Python course in Bioinformatics

by Katja Schuerer and Catherine Letondal

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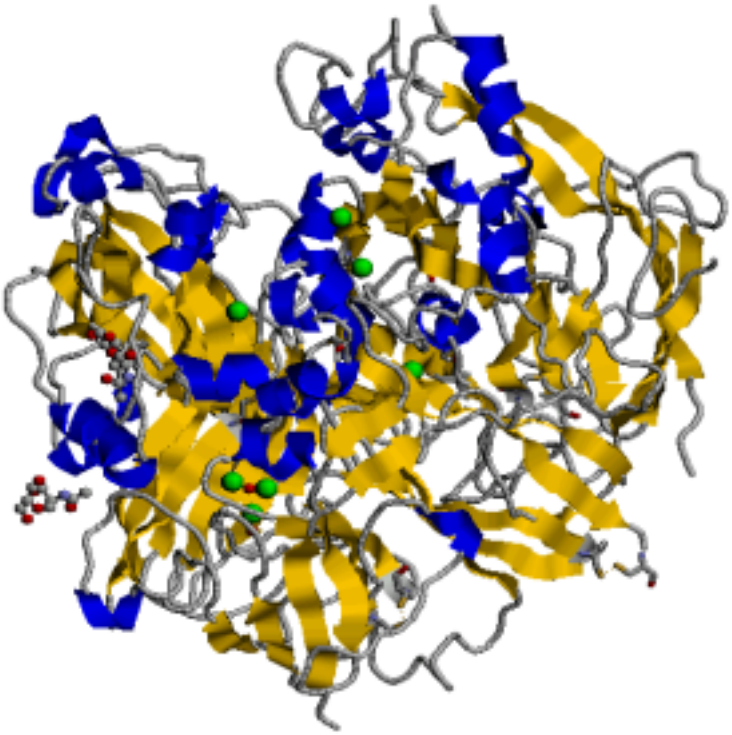
Introduction to Python [http://www.python.org/] and Biopython [http://www.biopython.org/] with biological examples.



The picture above represents the 3D structure of the Human Ferroxidase [http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-id+4SU6q1IomZ3+-e+[SWALL:'CERU_HUMAN']] protein, that we use in some of the exercises in this course.

This course is designed for biologists who already have some programming knowledge, in other languages such as perl or C. For this reason, while presenting a substantial introduction to the Python language, it does not constitute an introduction to programming itself (as [Tis2001] or our course in informatics for biology [http://www.pasteur.fr/formation/infobio/infobio-en.html], with an online programming course [http://www.pasteur.fr/formation/infobio/python/] in Python). What distinguishes this course from general Python introductory courses, is however the important focus on biological examples that are used throughout the course, as well as the suggested exercises drawn from the field of biology. The second half of the course describes the Biopython (http://www.biopython.org/) set of modules. This course can be considered a complement to the Biopython tutorial, and what's more often refers to it, by bringing practical exercises using these components.

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Comments are welcome.

PDF version of this course [support.pdf]

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Chapter 1. General introduction

1.1. Running Python

There are several ways to run Python code:

1. from the interpreter:

```
>>> dna = 'gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg'
>>> dna
'gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg'
```

2. from a file:
   If file `mydna.py` contains:

```
#! /local/bin/python

dna = 'gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg'
print dna
```

   it can be executed from the command line:

```
caroline:~> python mydna.py
gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg
```

   or using the `#!` notation:

```
caroline:~> ./mydna.py
gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg
```

   It is also possible to execute files during an interactive interpreter session:

```
caroline:~> python
Python 2.2.1c1 (#1, Mar 27 2002, 13:20:02)
[GCC 2.95.4  (Debian prerelease)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> execfile('mydna.py')
gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg
```

   or to load a file from the command line before entering Python in interactive mode (-i):

```
caroline:~> python -i mydna.py
gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg
>>>
```

this is very convenient when your Python file contains definitions (functions, classes,...) that you want to test interactively.

