Scientific Programming

# Lecture A03 – Structured programming

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# Structured programming

After having surveyed the basic data items, we now survey the basic control structures:



# Structured programming

#### Blocks

Blocks are used to enable groups of statements to be treated as if they were one statement.

Block-structured languages have a syntax for enclosing blocks in some formal way.



### Some simple examples

```
for loop
L = [1,2,3,4]
print("-----")
for val in L:
    print(">> ", end="")
    print(val, val*val)
print("-----")
```

## Some simple examples

for loop
L = [1,2,3,4] -----print("------") >> 1 1
for val in L: >> 2 4
 print(">> ", end="") >> 3 9
 print(val, val\*val) >> 4 16
print("-----") -----

if - else statement

```
answer = input()
if (answer.lower() == "yes"):
    print("Good!")
else:
    print("Too bad!")
```

```
Andrea Passerini (UniTN)
```

# Python vs rest-of-the-world: Indentation

#### Python

Blocks are identified by indentation

```
L = [1,2,3,4]
print("----")
for val in L
    print("** ", end="")
    print(val, val*val)
print("----")
```

#### Java

Blocks are identified by curly braces

#### Rules

- End-of-line is end of statement
- End-of-indentation is end of block

### Common errors

```
L = [1,2,3,4]
print("-----")
for val in L:
print("** ", end="")
print(val, val**2)
print("-----")
```

```
[andrea@praha ~]$ python errors.py
File "errors.py", line 4
    print("** ", end="")
    ^
```

IndentationError: expected an indented block

### Common errors

```
L = [1, 2, 3, 4]
print("-----")
for val in L:
     print("** ", end="")
   print(val, val**2)
print("-----")
[andrea@praha ~]$ python errors.py
  File "errors.py", line 5
   print(val, val**2)
IndentationError: unindent does not match any
outer indentation level
```

### Common errors

```
L = [1,2,3,4]
print("-----")
for val in L:
    print("** ", end="")
    print(val, val**2)
print("-----")
[andrea@praha ~]$ python errors.py
```

```
File "errors.py", line 5
    print(val, val**2)
```

~

IndentationError: unexpected indent

# Other formatting quirks

Content of parenthesis (), [], { } can be split among multiple lines. Without parenthesis, you get an error.

]

- S2 = "abcefghijklmnopqrstuvwxyz" + "ABCDEFGHIJKLMNOPQRSTUVWXYZ"

```
[andrea@praha ~]$ python prova.py
File "prova.py", line 12
    S2 = "abcefghijklmnopqrstuvwxyz" +
SyntaxError: invalid syntax
```

# Other formatting quirks

In-line sequences

Multiple statements are normally written one per line. Is it possible to use ; to separate multiple statements in a single line.

a = 1; b = 2; c = a + b

In-line structured commands

It is possible to avoid indentation in structured statements, by writing a single statement on the same line

if val > maximum: maximum = val; pos = i

Both approaches are considered non-pythonic and advised against

#### if - else statements

#### **Conditional statement**

A conditional statement allows to write code that gets executed if and only if some condition is satisfied.

```
print("Guess what number I'm thinking: ")
guess = input()
if guess == 5633839494:
    print("It's correct!")
else:
    print("Sorry, wrong number")
BTW, do you see a problem in this code?
```

### if - elsestatements

#### **Conditional statement**

The conditional statements allow to write code that gets executed if and only if some condition is satisfied.

```
print("Guess what number I'm thinking: ")
guess = int(input())
if guess == 5633839494:
    print("It's correct!")
else:
    print("Sorry, wrong number")
```

The return of input() is a string, compared to a number returns False

if, elif and else form a "chain": only one of the branches is executed.

```
print("Insert a number between 1 and 4")
value = int(input())
if value == 1:
    print("Very good choice")
elif value == 2:
    print("The first even number")
elif value == 3:
    print("The first Fermat number")
elif value == 4:
    print("A highly totient number")
else:
    print("I said, between 1 and 4")
```

if, elif and else form a "chain": only one of the branches is executed. The first one that matches is executed.

