Scientific Programming Practical 10

Introduction

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Ex 6

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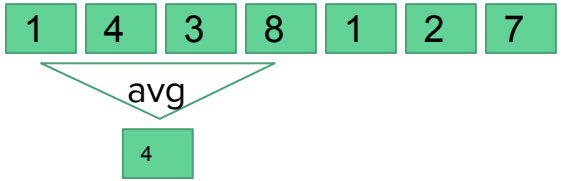

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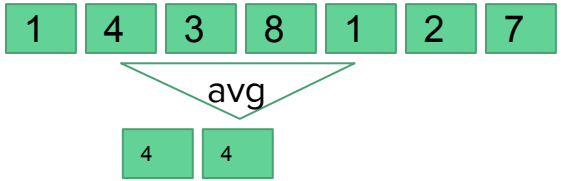

[4. 4. 3.5 4.5]

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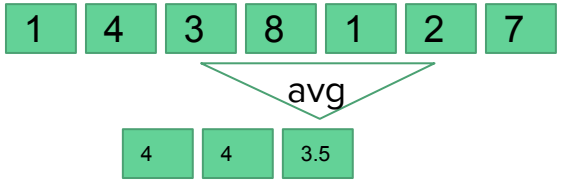

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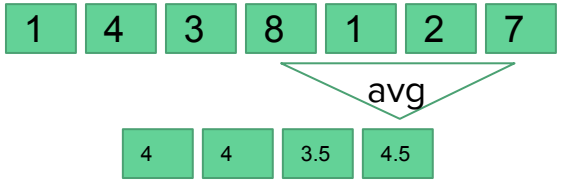

Cumulative sum:

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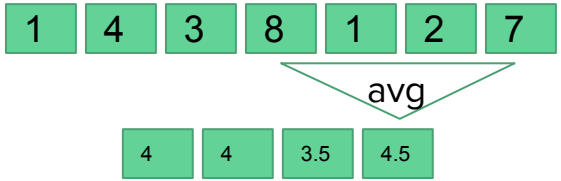

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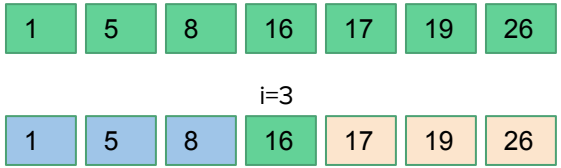

Clever bit: when we move to the right with the window we need to disregard (i.e. subtract) the blue elements one after the other

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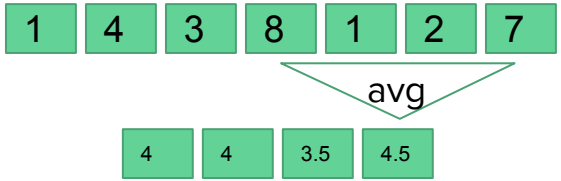

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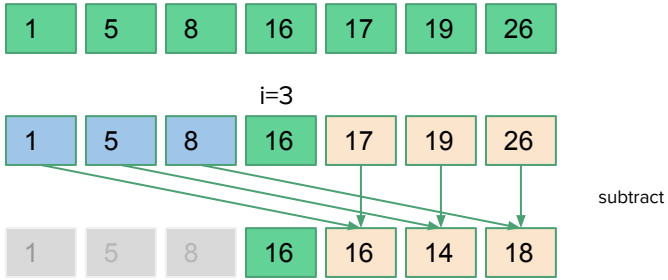

Clever bit: when we move to the right with the window we need to disregard (i.e. subtract) the blue elements one after the other
Let's subtract them after the starting point (i=3)

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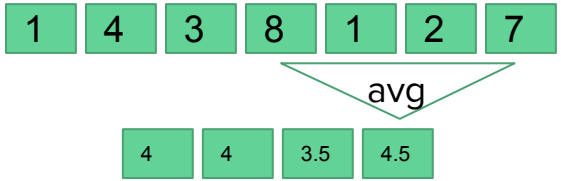
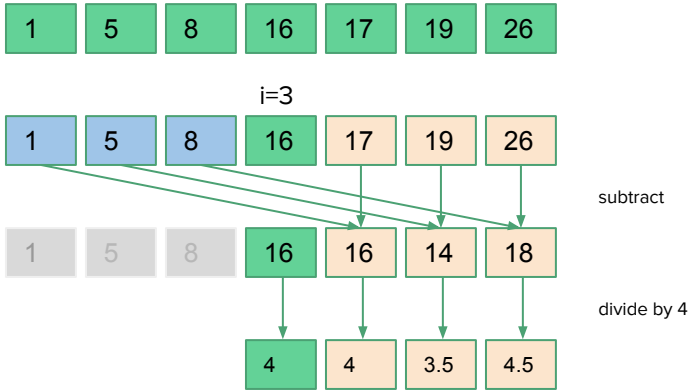


Cumulative sum:



Clever bit: when we move to the right with the window we need to disregard (i.e. subtract) the blue elements one after the other

Let's subtract them after the starting point (i=3)

Finally, let's compute the mean value (i.e. divide by 4)

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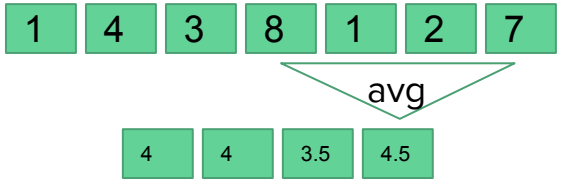
```python
def movingAvg(v, n):
    """computes the moving average of n values in the array v"""
    cs = np.cumsum(v)
    #print(cs)
    #print("\t",cs[n:])
    #print("\t", cs[:-n])
    cs[n:] = cs[n:] - cs[:-n]
    #print("CS:", cs)
    return cs[n - 1:] / n
```

Example:



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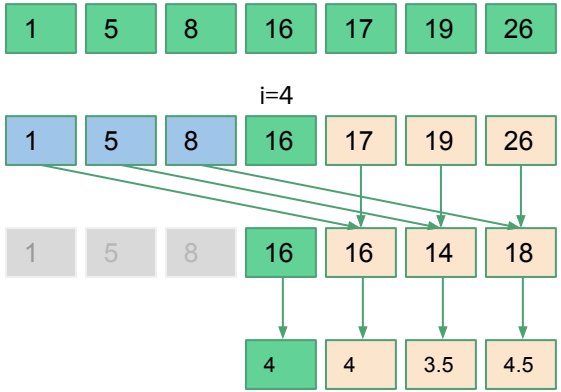


```python
X = np.arange(0, 5, 0.005)
#B = np.random(100)
B = np.sin(2*np.pi*X)

#Let's add random numbers uniformly distributed in [0,1)
B += np.random.random_sample(1000)
#B += np.random.rand(1000)
C = movingAvg(B,5)
D = movingAvg(B,10)
E = movingAvg(B,50)
#X = np.arange(0,B.shape[0])

plt.plot(X,B)
plt.title("No moving average")
plt.show()
plt.close()
plt.plot(np.arange(0,C.shape[0]),C)
plt.title("Window size: 5")
plt.show()
plt.close()
plt.title("Window size: 10")
plt.plot(np.arange(0,D.shape[0]),D)
plt.show()
plt.close()
plt.title("Window size: 50")
plt.plot(np.arange(0,E.shape[0]),E)
plt.show()
```

