Introduction to Python

SIT training program

What is Python?

- Open source software
 - Open Source Initiative (OSI) organisation
- Interpreted language, not compiled
- High level language
- Clean syntax
- Object Oriented Programming language (OOP)
- Differences with other PLs: R
 - Syntax, speed
- Programming environments
 - Visual Studio Code
- Anaconda (Python 3.7)
 - Jupyter Notebook



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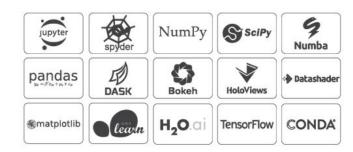
Anaconda Distribution

The World's Most Popular Python/R Data Science Platform

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The open-source Anaconda Distribution is the easiest way to perform Python/R data science and machine learning on Linux, Windows, and Mac OS X. With over 15 million users worldwide, it is the industry standard for developing, testing, and training on a single machine, enabling *individual data scientists* to:

- · Quickly download 1,500+ Python/R data science packages
- · Manage libraries, dependencies, and environments with Conda
- Develop and train machine learning and deep learning models with scikitlearn, TensorFlow, and Theano
- Analyze data with scalability and performance with Dask, NumPy, pandas, and Numba
- · Visualize results with Matplotlib, Bokeh, Datashader, and Holoviews









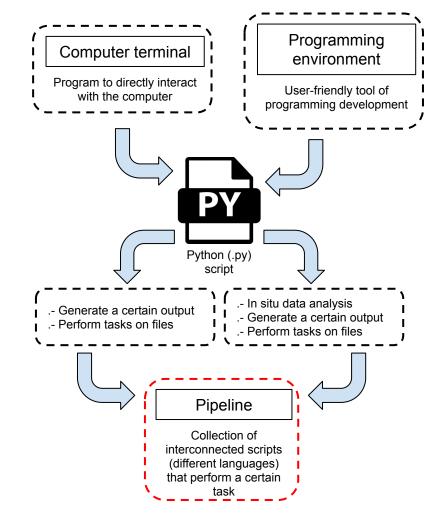
Jupyter notebook

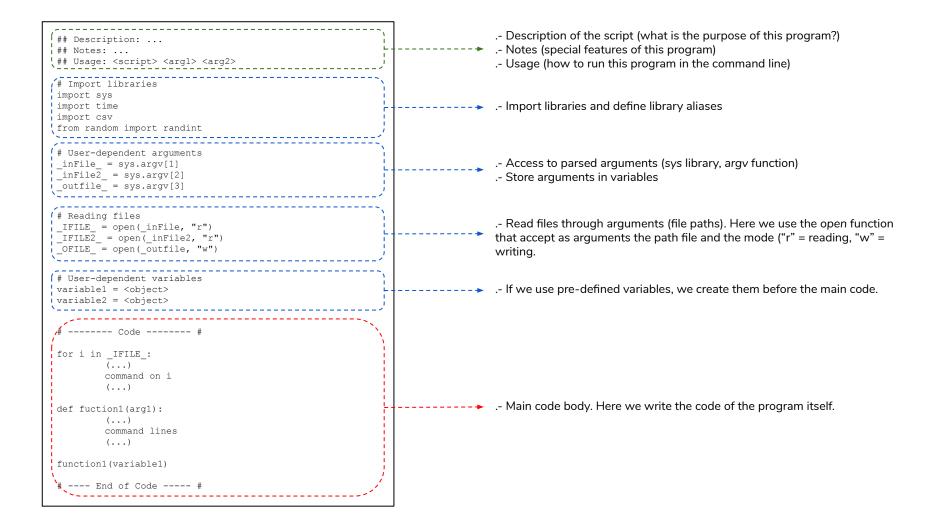
Web-based interactive development environment. Integrates Markdown and Python kernels





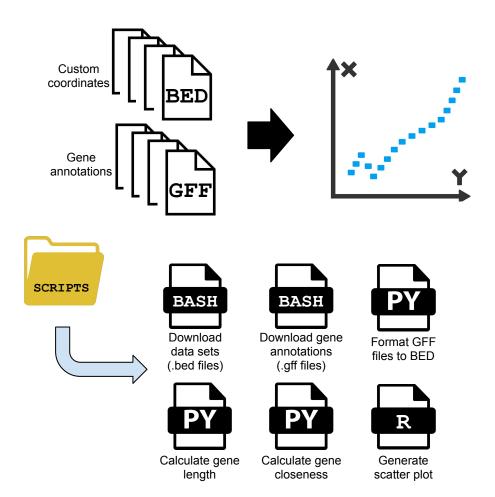
- .- In situ data analysis
- .- Teaching
- .- Electronic notebook (Markdown)