3. from other programs embedding the Python interpreter:

```
#include <Python.h>

int main(int argc, char** argv) {

  Py_Initialize();
  PyRun_SimpleString("dna = 'atgagag' + 'tagagga'");
  PyRun_SimpleString("print 'Dna is:', dna");

  return 0;
}
```

1.2. Documentation

1.2.1. General informations

General informations about Python and BioPython can be found:

- on the Python [http://www.python.org] home page
- in the Python tutorial [http://www.python.org/doc/2.2.1/tut/tut.html] written by Guido van Rossum, the author of the Python language.
- in “The Python - Essential Reference” book ([Beaz2001]) - a compact but understandable reference guide
- on the BioPython [http://www.biopython.org] home page
- in the BioPython tutorial (PDF [http://www.bioinformatics.org/bradstuff/bp/tut/Tutorial.pdf], HTML [http://www.bioinformatics.org/bradstuff/bp/tut/Tutorial.html])

1.2.2. Getting information

There are several ways to obtain documentation within the Python environment:

- from the command line using the **pydoc** command
- by the `help()` function during an interactive interpreter session

The **pydoc** command and the `help()` function provided with a string argument search the `PYTHONPATH` for an object of this name. But the `help()` function can also be applied directly on an object.

```
>>> def ambiguous_dna_alphabet():
...     " returns a string containing all ambiguous dna bases "
...     return "bdhkmnrsuvwxy"
...
>>> help('ambiguous_dna_alphabet')                                    ❶
no Python documentation found for 'ambiguous_dna_alphabet'

>>> help(ambiguous_dna_alphabet)
Help on function ambiguous_dna_alphabet in module __main__:

ambiguous_dna_alphabet()
     returns a string containing all ambiguous dna bases
```

❶ `ambiguous_dna_alphabet` is not defined in a module on the `PYTHONPATH`.

- by the function `dir(obj)` which displays the names defined in the local namespace (see Section 4.3.1) of the object `obj`. If no argument is specified `dir` shows the definitions of the current module.

```
>>> dir()
['__builtins__', '__doc__', '__name__']

>>> dna = 'atgacgatagacataga'
>>> dir(dna)
['__add__', '__class__', '__contains__', '__delattr__', '__eq__',
'__ge__', '__getattribute__', '__getitem__', '__getslice__', '__gt__',
'__hash__', '__init__', '__le__', '__len__', '__lt__', '__mul__',
'__ne__', '__new__', '__reduce__', '__repr__', '__rmul__', '__setattr__',
'__str__', 'capitalize', 'center', 'count', 'decode', 'encode',
'endswith', 'expandtabs', 'find', 'index', 'isalnum', 'isalpha',
'isdigit', 'islower', 'isspace', 'istitle', 'isupper', 'join', 'ljust',
'lower', 'lstrip', 'replace', 'rfind', 'rindex', 'rjust', 'rstrip',
'split', 'splitlines', 'startswith', 'strip', 'swapcase', 'title',
'translate', 'upper']
```

```
>>> dir()
['__builtins__', '__doc__', '__name__', 'dna']
```

1.2.3. Making documentation

If the first statement of a module, class or function is a string, it is used as the documentation which can be accessed by the `__doc__` attribute of the object. The `__doc__` attribute contains the raw documentation string whereas the `help()` function prints it in a human readable format.

```
>>> ambiguous_dna_alphabet.__doc__
' returns a string containing all ambiguous dna bases '

>>> help(ambiguous_dna_alphabet)
Help on function ambiguous_dna_alphabet in module __main__:

ambiguous_dna_alphabet()
     returns a string containing all ambiguous dna bases
```

If a string is enclosed by triple quotes or triple double-quotes it can span several lines and the line-feed characters are retained in the string.

1.3. Working environment

1.3.1. Emacs

Python provides an editing mode for emacs, which will be automatically loaded if the following lines are present in the `.emacs` file.

```
(autoload 'python-mode "python-mode" "Python editing mode." t)
(setq auto-mode-alist
      (cons '("\\.py$" . python-mode) auto-mode-alist))
(setq interpreter-mode-alist
      (cons '("python" . python-mode)
            interpreter-mode-alist))
```

Whithin this emacs mode, from the "Python" menu, you can start an interactive interpreter session or (re)execute the python buffer, functions and classes definitions.

Important

The python-mode is very useful because it resolves indentation problems occurring if tab and space characters are mixed (see Section 3.1.2).

Caution

You can copy-paste a block of correct indented code into an interactive interpreter session. But take care, that the block does not contain empty lines.

Chapter 2. Introduction to basic types in Python

2.1. Strings

We are going to start the introduction to strings with some examples of DNA manipulations. Execute the following lines in the Python interpreter and look at the results:

Example 2.1. Introduction to strings

```
>>> dna = 'gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg'
>>> dna
'gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg'

>>> dnasuite = 'cctttacttcgcctccgcgccctgcattccgttcctggcctcg'
>>> dna = dna + dnasuite
>>> dna
'gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctgggcctttactt
cgcctccgcgccctgcattccgttcctggcctcg'

>>> from string import *                                                    ❶

>>> len(dna)
103
>>> 'n' in dna
0
>>> count(dna, 'a')
10
>>> replace(dna, 'a', 'A')
'gcAtgAcgttAttAcgActctgtcAcgccgcggtgcgActgAggcgtggcgtctgctgggcctttActt
cgcctccgcgccctgcAttccgttcctggcctcg'
```

❶ This will be explained later (Section 9.1).

