SEE1002 Introduction to Computing for Energy and Environment

Part 2: Elements of Python programming

Sec. 4: Repeating tasks 1: Loops

Course Outline

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Part 2: Elements of Python programming

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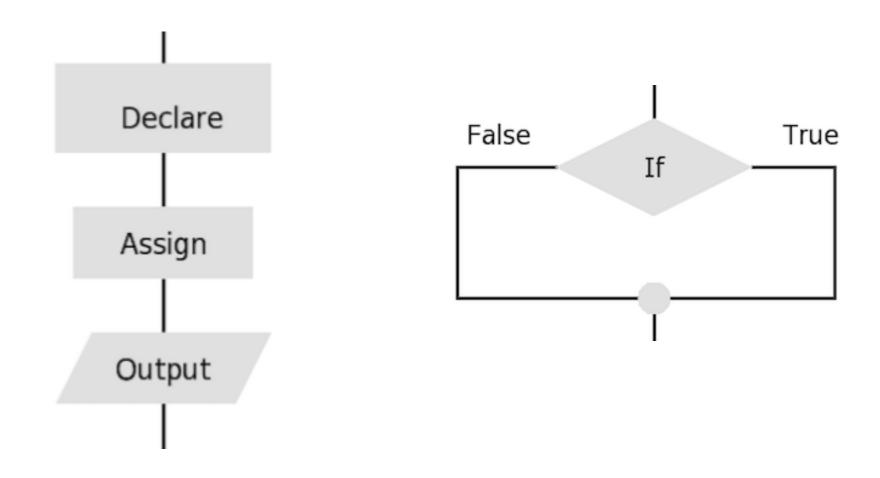
Outline

- I. Motivation
- 2. while loop
- 3. for loop

I. Motivation

Recap

We have been introduced to two basic types of program flow:



Linear flow

Branching

Limitations

- We can get pretty far with what we've learned so far.
- But it will take us a lot of work to solve all but the simplest problems!
- This is because we yet to introduce a method for repeating tasks.

Example 1: manual counting

How would you write a program to print integers from I to 3? How would your approach change if you had to consider I to 20? I to 1000000?

Repeating tasks efficiently

- Most problems solved on a computer differ a lot from the sort of problems we've examined so far.
- Generally the computer spends most of its time carrying out the same set of tasks. Remember that computers are good at doing things quickly and accurately!
- By contrast humans are error prone. So we want to write simple programs that allow computers to do what they're good at.
- We need an efficient way of repeating tasks. The easiest way is with a loop.

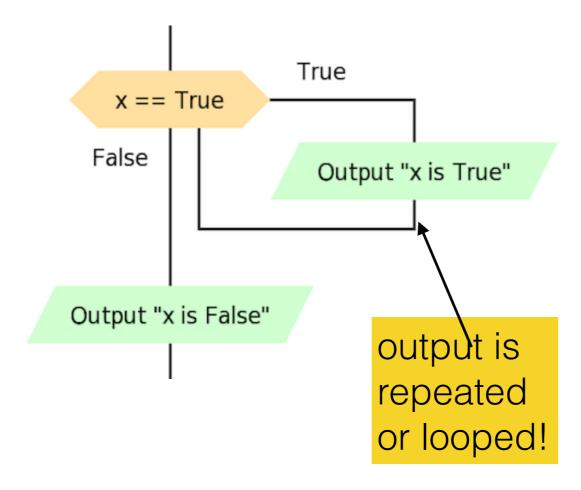
2. while loop

Motivation

- The simplest way of repeating a task is to keep doing the same thing until the situation changes (i.e. while a certain condition holds)
- Examples
 - Keep going straight until you reach the corner.
 - Boil the pasta until it becomes tender
 - Apply for a job until you're hired

<u>Overview</u>

The while loop executes a series of statements while a condition is true.



```
x=True
while x==True:
    print('x is True')
else:
    print('x is False')
```

Flowgorithm

Python

Syntax of the while statement

More precisely, the while statement has the following syntax:

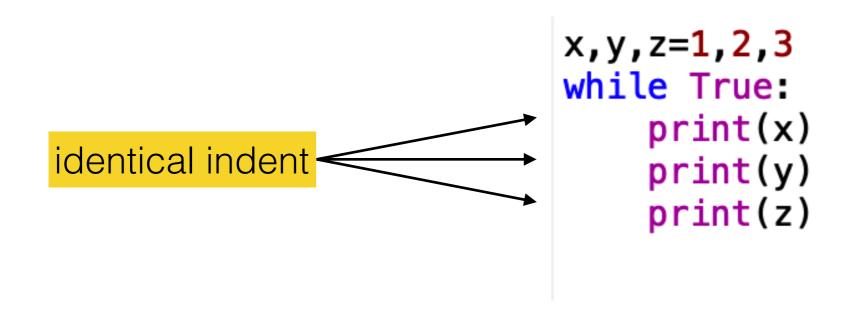
```
while <expression>:
    statement 1.1
    [...] executed if expression==True
else:
    statement 2.1
    [...]
    executed if expression==False
```

Comments on the syntax

- The syntax is essentially identical to that of if-else.
 So the same rules need to be observed:
 - I. Colon follows while and else
 - 2. The statements to be executed following while and else must be indented by the same amount (typically 4 spaces).
- If these rules are not followed, the program will not behave as expected:

Multiple statements

- As with if-else, multiple statements can be executed for the true and false conditions.
- Statements that are executed sequentially must be indented by the same amount.