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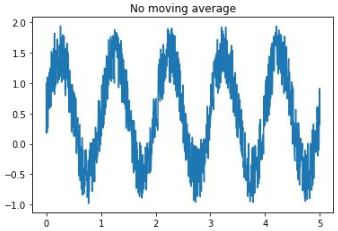

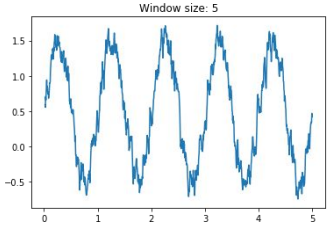

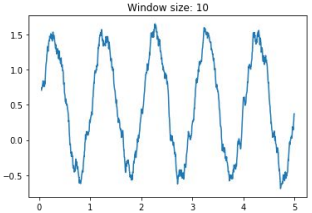

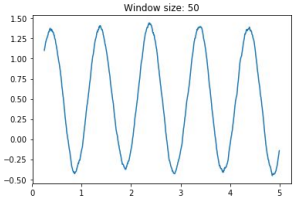


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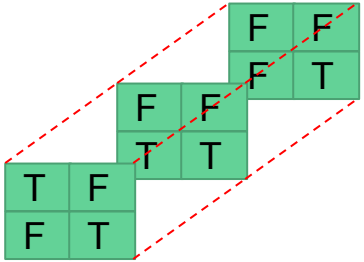
D = movingAvg(B,10)
E = movingAvg(B,50)
#X = np.arange(0,B.shape[0])

plt.plot(X,B)
plt.title("No moving average")
plt.show()
plt.close()
plt.plot(X[4:],C) # X has 1000- 5 -1 elements
plt.title("Window size: 5")
plt.show()
plt.close()
plt.title("Window size: 10")
plt.plot(X[9:],D) # X has 1000- 9 -1 elements
plt.show()
plt.close()
plt.title("Window size: 50")
plt.plot(X[49:],E) # X has 1000- 49 -1 elements
plt.show()
```

Axis on 3D arrays




```
vals:
[[[ True False]
  [False  True]]

 [[False False]
  [ True  True]]

 [[False False]
  [False  True]]]

The matrix is 3D
First matrix:
[[ True False]
 [False  True]]

First row, all matrices:
[[ True False]
 [False False]
 [False False]]

Second column, all matrices:
[[False  True]
 [False  True]
 [False  True]]
```

```python
import numpy as np

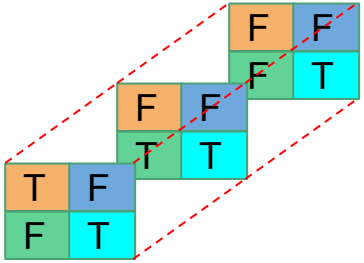
v1 = [[True, False],[False, True]]
v2 = [[False, False],[True, True]]
v3 = [[False, False], [False, True]]
print("vals:")
vals = np.array([v1,v2,v3])
print(vals)
print("\nThe matrix is {}D".format(vals.ndim))
print("First matrix:")
print(vals[0,:,:])
print("\nFirst row, all matrices:")
print(vals[:,0,:])
print("\nSecond column, all matrices:")
print(vals[:,:,1])

print("\nAXIS=0")
print("ANY:")
print(np.any(vals, axis=0))
print("ALL ")
print(np.all(vals, axis=0))

print("\nAXIS=1")
print("ANY:")
print(np.any(vals, axis=1))
print("ALL:")
print(np.all(vals, axis=1))

print("\nAXIS=2")
print("ANY:")
print(np.any(vals, axis=2))
print("ALL:")
print(np.all(vals, axis=2))
```

Axis on 3D arrays



axis = 0

```
AXIS=0
ANY:
[[ True False]
 [ True  True]]
ALL
[[False False]
 [False  True]]
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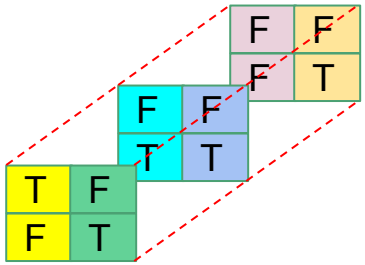
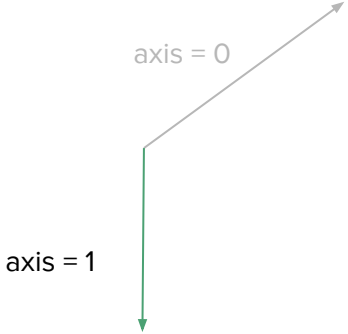
print("\nAXIS=2")
print("ANY:")
print(np.any(vals, axis=2))
print("ALL:")
print(np.all(vals, axis=2))
```

Axis on 3D arrays




```
AXIS=1
ANY:
[[ True  True]
 [ True  True]
 [False  True]]
ALL:
[[False False]
 [False False]
 [False False]]
```

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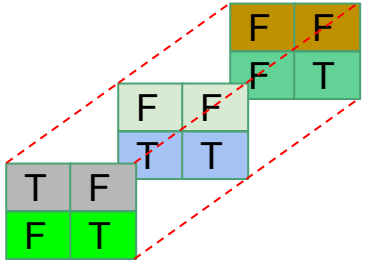
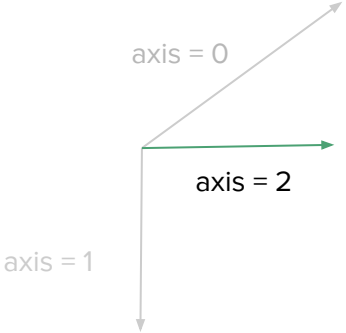



```
AXIS=2
ANY:
[[ True  True]
 [False  True]
 [False  True]]
ALL:
[[False False]
 [False  True]
 [False False]]
```

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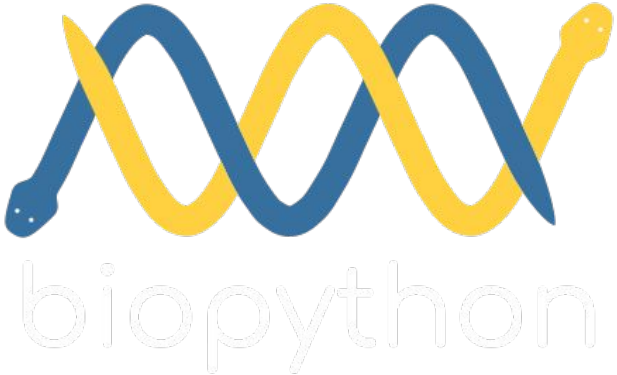
print("ALL:")
print(np.all(vals, axis=1))

print("\nAXIS=2")
print("ANY:")
print(np.any(vals, axis=2))
print("ALL:")
print(np.all(vals, axis=2))
```

Biopython



The Biopython Project is an international association of developers of freely available **Python tools for computational molecular biology**.