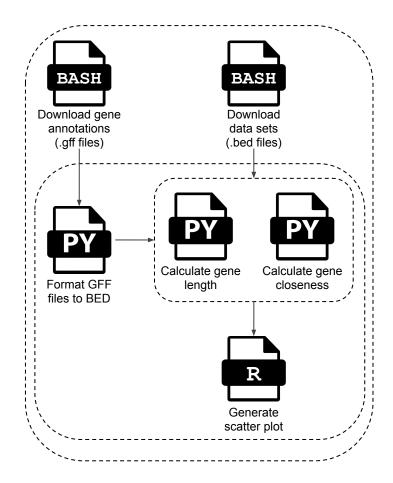




```
## Description: ...
## Notes: ...
## Usage: <script> <arg1> <arg2>
# Import libraries
import sys
import time
import csv
from random import randint
# User-dependent arguments
inFile = sys.argv[1]
inFile2 = sys.argv[2]
outfile = sys.argv[3]
# Reading files
IFILE = open( inFile, "r")
IFILE2 = open( inFile2, "r")
OFILE = open( outfile, "w")
# User-dependent variables
variable1 = <object>
variable2 = <object>
# ----- Code ----- #
for i in IFILE:
        (...)
        command on i
        (...)
def fuction1(arg1):
        ( . . . )
        command lines
        (...)
function1(variable1)
# ---- End of Code ----- #
```

```
## Script to get the distance (pair-wise) of an element in a BED file
## to the closest element in another BED file. As output
## it generates another BED file of the target elements (first file)
## plus the closest element and the distance between them.
## Usage: python <script> <input BED file> <input BED file 2> <output file name index>
import sys
import re
import csv
import math
from random import randint
 inFile=sys.argv[1]
inFile2=sys.argv[2]
outfile=sys.argv[3]+".closeness.bed"
IFILE =open( inFile, "r")
IFILE2 =open( inFile2, "r")
OFILE =open( outfile, "w")
## Calculate empirical closeness
inFileLines= IFILE .readlines()
inFileLines2= IFILE2 .readlines()
for i in range(0, len(inFileLines)):
        line=inFileLines[i].replace("\n", "").split("\t")
        chr=line[0]; start=line[1]; end=line[2]; label=line[3]; score=line[4]; strand=line
[5]; ID=line[6]
        length=int(end)-int(start)
        closeness=[]: ids=[]
       for j in range(0, len(inFileLines2)):
                line2=inFileLines2[j].replace("\n", "").split("\t")
                chr2=line2[0]; start2=line2[1]; end2=line2[2]; label2=line2[3]; score2=lin
e2[4]; strand2=line2[5]; ID2=line2[6]
                length2=int(end)-int(start)
                boundaries=[]
                if chr == chr2 and strand == strand2 and ID != ID2: # only consider same
chromosome, strand and different ids
                        boundaries.append(abs(int(start)-int(start2))); boundaries.append(a
bs(int(start)-int(end2)))
                        boundaries.append(abs(int(end)-int(end2))); boundaries.append(abs(i
nt(end)-int(start2)))
                        closeness.append(min(boundaries)); ids.append(ID2)
        if len(closeness) != 0:
                OFILE .write( chr + "\t" + start + "\t" + end + "\t" + ID + "\t" + ids[c]
oseness.index(min(closeness))| + "\t" + str(min(closeness)) + "\n")
        else:
                continue
```





How to solve a problem in programming?

- 1. What do you want to solve? **Understand** the goal of the problem, the final result.
- 2. In Object-Oriented-Programming this means: understand in **what kind of object** you want to store the result.
- 3. In order to reach that result, there is a process that goes from the input (e. arguments) to the output (result). Try to divide that process in **simple steps**. If you need to create smaller functions within the main one, do it.
- 4. Write down these steps: **pseudocode**. This is a way to describe each step: what each step does and how.
- 5. **Translate** the pseudocode into real code, line by line.
- 6. **Comment** your code!
- 7. **Try** your code with simple examples

Example 1

Exercise: Can you create a function that identifies the variant position between these two DNA sequences of the same length?