Types of while loops

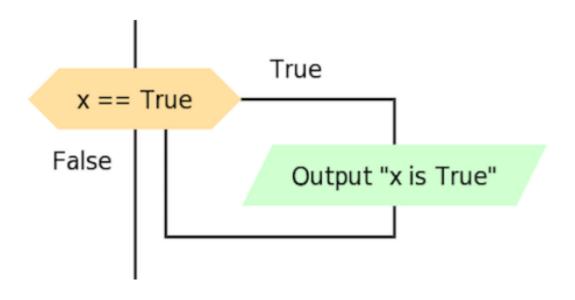
There are essentially 3 different types of while loops:

- i. infinite loop
- II. finite loop
- III. loop over index

i. Infinite loop

- An infinite loop is constructed using a condition that's always true.
- The only way to get out of a infinite loop is to hit control-c or the stop button.
- An infinite loop is one of the first things learned by any programming student. But its practical applications are fairly limited.

<u>Implementation</u>



```
x=True
while x==True:
    print( 'x is True' )
x is True
```

x is True

Example 2: infinite loop with multiple statements

Consider this Python program. What do you think it does?

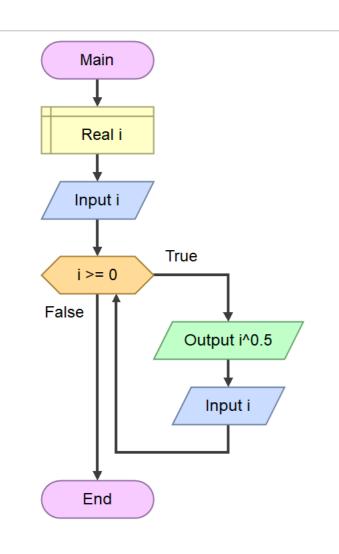
```
x=1
y=2
z=3
while True:
    print(x)
    print(y)
    print(z)
```

ii. Finite loop

- A much more useful while loop is one in which the test condition isn't always true.
- Hence the loop only runs for a finite number of times.
- This is the most common use of the while loop.
 One often wants to continue testing a condition until it has changed.

<u>Implementation</u>

Typically we stop looping once a condition is met.

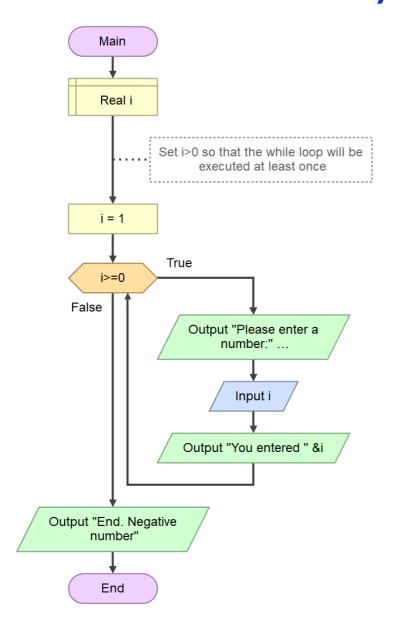


```
i=float(input('please enter a number: '))
while i >=0:
    print(i**0.5)
    i=float(input('please enter a number: '))
```

The program exits the loop once a negative number is input, i.e., the loop is finite

Repeated testing

The most common finite loop is the one we just saw, in which we repeatedly test for a condition. To save typing, we can use an arbitrary value for the first test.



```
i=1 # positive value to get inside loop
 while i \ge 0:
      i=float(input('Please enter a number: '))
      print('You entered', i)
 print( 'End. Negative number' )
Please enter a number: 4.3
You entered 4.3
Please enter a number: -1.2
You entered -1.2
End. Negative number
```

Alternative version

We can rewrite our program using an else block to highlight what happens when a negative number is input. Both versions are equivalent.