The goal of Biopython is to make it as easy as possible to use **Python for bioinformatics** by creating high-quality, reusable modules and classes.

https://biopython.org/wiki/Documentation

Biopython

Biopython:

1. Provides tools to **parse several common bioinformatics formats** (e.g. FASTA, FASTQ, BLAST, PDB, Clustalw, Genbank,..).

2. Provides an **interface towards biological data repositories** (e.g. NCBI, Expasy, Swiss-Prot,..)

3. Provides an **interface towards some bioinformatic tools** (e.g. clustalw, MUSCLE, BLAST,…)

4. **Implements some tools** like pairwise alignment **and data structures** to deal with biological data.

More material at:

http://biopython.org/DIST/docs/tutorial/Tutorial.pdf

Seq objects

Seq objects are more powerful than strings to deal with sequences and are defined in the module **Bio.Seq**.

They are **immutable objects**. The mutable version is **MutableSeq**.

```
from Bio.Seq import Seq

s = Seq("GATTACATAATA")
dna_seq = Seq("GATTATACGTAC")
print("S:", s)

print("dna_seq:", dna_seq)


my_prot = Seq("MGNAAAAKKGSEQE")
print("my_prot:", my_prot)
```

```
S: GATTACATAATA
dna_seq: GATTATACGTAC
my_prot: MGNAAAAKKGSEQE
```

Seq objects

Seq objects behave like strings.

In the latest release the description of the Alphabet associated to the sequence has been dropped therefore there is no consistency check...

```
from Bio.Seq import Seq

dna_seq = Seq("GATTATACGTAC")
my_prot = Seq("MGNAAAAKKGSEQE")


#Does it really make sense though?!?
print(dna_seq + my_prot)
```

```
GATTATACGTACMGNAAAAKKGSEQE
```

Seq objects

Seq objects behave like strings, but the consistency of the alphabet is checked too.

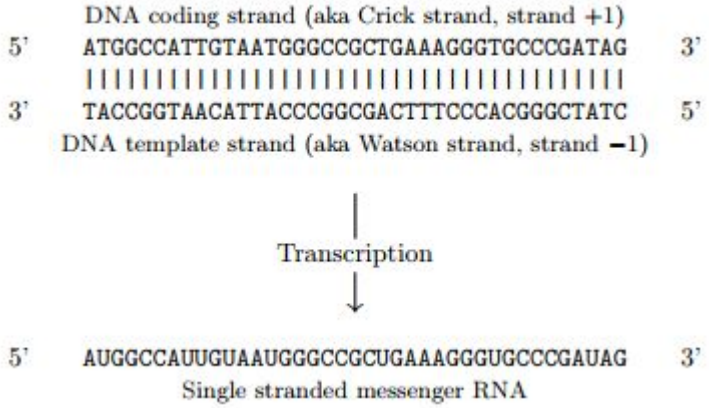
We can loop through the elements of the sequence and perform slicing...

```python
from Bio.Seq import Seq

dna_seq = Seq("GATTATACGTACGGCTA")

for base in dna_seq:
    print(base, end = " ")

print("")

sub_seq = dna_seq[4:10]
print(sub_seq)

#Let's reverse the string:

print("Reversed: ", dna_seq[::-1])
#from Seq to string:
dna_str = str(dna_seq)
print("As string:", dna_str)
print(type(dna_str))
```

```
G A T T A T A C G T A C G G C T A
ATACGT
Reversed:  ATCGGCATGCATATTAG
As string: GATTATACGTACGGCTA
<class 'str'>
```

Seq objects

Biopython provides several methods working on Seq objects
(remember Seq are immutable!)



General methods (return **int** and **Seq** objects):

`Seq.count(s)` : counts the number of times s appears in the sequence;
`Seq.upper()` : makes the sequence of the object Seq in upper case
`Seq.lower()` : makes the sequence of the object Seq in lower case

Only for DNA/RNA (return **Seq** objects):

`Seq.complement()` to complement the sequence
`Seq.reverse_complement()` to reverse complement the sequence.
`Seq.transcribe()` transcribes the DNA into mRNA
`Seq.back_transcribe()` back transcribes mRNA into DNA
`Seq.translate()` translates mRNA or DNA into proteins

Other functions are in **SeqUtils**
(ex. use from Bio.SeqUtils import molecular_weight**):**

`SeqUtils.GC(Seq)` computes GC content
`SeqUtils.molecular_weight(Seq)` computes the molecular weight of the seq
….

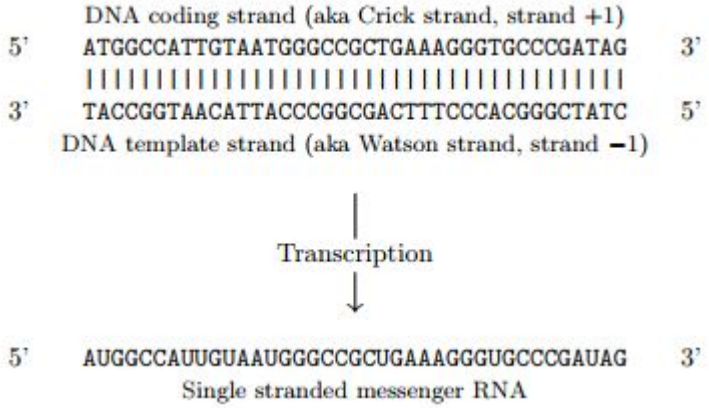
Check out: http://biopython.org/DIST/docs/api/

Seq objects

Biopython provides several methods working on Seq objects
(remember Seq are immutable!)

```python
from Bio.Seq import Seq

my_seq = Seq("GATCGATGGGCCTATATAGGATCGAAAATCGC")

print("Original sequence:\t{}".format(my_seq) )
comp  = my_seq.complement()
print("")
print("Complement:\t\t{}".format(comp))
print("")
revcomp = my_seq.reverse_complement()
print("Reverse complement:\t{}".format(revcomp))
```

```
Original sequence:      GATCGATGGGCCTATATAGGATCGAAAATCGC

Complement:             CTAGCTACCCGGATATATCCTAGCTTTTAGCG

Reverse complement:     GCGATTTTCGATCCTATATAGGCCCATCGATC
```



Check out: http://biopython.org/DIST/docs/api/

Seq objects

Biopython provides several methods working on Seq objects
(remember Seq are immutable!)

```python
from Bio.Seq import Seq

coding_dna = Seq("ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG")
print(coding_dna)

mrna = coding_dna.transcribe()
print(mrna)
print("")
print("... and back")
print(mrna.back_transcribe())
print("")
print("Translation to protein:")
prot = mrna.translate()
print(prot)
print("")
print("Up to first stop:")
print(mrna.translate(to_stop = True))
print("")
print("Mitocondrial translation: (TGA is W!)")
mit_prot = mrna.translate(table=2)
print(mit_prot)
#The following produces a translation error!
#print("RE-Translated protein: {}".format(prot.translate()))
```

```
ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG
AUGGCCAUUGUAAUGGGCCGCUGAAAGGGUGCCCGAUAG

... and back
ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG

Translation to protein:
MAIVMGR*KGAR*

Up to first stop:
MAIVMGR

Mitocondrial translation: (TGA is W!)
MAIVMGRWKGAR*
```

Sequence annotations

The **SeqRecord** object is used to store annotations associated to sequences. They might provide:

1. `SeqRecord.seq` : the sequence (the Seq object)
2. `SeqRecord.id` : the identifier of the sequence, typically an accession number
3. `SeqRecord.name` : a "common" name or identifier sometimes identical to the accession number
4. `SeqRecord.description` : a human readable description of the sequence
5. `SeqRecord.letter_annotations` : a per letter annotation using a restricted dictionary (e.g. quality)
6. `SeqRecord.annotations` : a dictionary of unstructured annotation (e.g. organism, publications,...)
7. `SeqRecord.features` : a list of SeqFeature objects with more structured information (e.g. genes pos).
8. `SeqRecord.dbxrefs` : a list of database cross references.