Sequence 1: CGATCGATGCTA

Sequence 2: CGATCGAGGCTA

Report the results in the following manner: CGATCGA[T/G]GCTA

Example 1: pseudocode

- 1. What do I have as inputs? Two sequences, which are the arguments of my function.
- 2. We need an empty string to store the result sequence: create segResult variable
- 3. We need to compare the elements of the sequences at each position, therefore we have to iterate through all the elements by using a loop.
- 4. We need to determine at the current position (index i) if these alleles are equal or not, therefore we perform two checks:
 - a. Check if both alleles are different
 - b. Check if both alleles are equal
- 5. At each check we do different things on the growing sequence:
 - a. If they are different, append "variant string" at the current position (i) to segResult.
 - b. If they are equal, append allele at the current position (i) to segResult.
- Once finished the sequence, provide seqResult variable.

Example 1: translate pseudocode

- What do I have as inputs? Two sequences, which are the arguments of my function.
- We need an empty string to store the result sequence: create seqResult variable
- 3. We need to compare the elements of the sequences at each position, therefore we have to iterate through all the elements by using a loop.
- 4. We need to determine at the current position (index i) if these alleles are equal or not, therefore we perform two checks:
 - a. Check if both alleles are different
 - b. Check if both alleles are equal
- 5. At each check we do different things on the growing sequence:
 - a. If they are different, append "variant string" at the current position (i) to segResult.
 - b. If they are equal, append allele at the current position (i) to segResult.
- Once finished the sequence, provide seqResult variable.

```
def variation(seq1, seq2):
      segResult = ""
      for i in range(len(seq1)):
            if seq1[i] != seq2[i]:
                  var = "["+seq1[i]+"/"+seq2[i]+"]"
                  segResult = segResult + var
            else:
                  seqResult = seqResult + seq1[i]
      return(seqResult)
```

Index												
Sequence 1	С	G	Α	Т	С	G	Α	Т	G	С	Т	Α
Sequence 2	С	G	Α	Т	С	G	Α	G	G	С	Т	Α

```
Input objects  
    sequence1 = "CGATCGATGCTA"  
    sequence2 = "CGATCGAGGCTA"
```

```
        Index
        C
        G
        A
        T
        C
        G
        A
        T
        G
        C
        T
        A

        Sequence 2
        C
        G
        A
        T
        C
        G
        A
        G
        G
        C
        T
        A
```

```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
         def variation(seq1, seq2):
               seqResult = " "
               for i in range(len(seq1)):
                     if seq1[i] != seq2[i]:
Define
                           var = "[" + seq1[i] + "/" + seq2[i] + "]"
function
                           seqResult = seqResult + var
                     else:
                           seqResult = seqResult + seq1[i]
               return(seqResult)
Call the
         result = variation(sequence1, sequence2)
function
```

Index												
Sequence 1	С	G	Α	Т	С	G	Α	Т	G	С	Т	Α
Sequence 2	С	G	Α	Т	С	G	Α	G	G	С	Т	Α
seqResult												

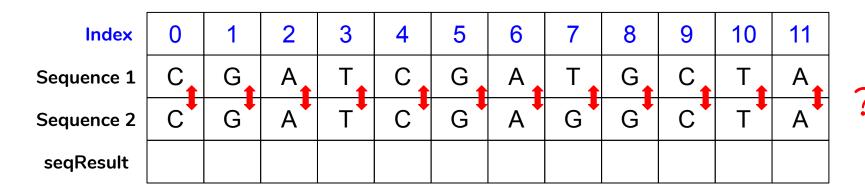
```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
         def variation(seq1, seq2):
               seqResult = " "
               for i in range(len(seq1)):
                     if seq1[i] != seq2[i]:
Define
                          var = "[" + seq1[i] + "/" + seq2[i] + "]"
function
                          seqResult = seqResult + var
                     else:
                          seqResult = seqResult + seq1[i]
               return(seqResult)
Call the
         result = variation(sequence1, sequence2)
```

```
3
                                         5
                                                          8
                                               6
                                                                9
                                                                     10
                                                                           11
    Index
                  G
                                         G
                                                          G
                        Α
                                               Α
                                                                           Α
Sequence 1
                                                     G
                  G
                                         G
                                                          G
Sequence 2
                        Α
                                               Α
                                                                           Α
seqResult
```