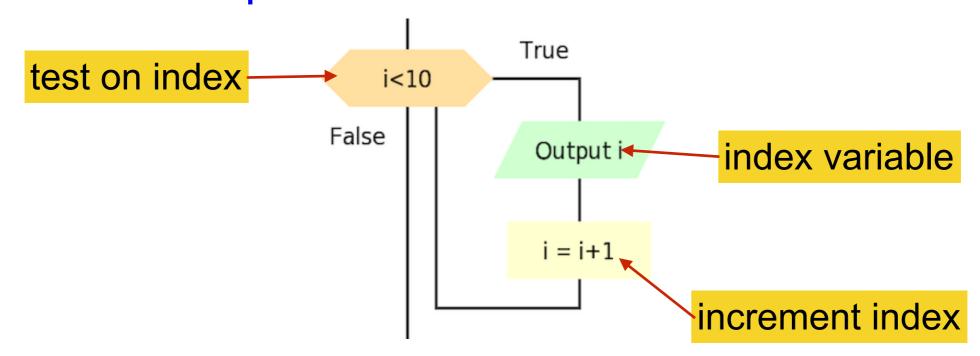
```
i=1 # positive value to get inside loop
while i >= 0:
    i=float(input('Please enter a number: '))
    print('You entered', i)
print( 'End. Negative number' )

i=1 # positive value to get inside loop
while i >= 0:
    i=float(input('Please enter a number: '))
    print('You entered', i)
else: # exit loop for negative number
    print( 'End. Negative number' )
```

iii. Loop over index

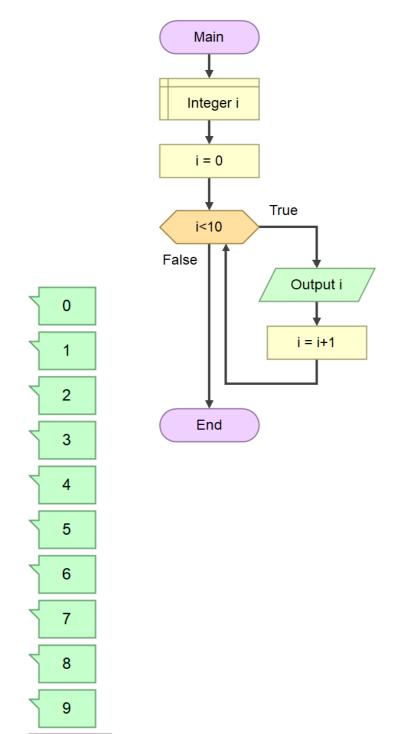
Instead of repeated testing, we can perform a specified number of loops. To this we need to count the number of loops using an index or counter variable.

- The index variable defines the condition under which the while loop is executed.
- The index variable must be increased or incremented inside the loop



Python implementation

The Python implementation exactly follows the Flowgorithm one almost identically.



```
i=0
while i<10:
    i = i + 1
    print( i )</pre>
```

```
1
2
3
4
5
6
7
8
9
10
```

Example 3: return on an investment

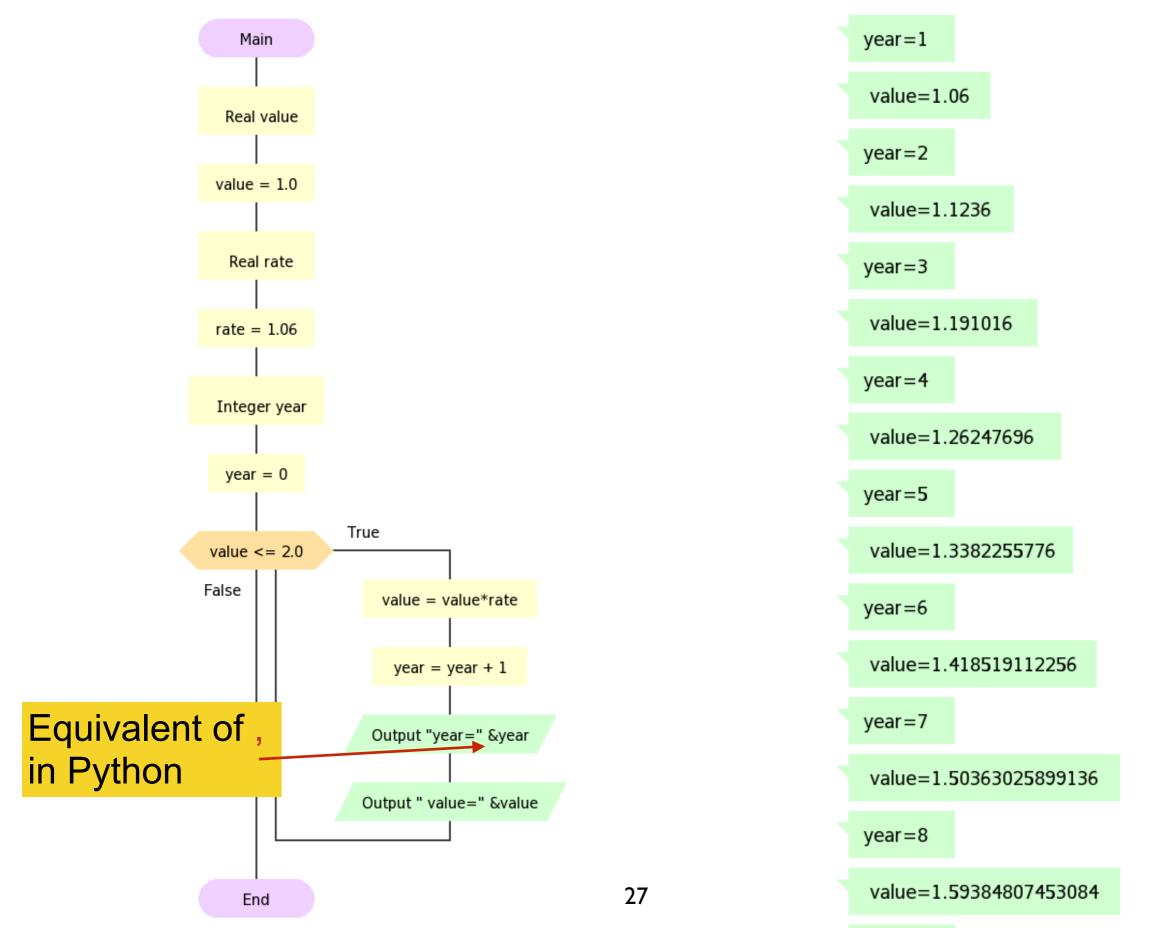
- There are simple formulas for calculating compound interest and the return on an investment, but let's pretend that we don't know them.
- Use a while loop to calculate the number of years required for an investment to more than double in value given an interest rate of 6%.
 Output the value of the investment after each year.
- We will use this example to illustrate various features of Python!

