Scientific Programming Practical 3

Introduction

Ordered collections of (homogeneous) objects

Mutable objects

Defined using the [] items separated by commas

```
my first list = [1,2,3]
print("first:", my first list)
my second list = [1,2,3,1,3] #elements can appear several times
print("second: ", my second list)
fruits = ["apple", "pear", "peach", "strawberry", "cherry"] #elements can be strings
print("fruits:", fruits)
an empty list = []
print("empty:" , an empty list)
another empty list = list()
print("another empty:", another empty list)
a list containing other lists = [[1,2], [3,4,5,6]] #elements can be other lists
print("list of lists:", a list containing other lists)
my final example = [my first list, a list containing other lists]
print("a list of lists of lists:", my final example)
```

```
first: [1, 2, 3]
second: [1, 2, 3, 1, 3]
fruits: ['apple', 'pear', 'peach', 'strawberry', 'cherry']
empty: []
another empty: []
list of lists: [[1, 2], [3, 4, 5, 6]]
a list of lists of lists: [[1, 2, 3], [[1, 2], [3, 4, 5, 6]]]
```

Operators and functions

NOTE: as in strings, list indexing starts from 0!

Result	Operator	Meaning
bool	ool =, != Check if two lists are equal or differ	
int	len(list)	Return the length of the list
list	list + list	Concatenate two lists (returns a new list)
list	list * int	Replicate the list (returns a new list)
list	list[int:int]	Extract a sub-list

The whole object must be there!

Result	Operator	Meaning
bool	obj in list	Check if an element is present in a list

Lists are mutable so now we can change values!

Result	Operator	Meaning	
obj	list[int]	Read/write an element at a specified index	

Operators and functions NOTE: as in strings, list indexing starts from 0!

in slicing list[S:E]

S is included

E is excluded

```
A = [1, 2, 3]
B = [1, 2, 3, 1, 2]
print("A is a ", type(A))
print(A, " has length: ", len(A))
print("A[0]: ", A[0], " A[1]:", A[1], " A[-1]:", A[-1])
print(B, " has length: ", len(B))
print("Is A equal to B?", A == B)
C = A + [1, 2]
print(C)
print("Is C equal to B?", B == C)
D = [1, 2, 3]*8
print(D)
E = D[12:18] #slicing
print(E)
print("Is A*2 equal to E?", A*2 == E)
```

```
A is a <class 'list'>
[1, 2, 3] has length: 3
A[0]: 1 A[1]: 2 A[-1]: 3
[1, 2, 3, 1, 2] has length: 5
Is A equal to B? False
[1, 2, 3, 1, 2]
Is C equal to B? True
[1, 2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3, 1, 2, 3]
[1, 2, 3, 1, 2, 3]
Is A*2 equal to E? True
```

Operators and functions

NOTE: as in strings, list indexing starts from 0!

IN operator: the whole element must be there!

Lists are **mutable objects** so now we can **change values**!

```
A = [1, 2, 3, 4, 5, 6]
B = [1, 3, 5]
print("A:", A)
print("B:", B)

print("Is B in A?", B in A)
print("A\'s ID:", id(A))
A[5] = [1,3,5] #we can add elements
print(A)
print("A\'s ID:", id(A))
print("A\'s ID:", id(A))
print("A has length:", len(A))
print("Is now B in A?", B in A)
```

```
A: [1, 2, 3, 4, 5, 6]

B: [1, 3, 5]

Is B in A? False

A's ID: 140419415368200

[1, 2, 3, 4, 5, [1, 3, 5]]

A's ID: 140419415368200

A has length: 6

Is now B in A? True
```

ERROR: do not exceed boundaries with indexing!

```
A = [1, 2, 3, 4, 5, 6]
print("A has length:", len(A))
print("First element:", A[0])
print("7th-element: ", A[6])
A has length: 6
First element: 1
IndexError
                                          Traceback (most recent call last)
<ipython-input-5-699e5f04cae0> in <module>()
      4 print("First element:", A[0])
----> 5 print("7th-element: ", A[6])
IndexError: list index out of range
```

Slicing can cope with indexes:

```
A = [1, 2, 3, 4, 5, 6]
print("A has length:", len(A))

print("First element:", A[0])
print("last element: ", A[-1])

print("3rd to 10th: ", A[2:10])

print("8th to 11th:", A[7:11])

A has length: 6
First element: 1
last element: 6
3rd to 10th: [3, 4, 5, 6]
8th to 11th: []
```