What is the difference between these two pieces of code?

```
value = 2
if (value == 2):
    print("Even and prime")
elif (value % 2 == 0):
    print("Even")
```

Even and prime

value = 2
if (value == 2):
 print("Even and prime")
if (value % 2 == 0):
 print("Even")

```
Even and prime
Even
```

What is printed by this piece of code?

```
if condition1:
    print("A")
elif condition2:
    print("B")
else:
    print("C")
```

	condition2==True	condition2==False
condition1==True	А	А
condition1==False	В	С

How we can re-obtain the behavior described by the table, without using elif / else, but using and/or/not operators?

	condition2==True	condition2==False
condition1==True	А	А
condition1==False	В	С

if condition1:

```
print("A")
```

if not condition1 and condition2:

print("B")

```
if not condition1 and not condition2:
    print("C")
```

# For Loop

#### For loop

The for loop is a generic iterator in Python: it can step through the items of any ordered sequence or other iterable object.

- Works on strings, lists, tuples, dictionaries, and other built-in iterables
- Is it possible to define new iterable objects
- L = ["Venezia", "Verona", "Padova", "Vicenza", "Treviso", "Belluno", "Rovigo"] for provincia in L: print(provincia, "si trova in Veneto")

### For loop

. . .

- for var in sequence:
   statement1
   statement2
  - var is the loop variable; it is assigned to each of the values in the list, until all the values are used
  - sequence is the loop sequence;
  - the statements to be executed are called the loop body

Codelens



### Iteration

str	for iterates over the characters
list	for iterates over the elements
tuple	for iterates over the elements
dict	for iterates over the keys

# Range

#### Range

The range() built-in function returns an iterable object that can be used to obtain a list of integers.

#### range(stop)

Returns a list of integers between 0 and stop-1

```
for k in range(4):
    print(k, end = ' ')
print("")
```

0 1 2 3

# Range

#### Range

The range() built-in function returns an iterable object that can be used to obtain a list of integers.

range(start, stop)

Returns a list of integers between start and stop-1

```
for k in range(1,5):
    print(k, end = ' ')
    1 2 3 4
print("")
```

# Range

#### Range

The range() built-in function returns an iterable object that can be used to obtain a list of integers.

range(start, stop, increment)

Returns a list of integers between start and stop-1, with increment increment

```
for k in range(2,10,2):
    print(k, end = ' ')
print("")
```

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### Range - Differences between 2.x and 3.x

```
Python 2.7.13 (default, Apr 23 2017, 16:50:35)
[GCC 4.2.1 Compatible Apple LLVM 8.0.0 (clang-800.0.42.1)] on of
Type "help", "copyright", "credits" or "license" for more infon
>>> L = range(10)
>>> print(L)
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

```
Python 3.5.3 |Anaconda 4.4.0 (x86_64)| (default, Mar 6 2017, 1
[GCC 4.2.1 Compatible Apple LLVM 6.0 (clang-600.0.57)] on darwi
Type "help", "copyright", "credits" or "license" for more infor
>>> L = range(10)
>>> print(L)
range(0, 10)
```

# Range - Differences between 2.x and 3.x

#### Python 2.x

range() returns a list that contains the desired integers. The list is stored in memory, making it inefficient to use range() for a very large number of iterations.

If you want to use the 3.x approach in 2.x, use xrange() instead.

#### Python 3.x

In Python 3.x, range() generates the numbers as the iterator for ask for them, without storing the list.

If you do want to create the list, use the list() built-in function:

```
L = list(range(10))
print(L)
[0.1.2.3.4.5.6.7.8.9]
```

# Examples of for – Summation

The following code sums the numbers contained in the list L

```
L = [1, 25, 6, 27, 57, 12]
total = 0
for number in L:
    total = total + number
print("The sum is", total)
```

Alternative code (using built-in functions)

```
L = [1, 25, 6, 27, 57, 12]
print(sum(L))
```

# Examples of for – Maximum

The following code returns the maximum value contained in L

```
L = [1, 25, 6, 27, 57, 12]
max_so_far = L[0]
for number in L:
    if number > max_so_far:
        max_so_far = number
print("The maximum is", max_so_far)
```

Alternative code (using built-in functions)