Exercise 2.1. GC content

Calculate the GC percent of `dna`. (Solution A.1)

Exercise 2.2. DNA complement

Calculate the complement of `dna` (Solution A.2).

Go to

See Section 6.2 and work on Section 6.3 before you continue here.

The following syntax enables the access of subparts of strings:

Example 2.2. slices

```
>>> EcoRI = 'gaattc'

>>> EcoRI[0]
'g'                                                    ❶
>>> EcoRI[-1]
'c'

>>> EcoRI[1:3]
'aa'
>>> EcoRI[3:]
'ttc'
>>> EcoRI[:]
'gaattc'
>>> EcoRI[:-1]
'gaatt'
                                                       ❷
>>> EcoRI[1:100]
'aattc'                                                ❷
>>> EcoRI[3:1]
''                                                     ❷
>>> EcoRI[100:101]
''
```

❷ Caution

If one of the start or end specification of a slice is out of range it is ignored. The result is empty if both are out of range or incompatible with each other.

❶ Negative indices access strings from the end.

Caution

Positive numbering starts with 0 but negative numbering with -1.

The next example searches for non ambiguous restriction sites:

Example 2.3. Find substrings

```
>>> dna = """ttcacctatgaatggactgtccccaaagaagtaggacccactaatgcagatcctgtg
tgtctagctaagatgtattattctgctgtggatcccactaaagatatattcactgggcttattgggccaa
tgaaaatatgcaagaaaggaagtttacatgcaaatgggagacagaaagatgtagacaaggaattctattt
gtttcctacagtatttgatgagaatgagagtttactcctggaagataatattagaatgtttacaactgca
cctgatcaggtggataaggaagatgaagactttcaggaatctaataaaatgcactccatgaatggattca
tgtatgggaatcagccgggtctcactatgtgcaaaggagattcggtcgtgtggtacttattcagcgccgg
aaatgaggccgatgtacatggaatatacttttcaggaaacacatatctgtggagaggagaacggagagac
acagcaaacctcttccctcaaacaagtcttacgctccacatgtggcctgacacagaggggacttttaatg
ttgaatgccttacaactgatcattacacaggcggcatgaagcaaaaatatactgtgaaccaatgcaggcg
gcagtctgaggattccaccttctacctgggagagaggacatactatatcgcagcagtggaggtggaatgg
gattattccccacaaagggagtgggaaaaggagctgcatcatttacaagagcagaatgtttcaaatgcat
ttttagataagggagagttttacataggctcaaagtacaagaaagttgtgtatcggcagtatactgatag
cacattccgtgttccagtggagagaaaagctgaagaagaacatctgggaattctaggtccacaacttcat
gcagatgttggagacaaagtcaaaattatctttaaaaacatggccacaaggccctactcaatacatgccc
atggggtacaaacagagagttctacagttactccaacattaccaggtgaaactctcacttacgtatggaa
aatcccagaaagatctggagctggaacagaggattctgcttgtattccatgggcttattattcaactgtg
gatcaagttaaggacctctacagtggattaattggccccctgattgtttgtcgaagaccttacttgaaag
tattcaatcccagaaggaagctggaatttgcccttctgtttctagttttgatgagaatgaatcttggta
cttagatgacaacatcaaaacatactctgatcaccccgagaaagtaaacaaagatgatgaggaattcata
gaaagcaataaaatgcatgctattaatggaagaatgtttggaaacct"""

>>> EcoRI = 'gaattc'
>>> BamHI = 'ggatcc'
>>> HindIII = 'aagctt'

>>> find (dna, EcoRI)
186
>>> index (dna,  EcoRI)
186

>>> find (dna,  HindIII)                                                    ❶
-1
>>> index (dna,  HindIII)
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
  File "/usr/local/lib/python2.2/string.py", line 141, in index
    return s.index(*args)
ValueError: substring not found in string.index

>>> find (dna, EcoRI, 187)
```

874

❶ If no match is found `find` returns -1 whereas `index` produce an error (For more explanations on exceptions see Chapter 8).

How to find all sites for *EcoRI*?

Go to

Work on the exercises in Section 5.2 to answer this question.

2.2. Lists

Lists are arbitrary collections of objects that can be nested. They are created by enclosing the comma separated items in square brackets. As strings they can be indexed and sliced, but as opposite to strings, it is also possible to modify them.