Methods	Return	Method	Meaning
	None	list.append(obj)	Add a new element at the end of the list
	None	list.extend(list)	Add several new elements at the end of the list
	None	list.insert(int,obj)	Add a new element at some given position
	None	list.remove(obj)	Remove the first occurrence of an element
	None	list.reverse()	Invert the order of the elements
can specify ———	None	list.sort()	Sort the elements
reverse = True	int	list.count(obj)	Count the occurrences of an element

Note that lists are **mutable objects** and therefore virtually all the previous methods (except *count*) do not have an output value, but **they modify the list**

Methods

```
print("\nDone with numbers, let's go strings...\n")
                                               #A string list
                                               fruits = ["apple", "banana", "pineapple", "cherry", "pear", "almond", "orange"]
                                               #Let's get a reverse lexicographic order:
[1, 2, 3]
                                               print(fruits)
[1, 2, 3, 72]
                                               fruits.sort()
[1, 2, 3, 72, 1, 5, 124, 99]
                                               fruits.reverse() # equivalent to: fruits.sort(reverse=True)
[99, 124, 5, 1, 72, 3, 2, 1]
                                               print(fruits)
[1, 1, 2, 3, 5, 72, 99, 124]
                                               fruits.remove("banana")
Min value: 1
                                               print(fruits)
Max value: 124
                                               fruits.insert(5, "wild apple") #put wild apple after apple.
Number 1 appears: 2 times
                                               print(fruits)
While number 837: 0
                                               print("\nSorted fruits:")
                                               fruits.sort() # does not return anything. Modifies list!
Done with numbers, let's go strings...
                                               print(fruits)
['apple', 'banana', 'pineapple', 'cherry', 'pear', 'almond', 'orange']
['pineapple', 'pear', 'orange', 'cherry', 'banana', 'apple', 'almond']
['pineapple', 'pear', 'orange', 'cherry', 'apple', 'almond']
['pineapple', 'pear', 'orange', 'cherry', 'apple', 'wild apple', 'almond']
```

#A numeric list
A = [1, 2, 3]
print(A)

print(A)

print(A)

print(A)
A.sort()
print(A)

print("A has id:", id(A))

print("A has id:", id(A))

A.append(72) #appends one and only one object

print("Number 1 appears:", A.count(1), " times")
print("While number 837: ", A.count(837))

A.reverse() #NOTE: NO RETURN VALUE!!!

A.extend([1, 5, 124, 99]) #adds all these objects, one after the other.

print("Min value: ", A[0]) # In this simple case, could have used min(A)
print("Max value: ", A[-1]) #In this simple case, could have used max(A)

Methods

lists are mutable objects and therefore virtually all the previous methods (except count) do not have an output value:

```
A = ["A", "B", "C"]
print("A:", A)

A_new = A.append("D")
print("A:", A)
print("A_new:", A_new)
A: ['A', 'B', 'C']
A: ['A', 'B', 'C', 'D']
```

A_new: None



Return	Method	Meaning
None	list.append(obj)	Add a new element at the end of the list
None	list.extend(list)	Add several new elements at the end of the list
None	<pre>list.insert(int,obj)</pre>	Add a new element at some given position
None	list.remove(obj)	Remove the first occurrence of an element
None	list.reverse()	Invert the order of the elements
None	list.sort()	Sort the elements
int	list.count(obj)	Count the occurrences of an element

Some important things on lists

1. append is different from extend

2. to remove an object it must exist

```
A = [1, 2, 3]

A.extend([4, 5])
print(A)
B = [1, 2, 3]
B.append([4,5])
print(B)

[1, 2, 3, 4, 5]
[1, 2, 3, [4, 5]]
```

Some important things on lists

3. a list is sortable if all its elements are (i.e. it is homogeneous)

```
A = [4,3, 1,7, 2]
print(A)
A.sort()
print(A)
A.append("banana")
print(A)
A.sort()
print(A)
[4, 3, 1, 7, 2]
[1, 2, 3, 4, 7]
[1, 2, 3, 4, 7, 'banana']
                                         Traceback (most recent call last)
TypeError
<ipython-input-1-91b77adb823f> in <module>
      5 A.append("banana")
      6 print(A)
----> 7 A.sort()
      8 print(A)
TypeError: '<' not supported between instances of 'str' and 'int'
```

REMEMBER:

Lists are MUTABLE objects...
... hence they hold references

to objects rather than objects.

```
A = ["hi", "there"]
B = A
print("A:", A)
print("B:", B)
A.extend(["from", "python"])
print("A now: ", A)
print("B now: ", B)
print("\n---- copy example -----")
#Let's make a distinct copy of A.
C = A[:] #all the elements of A have been copied in C
print("C:", C)
A[3] = "java"
print("A now:", A)
print("C now:", C)
print("\n---- be careful though -----")
#Watch out though that...
D = [A, A]
E = D[:]
print("D:", D)
print("E:", E)
D[0][0] = "hello"
print("D now:", D)
print("E now", E)
A: ['hi', 'there']
B: ['hi', 'there']
A now: ['hi', 'there', 'from', 'python']
B now: ['hi', 'there', 'from', 'python']
---- copy example -----
C: ['hi', 'there', 'from', 'python']
A now: ['hi', 'there', 'from', 'java']
C now: ['hi', 'there', 'from', 'python']
---- be careful though -----
D: [['hi', 'there', 'from', 'java'], ['hi', 'there', 'from', 'java']]
E: [['hi', 'there', 'from', 'java'], ['hi', 'there', 'from', 'java']]
D now: [['hello', 'there', 'from', 'java'], ['hello', 'there', 'from', 'java']]
E now [['hello', 'there', 'from', 'java'], ['hello', 'there', 'from', 'java']]
```

The split method. String → List

```
Syntax:

LIST = str.split(str)

split at characters

string to be split
```

```
text = "This is my sentence. How many words have I written?"
words = text.split(' ')
print(text)
print(words)
print("\nThe sentence contains ", len(words), "words")

This is my sentence. How many words have I written?
['This', 'is', 'my', 'sentence.', 'How', 'many', 'words', 'have', 'I', 'written?']
```

The sentence contains 10 words

The split method

Example Recall the protein seen in the previous practical:

chain_a = """SSSVPSQKTYQGSYGFRLGFLHSGTAKSVTCTYSPALNKM
FCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVV
RRCPHHERCSDSDGLAPPQHLIRVEGNLRVEYLDDRNTFR
HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG EPHHELPPGSTKRALPNNT"""

how can we split it into several lines?

```
chain a = """SSSVPSOKTYOGSYGFRLGFLHSGTAKSVTCTYSPALNKM
FCOLAKTCPVOLWVDSTPPPGTRVRAMAIYKQSOHMTEVV
RRCPHHERCSDSDGLAPPQHLIRVEGNLRVEYLDDRNTFR
HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG
EPHHELPPGSTKRALPNNT""
lines = chain a.split('\n')
print("Original sequence:")
print( chain a, "\n") #some spacing to keep things clear
print("line by line:")
# write the following and you will appreciate loops! :-)
print("1st line:" ,lines[0])
print("2nd line:" ,lines[1])
print("3rd line:" ,lines[2])
print("4th line:" ,lines[3])
print("5th line:" ,lines[4])
print("6th line:" ,lines[5])
print("\nSplit the 1st line in correspondence of FRL:\n",lines[0].split("FRL"))
Original sequence:
SSSVPSOKTYOGSYGFRLGFLHSGTAKSVTCTYSPALNKM
FCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVV
RRCPHHERCSDSDGLAPPOHLIRVEGNLRVEYLDDRNTFR
HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG
EPHHELPPGSTKRALPNNT
line by line:
1st line: SSSVPSOKTYOGSYGFRLGFLHSGTAKSVTCTYSPALNKM
2nd line: FCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVV
3rd line: RRCPHHERCSDSDGLAPPQHLIRVEGNLRVEYLDDRNTFR
4th line: HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
5th line: IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG
6th line: EPHHELPPGSTKRALPNNT
Split the 1st line in correspondence of FRL:
 ['SSSVPSQKTYQGSYG', 'GFLHSGTAKSVTCTYSPALNKM']
```

The split method

Example Recall the protein seen in the previous practical:

chain_a = """SSSVPSQKTYQGSYGFRLGFLHSGTAKSVTCTYSPALNKM
FCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVV
RRCPHHERCSDSDGLAPPQHLIRVEGNLRVEYLDDRNTFR
HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG EPHHELPPGSTKRALPNNT"""