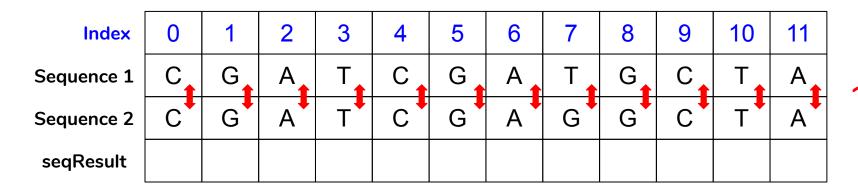
```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
         def variation(seq1, seq2):
               seqResult = " "
               for i in range(len(seq1)):
                     if seq1[i] != seq2[i]:
Define
                           var = "[" + seq1[i] + "/" + seq2[i] + "]"
function
                           seqResult = seqResult + var
                     else:
                           seqResult = seqResult + seq1[i]
               return(seqResult)
Call the
         result = variation(sequence1, sequence2)
function
```

```
3
                                          5
                                                            8
                                                6
                                                                       10
                                                                             11
    Index
                   G
                                          G
                                                Α
                                                            G
Sequence 1
                                                                             Α
                                                      G
                                          G
Sequence 2
seqResult
```

```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
         def variation(seq1, seq2):
               seqResult = " "
               for i in range(len(seq1)):
                     if seq1[i] != seq2[i]:
Define
                           var = "[" + seq1[i] + "/" + seq2[i] + "]"
function
                           seqResult = seqResult + var
                     else:
                           seqResult = seqResult + seq1[i]
               return(seqResult)
Call the
         result = variation(sequence1, sequence2)
function
```



```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
Input objects
          def variation(seq1, seq2):
                seqResult = " "
                                                    TRUE!
                for i in range(len(seq1)):
                      if seq1[i] != seq2[i]:
 Define
                            var = "[" + seq1[i] + "/" + seq2[i] + "]"
 function
                            seqResult = seqResult + var
                      else:
                            seqResult = seqResult + seq1[i]
                return(seqResult)
 Call the
          result = variation(sequence1, sequence2)
 function
```



```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
Input objects
          def variation(seq1, seq2):
                seqResult = " "
                                                   FALSE!
                for i in range(len(seq1)):
                      if seq1[i] != seq2[i]:
 Define
                           var = "[" + seq1[i] + "/" + seq2[i] + "]"
 function
                            seqResult = seqResult + var
                      else:
                            seqResult = seqResult + seq1[i]
                return (seqResult)
 Call the
          result = variation(sequence1, sequence2)
 function
```

```
3
                                         5
                                                          8
                                               6
                                                                9
                                                                     10
                                                                           11
    Index
                  G
                                         G
                                                          G
                        Α
                                               Α
                                                                           Α
Sequence 1
                                                     G
                  G
                                         G
                                                          G
Sequence 2
                        Α
                                               Α
                                                                           Α
seqResult
```

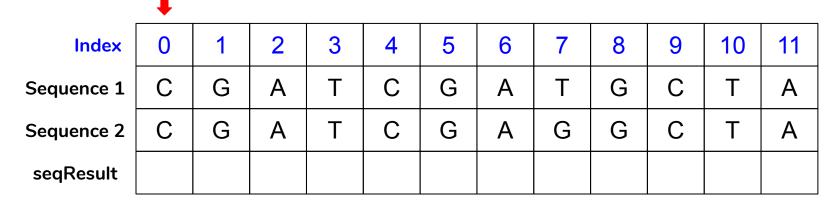
```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
         def variation(seq1, seq2):
               seqResult = " "
               for i in range(len(seq1)):
                     if seq1[i] != seq2[i]:
Define
                          var = "[" + seq1[i] + "/" + seq2[i] + "]"
function
                           seqResult = seqResult + var
                     else:
                           seqResult = seqResult + seq1[i]
               return(seqResult)
Call the
         result = variation(sequence1, sequence2)
function
```