```
L = [1, 25, 6, 27, 57, 12]
print(max(L))
```

## Examples of for – Fibonacci

The following code computes the first 20 Fibonacci numbers

$$F[n] = \begin{cases} F[n-1] + F[n-1] & n > 2\\ 1 & n \le 2 \end{cases}$$

```
F = [1,1]
for k in range(18):
    F.append(F[-1]+F[-2])
print(F)
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377,
610, 987, 1597, 2584, 4181, 6765]
```

Two or more loops may be "nested", meaning that one is contained in the other.

Consider the following example, that lists all possible "quarters of hour"

```
L = []
for h in range(24):
    for m in range(0, 60, 15):
        L.append(str(h)+":"+str(m))
print(L)
['0:0', '0:15', '0:30', '0:45', '1:0', '1:15', '1:30',
    '1:45','2:0', '2:15', '2:30', '2:45', '3:0', '3:15',
    '3:30', '3:45', ...
```

The following code should check whether there are two repeated values inside a list

```
L = [1,3,5,6]
for x in L:
    for y in L:
        if x == y:
            print(x, "is repeated")
```

Do you see any problems?

- 1 is repeated
- 3 is repeated
- 5 is repeated
- 6 is repeated

The following code checks whether there are two repeated values inside a list

```
L = [1,3,5,6,1,8,3]
for i in range(len(L)):
    for j in range(i+1,len(L)):
        if L[i] == L[j]:
            print(L[i], "is repeated at ", i, j)
```

1 is repeated at 0 4 3 is repeated at 2 6

The following code checks whether there are two repeated values inside a list

```
L = [1,3,5,6,1,8,3,4,3]
for i in range(len(L)):
    for j in range(i+1,len(L)):
        if L[i] == L[j]:
            print(L[i], "is repeated at ", i, j)
```

What is printed?

- 1 is repeated at 0 4
- 3 is repeated at 2 6
- 3 is repeated at 2 8
- 3 is repeated at 6 8

#### Exercise

Given a list L of integers, print True if L contains two distinct values whose sum is equal to 17

Example: If L=[3,7,12,10,8,32,7,5], print True because 7+10=17.

```
found = False
for i in range(len(L)):
    for j in range(i+1,len(L)):
        if L[i]+L[j] == 17:
            found = True
print(found)
```

#### Exercise

Given a list L of integers, print the indexes of a couple of values whose sum is equal to 17

Example: If L=[3,7,12,10,8,32,7,5], print either 2,7 or 1,3 because L[2]+L[7]=17 and L[1]+L[3]=17.

```
found = False
for i in range(len(L)):
    for j in range(i+1,len(L)):
        if L[i]+L[j] == 17:
            found = True
            pos_i = i
            pos_j = j
if found:
    print(pos_i, pos_j)
```

#### Exercise

Given a list L of integers, print the indexes of the first couple of values whose sum is equal to 17

```
Example: If L=[3,7,12,10,8,32,7,5], print 1,3 because L[1]+L[3]=17.
```

```
found = False
for i in range(len(L)):
    for j in range(i+1,len(L)):
        if L[i]+L[j] == 17 and not found:
            found = True
            pos_i = i
            pos_j = j
if found:
    print(pos_i, pos_j)
```
# While loops

### While

The while statement allows to write code that repeats as long as a certain condition is true. while stops iterating as soon as the condition is not true anymore.

#### while condition:

- # statements that may change
- # the condition from
- # True to False





# While loops

Differences between while and for

- for element in collection: executes *n* times, where *n* is the length of collection.
- while condition: executes an indefinite number of times, as long as the condition is true.

## Use of while

The while statement is useful when the value of condition can not be known beforehand, for instance when interacting with a user

```
while input("Do you want me to stop? ").lower() != "yes":
    print("Then I'll keep going!")
```

Write a program that ask the user a question (e.g., what is the capital of Italy) and keep repeating the question until the answer is correct

```
answer = ""
while (answer != "rome"):
    print("What is the capital of Italy?")
    answer = input().lower()
    if answer != "rome":
        print("Sorry, wrong answer; retry")
```

Write a program that ask the user a question (e.g., what is the capital of Italy) and repeats the question three times or until the answer is correct.