Sequence annotations

Read a fasta file NC005816.fna containing the whole sequence for Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1 and retrieve some information about the sequence.

```
>gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence
TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGGGGGTAATCTGCTCTCC
TGATTCAGGAGAGTTTATGGTCACTTTTGAGACAGTTATGGAAATTAAAATCCTGCACAAGCAGGGAATG
AGTAGCCGGGCGATTGCCAGAGAACTGGGGATCTCCCGCAATACCGTTAAACGTTATTTGCAGGCAAAAT
CTGAGCCGCCAAAATATACGCCGCGACCTGCTGTTGCTTCACTCCTGGATGAATACCGGGATTATATTCG
TCAACGCATCGCCGATGCTCATCCTTACAAAATCCCGGCAACGGTAATCGCTCGCGAGATCAGAGACCAG
GGATATCGTGGCGGAATGACCATTCTCAGGGCATTCATTCGTTCTCTCTCGGTTCCTCAGGAGCAGGAGC
CTGCCGTTCGGTTCGAAACTGAACCCGGACGACAGATGCAGGTTGACTGGGGCACTATGCGTAATGGTCG
CTCACCGCTTCACGTGTTCGTTGCTGTTCTCGGATACAGCCGAATGCTGTACATCGAATTCACTGACAAT
ATGCGTTATGACACGCTGGAGACCTGCCATCGTAATGCGTTCCGCTTCTTTGGTGGTGTGCCGCGCGAAG
TGTTGTATGACAATATGAAAACTGTGG....
```

https://www.ncbi.nlm.nih.gov

https://www.ncbi.nlm.nih.gov/nuccore/NC_005816

NCBI Resources How To

Nucleotide | Nucleotide | NC005816

Advanced

Learn more about upcoming changes to the Nucleotide, EST, and GSS databases.

GenBank Send to:

Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence

NCBI Reference Sequence: NC_005816.1

FASTA Graphics

Go to:

```
LOCUS       NC_005816               9609 bp    DNA     circular CON 11-JAN-2018
DEFINITION  Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete
            sequence.
ACCESSION   NC_005816
VERSION     NC_005816.1
DBLINK      BioProject: PRJNA224116
            BioSample: SAMN02602970
            Assembly: GCF_000007885.1
KEYWORDS    RefSeq.
SOURCE      Yersinia pestis biovar Microtus str. 91001
  ORGANISM  Yersinia pestis biovar Microtus str. 91001
            Bacteria; Proteobacteria; Gammaproteobacteria; Enterobacterales;
            Yersiniaceae; Yersinia.
REFERENCE   1  (bases 1 to 9609)
  AUTHORS   Zhou,D., Tong,Z., Song,Y., Han,Y., Pei,D., Pang,X., Zhai,J., Li,M.,
            Cui,B., Qi,Z., Jin,L., Dai,R., Du,Z., Wang,J., Guo,Z., Wang,J.,
            Huang,P. and Yang,R.
  TITLE     Genetics of metabolic variations between Yersinia pestis biovars
```

Sequence annotations

Read a fasta file NC005816.fna containing the whole sequence for Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1 and retrieve some information about the sequence.

```
ID: gi|45478711|ref|NC_005816.1|
Name: gi|45478711|ref|NC_005816.1|
Description: gi|45478711|ref|NC_005816.1| Yersinia
pestis biovar Microtus str. 91001 plasmid pPCP1,
complete sequence
Number of features: 0
Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGAT
CCAGG...CTG', SingleLetterAlphabet())

Sequence [first 30 bases]:
TGTAACGAACGGTGCAATAGTGATCCACAC

The id:
gi|45478711|ref|NC_005816.1|

The description:
gi|45478711|ref|NC_005816.1| Yersinia pestis biovar
Microtus str. 91001 plasmid pPCP1, complete sequence

The record is a:  <class 'Bio.SeqRecord.SeqRecord'>
```

```python
from Bio import SeqIO

record =
SeqIO.read("file_samples/NC_005816.fna",
"fasta")

print(record)
print("")
print("Sequence [first 30 bases]:")
print(record.seq[0:30])
print("")
print("The id:")
print(record.id)
print("")
print("The description:")
print(record.description)
print("")
print("The record is a: ", type(record))
```

SeqIO.parse

The `Bio.SeqIO` module aims to provide a simple way to work with several different sequence file formats

The method `Bio.SeqIO.parse` is used to parse some sequence data into a **SeqRecord iterator**. In particular, the basic syntax is:

```
SeqRecordIterator = Bio.SeqIO.parse(filename, file_format)
```

where `filename` is typically an open handle to a file and `file_format` is a lower case string describing the file format. Possible options include **fasta, fastq-illumina, abi, ace, clustal...** all the

Note that `Bio.SeqIO.parse` returns an iterator, therefore it is possible to manually fetch one SeqRecord after the other with the `next(iterator)` method.

Formats available:
https://biopython.org/wiki/SeqIO

WARNING: When dealing with very large FASTA or FASTQ files, the overhead of working with all these objects can make scripts too slow. In this case `SimpleFastaParser` and `FastqGeneralIterator` parsers might be better as they return just a tuple of strings for each record.

SeqIO

Example: Let's read the first 3 entries of the .fasta file contigs82.fasta printing off the length of the sequence and the first 50 bases of each sequence followed by "...".

```
from Bio import SeqIO

seqIterator = SeqIO.parse("file_samples/contigs82.fasta", "fasta")

labels = ["1st","2nd","3rd"]
for l in labels:
    seqRec = next(seqIterator)
    print(l, "entry:")
    print(seqRec.id, " has size ", len(seqRec.seq))
    print(seqRec.seq[:50]+"...")
    print("")
```

SeqIO.parse returns an iterator, we can get the next element with next(iterator)

```
1st entry:
MDC020656.85  has size  2802
GAGGGGTTTAGTTCCTCATACTCGCAAAGCAAAGATACATAAATTTAGAA...

2nd entry:
MDC001115.177  has size  3118
TGAATGGTGAAAATTAGCCAGAAGATCTTCTCCACACATGACATATGCAT...

3rd entry:
MDC013284.379  has size  5173
TATCGTTTCCTCTGAGTAGAATATCGTTATAACAAGATTTTTTTTTTCCT...
```

Do you remember all the “pain” to parse the header, concatenate the sequence etc... ?