Index	0	1	2	3	4	5	6	7	8	9	10	11
Sequence 1	С	G	А	Τ	С	G	Α	Τ	Ŋ	О	7	Α
Sequence 2	С	G	Α	Т	С	G	Α	G	G	С	Т	Α
seqResult												

```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
         def variation(seq1, seq2):
               seqResult = " "
               for i in range(len(seq1)):
                     if seq1[i] != seq2[i]:
Define
                          var = "[" + seq1[i] + "/" + seq2[i] + "]"
function
                          seqResult = seqResult + var
                     else:
                          seqResult = seqResult + seq1[i]
               return(seqResult)
Call the
         result = variation(sequence1, sequence2)
```

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

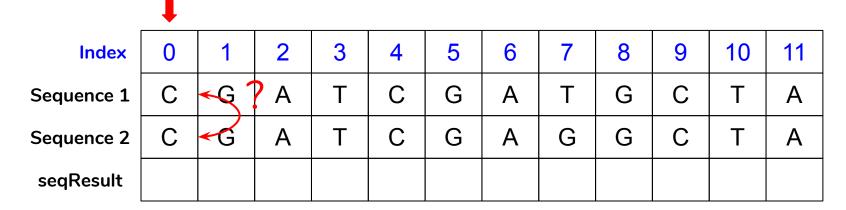


result = variation(sequence1, sequence2)

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

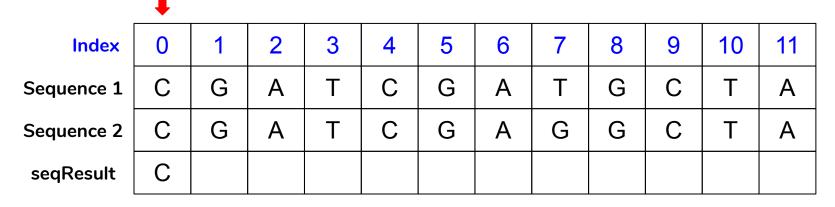


result = variation(sequence1, sequence2)

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

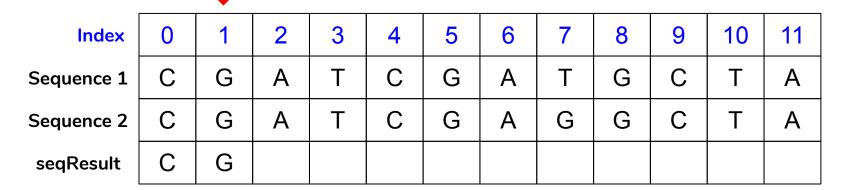


```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
Input objects
          def variation(seq1, seq2):
                seqResult = " "
                                               (iteration 1)
                for i in range(len(seq1)):
                      if seq1[i] != seq2[i]:
 Define
                            var = "[" + seq1[i] + "/" + seq2[i] + "]"
 function
                            seqResult = seqResult + var
                      else:
                            seqResult = seqResult + seq1[i]
                return (seqResult)
 Call the
          result = variation(sequence1, sequence2)
```

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

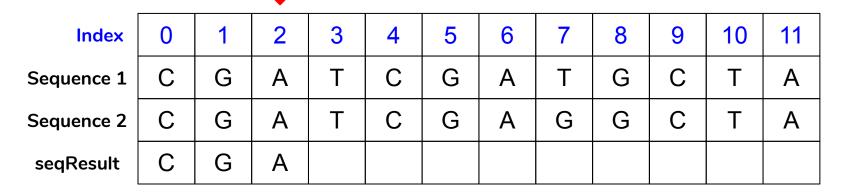


```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
Input objects
          def variation(seq1, seq2):
                seqResult = " "
                                               (iteration 2)
                for i in range(len(seq1)):
                      if seq1[i] != seq2[i]:
 Define
                            var = "[" + seq1[i] + "/" + seq2[i] + "]"
 function
                            seqResult = seqResult + var
                      else:
                            seqResult = seqResult + seq1[i]
                return (seqResult)
 Call the
          result = variation(sequence1, sequence2)
```