Example 3: approach

How do we use a while loop? Continue calculating the value of the investment so long as the value hasn't increased by more than a factor of 2. This is a finite loop in which we test on a condition.

- Needed variables:
 - value (current value of investment)
 - years (number of years elapsed)
- Needed constant
 - rate (interest rate +1)

Implementation in Flowgorithm



Basic Python solution

```
value = 1.0
rate = 1.06
year = 0

while value <= 2.0:
    value = value * rate
    year = year + 1
    print( 'year: ',year,'value:',value )
else:
    print( 'It takes',year,'years for the investment to double in value' )</pre>
Final output message
```

```
year: 1 value: 1.06
year: 2 value: 1.1236
year: 3 value: 1.191016
year: 4 value: 1.26247696
year: 5 value: 1.3382255776
year: 6 value: 1.41851911226
year: 7 value: 1.50363025899
year: 8 value: 1.59384807453
year: 9 value: 1.689478959
year: 10 value: 1.79084769654
year: 11 value: 1.89829855834
year: 12 value: 2.01219647184
It takes 12 years for the investment to double in value
```

Extensions

This is our first non-trivial example. It illustrates a few important Python topics:

- I. Initialisation of variables
- 2. Updating variables
- 3. Formatted output

Python solution

```
value = 1.0
rate = 1.06
year = 0

while value <= 2.0:
    value = value * rate
    year = year + 1
    print( 'year: ',year,'value:',value )
else:
    print( 'It takes',year,'years for the investment to double in value'</pre>
```

```
year: 1 value: 1.06
year: 2 value: 1.1236
year: 3 value: 1.191016
year: 4 value: 1.26247696
year: 5 value: 1.3362255776
year: 6 value: 1.41851911226
year: 7 value: 1.50363025899
year: 8 value: 1.59384807453
year: 9 value: 1.689478959
year: 10 value: 1.79084769654
year: 11 value: 1.89829855834
year: 12 value: 2.01219647184
It takes 12 years for the investment to double in value
```

i) Initialisation

- It's good programming practice to define one's variables at the beginning of the program.
- In Python we need to initialise the variables by assigning a value (often, though not always, 0). This must be done manually.
- In Flowgorithm the situation is different:
 - I. Declare variables.
 - 2. Assign values

These steps are combined in Python

Modification: undefined variable

```
value=1.0
rate=1.06

while value <= 2.0:
    value = value * rate
    year = year + 1
    print( 'year: ',year, 'value:',value )
else:
    print( 'It takes',year, 'years for the investment to double in value')</pre>
```

```
Sec2.4-Loops/code/interest-undefined.py", line 6,
    year = year + 1
NameError: name 'year' is not defined
```

Python tells us where the problem first appears, but not where year should be defined

Modification: incorrect initial value

```
rate = 1.0
rate = 2.06
year = 0

while value <= 2.0:
   value = value * rate
   year = year + 1
   print( 'year: ',year,'value:',value )
else:
   print( 'It takes',year,'years for the investment to double in value')</pre>
```

```
year: 1 value: 2.06
It takes 1 years for the investment to double in value
```

This is a bug rather than a (syntax) error. While the program still runs, the output is incorrect.

ii) Updating variables

- In science and engineering, many programs involve statements of the form x = x +increment or x = x*scale.
- This is sometimes referred to as an accumulator pattern.
- The interpretation is that we are updating a variable.
- Examples:
 - Position of an object as a function of time
 - Number of bacteria after a time interval

Assignment operators

We can abbreviate accumulator patterns using assignment operators:

```
x = x + step → x += step
x = x - step → x -= step
x = x * constant → x *= constant
x = x / constant → x /= constant
```

• As usual = refers to assignment not equality!