Example 2.4. Introduction of lists

```
>>> EcoRI = 'gaattc'
>>> BamHI = 'ggatcc'
>>> HindIII = 'aagctt'

>>> renz = [ EcoRI, BamHI, HindIII ]                                    ❶
>>> renz
['gaattc', 'ggatcc', 'aagctt']

>>> tree = [ 'Bovine', [ 'Gibbon', ['Orang', [ 'Gorilla',
[ 'Chimp', 'Human' ]]]], 'Mouse' ]
>>> tree
['Bovine', ['Gibbon', ['Orang', ['Gorilla', ['Chimp', 'Human']]]],
'Mouse']

>>> digest = [ renz[0], renz[1] ]
>>> digest
['gaattc', 'ggatcc']

>>> digest[1] = renz[2]
>>> digest                                                              ❷
['gaattc', 'aagctt']

>>> EcoRI[1] = 'A'
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
TypeError: object doesn't support item assignment

>>> del digest[1]
```

```
>>> digest                                                          ❸
['gaattc']

>>> digest = digest + renz[1:3]
>>> digest                                                          ❹
['gaattc', 'ggatcc', 'aagctt']

>>> digest.append(EcoRI)
>>> digest
['gaattc', 'ggatcc', 'aagctt', 'gaattc']

>>> digest.pop()
'gaattc'
>>> digest
['gaattc', 'ggatcc', 'aagctt']

>>> digest.insert(2, 'ttcgaa')                                      ❺
>>> digest
['gaattc', 'ggatcc', 'ttcgaa', 'aagctt']

>> digest.reverse()
>>> digest
['aagctt', 'ttcgaa', 'ggatcc', 'gaattc']
```

❶ list creation
❷ replace an element or a slice
❸ deletion of an element

❹ concatenation of two lists via the + operator.

Caution

This merges the two list whereas the method `append()` includes its argument in the list.

❺ insertion of an element

Example 2.5. Functions returning a list

```
>>> range(3)
[0, 1, 2]
>>> range(10,20,2)
[10, 12, 14, 16, 18]
>>> range(5,2,-1)
[5, 4, 3]

>>> aas = "ALA TYR TRP SER GLY".split()
>>> aas
['ALA', 'TYR', 'TRP', 'SER', 'GLY']
```

```
>>> " ".join(aas)
'ALA TYR TRP SER GLY'

>>> l = list('atgatgcgcccacgtacga')
['a', 't', 'g', 'a', 't', 'g', 'c', 'g', 'c', 'c', 'c', 'a', 'c', 'g',
't', 'a', 'c', 'g', 'a']
```

The next example generates all possibilities of digests using two enzymes from a list of enzymes. It is more complex and use a nested list and the `range` function introduced above (Example 2.5).

Example 2.6. Generate all possible digests with two enzymes

```
def all_2_digests(enzymes):
    """ generate all possible digests with 2 enzymes """                ❶

    digests = []
    for i in range(len(enzymes)):
        for k in range(i+1, len(enzymes)):
            digests.append( [enzymes[i], enzymes[k]] )
    return digests
```

❶ If the first statement of a function definition is a string, this string is used as documentation (see Section 1.2.3).

```
>>> all_2_digests(['EcoRI', 'HindIII', 'BamHI'])
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]
```

Exercise 2.3. Restriction site occurrences as a list

Transform Example 5.3 that finds restriction sites to return a list containing all restriction site occurences instead of printing them (Solution A.3) .

Exercise 2.4. Restriction digest

Write a function that returns the length of all restriction fragments of a DNA sequence and that takes a list of restriction enzymes and the DNA sequence. (Solution A.4)

Tip

For each enzyme you need two informations, the restriction pattern and the position where the enzyme cuts its pattern. You can model an enzyme as a list containing this two informations, for example:

```
EcoRI = [ 'gaattc', 1 ]
```

Tip

If you to do something with list, try to find out if there is a method of list objects that even implements your task. You can use the `dir` function to get all methods of a list object (Section 1.2.2).

Exercise 2.5. Get the codon list from a DNA sequence

Write a function that returns the list of codons for a DNA sequence and a given frame (Solution A.5).

Exercise 2.6. Reverse Complement of DNA

Write a function returning the reverse complement of a DNA. Remember Exercise 2.2 that calculates the complement of DNA. (Solution A.6)

Go to

Before you continue see Section 4.2 to get a deeper inside in variable assignments and read also Section 6.4 that explain how arguments can be passed to the function parameters.