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

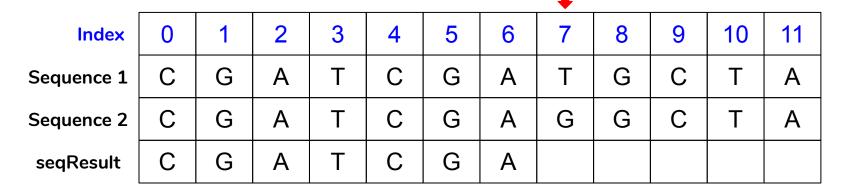


result = variation(sequence1, sequence2)

function

Environment

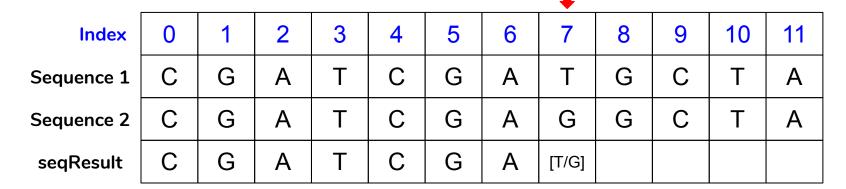
```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```



```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
Input objects
          def variation(seq1, seq2):
                 seqResult = " "
                                                 (iteration 8)
                 for i in range(len(seq1)):
                       if seq1[i] != seq2[i]:
 Define
                             var = "[" + seq1[i] + "/" + seq2[i] + "]"
 function
                             seqResult = seqResult + var
                       else:
                             seqResult = seqResult + seq1[i]
                 return (seqResult)
 Call the
           result = variation(sequence1, sequence2)
 function
```

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```



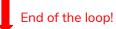
```
sequence1 = "CGATCGATGCTA"
sequence2 = "CGATCGAGGCTA"
Input objects
          def variation(seq1, seq2):
                seqResult = " "
                                                (iteration 8)
                for i in range(len(seq1)):
                       if seq1[i] != seq2[i]:
                            var = "[" + seq1[i] + "/" + seq2[i] + "]"
 Define
 function
                            seqResult = seqResult + var
                      else:
                            seqResult = seqResult + seq1[i]
                return (seqResult)
 Call the
          result = variation(sequence1, sequence2)
```

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

```
seqResult =
"CGATCGA[T/G]"
i = 7
```



Index	0	1	2	3	4	5	6	7	8	9	10	11
Sequence 1	С	G	Α	Η	С	G	Α	7	G	С	Т	Α
Sequence 2	С	G	Α	Т	С	G	Α	G	G	С	Т	Α
seqResult	С	G	Α	Т	С	G	Α	[T/G]	G	С	Т	Α

result = variation(sequence1, sequence2)

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
```

```
seqResult =
"CGATCGA[T/G]GCTA"
i = 11
```

Index	0	1	2	3	4	5	6	7	8	9	10	11
Sequence 1	С	Ŋ	А	Η	С	G	Α	Т	G	С	7	Α
Sequence 2	С	G	Α	Т	С	G	Α	G	G	С	Т	Α
seqResult	С	G	Α	Т	С	G	Α	[T/G]	G	С	Т	Α

```
Input objects  

sequence1 = "CGATCGATGCTA"

sequence2 = "CGATCGAGGCTA"

def variation(seq1, seq2):
    seqResult = " "
    for i in range(len(seq1)):
        if seq1[i] != seq2[i]:
            var = "[" + seq1[i] + "/" + seq2[i] + "]"
            seqResult = seqResult + var
        else:
            seqResult = seqResult + seq1[i]

return(seqResult)

Call the
```

result = variation(sequence1, sequence2)

function

Environment

```
sequence1 = "CGAT..."
sequence2 = "CGAT..."
variation
result
```

```
seqResult =
"CGATCGA[T/G]GCTA"
i = 11
```

Example 2

Exercise: Write a function that counts the number of occurrences of a certain subsequence (e. "ATG") in a longer sequence.

Sequence 1: CGATCGATGCTA

Example 2: pseudocode

- 1. What do I have as inputs? One sequence and one subsequence (arguments of my function).
- 2. Our goal is to count occurrences, which means that our result will be an integer. This is a growing number, therefore we need to initialize an integer variable.
- 3. We go through the sequence (iterable) in order to see all the possible subsequences. We use a loop.
- 4. At each position (i) of the sequence we obtain a chunk of length equal to the subsequence.
- 5. At each chunk that we extract from the sequence, we test if is equal to the subsequence we are testing.
 - a. If the chunk is equal to the subsequence, our result variable (integer) grows by 1.
 - b. If not, we continue looking for occurrences.