SeqIO

With SimpleFastaParser...

```
labels = ["1st","2nd","3rd"]

with open("file_samples/contigs82.fasta") as cont_handle:
    for l in labels:
        ID, seq  = next(SimpleFastaParser(cont_handle))

        print(l, "entry:")
        print(ID, " has size ", len(seq))
        print(seq[:50]+"...")
        print("")
```

```
1st entry:
MDC020656.85  has size  2802
GAGGGGTTTAGTTCCTCATACTCGCAAAGCAAAGATACATAAATTTAGAA...

2nd entry:
MDC013284.379  has size  5173
TATCGTTTCCTCTGAGTAGAATATCGTTATAACAAGATTTTTTTTTTCCT...

3rd entry:
MDC018185.241  has size  23761
AAAACGAGGAAAATCCATCTTGATGAACAGGAGATGCGGAGGAAAAAAAT...
```

SeqIO

The module `Bio.SeqIO` also has three different ways to allow random access to elements:

1. `Bio.SeqIO.to_dict(file_handle/iterator)` : builds a dictionary of all the SeqRecords keeping them in memory and allowing modifications to the records. **This potentially uses a lot of memory but is very fast;**
2. `Bio.SeqIO.index(filename,file_type)` : builds a sort of read-only dictionary, parses the elements into SeqRecords on demand (i.e. it returns an iterator!). **This method is slower, but more memory efficient;**
3. `Bio.SeqIO.index_db(indexName.idx,filenames, file_format)` : builds a read-only dictionary, but stores ids and offsets on a SQLite3 database. **It is slower but uses less memory.**

Examples are given on the notes of the practical sheet

SeqIO.write

The module `Bio.SeqIO` provides also a way to write sequence records to files in various formats (like fasta, fastq, genbank, pfam…)

SeqRecords can be written out to files by using

```
N = Bio.SeqIO.write(records,out_filename, file_format)
```

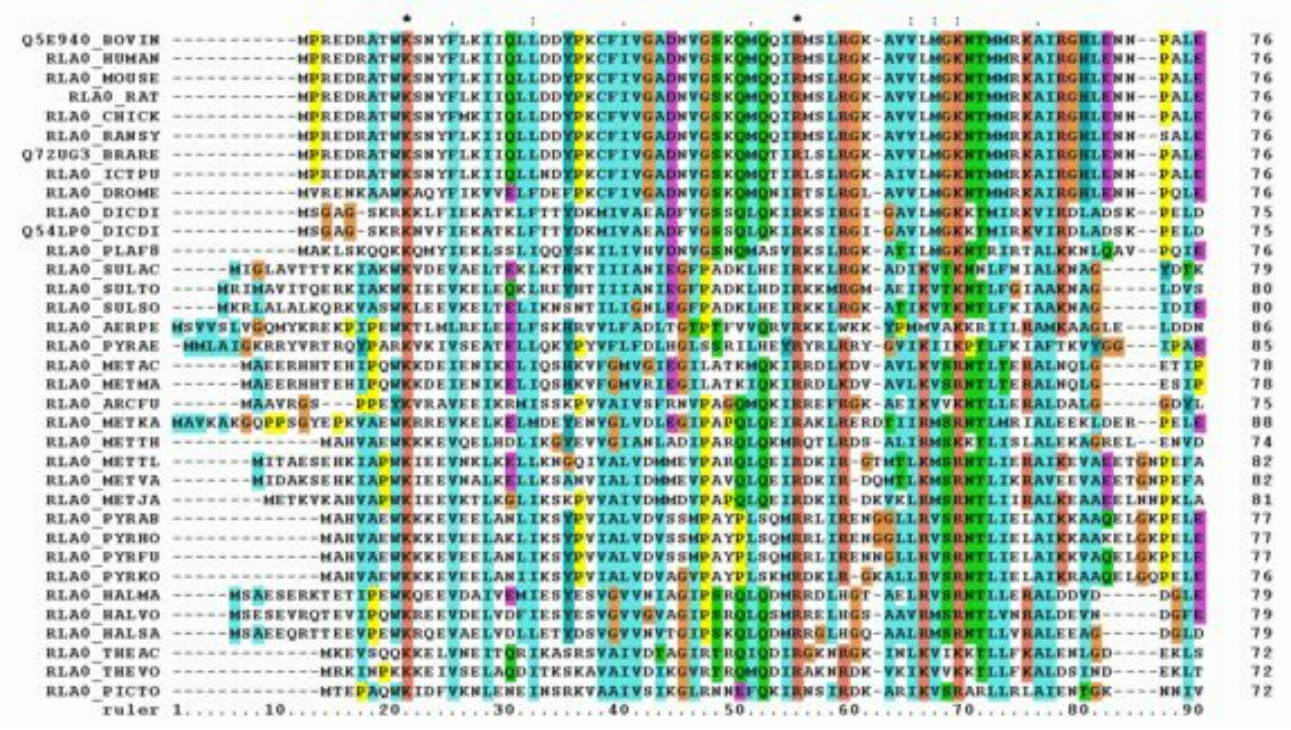
where **records** is a list of the SeqRecords to write, **out_filename** is the string with the filename to write and **file_format** is the format of the file to write. **N** is the number of sequences written.

WARNING: If you write a file that is already present, `SeqIO.write` will just rewrite it without telling you.

Examples are given on the notes of the practical sheet

Multiple sequence alignment

Multiple Sequence Alignments are a collection of **multiple sequences which have been aligned together** – usually with the insertion of gap characters, and addition of leading or trailing gaps – such that all the sequence strings have the same length.



In Biopython, each row is a `SeqRecord` object and alignments are stored in an object `MultipleSeqAlignment`

Parsing MSAs: AlignIO

The basic syntax of the two functions:

```
Bio.AlignIO.parse(file_handle, alignment_format)
Bio.AlignIO.read(file_handle, alignment_format)
```

where `file_handle` is the handler to the opened file, while the `alignment_format` is a lower case string with the alignment format (e.g. fasta, clustal, stockholm, mauve, phylip,...).

```
from Bio import AlignIO

alignments = AlignIO.read("file_samples/PF02171_seed.sth", "stockholm")


for align in alignments:
    start = align.annotations["start"]
    end = align.annotations["end"]
    seq = align.seq
    desc = align.description
    dbref = ",".join([x for x in align.dbxrefs])
    print("{} S:{} E:{}".format(desc, start, end))
    if(len(dbref) > 0):
        print(dbref)
    print("{}".format(seq))
    print("")
```

```
AGO1_SCHPO/500-799 S:500 E:799
YLFFILDK-NSPEP-YGSIKRVCNTMLGVPSQCAISKHILQS---------KPQYCANLGMKINVKVGGIN-CSLIPKSNP----L

AGO6_ARATH/541-851 S:541 E:851
FILCILPERKTSDI-YGPWKKICLTEEGIHTQCICPIKI------------SDQYLTNVLLKINSKLGGIN-SLLGIEYSYNIPLI

AGO4_ARATH/577-885 S:577 E:885
FILCVLPDKKNSDL-YGPWKKKNLTEFGIVTQCMAPTRQPND-----------QYLTNLLLKINAKLGGLN-SMLSVERTPAFTVI

TAG76_CAEEL/660-966 S:660 E:966
CIIVVLQS-KNSDI-YMTVKEQSDIVHGIMSQCVLMKNVSRP---------TPATCANIVLKLNMKMGGIN--SRIVADKITNKYL
```

The function `Bio.AlignIO.parse()` returns an iterator of `MultipleSeqAlignment` objects that is a collection of `SeqRecords`.

