

Scientific Programming

Practical 4

Introduction

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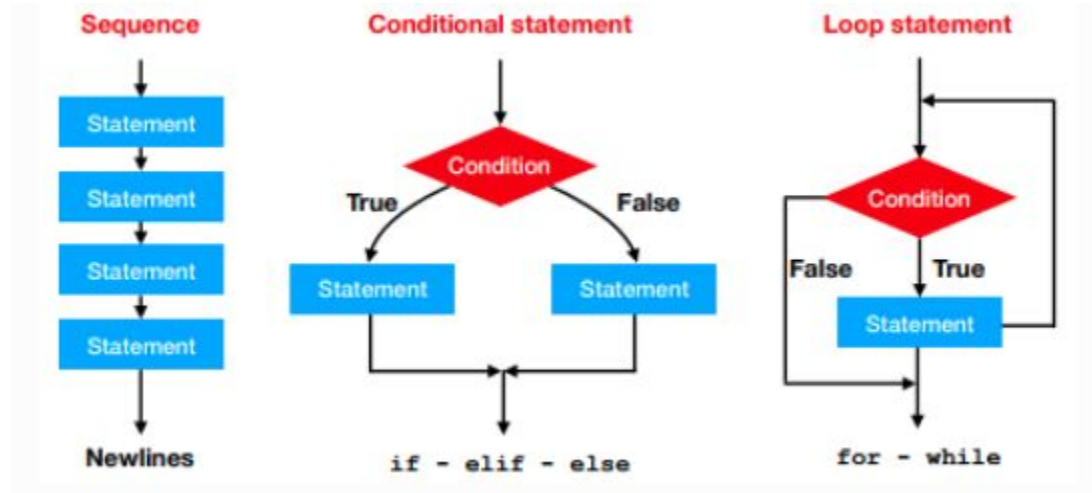
Execution flow

Three types:

Sequential

Conditional branch

Loop



If statement - basic

```
if condition :  
    #This is the True branch  
    #do something  
  
else:  
    #This is the False branch (or else branch)  
    #do something else
```

Indentation is important in python!

If statement - basic

Example: Let's get an integer from the user and test if it is even or odd, printing the result to the screen.

```
print("Dear user give me an integer:")
num = int(input())
res = ""
if num % 2 == 0:
    #The number is even
    res = "even"
else:
    #The number is odd
    res = "odd"

print("Number ", num, " is ", res)
```

```
Dear user give me an integer:
3
Number 3 is odd
```

If - elif - else

```
if condition :  
    #This is branch 1  
    #do something  
  
elif condition1 :  
    #This is branch 2  
    #do something  
  
elif condition2 :  
    #This is branch 3  
    #do something  
  
else:  
    #else branch. Executed if all other conditions are false  
    #do something else
```

Note that **branch 1** is executed if condition is **True**, **branch 2** if and only if **branch 1** is **False** and **branch 1** is **True**, **branch 3** if condition is **False**, **condition 1** is **False** and **condition2** is **True**. If all conditions are **False** the **else** branch is executed.

If - elif - else

Example: The tax rate of a salary depends on the income. If the income is < 10000 euros, no tax is due, if the income is between 10000 euros and 20000 the tax rate is 25%, if between 20000 and 45000 it is 35% otherwise it is 40%. What is the tax due by a person earning 35000 euros per year?

```
income = 35000
rate = 0.0

if income < 10000:
    rate = 0
elif income < 20000:
    rate = 0.2
elif income < 45000:
    rate = 0.35
else:
    rate = 0.4

tax = income*rate

print("The tax due is ", tax, " euros (i.e ", rate*100, "%)")
```

The tax due is 12250.0 euros (i.e 35.0 %)

Spot the difference!

#Example 1

```
val = 10
```

```
if val > 5:  
    print("Value >5")  
elif val > 5:  
    print("I said value is >5!")  
else:  
    print("Value is <= 5")
```

#Example 2

```
val = 10
```

```
if(val > 5):  
    print("\n\nValue is >5")  
  
if(val > 5):  
    print("I said Value is >5!!!")
```

Spot the difference!

#Example 1

```
val = 10
```

```
if val > 5:  
    print("Value >5")  
elif val > 5:  
    print("I said value is >5!")  
else:  
    print("Value is <= 5")
```

Output:

Value >5

#Example 2

```
val = 10
```

```
if(val > 5):  
    print("\n\nValue is >5")  
  
if(val > 5):  
    print("I said Value is >5!!!")
```

Output:

Value is >5
I said Value is >5!!!