Modification: assignment operators

```
value=1.0
rate=1.06
year = 0

while value <= 2.0:
    value *= rate
    vear += 1
    print( 'year: ',year,'value:',value )
else:
    print( 'It takes',year,'years for the investment to double in value' )</pre>
```

```
year: 1 value: 1.06
year: 2 value: 1.1236
year: 3 value: 1.191016
year: 4 value: 1.26247696
year: 5 value: 1.3382255776
year: 6 value: 1.41851911226
year: 7 value: 1.50363025899
year: 8 value: 1.59384807453
year: 9 value: 1.689478959
year: 10 value: 1.79084769654
year: 11 value: 1.89829855834
year: 12 value: 2.01219647184
It takes 12 years for the investment to double in value
```

Results are unchanged.

iii) Formatting

The output of our program is a little messy.

- I. Python prints more digits than we need.
- 2. The output isn't nicely aligned.

We can correct these problems using formatted output.

Formatted output

 Up till now we've used this form of the print command:

```
print( string1, variable1, string2, variable, [...])
```

- Recall however the the general form of print:
 - print(<expression>)
- We can choose an expression that allows us to specify the precision of the output. In its simplest form:

```
print('[text1] {spec}'.format(X))
```

where spec specifies the format string or how the variable x is to be formatted.

Format strings

There there are many ways of specifying the format string. The general syntax is complicated. For now, let's consider some typical examples.

```
x=1.2345
y=2
z=3.1415
t='test'
print( 'x=',x ) # original
                                                                                x = 1.2345
print('x= {:.2f}'.format(x)) # 2 decimal places
                                                                                x = 1.23
print('x= {:.3f}, y={:d}'.format(x,y)) # 3 decimal places + integer
                                                                                x = 1.234, y = 2
print('x=\{1:.3f\}, z=\{0:.0f\}'.format(z,x)) # can specify position
                                                                                x = 1.234, z = 3
print('x= \{x0:.3f\}, z=\{z0:.0f\}'.format(x0=x,z0=z)) # named arguments
                                                                                x = 1.234, z = 3
print()
                                                                                text=test
print('text={:s}'.format(t)) # we can also print strings
```

Basic syntax

- I. The value of a variable is substituted inside { }.
- 2. By default, the variables are assigned to the matching braces in the order in which they appear inside . format().
- 3. Variables can be used in a different order by specifying the position with {n} where n is the order of the variable inside .format().
- 4. The datatype can be specified as {n:f}, {n:d}, {n:s} for float, ints and strings.
- 5. The number of decimal places can be specified as {n:.#f} where # is the number of digits.

Modification: formatted output

```
value=1.0
rate=1.06
year = 0
while value <= 2.0:
   value *= rate
   year += 1
    print( 'year: {:d}, value: {:.2f}'.format(year,value) )
else:
   print( 'It takes', year, 'years for the investment to double in value' )
  year: 1, value: 1.06
  year: 2, value: 1.12
  year: 3, value: 1.19
  year: 4, value: 1.26
                                   The output looks nicer! But
  year: 5, value: 1.34
  year: 6, value: 1.42
                                   it's not perfect
  year: 7, value: 1.50
  year: 8, value: 1.59
  year: 9, value: 1.69
  year: 10, value: 1.79
  year: 11, value: 1.90
  year: 12, value: 2.01
  It takes 12 years for the investment to double in value
```

Columns aren't aligned

Alignment

There are various ways of aligning the text.

- Specify the number of digits of output as {n:#d} where # is the number of digits. This ensures that the output has a fixed number of digits.
- 2. Add a tab character with \t. This is equivalent to using a tab stop in a word processor like Word.

Modification: padding

```
value=1.0
 rate=1.06
 year = 0
 while value <= 2.0:
     value *= rate
     vear += 1
     print( 'year: {:3d}, value: {:.2f}'.format(year,value) )
 else:
     print( 'It takes', year, 'years for the investment to double in value' )
       1, value: 1.06
year:
      2, value: 1.12
year:
      3, value: 1.19
year:
      4, value: 1.26
year:
                                     Columns are now aligned!
      5, value: 1.34
year:
      6, value: 1.42
year:
      7, value: 1.50
year:
      8, value: 1.59
year:
       9, value: 1.69
year:
year: 110, value: 1.79
      11, value: 1.90
vear:
      12, value: 2.01
It takes 12 years for the investment to double in value
```

Output is padded with extra blank spaces.