```
answer = ""
attempts = 0
while (answer != "rome" and attempts < 3):
    print("What is the capital of Italy?")
    answer = input().lower()
    if answer != "rome":
        print("Sorry, wrong answer; retry")
        attempts = attempts+1
if (attempts == 3):
    print("The capital is Rome! Goat!")
else:
    print("Very good")</pre>
```

Let L be a list of integers and let  $L_{sum}(k) = \sum_{i=0}^{k-1} L[i]$ . Write a program that takes L and an integer value threshold as input and prints the number of elements k such that  $L_{sum}(k) \geq threshold$ . Print -1 if the sum of all elements is smaller than threshold.

For example,

- If L = [1, 4, 3, 12, 7] and threshold = 7, the output should be 3, meaning that the sum of the first three elements (8) is larger than threshold.
- If L = [1, 2, 3, 4] and threshold = 11, the output should be -1, meaning that the sum of all elements (10) is smaller than threshold.

```
L = list(range(10))
threshold = 20
tot = 0
i = 0
while (tot <= threshold and i < len(L)):
    tot = tot + L[i]
    i = i+1
if (tot >= threshold):
    print(i-1)
else:
    print(-1)
```

Write a program that creates a list with all the Fibonacci number smaller than 1,000,000.

```
F = [1,1]
over = False
while not over:
    next = F[-1]+F[-2]
    if next > 1000000:
        over = True
    else:
        F.append(next)
```

```
F = [1,1]
while F[-1]<1000000:
    F.append(F[-1]+F[-2])
F.pop(-1)</pre>
```

#### Exercise

The 3n + 1 sequence is defined like this: given a number n, compute a new value for n as follow: if n is even, divide n by 2. If n is odd, multiply it by 3 and add 1. Stop when you reach the value of 1. Example: for n = 3, the sequence is [3, 10, 5, 16, 8, 4, 2, 1]. Write a program that creates a list D, such that for each value n between 1 and 50, D[n] contains the length of the sequence so generated. In case of n = 3, the length is 8. In case of n = 27, the length is 111.

## Use of while - Exercise

```
MAX = 51
L = [0] * MAX
for n in range(1,MAX):
    count = 0
    start = n
    while n > 1:
        if (n \% 2 == 0):
            n = n // 2
        else:
            n = 3*n+1
        count = count + 1
    L[start] = count
print(L[1:])
```

### break

Inside a loop (either for or while), a break statement interrupts the execution of the loop.

```
sums = []
tot = 0
for x in range(1,100):
    tot = tot+x
    if tot>300:
        break
    sums.append(tot)
print(sums)
```

```
[1, 3, 6, 10, 15, 21, 28,
36, 45, 55, 66, 78, 91,
105, 120, 136, 153, 171,
190, 210, 231, 253, 276,
300]
```

### break

This version prints the same output as before; it is much better without a break!

```
sums = []
tot = 0
x = 1
while (tot+x <= 300):
    tot = tot + x
    sums.append(tot)
    x = x + 1
print(sums)</pre>
```

```
[1, 3, 6, 10, 15, 21, 28,
36, 45, 55, 66, 78, 91,
105, 120, 136, 153, 171,
190, 210, 231, 253, 276,
300]
```

#### continue

Inside a loop (either for or while), a continue statement interrupts the current iteration of the loop and skip to the next one.

#### continue

This version prints the same output as before; it is much better without a continue!

LS = [] [2, 3, 4, 6, 8, 9, 10, 12, for x in range(1,31): 14, 15, 16, 18, 20, 21, if x%2 == 0 or x%3 == 0: 22, 24, 26, 27, 28, 30] LS.append(x) print(LS)

## Break and continue behavior

```
for number in range(10):
    print(number, end=" ")
print("")
                                0 1 2 3 4 5 6 7 8 9
for number in range(10):
    print(number, end=" ")
    break
print("")
                                0
for number in range(10):
    print(number, end=" ")
    continue
print("")
                                0 1 2 3 4 5 6 7 8 9
```

## Break and continue behavior