Each `SeqRecord` contains several information like the **ID, Name, Description, Number of features, start, end** and **sequence**.

In the frequent case that we have to deal with a **single multiple alignment** we will have to use the `Bio.AlignIO.read()` function.

Writing and converting MSAs

Biopython provides a function `Bio.AlignIO.write()` to write alignments to file

and

`Bio.AlignIO.convert()` to convert one format into the other (provided that all information needed for the second format is available)

```
N = Bio.AlignIO.write(alignments,outfile,file_format)
```

where `alignments` are a MultipleSeqAlignment object with the alignments to write to the output file with name `outfile` that has format `file_format` (a low case string with the file format). N is the number of entries written to the file.

Ex.

```
my_alignments = [align1, align2, align3]
N = AlignIO.write(my_alignments, "file_samples/my_malign.phy", "phylip")
```

```
Bio.AlignIO.convert(input_file, input_file_format, output_file, output_file_format)
```

basically by passing the input file name and format and output file name and format.

Ex:

```
Bio.AlignIO.convert("PF05371_seed.sth", "stockholm", "PF05371_seed.aln", "clustal")
```

Example: Convert the seed alignment of the Piwi (PF02171) family stored in the pfam (stockholm) format PF02171_seed.sth into phylip format. Print some stats on the data.

```
N. of seq: 16
Len of seq: 395
1 multiple alignments converted to phylip
```

```
# STOCKHOLM 1.0
#=GS AGO1_SCHPO/500-799    AC O74957.1
#=GS AGO6_ARATH/541-851    AC O48771.2
#=GS AGO4_ARATH/577-885    AC Q9ZVD5.2
#=GS TAG76_CAEEL/660-966   AC P34681.2
#=GS O16720_CAEEL/566-867  AC O16720.2
#=GS O62275_CAEEL/594-924  AC O62275.1
#=GS YQ53_CAEEL/650-977    AC Q09249.1
#=GS NRDE3_CAEEL/673-1001  AC Q21691.1
#=GS Q17567_CAEEL/397-708  AC Q17567.1
#=GS AUB_DROME/555-852     AC O76922.1
#=GS PIWI_DROME/538-829    AC Q9VKM1.1
#=GS PIWL1_HUMAN/555-847   AC Q96J94.1
#=GS PIWI_ARCFU/110-406    AC O28951.1
#=GS PIWI_ARCFU/110-406    DR PDB; 2W42 B; 110-406;
#=GS PIWI_ARCFU/110-406    DR PDB; 1YTU B; 110-406;
#=GS PIWI_ARCFU/110-406    DR PDB; 2BGG B; 110-406;
#=GS PIWI_ARCFU/110-406    DR PDB; 1W9H A; 110-406;
#=GS PIWI_ARCFU/110-406    DR PDB; 2BGG A; 110-406;
#=GS PIWI_ARCFU/110-406    DR PDB; 1YTU A; 110-406;
#=GS PIWI_ARCFU/110-406    DR PDB; 2W42 A; 110-406;
#=GS Y1321_METJA/426-699   AC Q58717.1
#=GS O67434_AQUAE/419-694  AC O67434.1
#=GS O67434_AQUAE/419-694  DR PDB; 1YVU A; 419-694;
#=GS O67434_AQUAE/419-694  DR PDB; 2F8S A; 419-694;
#=GS O67434_AQUAE/419-694  DR PDB; 2F8T A; 419-694;
#=GS O67434_AQUAE/419-694  DR PDB; 2F8S B; 419-694;
#=GS O67434_AQUAE/419-694  DR PDB; 2NUB A; 419-694;
#=GS O67434_AQUAE/419-694  DR PDB; 2F8T B; 419-694;
#=GS AGO10_ARATH/625-946   AC Q9XGW1.1
AGO1_SCHPO/500-799
YLFFILDK.NSPEP.YGSIKRVCNTMLGVPSQCAISKHILQS........KPQYCANLGMKINVKVGGIN.CSLIPKSNP....LGNVPTL.........ILGGDVYHPG\
AGO6_ARATH/541-851
FILCILPERKTSDI.YGPWKKICLTEEGIHTQCICPIKI...........SDQYLTNVLLKINSKLGGIN.SLLGIEYSYNIPLINKIPTL.........ILGMDVSHGPF
AGO4_ARATH/577-885
FILCVLPDKKNSDL.YGPWKKKNLTEFGIVTQCMAPTRQPND..........QYLTNLLLKINAKLGGLN.SMLSVERTPAFTVISKVPTI.........ILGMDVSHGSF
TAG76_CAEEL/660-966
CIIVVLQS.KNSDI.YMTVKEQSDIVHGIMSQCVLMKNVSRP........TPATCANIVLKLNMKMGGIN..SRIVADKITNKYLVDQPTM.........VVGIDVTHPT(
O16720_CAEEL/566-867
LIVVVLPG..KTPI.YAEVKRVGDTVLGIATQCVQAKNAIRT........TPQTLSNLCLKMNVKLGGVN.SILLPNVRPR...IFNEPVI.........FLGCDITHPA/
O62275_CAEEL/594-924
TFVFIITD.DSITT.LHQRYKMIEKDTKMIVQDMKLSKALSV..IN...AGKRLTLENVINKTNVKLGGSN..YVFVDAKKQL.....DSHL.........IIGVGISAPP/
```

```
from Bio import AlignIO

alignments = AlignIO.read("file_samples/PF02171_seed.sth", "stockholm")

out = AlignIO.convert("file_samples/PF02171_seed.sth",
                      "stockholm",
                      "file_samples/PF05371_seed.aln",
                      "clustal")

print("N. of seq: {}\nLen of seq: {}".format(
                                            len(alignments),
                                            len(alignments[0])))
print("{} multiple alignments converted to phylip".format(out))
```

```
CLUSTAL X (1.81) multiple sequence alignment


AGO1_SCHPO/500-799                  YLFFILDK-NSPEP-YGSIKRVCNTMLGVPSQCAISKHILQS--------
AGO6_ARATH/541-851                  FILCILPERKTSDI-YGPWKKICLTEEGIHTQCICPIKI-----------
AGO4_ARATH/577-885                  FILCVLPDKKNSDL-YGPWKKKNLTEFGIVTQCMAPTRQPND--------
TAG76_CAEEL/660-966                 CIIVVLQS-KNSDI-YMTVKEQSDIVHGIMSQCVLMKNVSRP--------
O16720_CAEEL/566-867                LIVVVLPG--KTPI-YAEVKRVGDTVLGIATQCVQAKNAIRT--------
O62275_CAEEL/594-924                TFVFIITD-DSITT-LHQRYKMIEKDTKMIVQDMKLSKALSV--IN---A
YQ53_CAEEL/650-977                  DILVGIAR-EKKPD-VHDILKYFEESIGLQTIQLCQQTVDKMMGG----Q
NRDE3_CAEEL/673-1001                TIVFGIIA-EKRPD-MHDILKYFEEKLGQQTIQISSETADKFMRD----H
Q17567_CAEEL/397-708                MLVVMLAD-DNKTR-YDSLKKYLCVECPIPNQCVNLRTLAGKSKDGGENK
AUB_DROME/555-852                   IVMVVMRS-PNEEK-YSCIKKRTCVDRPVPSQVVTLKVIAPRQQKP---T
PIWI_DROME/538-829                  LILCLVPN-DNAER-YSSIKKRGYVDRAVPTQVVTLKTTKNRSL------
PIWL1_HUMAN/555-847                 IVVCLLSS-NRKDK-YDAIKKYLCTDCPTPSQCVVARTLGKQQT------
PIWI_ARCFU/110-406                  GIMLVLPE-YNTPL-YYKLKSYLINS--IPSQFMRYDILSNRNL------
Y1321_METJA/426-699                 CFALIIGKEKYKDNDYYEILKKQLFDLKIISQNILWENWRKDDK------
O67434_AQUAE/419-694                LVIVFLEEYPKVDP-YKSFLLYDFVKRELLKKMIPSQVILNRTLKN---E
AGO10_ARATH/625-946                 LLLAILPD-NNGSL-YGDLKRICETELGLISQCCLTKHVFKI--------

AGO1_SCHPO/500-799                  -KPQYCANLGMKINVKVGGIN-CSLIPKSNP----LGNVPTL--------
```