how can we split it into several lines?

```
chain a = """SSSVPSOKTYOGSYGFRLGFLHSGTAKSVTCTYSPALNKM
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RRCPHHERCSDSDGLAPPQHLIRVEGNLRVEYLDDRNTFR
HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG
EPHHELPPGSTKRALPNNT""
lines = chain a.split('\n')
print("Original sequence:")
print( chain a, "\n") #some spacing to keep things clear
print("line by line:")
# write the following and you will appreciate loops! :-)
print("1st line:" ,lines[0])
print("2nd line:" ,lines[1])
print("3rd line:" ,lines[2])
print("4th line:" ,lines[3])
print("5th line:" ,lines[4])
print("6th line:" ,lines[5])
print("\nSplit the 1st line in correspondence of FRL:\n",lines[0].split("FRL"))
Original sequence:
SSSVPSOKTYOGSYGFRLGFLHSGTAKSVTCTYSPALNKM
FCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVV
RRCPHHERCSDSDGLAPPOHLIRVEGNLRVEYLDDRNTFR
HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG
EPHHELPPGSTKRALPNNT
line by line:
1st line: SSSVPSOKTYOGSYGFRLGFLHSGTAKSVTCTYSPALNKM
2nd line: FCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVV
3rd line: RRCPHHERCSDSDGLAPPQHLIRVEGNLRVEYLDDRNTFR
4th line: HSVVVPYEPPEVGSDCTTIHYNYMCNSSCMGGMNRRPILT
5th line: IITLEDSSGNLLGRNSFEVRVCACPGRDRRTEEENLRKKG
6th line: EPHHELPPGSTKRALPNNT
Split the 1st line in correspondence of FRL:
 ['SSSVPSQKTYQGSYG', 'GFLHSGTAKSVTCTYSPALNKM']
```

where is FRL gone?



The join method. List → String

Example Given the list ['Oct', '5', '2018', '15:30'], let's combine all its elements in a string joining the elements with a dash ("-") and print them. Let's finally join them with a tab ("\t") and print them.

Syntax: str.join(list) elements to join string used to join them

```
vals = ['Oct', '5th', '2018', '15:30']
print(vals)
myStr = "-".join(vals)
print("\n" + myStr)
myStr = "\t".join(vals)
print("\n" + myStr)

['Oct', '5th', '2018', '15:30']
Oct-5th-2018-15:30
Oct 5th 2018 15:30
```

Tuples are the IMMUTABLE version of lists (ordered sequence of objects)

```
first tuple = (1,2,3)
print(first tuple)
second tuple = (1,) #this contains one element only, but we need the comma!
var = (1) #This is not a tuple!!!
print(second_tuple, " type:", type(second_tuple))
print(var, "type:", type(var))
empty tuple = () #fairly useless
print(empty tuple)
third tuple = ("January", 1 ,2007) #heterogeneous info
print(third tuple)
days = (third tuple, ("February", 2, 1998), ("March", 2, 1978), ("June", 12, 1978))
print(days, "\n")
#Remember tuples are immutable objects...
print("Days has id: ", id(days))
days = ("Mon", "Tue", "Wed", "Thu", "Fri", "Sat", "Sun")
#...hence reassignment creates a new object
print("Days now has id: ", id(days))
(1, 2, 3)
(1.) type: <class 'tuple'>
1 type: <class 'int'>
()
('January', 1, 2007)
(('January', 1, 2007), ('February', 2, 1998), ('March', 2, 1978), ('June', 12, 1978))
Days has id: 140419415813880
Days now has id: 140419416147240
```

Tuples are the IMMUTABLE version of lists (ordered sequence of objects)

Tuples can be used as keys of dictionary, whereas lists cannot

```
a = [1, 2, [1,2,3]] # a list
b = (1, 2, [1,2,3]) # a tuple
print("a:", a)
print("b:", b)
print("")
print("a[0]:", a[0], "b[0]:", b[0])
print("a[2]:", a[2], "b[2]:", b[2])

a: [1, 2, [1, 2, 3]]
b: (1, 2, [1, 2, 3])
a[0]: 1 b[0]: 1
a[2]: [1, 2, 3] b[2]: [1, 2, 3]
```

Tuples are the IMMUTABLE version of lists (ordered sequence of objects)

```
a = [1, 2, [1,2,3]] # a list
b = (1, 2, [1,2,3]) # a tuple
print("a:", a)
print("b:", b)
print("")
print("a[0]:", a[0], "b[0]:", b[0])
print("a[2]:", a[2], "b[2]:", b[2])
print("")
a[1] = [7,8,9]
print(a)
b[1] = [7,8,9]
print(b)
a: [1, 2, [1, 2, 3]]
b: (1, 2, [1, 2, 3])
a[0]: 1 b[0]: 1
a[2]: [1, 2, 3] b[2]: [1, 2, 3]
[1, [7, 8, 9], [1, 2, 3]]
                                          Traceback (most recent call last)
TypeError
<ipython-input-2-549ff0d2c315> in <module>
      9 a[1] = [7,8,9]
     10 print(a)
---> 11 b[1] = [7,8,9]
     12 print(b)
     13
```

TypeError: 'tuple' object does not support item assignment

Tuples Functions

working as in lists...