```
for number in range(1,11):
    print(number, end=" ")
    if number \% 4 == 0:
        break
print("")
                                1 2 3 4
for number in range(1,11):
    if number % 4 == 0:
        break
                                123
    print(number, end=" ")
print("")
```

# Avoid break and continue!

Using break and continue frequently makes code hard to follow. But if replacing them makes the code even harder to follow, then that's a bad change.

E.W. Dijkstra. Go To Statement Considered Harmful. Communications of the ACM, Vol. 11 (1968) 147-148



# List Comprehension

### List comprehension

The list comprehension operator allows to filter or transform a list. The original list is left unchanged. A new list is created instead.

The abstract syntax is:

# List Comprehension

### List comprehension as a filter

Given an arbitrary iterable object original, we can create a new list that only contains those elements of original that satisfy a given condition.

The abstract syntax is:

```
filtered = [element
    for element in original
    if condition(element)]
```

# List comprehension - example

#### Example

Generate the list of natural numbers smaller or equal to 30 that are divisible by either 2 or 3

 $L = \{n : 1 \le n \le 30 \text{ and } (n \mod 2 = 0 \text{ or } n \mod 3 = 0)\}$ 

L = [n for n in range(1,31) if n%2 == 0 or n%3 == 0]

[2, 3, 4, 6, 8, 9, 10, 12, 14, 15, 16, 18, 20, 21, 22, 24, 26, 27, 28, 30]

## List comprehension - exercise

### Exercise

Given a list of DNA sequences represented as strings, returns only those sequences that contain at least one adenosine ("A")

```
sequences = ["ACTGG", "CCTGT", "ATTTA", "TATAGC"]
L = [seq for seq in sequences if "A" in seq]
```

```
['ACTGG', 'ATTTA', 'TATAGC']
```

## List comprehension - exercise

#### Exercise

Given a list of telephone numbers represented as strings, returns only those that are from Verona (prefix "045")

numbers = ["04599904523", "0461304534", "0288662244", "0458346157"]

L = [number for number in numbers if number.startswith("045")]

['04599904523', '0458346157']

## Note

The name of the "temporary" variable holding the current element (in the examples above, **n** and **seq**, respectively) is arbitrary.

These pieces of code are identical:

L = [n for n in range(1,31) if n%2 == 0 or n%3 == 0]

The name of the variable does not make any difference. You are free to pick any name you like, but choose something meaningful.

# List Comprehension

### List comprehension as transformation

Given an arbitrary list original, we can use a list comprehension to also transform the elements in the list in some way.

The abstract syntax is:

The expression should be based on element, but sometimes it is possible that they are completely independent.

## List comprehension - exercises

#### Exercise

Generate the list of the squares of the natural numbers between 1 and 30.

$$L = \{ n^2 : 1 \le n \le 30 \}$$

L = [n\*n for n in range(1,31)]
print(L)

[1, 4, 9, 16, 25, 36, 49, 64, 81, 100, 121, 144, 169, 196, 225, 256, 289, 324, 361, 400, 441, 484, 529, 576, 625, 676, 729, 784, 841, 900]

## List comprehension – exercises

#### Exercise

Given the list of strings representing (part of) the 3D structure of a protein chain, compute a list of lists which should hold, for each residue (that is, for every row of atoms), its coordinates.

```
atoms = [
    "SER A 96 77.253 20.522 75.007",
    "VAL A 97 76.066 22.304 71.921",
    "PRO A 98 77.731 23.371 68.681",
    "SER A 99 80.136 26.246 68.973",
    "GLN A 100 79.039 29.534 67.364",
    "LYS A 101 81.787 32.022 68.157",
]
coords = [row.split()[-3:] for row in atoms]
print(coords)
```

## List comprehension – example

But! The results is a list of list of strings, I need float coordinates! What we can do?

```
coords = [
    [float(coord) for coord in row.split()[-3:]]
    for row in atoms]
print(coords)
```

 $[[77.253, 20.522, 75.007], [76.066, 22.304, 71.921], \ldots$ 

## $List\ comprehension-example$

But! Nice list of lists, but I need a list of tuples - I will use them later in a dictionary!