Manipulating/writing MSA

It is possible to slice alignments using the [] operator applied on a `SeqRecord`.

Think about it as a matrix

1. `SeqRecord[i,j]` returns the jth character of alignment i as a string;
2. `SeqRecord[:,j]` returns all the jth characters of the multiple alignment as a string;
3. `SeqRecord[:,i:j]` returns a MultipleSeqAlignment with the sub-alignments going for i to j (excluded)
4. `SeqRecord[a:b,i:j]` similar to 3. but for alignments going from a to b (excluded) only

```
YLFFILDK-NSPEP-YGSIKLVPPVYYAHLVSNLARYQDV
FILCILPERKTSDI-YGPWKIVAPVRYAHLAAAQVAQFTK
FILCVLPDKKNSDL-YGPWKVVAPICYAHLAAAQLGTFMK
CIIVVLQS-KNSDI-YMTVKIPTPVYYADLVATRARCHVK
LIVVVLPG--KTPI-YAEVKIPAPAYYAHLVAFRARYHLV
TFVFIITD-DSITT-LHQRYLPTPLYVANEYAKRGRNLWN
DILVGIAR-EKKPD-VHDILVPDVLYAAENLAKRGRNNYK
TIVFGIIA-EKRPD-MHDILIPNVSYAAQNLAKRGHNNYK
MLVVMLAD-DNKTR-YDSLKVPAPCQYAHKLAFLTAQSLH
IVMVVMRS-PNEEK-YSCIKVPAVCHYAHKLAFLVAESIN
LILCLVPN-DNAER-YSSIKVPAVCQYAKKLATLVGTNLH
IVVCLLSS-NRKDK-YDAIKVPAPCQYAHKLAFLVGQSIH
GIMLVLPE-YNTPL-YYKLKLPVTVNYPKLVAGIIANVNR
CFALIIGKEKYKDNDYYEILIPAPIHYADKFVKALGKNWK
LVIVFLEEYPKVDP-YKSFLLPATVHYSDKITKLMLRGIE
LLLAILPD-NNGSL-YGDLKIVPPAYYAHLAAFRARFYLE
```

align[0,0] is Y
align[2,1] is I
align[:,0] is YFFCLTDTMILIGCLL

align[:,0:3] gets first 3 rows (SeqRecords)
YLFFILDK-N...
FILCILPERK…
FILCVLPDK…

align[0:3,0:3] first 3 cols of first 3 rows (SeqRecords):
YLF
FIL
FIL

Pairwise alignment

Biopython has its own module to make pairwise alignment. It provides two algorithms: Smith-Waterman for **local alignment** and Needleman-Wunsch for **global alignment**. These methods are implemented in two Biopython functions of the `Bio.pairwise2` module:

```
pairwise2.align.globalxx()
pairwise2.align.localxx()
```

```
aligns = pairwise2.align.globalxx(seq1,seq2)
aligns = pairwise2.align.localxx(seq1,seq2)
```

where seq1 and seq2 are two `str` objects. These methods return a list of alignments (at least one) that have the same **optimal score**. Each alignment is represented as tuples with the following 5 elements in order:

1. The alignment of the first sequence;
2. The alignment of the second sequence;
3. The alignment score;
4. The start of the alignment (for global alignments this is always 0);
5. The end of the alignment (for global alignments this is always the length of the alignment).

```
Example:
alignments = pairwise2.align.globalxx("ACCGTTATATAGGCCA", "ACGTACTAGTATAGGCCA")
for i in range(len(alignments)):
    print(alignments[i])

('ACCGT--TA-TATAGGCCA', 'A-CGTACTAGTATAGGCCA', 15.0, 0, 19)
('ACCGT--TA-TATAGGCCA', 'AC-GTACTAGTATAGGCCA', 15.0, 0, 19)
```

Pairwise alignment

OPTIONS FOR MATCHES/MISMATCHES
AND GAP OPENS/EXTENSIONS

```
pairwise2.align.globalxx
pairwise2.align.globalmx
pairwise2.align.globalms
pairwise2.align.globalmd
pairwise2.align.globalxd
pairwise2.align.globalxs
pairwise2.align.localxx
pairwise2.align.localmx
pairwise2.align.localms
pairwise2.align.localmd
pairwise2.align.localxd
pairwise2.align.localxs
```

Match parameters can be:

- `x` : means that a match scores 1 a mismatch 0;
- `m` : the match and mismatch score are passed as additional params after the sequence (es. `aligns = pairwise2.align.globalmx(seq1,seq2, 1, -1)` to set 1 as match score and -1 as mismatch penalty.

Gap parameters can be:

- `x` : gap penalty is 0;
- `s` : same gap open and gap extend penalties for the 2 sequences (passed as additional params after seqs).
- `d` : different gap open and gap extend penalties for the 2 seqs (additional params after the seqs).