Result	Operator	Meaning
bool	=, !=	Check if two tuples are equal or different
int	len(tuple)	Return the length of the tuple
tuple	tuple + tuple	Concatenate two tuples (returns a new tuple)
tuple	tuple * int	Replicate the tuple (returns a tuple)
tuple	tuple[int]	Read an element of the tuple
tuple	<pre>tuple[int:int]</pre>	Extract a sub-tuple

Functions

```
practical1 = ("Wednesday", "23/09/2020")
practical2 = ("Monday", "28/09/2020")
practical3 = ("Wednesday", "30/09/2020")
#A tuple containing 3 tuples
lectures = (practical1, practical2, practical3)
#One tuple only
mergedLectures = practical1 + practical2 + practical3
print("The first three lectures:\n", lectures, "\n")
print("mergedLectures:\n", mergedLectures)
#This returns the whole tuple
print("1st lecture was on: ", lectures[0], "\n")
#2 elements from the same tuple
print("1st lecture was on ", mergedLectures[0], ", ", mergedLectures[1], "\n")
# Return type is tuple!
print("3rd lecture was on: ", lectures[2])
#2 elements from the same tuple returned in tuple
print("3rd lecture was on ", mergedLectures[4:], "\n")
The first three lectures:
 (('Wednesday', '23/09/2020'), ('Monday', '28/09/2020'), ('Wednesday', '30/09/2020'))
mergedLectures:
('Wednesday', '23/09/2020', 'Monday', '28/09/2020', 'Wednesday', '30/09/2020')
1st lecture was on: ('Wednesday', '23/09/2020')
1st lecture was on Wednesday , 23/09/2020
3rd lecture was on: ('Wednesday', '30/09/2020')
3rd lecture was on ('Wednesday', '30/09/2020')
```

Tuples Methods

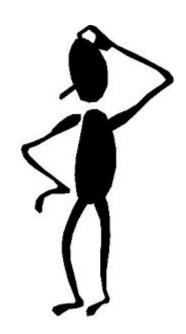
working as in lists...

Return	Method	Meaning
int	tuple.count(obj)	Count the occurrences of an element
int	tuple.index(obj)	Return the index of the first occurrence of an object

Methods

```
practical1 = ("Wednesday", "23/09/2020")
practical2 = ("Monday", "28/09/2020")
practical3 = ("Wednesday", "30/09/2020")
mergedLectures = practical1 + practical2 + practical3 #One tuple only
print(mergedLectures.count("Wednesday"), " lectures were on Wednesday")
print(mergedLectures.count("Monday"), " lecture was on Monday")
print(mergedLectures.count("Friday"), " lectures was on Friday")
print("Index:", practical2.index("Monday"))
#You cannot look for an element that does not exist
print("Index:", practical2.index("Wednesday"))
2 lectures were on Wednesday
1 lecture was on Monday
0 lectures was on Friday
Index: 0
ValueError
                                         Traceback (most recent call last)
<ipvthon-input-19-20063b595bbc> in <module>
     10
     11 print("Index:", practical2.index("Monday"))
---> 12 print("Index:", practical2.index("Wednesday"))
     13
ValueError: tuple.index(x): x not in tuple
```

Questions?



https://qcbsciprolab2020.readthedocs.io/en/latest/practical3.html

Go quickly through the text and do the exercises at the end

Exercises

1. Given the following text string:

```
"""this is a text
string on
several lines that does not say anything."""
```

a. print it; b) print how many lines, words and characters it contains. Finally, c)sort the words alphabetically and print the first and the last in lexicographic order.

Show/Hide Solution

2. The variant calling format (VCF) is a format to represent structural variants of genomes (i.e. SNPs, insertions, deletions). Each line of this format represents a variant, every piece of information within a line is separated by a tab (\t in python). The first 5 fields of this format report the chromosome (chr), the position (pos), the name of the variant (name), the reference allele (REF) and the alternative allele (ALT). Assuming to have a variable VCF defined containing the following three lines (representing three SNPs):

```
VCF = """MDC000001.124\\t7112\\tFB_AFFY_0000024\\tG\\tA
MDC000002.328\\t941\\tFB_AFFY_0000144\\tC\\tT
MDC000004.272\\t2015\\tFB_AFFY_0000222\\tG\\tA"""
```

- Store these three variants as a list of lists, where each one of the fields is kept separate (e.g. the list should be similar to: [[chr1,pos1,name1,ref1,alt1], [chr2, pos2, name2, ref2, alt2], ...] where all the elements are as specified in the string VCF (note that "..." means that the list is not complete).
- 2. Print each variant changing its format in: "name|chr|pos|REF/ALT".