For loops

```
for elem in collection :  
    #OK, do something with elem  
    # instruction 1  
    # instruction 2
```

Depending on the type of the collection `elem` will get different values. Recall from the lecture that:

<code>str</code>	<code>for</code> iterates over the characters
<code>list</code>	<code>for</code> iterates over the elements
<code>tuple</code>	<code>for</code> iterates over the elements
<code>dict</code>	<code>for</code> iterates over the keys

For loops

```
S = "Hi there from python"
Slist = S.split(" ")
Stuple = ("Hi","there","from","python")
print("String:", S)
print("List:", Slist)
print("Tuple:", Stuple)

#for loop on string
print("On strings:")
for c in S:
    print(c)

print("\nOn lists:")
#for loop on list
for item in Slist:
    print(item)

print("\nOn tuples:")
#for loop on list
for item in Stuple:
    print(item)
```

```
String: Hi there from python
List: ['Hi', 'there', 'from', 'python']
Tuple: ('Hi', 'there', 'from', 'python')
On strings:
H
i

t
h
e
r
e

f
r
o
m

p
y
t
h
o
n

On lists:
Hi
there
from
python

On tuples:
Hi
there
from
python
```

Looping over a range

Remember:

S included,
E excluded!

```
range(E)          # ranges from 0 to E-1
range(S,E)        # ranges from S to E-1
range(S,E,step)   # ranges from S to E-1 with +step jumps
```

Example: Given a list of integers, return a list with all the even numbers.

```
myList = [1, 7, 9, 121, 77, 82]
onlyEven = []

for i in range(0, len(myList)): #this is equivalent to range(len(myList)):
    if( myList[i] % 2 == 0 ):
        onlyEven.append(myList[i])

print("original list:", myList)
print("only even numbers:", onlyEven)
```

```
original list: [1, 7, 9, 121, 77, 82]
only even numbers: [82]
```

Looping over a range

Example: Let's consider the two DNA strings `s1 = "ATACATATAGGGCCAATTATTATAAGTCAC"` and `s2 = "CGCCACTTAAGCGCCCTGTATTAAAGTCGC"` that have the same length. Let's create a third string `out` such that `out[i]` is `"|"` if `s1[i] == s2[i]`, `" "` otherwise.

```
s1 = "ATACATATAGGGCCAATTATTATAAGTCAC"
s2 = "CGCCACTTAAGCGCCCTGTATTAAAGTCGC"

outSTR = ""
for i in range(len(s1)):
    if(s1[i] == s2[i]):
        outSTR = outSTR + "|"
    else:
        outSTR = outSTR + " "

print(s1)
print(outSTR)
print(s2)
```

```
ATACATATAGGGCCAATTATTATAAGTCAC
  ||  ||  |  |  |  |  ||||  |
CGCCACTTAAGCGCCCTGTATTAAAGTCGC
```

Nested for loops

It is possible to place
one for loop into
another one

```
for i in collection:  
    for j in another_collection:  
        #do some stuff with i and j
```

Nested for loops

Given the matrix $\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$ stored as a list of lists (i.e. `matrix = [[1, 2, 3], [4, 5, 6], [7, 8, 9]]`).

Print it out as:

1	2	3
4	5	6
7	8	9

```
matrix = [[1, 2, 3], [4, 5, 6], [7, 8, 9]]

for i in range(len(matrix)):
    line = ""
    for j in range(len(matrix[i])):
        line = line + str(matrix[i][j]) + " " #note int --> str conversion!
    print(line)
```

```
1 2 3
4 5 6
7 8 9
```

While loops

Useful to loop until a
specific condition is
True

```
while (condition):  
  
    #do something  
    #update the value of condition
```

Print the numbers from 0 to 4

Anything wrong with
this?

```
i = 0  
while (i < 5):  
    print("i now is:", i)  
    i = i + 1 #THIS IS VERY IMPORTANT!  
  
i now is: 0  
i now is: 1  
i now is: 2  
i now is: 3  
i now is: 4
```

Note: The loop will continue until *condition* holds true and the only code executed is the block defined through the indentation. This block of code must update the value of condition otherwise the interpreter will get stuck in the loop and will never exit.

Nesting while and for loops

```
for i in range(1,10):  
    j = 1  
    output = ""  
    while(j<= i):  
        output = str(j) + " " + output  
        j = j + 1  
    print(output)  
  
# or without string output  
# for i in range(1,10):  
#     j = 1  
#     while(j<=i):  
#         print(j, end = " ")  
#         j = j + 1  
#     print("")
```

```
1  
2 1  
3 2 1  
4 3 2 1  
5 4 3 2 1  
6 5 4 3 2 1  
7 6 5 4 3 2 1  
8 7 6 5 4 3 2 1  
9 8 7 6 5 4 3 2 1
```

Let's print the following picture to std out

```
1  
2 1  
3 2 1  
4 3 2 1  
5 4 3 2 1  
6 5 4 3 2 1  
7 6 5 4 3 2 1  
8 7 6 5 4 3 2 1  
9 8 7 6 5 4 3 2 1
```


<http://qcbsciprolab.readthedocs.io/en/latest/practical4.html>

Exercises

1. Write a python script that creates the following pattern:

```
+
++
+++
++++
+++++
++++++
+++++++ <-- 7
+++++++
+++++++
+++++
+++
++
+
```

Show/Hide Solution

2. Count how many of the first 100 integers are divisible by 2, 3, 5, 7 but not by 10 and print these counts. Be aware that a number can be divisible by more than one of these numbers (e.g. 6) and therefore it must be counted as divisible by 2 and 3.

Show/Hide Solution

3. Write a Python script that reverse-complements a string of DNA. To reverse-complement a string of DNA, one needs to replace and A with T, T with A, C with G and G with C, while any other character is complemented in N. Finally, reverse the sequence (e.g. the first base becomes the last). Example: ATCG becomes CGAT. Apply the code to the string:
"GATTACATATATCAGTACAGATATATACGCGCGGGCTTACTATTAAAAACCCC"