The first letter is **the score for a match**
the second letter is **the penalty for a gap**

Pairwise alignment

Example. Let's perform the alignment of the two sequences "ACCGTTATATAGGCCA" and "ACGTACTAGTATAGGCCA"

```
('ACCGT--TA-TATAGGCCA', 'A-CGTACTAGTATAGGCCA', 15.0, 0, 19)
('ACCGT--TA-TATAGGCCA', 'AC-GTACTAGTATAGGCCA', 15.0, 0, 19)

Looping through aligns
ACCGT--TA-TATAGGCCA
A-CGTACTAGTATAGGCCA
Score: 15.0, Start: 0, End: 19

ACCGT--TA-TATAGGCCA
AC-GTACTAGTATAGGCCA
Score: 15.0, Start: 0, End: 19


Match: 1, Mismatch: -1, Gap open: -0.5, Gap extend: -0.2
ACCGT--TA-TATAGGCCA
A-CGTACTAGTATAGGCCA
Score: 13.3, Start: 0, End: 19

ACCGT--TA-TATAGGCCA
AC-GTACTAGTATAGGCCA
Score: 13.3, Start: 0, End: 19
```

```python
from Bio import pairwise2
from Bio import SeqIO


alignments = pairwise2.align.globalxx("ACCGTTATATAGGCCA",
                                      "ACGTACTAGTATAGGCCA")

for i in range(len(alignments)):
    print(alignments[i])

print("")
print("Looping through aligns")
for align in alignments:
        print(align[0])
        print(align[1])
        print("Score: {}, Start: {}, End: {}".format(align[2],
                                                     align[3],
                                                     align[4]))

        print("")

alignments = pairwise2.align.globalms("ACCGTTATATAGGCCA",
                                      "ACGTACTAGTATAGGCCA",
                                      1,-1,-0.5,-0.2)
print("")
print("Match: 1, Mismatch: -1, Gap open: -0.5, Gap extend: -0.2")
for align in alignments:
    print(align[0])
    print(align[1])
    print("Score: {}, Start: {}, End: {}".format(align[2],
                                                 align[3],
                                                 align[4]))

    print("")
```

http://biopython.org

biopython

Python Tools for Computational Molecular Biology

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Biopython version 1.78

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Biopython

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Introduction

Biopython is a set of freely available tools for biological computation written in Python by an international team of developers.

It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics. The source code is made available under the Biopython License, which is extremely liberal and compatible with almost every license in the world.

We are a member project of the Open Bioinformatics Foundation (OBF), who take care of our domain name and hosting for our mailing list etc. The OBF used to host our development repository, issue tracker and website but these are now on GitHub.

This page will help you download and install Biopython, and start using the libraries and tools.

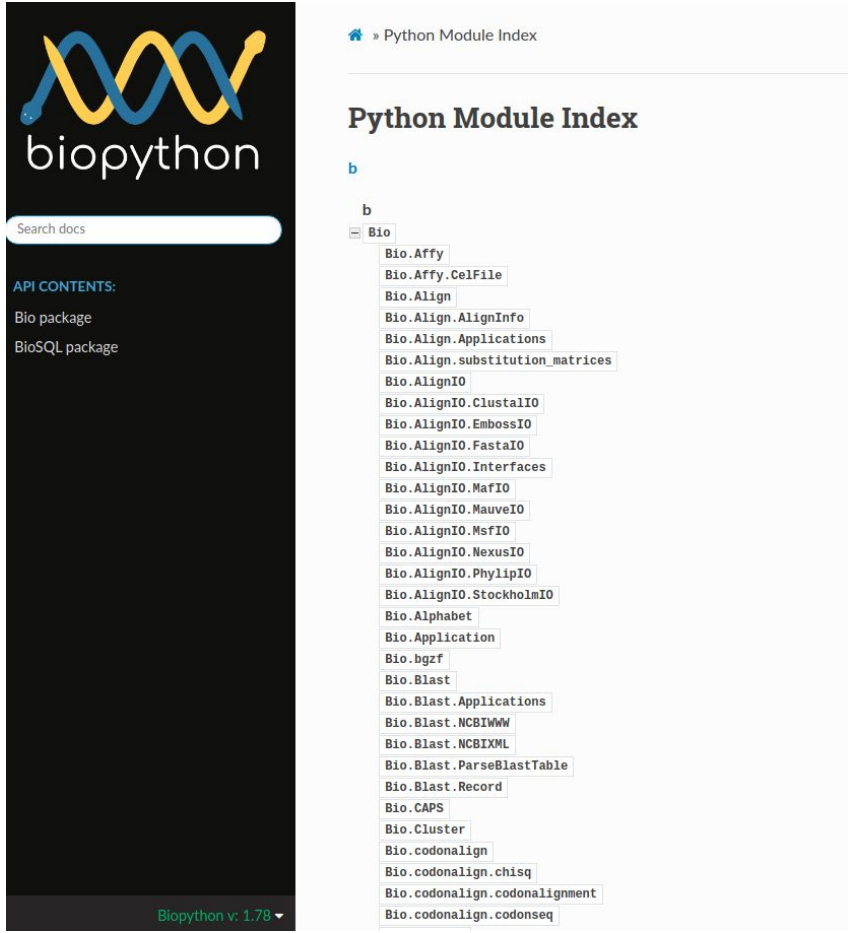
Get Started	Get help	Contribute
Download Biopython	Tutorial (PDF)	What's being worked on
Main README	Documentation on this wiki	Developing on Github
	Cookbook (working examples)	Google Summer of Code
	Discuss and ask questions	Report bugs

The latest release is Biopython 1.78, released on 4 September 2020.

https://biopython.org/docs/1.78/api/py-modindex.html

Check:

Seq
SeqRecord
MultipleSeqAlignment



Installing biopython

```
import Bio
```

```
---------------------------------------------------------------------------
ImportError                               Traceback (most recent call last)
<ipython-input-1-f227b1b7f7f3> in <module>()
----> 1 import Bio

ImportError: No module named 'Bio'
```

In windows installing Biopython should be as easy as opening the command prompt as admininstrator (typing `cmd` and then right clicking on the link choosing run as admininstrator) and then `pip3 install biopython`.

In linux `sudo pip3 install biopython` will install biopython for python3 up to python3.5. On python 3.6, the command is: `python3.6 -m pip install biopython`.

http://qcbsciprolab2020.readthedocs.io/en/latest/practical10.html

Exercises

1. Write a python function that reads a genebank file given in input and prints off the following information:
    1. Identifier, name and description;
    2. The first 100 characters of the sequence;
    3. Number of external references (dbxrefs) and ids of the external refs.
    4. The name of the organism (hint: check the annotations dictionary at the key "organism")
    5. Retrieve and print all (if any) associated publications (hint: annotation dictionary, key:"references")
    6. Retrieve and print all the locations of "CDS" features of the sequence (hint: check the features)

Hint: go back and check the details of the `SeqRecord` object.

Test the program downloading some files from genebank like this

Show/Hide Solution

2. Write a python program that loads a pfam file (stockholm format .sth) and reports for each record of the alignment:
    1. the id of the entry
    2. the start and end points
    3. the number of gaps and the % of gaps on the total length of the alignment
    4. the number of external database references (dbxrefs), and the first 3 external references comma separated (hint: use join).

Print these information to the screen. Finally, write this information in a tab separated file (.tsv) having the following format: `#ID\tstart\tend\tnum_gaps\tpercentage_gaps\tdbxrefs`.