```
coords = [
   tuple([float(coord) for coord in row.split()[-3:]])
   for row in atoms]
print(coords)
```

 $[(77.253, 20.522, 75.007), (76.066, 22.304, 71.921), \ldots$ 

# List Comprehension

### All together, now!

Given an arbitrary list original, we can use a list comprehension to transform and filter the elements in the list at the same time

The abstract syntax is:

# List Comprehension

Using the example developed so far, we want just to list the coordinates of serines.

```
coords = [
   tuple([float(coord) for coord in row.split()[-3:]])
   for row in atoms
   if row.startswith("SER")]
print(coords)
```

[(77.253, 20.522, 75.007), (80.136, 26.246, 68.973)]

# List comprehension and lists of lists

Let's say that we want to create a bi-dimensional matrix  $n \times n$ , initialized to zero. Let's write in this way

n = 4
L = [[0]\*n]\*n
print(L)

[[0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0]] What happens if I execute L[1][1] = 5? [[0, 5, 0, 0], [0, 5, 0, 0], [0, 5, 0, 0], [0, 5, 0, 0]] Why?

# List comprehension and lists of lists

The correct way of initializing a list of lists is to use list comprehension (or a loop)

```
n = 4
L = [[0]*n for i in range(n)]
L[1][1] = 5
print(L)
```

[[0, 0, 0, 0], [0, 5, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0]]

#### Exercise

Given a number n, print all the possible ways to obtain it as a products of two integers. Pay attention at commutative repetitions (e.g., 4x9 and 9x4)

```
n = 36
L = []
for i in range(n+1):
    for j in range(i,n+1):
        if (i*j==n):
            L.append((i,j))
print(L)
# Through list comprehension
L = [(i,j) for i in range(n+1) for j in range(i,n+1) if i*j==n]
```

### Problem

Given a list of values, generate the sublist of values that only appear once in the list. For example, L = [1,3,2,3,5,4,5,3,3] should generate [1, 2, 4]

L = [1,3,2,3,5,4,5,3,3] SL = [n for n in L if L.count(n)==1] print(SL)

### Problem

Given a list of values, potentially with repeated values, generate the ordered sublist of values where repeated value are removed. For example, L = [1,3,2,3,5,4,5,3,3] should generate L = [1,2,3,4,5]

```
L = [1,3,2,3,5,4,5,3,3]
SL = []
for n in L:
    if (n not in SL):
        SL.append(n)
print(SL.sort())
```

### Problem

Given two lists of values (with no repetitions), generate the sublist of values that appear in both of them.

L1 = [1,7,9,3,23,11] L2 = [7,23,2,4,8,16] SL = [] for v in L1: if v in L2: SL.append(v) print(SL)
### Problem

Given two lists of ordered values, generate the sublist of values that appear in both of them. Exploit the fact that the lists are ordered.

```
A = [1, 2, 4, 8, 16, 32]
B = [4, 8, 12, 16, 20]
LS = []
a = b = 0
while (a < len(A) and b < len(B)):
    if A[a] == B[b]:
        LS.append(A[a])
         a = a+1
         b = b+1
    elif A[a] < B[b]:
         a = a + 1
    else:
         b = b+1
print(LS)
```

#### Exercise - Sudoku

Given a matrix  $9 \times 9$ , print True if the matrix is an acceptable Sodoku solution, print False otherwise.

Given the list of strings:

```
table = [
   "protein domain start end",
   "YNL275W PF00955 236 498",
   "YHR065C SM00490 335 416",
   "YKL053C-A PF05254 5 72",
   "YOR349W PANTHER 353 414",
]
```

- write a program that takes the column names from the first row of table;
- for each row creates a dictionary like this:

```
dictionary = {
    "protein": "YNL275W",
    "domain": "PF00955",
    "start": "236",
    "end":, "498"
}
```

• append each of these dictionaries to a list.

Given a long text represented as a string, compute the frequencies of each words that appear in it and store it in a dictionary that associates words to frequencies.

text = """Nel pozzo di San Patrizio c'e' una pazza che lava una pezza. Arriva un pazzo, con un pezzo di pizza e chiede alla pazza se ne vuole un pezzo. La pazza rifiuta. Allora il pazzo prende la pazza, la pezza e la pizza e li butta nel pozzo di San Patrizio, protettore dei pazzi. """