Index	0	1	2	3	4	5	6	7	8	9	10	11
Sequence	С	G	Α	Т	С	G	Α	Т	G	С	Т	A

Subsequence: ATG

Example 3

Exercise: Given a sorted list of numbers $test_list$, try to find the index of a certain number $test_number$ within that list. Here we are going to make use of a binary search algorithm (methodology of **divide and conquer**).

test_list: [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20]

test_number: 8

- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem

test element = 5



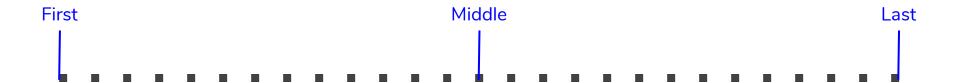
- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem

test element = 5

First Last

- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem

test element = 5



- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem

```
test element = 5

5 == Middle? FALSE!

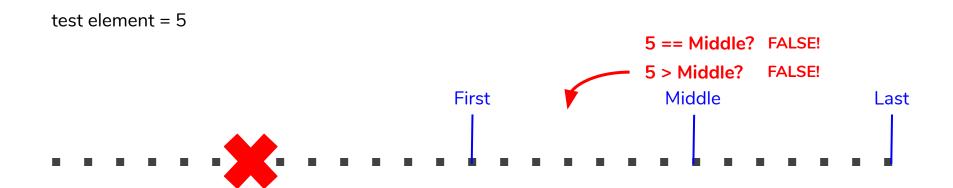
5 > Middle? TRUE!

First

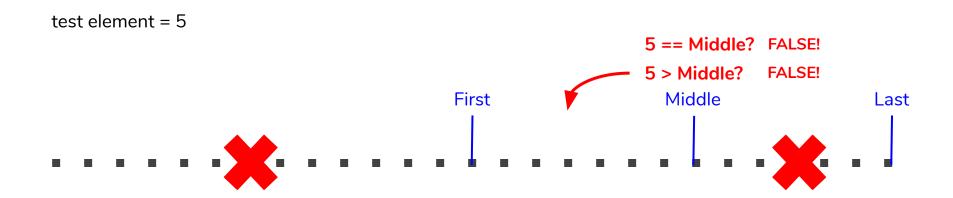
Middle

Last
```

- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem



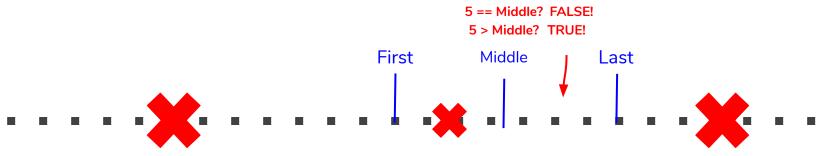
- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem





- 1. Break down a problem into two or more subproblems
- 2. Subproblems are easier to solve
- 3. Combination of subproblem results solve the global problem

test element = 5



Example 3: pseudocode

- 1. What do I have as inputs? One numeric list and the number I want to find
- 2. Since the beginning we need to use three variables in order to compare our number with the middle number: the index of the first element of the list, the last index and the index of the number we want to find.
 Why do we need this last one?
- 3. Each time we are choosing between the upper/lower half of the list where to look for our number. However, the first and the last indexes of these lists must be always like first <= last. What happens when we finally reach a list of two numbers? What is the middle number of this list?
- 4. We need to find the element in the middle of the list. We use the indexes to find it (first+last/2).
- 5. We have to check if our number is equal to the number in the middle. In this check we have two possibilities:
 - a. Our number is equal to the middle number. We can return the index!
 - b. Our number is different to the middle number. Then we have to **update** (change) the extreme indexes (first or last) in order to take the upper or lower half list. How?
 - i. If our number is lower than the middle number, the last index is equal to the middle index minus 1
 - ii. Else (our number is higher than the middle number), the first index is equal to the middle index plus 1

Example 3: pseudocode

- 1. What do I have as inputs? One numeric list and the number I want to find
- 2. Since the beginning we need to use three variables in order to compare our number with the middle number: the index of the first element of the list, the last index and the index of the number we want to find.
 Why do we need this last one?
- 3. Each time we are choosing between the upper/lower half of the list where to look for our number. However, the first and the last indexes of these lists must be always like first <= last. What happens when we finally reach a list of two numbers? What is the middle number of this list?

Index

List

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20