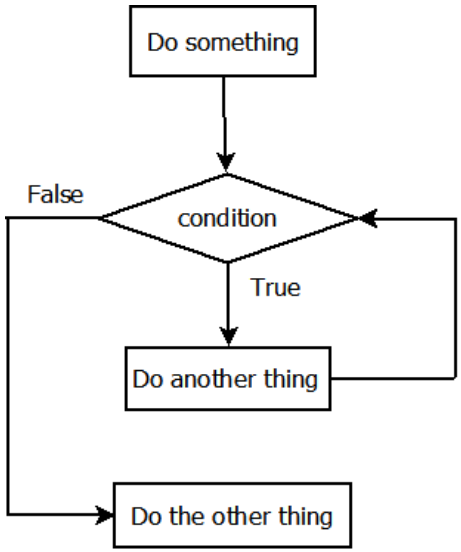
Example:

```
x=int(input("Enter the value smaller than 10: "))
if x>10:
  print("Your number is greater than 10")
  print("I will fix your number.")
  x=5
print("x=",x)
```

The if statement: more elaborate example

```
if x>10:
  print("Your number is greater than 10")
elif x>9:
  print("Your number is OK, but you're cutting it close.")
else:
   print("Your number is fine.")
```

While



Example:

```
x=int(input("Enter the value smaller than 10: "))
while x>10:
  print("Your number is greater than 10")
  x=int(input("Enter the value smaller than 10: "))
print("x=",x)
```

Break and continue

Stop the loop.

```
while x>10:
  print("the number is larger than 10. Please try again")
  x=int(input("x="))
  if x==100:   # nested loop
    break
```

- `continue`: If there is `continue` in a loop will make the program skip the rest of the indented code in the loop and goes back to the beginning of the loop.
- The continue statement is used rather rarely in practice.

Example 2.4: Fibonacci sequence

Lists and Arrays

- In physics, we frequently use collectively a set of numbers $A = \{a_i\}$.
- Examples are a vector, matrix, and so on.
- Python provides standard features, called containers, for storing collections of numbers.
- **list, array**, dictionary, tuple, set

Lists

- List is the most basic type of container in python.
- List is a list of quantities.
- The quantities can be any type of data: integers, floats, strings, and so on.

elements

- The quantities in a list.
- Do not have to be all of the same type.
- However, in most of the cases, we will deal with the elements with the same type.

Usage

```
r=[1,1,2,3,5,8.13,21]
print(r)
```

Lists

Usage II

```
x=1.0
y=1.4
z=-3.1
r=[x,y,z]
print(r)
```

NOTE: The vale of `x` is changed later in the program the value of `r` will change as well.

Change the value of element

```
r=[1.0,1.5,-2.2]
r[1]=3.2
print(r)
```

Note: The index for the elements starts from zero.

Lists

Built-in Function related to list

```
sum, max, min, len

r=[1.0,1.5,-2.2]
total=sum(r)
mean=sum(r)/len(r)
print(total)
print(mean)
```

map

- a kind of meta-function
- map creates a specialized object in the computer memory, called an iterator

```
from math import log
r=[1.0,1.5,-2.2]
logr=list(map(log,r))
print(logr)
```

Lists

append

Add a new element to the end of the list.

```
r.append(2.3)
```

del

Delete an element by offset.

```
del r[-1]
```

- The negative index counts backward from the end of the list.
- `del` is not a list method (OOP), but it is a python *statement*.

Lists

Create an empty list

```
r=[]
r.append(1.0)
r.append(1.4)
r.append(-3.2)
print(r)
```

pop method

Remove a value from the end of a list.

```
r=[1.0,1.5,-2.2,2.6]
r.pop()
print(r)
```

- `r.pop()` is the same as `r.pop(-1)`
- pop method is similar to the python statement `del`.
- `r.pop(0)` removes the first item from the list.

Arrays

Difference between lists and arrays:

1. The number of elements in an array is fixed. (One can not add or remove the elements of array.)
2. The elements of an array must all be of the same type.
3. Arrays can be two-dimensional, like matrices in algebra.
   - Contradiction: List of list is also possible:

```
a=[[1,2,3],[3,4,5],[6,3,2]]
print(a[0][1])
```

4. Arrays behave roughly like vectors or matrices.(One can do some arithmetic like adding them together, etc. But lists give some error message or unexpected(?) results.)
5. Arrays work faster than lists.
6. `numpy` package supports the array.

Arrays

Create one-dimensional array with n elements

All elements are initially equal to zero.

```
from numpy import zeros
a=zeros(4,float)
print(a)
```

Create two-dimensional array with n elements

All elements are initially equal to zero.

```
from numpy import zeros
a=zeros([3,4],float)
print(a)
```

Note that the first arguments of `zeros` in this case is itself a list.
similar function with `zeros`: `ones`

Arrays

Create one-dimensional empty array with n elements

```
from numpy import empty
a=empty(4,float)
print(a)
```

Faster than zeros or ones.

Covert list into array

```
from numpy import array
r=[1.0,1.5,-2.2]
a=array(r,float)
print(a)
```

or

```
from numpy import array
a=array([1.0,1.5,-2.2],float)
print(a)
```

Arrays

Covert list of list into $2-D$ array

```
from numpy import array
a=array([[1,2,3],[4,5,6]],float)
print(a)
```

Index of $2-D$ array

```
from numpy import zeros
a=zeros([2,2],float)
a[0,1]=1
a[1,0]=-1
print(a)
```

Reading an Array from a File

Use `loadtxt` function from the `numpy` package.