Modification: tab

```
value=1.0
 rate=1.06
year = 0
 while value <= 2.0:
    value *= rate
    year +=-1
    print( 'year: {:d}, \t value: {:.2f}'.format(year,value) )
 else:
    print( 'It takes', year, 'years for the investment to double in value' )
           value: 1.06
year: 1,
year: 2,
           value: 1.12
         value: 1.19
year: 3,
year: 4,
         value: 1.26
year: 5,
           value: 1.34
                                    Columns are now aligned!
year: 6,
         value: 1.42
year: 7, value: 1.50
year: 8, value: 1.59
         value: 1.69
year: 9,
year: 10, value: 1.79
year: 11,
           value: 1.90
           value: 2.01
year: 12,
It takes 12 Vears for the investment to double in value
   Output is shifted to
   the next 'tab stop'.
```

3. for loop

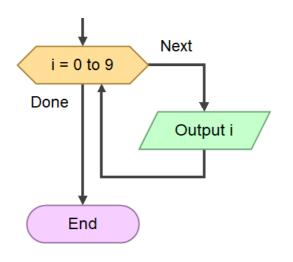
Motivation

- Another way of repeating a task is to do it for a specified number of times.
- Examples
 - Add 4 cups of flour
 - Buy 4 large apples
 - Send 4 text messages

Note: this is very similar to the while loop over an index. However, instead of specifying a loop condition (e.g., i<10), we specify the range of numbers.

<u>Overview</u>

The for loop also executes a series of statements while a condition is true. But it's simpler to associate the loop with certain iterations over values of the index variable.



for i in range(1,11):
 print(i)

Flowgorithm

Python

Simplest form of the for loop

Most of the time we'll use for with range:

```
for variable in range([start,]stop[,step]):
    statement 1.1
    statement 1.2
    [...]

[...]

executed for each number in the range
    statement 1.2
```

Syntax follows that of while and if

range

range effectively generates an integer **list** with a specified starting point, end point and spacing. Syntax:

```
range([start,]stop[,step])
```

where

- ▶ start is the optional starting point (default =0)
- stop is the end point (loop terminates at stop-I for increment >0)
- step is the optional spacing (default = I)

Comments

In Python 2, range generated an actual list. In Python 3, it generates an object with a special range data type.

equivalent to [0,1,2,3,4,5,6,7,8,9]

```
In [104]: x=range(10)
In [105]: print(x)
range(0, 10)
In [106]: print(x[0])
0
In [107]: print(x[1])
1
In [108]: print(x[9])
```



can access individual elements

Simple examples

Reminder about in

We have already introduced in! Recall that it's a way of testing for membership in a list.

```
In [115]: list3=[1,2,3]
In [116]: 1 in list3
Out[116]: True

In [117]: 4 in list3
Out[117]: False
```

Thus the for loop

```
for variable in range([start,]stop[,step]):
```

is executed for all variables belonging to the range list.

General syntax of the for statement

More precisely, the for statement has the following syntax:

```
for variable in list:
    statement 1.1
    statement 1.2
                        executed for each element in the list
    [...]
statement 2.1
                   executed after every item in the list
                   has been examined
statement 2.1
[...]
```

Comments

- For the simplest version of the for loop, the loop variable is an index or counter variable. In this case, it's almost always an integer.
- It's possible to modify the counter inside the loop, but this can lead to confusion.

```
for i in range(10):
    print(i)

for i in range(10):
    i = 1
    print(i)

Modification has no effect on loop

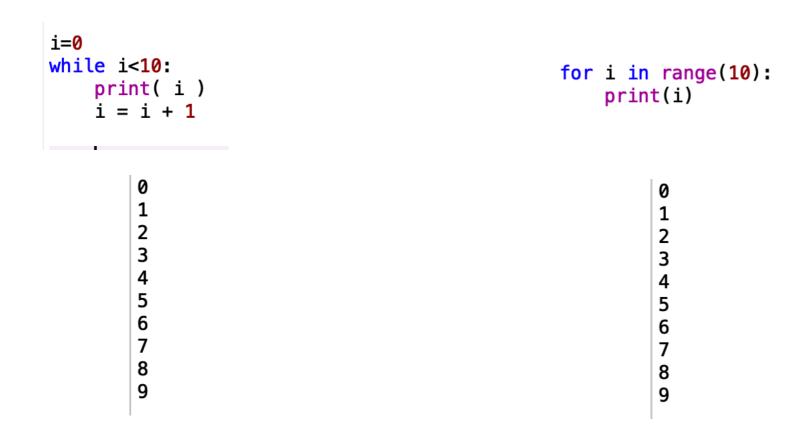
The program still runs but it can
be hard to understand what's
happening
happening
```

Why is the for loop useful?

- The for loop is probably the most commonly used loop in science and engineering.
- Why? In many applications, a set of tasks is repeated a certain number of times.
 - Examples: set of molecules or spatial locations.
- More concretely, many applications in science and engineering are related to counting.

Differences between while and for (1)

The while and for loops are very similar. Everything we can do with for we can do with while.



The for loop is more compact.