`loadtxt`

for any dimension of data!

```
from numpy import loadtxt
a=loadtxt("values.txt",float)
print(a)
```

Arithmetic with Arrays

- As with lists, the individual elements of the list (array) behave like ordinary variables.
- One can do arithmetic with entire arrays at once!

Simple example

```
from numpy import array
a=array([1,2,3,4],int)
b=2*a
print(b)
c=a+b
print(c)
print(a+1)
print(a*b)   # not a dot product!
print(dot(a,b))
```

Matrix multiplication (and multiplication of column vector to a matrix) can be obtained by the dot function (see the example in the book).

Functions for Arrays

- Built-in functions `sum`, `max`, `min`, `len`, `map` can be applied to array as well.

Simple example

```
b=array(list(map(sqrt,a)),float)
```

`size`, `shape` methods

```
a=array([[1,2,3],[4,5,6]], int)
print(a.size)
print(a.shape)   # the results is tuple
```

See also the examples in the book.

Warning for Arrays

- For array, if we use b=a, then the python does not make a new array n.
- The direct assignment of array a to new variable b results that the b also refer the same array of numbers with a, stored somewhere in the memory.

Simple example

```
from numpy import array
a=array([1,1],int)
b=a
a[0]=2
print(a)
print(b)
```

Warning for Arrays

copy function

To make a copy of array a use copy function

```
from numpy import copy,array
a=array([1,1],int)
b=copy(a)
a[0]=2
print(a)
print(b)
```

Slicing I

Slicing for lists

- Slicing works with both arrays and lists.
- Let `r` is a list.
- Then `r[m:n]` is another list composed of a subset of the elements of `r`.
- Starting with m and going up to but not including element n.

```
r=[1,3,5,7.9,11,13,15]
s=r[2:5]
print(s)
```

Slicing: variants

- `r[2:]`: all elements of the list from elements 2 up to the end of the list.
- `r[:5]`: all elements from the start of the list up to, but not including, element 5.
- `r[:]`: entire list.

Slicing II

Slicing for arrays

```
from numpy import array
a=array([2,4,6,8,10,12,14,16],int)
b=a[3:6]
print(b)
```

also `a[3:]`, `a[:7]`, `a[:]` work for the array.

Slicing for two-dimensional arrays

- `a[2,3:6]`: one-dimensional array with three elements equals to `a[2,3]`, `a[2,4]`, `a[2,5]`.
- `a[2:4,3:6]`: two dimensional array of size 2×3 with values drawn from the appropriate subblock of a, starting at `a[2,3]`.
- `a[2,:]`: the whole of row 2 of array a.
- `a[:,3]`: the whole of column 3 of array a.

for loops I

for loops

```
r=[1,3,5,7.9,11,13,15]
for n in r:
  print(n)
  print(n*2)
print("Finished")
```

range function

- range(5): generate a list [0,1,2,3,4]
- range(2,8): generate a list [2,3,4,5,6,7]
- range(2,20,3): generate a list [2,5,8,11,14,17]
- range(20,2,-3): generate a list [20,17,14,11,8,5]

Arguments of range should be integers.

for loops II

for loop with function range

```
for n in range(5):
  print(n**2)

for n in range(1,11):
print(2**n)
```

arange function from numpy package

- arange(1,8,2): generate an array [1,3,5,7]
- arange(1.0,8.0.2.0): generate an array [1.0,3.0,5.0,7.0]
- arange(2.0,2.8,0.2): generate an array [2.0,2.2,2.4,2.6]

arange function can be also used with for loops.

for loops III

`linspace` function from `numpy` package

- `linspace(2.0,8.0,5)`: divides the interval from 2.0 to 2.8 into 5 values, creating an array `[2.0,2.2,2.4,2.6,2.8]`
- `linspace(2.0,2.8,3)`: generate a list `[2.0,2.4,2.8]`
- `linspace` includes the last point in the range.

`linspace` function can be also used with `for` loops.

See the Examples in the textbook.
For loops and the `sum` function give us two different ways to compute sums of quantities.
For loops are in general more flexible and faster than the array operation.

User-Defined Function I

Simple Structure

```
def function_name(argument1, ...):
  do something
  return x
```

Example: Factorial

```
def factorial(n):
  f=1.0
  for k in range(1,n+1):
    f*=k
  return k

 a=factorial(10)
```

User-Defined Function II

Local variables

In the above example, `f`,`k` are local variables.
But if some variables are defined outside the function, those variables can be referred in the function.⇒ Solution: Use the different files.

Function can return a List

```
from math import cos, sin, pi
def cartesian(r,theta):
  x=r*cos(theta)
  y=r*sin(theta)
  position=[x,y]
  return position     # or equivalently return [x,y]

position_1=cartesian(10.2,pi/4.0)
```

User-Defined Function III

Function can return an Array

```
from math import cos, sin, pi
from numpy import arrray

def cartesian(r,theta):
  x=r*cos(theta)
  y=r*sin(theta)
  return array([x,y],float)

position=cartesian(10.2,pi/4.0)
```

User-Defined Function IV

Function can return two values

```
from math import cos, sin, pi
from numpy import arrray

def cartesian(r,theta):
x=r*cos(theta)
y=r*sin(theta)
return x,y

rx,ry=cartesian(10.2,pi/4.0)
```

User-Defined Function with map

```
def f(x):
  return 2*x-1

newlist=list(map(f,oldlist))
```

User-Defined Function V

User-Defined Function in a Different File

```
from mydefinitions import myfunction
```

See the examples and exercises:
Read also the rest of the chapter for good programming style.