Differences between while and for (2)

The while loop is more useful when we don't know how many times the loop will be executed (e.g. finite loop):

```
value=128.0
value=128.0
                                                    for i in range(6):
while value >2.0:
                                                        value /= 2.0
   value /= 2.0
                                                        print( 'current value=',value )
   print( 'current value=',value )
                                                    else:
else:
                                                         print( 'final value=',value )
     print( 'final value=',value )
                                                    current value= 64.0
 current value= 64.0
                                                    current value= 32.0
 current value= 32.0
                                                    current value= 16.0
 current value= 16.0
                                                    current value= 8.0
 current value= 8.0
                                                    current value= 4.0
 current value= 4.0
                                                    current value= 2.0
 current value= 2.0
                                                    final value= 2.0
 final value= 2.0
```

The version with the for loop isn't as useful in practice.

Use of else

- In theory we can add an else block after a for block.
- In practice, there's usually no need because the statements after the for will be automatically executed.

```
for i in range(3):
                            for i in range(3):
                                                             for i in range(3):
    print( i )
                                print(i)
                                                                 print( i )
print( "we're done" )
                            else:
                                                             else:
                                print( "we're done" )
                                                                 print( "we're done" )
                                                             print( "we're done" )
0
                              0
we're done
                              we're done
                                                             we're done
                                                             we're done
```

<u>Iteration</u>

- In traditional computer languages, for loops are limited to counting, e.g., for with an appropriately specified range.
- This is limiting because it isn't always convenient to think in terms of a counter variable.
- Sometimes it's more convenient to loop over items of a list. This is referred to as iteration rather than counting. Iteration is more general. In Python this is easily done using in.

Looping over a counter variable vs. iteration over a list

For some problems it's more natural to iterate over a list.

```
mylist= ['dog', 'cat', 'mouse', 'goldfish', 'turtle']
N=len(mylist)
for i in range(N):
    print( mylist[i] )
```

counter variable

```
dog
cat
mouse
goldfish
turtle
```

```
mylist= ['dog', 'cat', 'mouse', 'goldfish', 'turtle']
for animal in mylist:
    print( animal )
```

iteration over list

Iteration yields more compact code as there's no need to deal with a counter variable.

Extensions

It's easy to think of situations in which the basic for loop is inadequate.

Examples

- ▶ Want a counter variable when we iterate over a list
- Want to loop over multiple variables
- Want to stop repeating the task earlier than expected

We now consider several extensions.

i) Extracting a counter variable

On occasion we want to iterate over a list but still have access to a counter variable. This can be done using enumerate.

```
list1=['dog','cat','mouse']
list2=['bone','catnip','cheese']

for i,animal in enumerate(list1):
    print( i,animal,list2[i] )
```

```
0 dog bone
1 cat catnip
2 mouse cheese
```

ii) Iterating over multiple lists

Occasionally we can to iterate over multiple lists. This can be using zip.

```
list1=['dog','cat','mouse','elephant']
list2=['bone','catnip','cheese','peanuts']
for animal,food in zip(list1,list2):
    print( animal,food )
```

dog bone cat catnip mouse cheese elephant peanuts

iii) Nested loops

Just as with if, for loops can be nested arbitrarily many times.

```
for i in range(9):
    print ('i=',i)

i= 0
i= 1
i= 2
```

i=3

i=4

i=5

i=6

i=7

i=8

```
i= 0 j= 0
i= 0 j= 1
i= 0 j= 2
i= 1 j= 0
i= 1 j= 1
i= 1 j= 2
i= 2 j= 0
i= 2 j= 1
i= 2 j= 2
```

```
for i in range(3):
    for j in range(3):
        print( 'i=',i,'j=',j )
```

Why are nested loops useful?

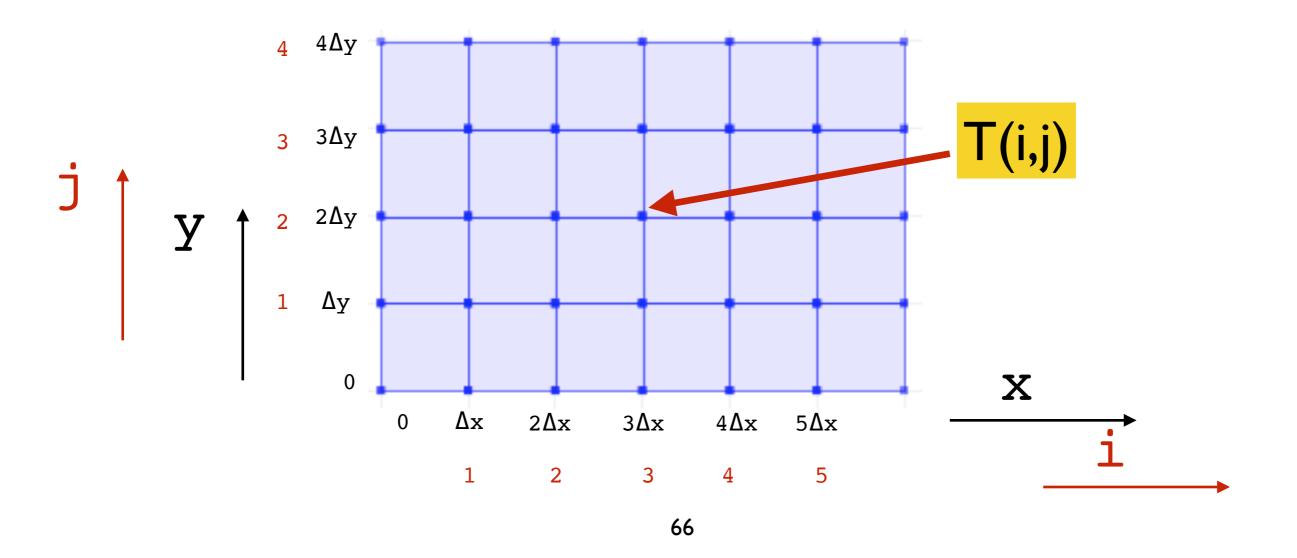
In many programs, each loop corresponds to a distinct direction. Examples:

- row, column
- **x**, y
- x,y,z

The nested loop allows us to sweep through all the points in the domain in a very natural way.

Application: defining a 2-D field

We can also define a field on our grid. This can be done by looping over (i, j).

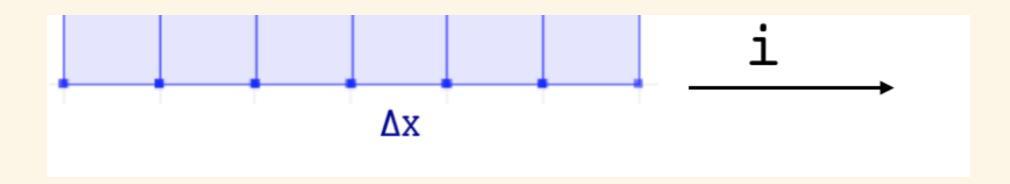


Grid spacing

- In the previous figure i and j are integers. In reality they correspond to locations x and y.
- In many situations we would like to convert (i, j)
 coordinates to (x, y) coordinates. This is easy to do!
 - $i=0 \rightarrow x=0$
 - i=1 → x=Δx Δx is the grid spacing
 - $i=2 \rightarrow x=2\Delta x$
 - etc.
- To have N points between x_1 and x_N , use $\Delta x = (x_N x_1) / (N-1)$. N includes endpoints.

Example 4: a I-D grid

Consider a one-dimensional grid with 20 evenly spaced points and endpoints at $x_i=0$ and $x_f=10$. Use a for loop to print the position of each grid point x_i .



iv) Speeding up execution of a loop

- By design, the same instructions are executed for every single pass through the loop. This can take a long time if there are many instructions to be carried out or many steps in the loop.
- There are two ways to speed things up:
 - I. Jump out of the loop (break)
 - 2. Proceed to the next iteration of the loop (continue)

break

- break causes Python to jump from the current loop to the (adjacent) outer loop. This amounts to being kicked out of the current/inner loop.
- It also applies to while.

current loop

current loop

```
for i in range(10):
    if i==2:
        break
    else:
        print( i )
print( 'we are finished' )
```

```
i= 0
i= 1
we are finished
```

j = 0 i = 0

break at i=2

```
for i in range(10):
    if i==3:
        break
    else:
```

print('j=',j,'i=',i)

for j in range(3):

print()

print('bye')

```
j= 0 i= 1
j= 0 i= 2

j= 1 i= 0
j= 1 i= 1
j= 1 i= 2

j= 2 i= 0
j= 2 i= 1
j= 2 i= 2
bye
break at i=3
```

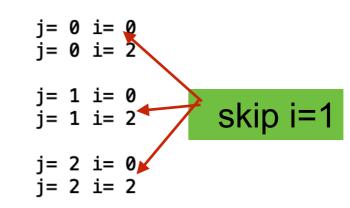
continue

continue causes Python to immediately proceed with the next iteration of the current loop. This amounts to skipping an iteration.

```
for i in range(5):
    if i==3:
        continue
    else:
        print('i=', i)
    print('bye')
```

```
i= 0
i= 1
i= 2
i= 4
bye
```

```
for j in range (3):
    print()
    for i in range(3):
        if i==1:
        continue
    else:
        print('j=',j,'i=',i)
```



<u>pass</u>

- pass causes Python to do nothing!
- It's effectively the same as a comment. However, a comment may generate a syntax error if there are no other statements. It's equivalent to continue if we have no other statements.
- It can also be used with while. In fact, it's more commonly used with while rather than for.

```
for i in range(0,10):
    if i==4:
        print( 'We have a match for i={}'.format(i) )
    else:
        pass
        do nothing

while input('Enter q or Q to quit: ').upper() != 'Q':
    pass
print( 'We are done!' )

do nothing

We have a match for i=4

Enter q or Q to quit: y

Enter q or Q to quit: q

we are done!
```

Difference between pass and continue

- In practice, we can use continue instead of pass.
- However, pass is more suggestive of doing nothing.

Summary

- 1. Loops are fundamental to computer programming.
- 2. while loops are useful for testing whether a condition has changed.
- 3. for loops are useful for counting or iterating over the items of a list.