2.3. Tuples

Tuples are like lists but they can not be modified. Items have to be enclosed by parentheses instead of square brackets to create a tuple instead of a list. In general all that can be done using tuples can be done with lists, but sometimes it is more secure to prevent internal changes.

An appropriate use of tuples in a biological example could be the 3D-coordinates of an atom in a structure. The example calculates distances between atoms in protein structures. Atoms are represented as tuples of their coordinates x,y,z in space.

Example 2.7. Distance of two points in space

```
from math import *

def distance(atom1, atom2):
    dx = atom1[0] - atom2[0]
    dy = atom1[1] - atom2[1]
    dz = atom1[2] - atom2[2]
    return sqrt(dx*dx + dy*dy + dz*dz)
```

```
>>> atom1 = (1.5, 2.0, 5.1)
>>> atom1
(1.5, 2.0, 5.0999999999999996)
>>> atom2 = (1.4, 4.6, 6.1)

>>> distance(atom1, atom2)
2.7874719729532704
```

but:

```
>>> atom1[0] = 1.0
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
TypeError: object doesn't support item assignment
```

Caution

When you create a tuple with only one value, a comma has to follow the value. This is necessary to make difference with parentheses that group expression. Look at the following example:

```
>>> renz = ('EcoRI')
>>> renz
'EcoRI'
```

```
>>> renz = ('EcoRI',)
>>> renz
('EcoRI',)
```

Note

Tuples are used internally to pass arguments to the string format operator % (Section 6.2.4) and to pass a variable number of arguments to a function (Section 6.6).

Go to

Follow the last links in the note above to learn how you can pass a variable list of arguments to a function. You can also look at Section 4.1.1 which describes a special syntax of assignments using tuples.

2.4. Sequence types: Summary

Sequences hold ordered sets of objects. In the first three sections of this chapter we have introduced strings, lists and tuples. Table 2.1 completes the list of built-in sequences types of Python. Table 2.2 gives a list of operators and functions which can be applicated to all sequence types. Table 2.3 gives the additional manipulation possibilities of mutable sequence types.

Table 2.1. Built-in sequence types

Type	Description	Elements	Mutable
StringType	Character string	Characters only	no
UnicodeType	Unicode character string	Unicode characters only	no
ListType	List	Arbitrary objects	yes
TupleType	Immutable List	Arbitrary objects	no
XRangeType	return by `xrange()`	Integers	no
BufferType	Buffer, return by `buffer()`	arbitrary objects of one type	yes/no

Table 2.2. Sequence types: Operators and Functions

Operator/Function	Action	Action on Numbers
`[ ... ], ( ... ), " ... "`	creation	
`s + t`	concatenation	addition
`s * n`	repetition [a]	multiplication
`s[i]`	indexation	
`s[i:k]`	slice	
`x in s`	membership	
`x not in s`		
`for a in s`	iteration	
`len(s)`	length	

`min(s)`	return smallest element
`max(s)`	return greatest element

[a]

[a] **Important**
shallow copy (see Example 4.5)

Table 2.3. Operations on mutable sequence types

Operator/Function	Action
`s[i] = x`	index assignment
`s[i:k] = t`	slice assignment
`del s[i]`	deletion

2.4.1. Lists and Tuples

Lists and tuples are collections of objects. They can hold different sort of object and they can be nested to organise the objects. The main difference between them is that list can be modified whereas tuples can not. Table 2.4 contains a summary list of list and tuple methods.

Table 2.4. List methods

Method	Operation
`list(s)`	converts any sequence object to a list
`s.append(x)`	append a new element
`s.extend(t)`	concatenation[a]
`s.count(x)`	count occurences of `x`
`s.index(x)`	find smallest position where `x` occurs in s
`s.insert(i,x)`	insert `x` at position `i`
`s.pop([i])`	removes i-th element and return it
`s.remove(x)`	remove element
`s.reverse()`[b]	reverse
`s.sort([cmp])`[b]	sort according to the `cmp` function

[a] equal to the + operator
[b] in place operation

2.4.2. Xrange types

The `range([start,] end [, stride])` function creates a list of integers from optional `start` to `end` with the optional `stride` (see Example 2.5 for an example). The `xrange([start,] end [,stride])` function, rather than creating a list containing all values, returns an immutable sequence object that calculates the value when needed. This saves memory for long sequences.

Xrange objects has only the method `tolist()` that returns a list containing all values.

2.4.3. Strings and Unicode strings

Strings and Unicode strings are immutable collections of characters. They can be inclosed by quotes, double-quotes and triple-(double)-quotes. In double-quoted strings special characters are expanded and triple-quoted strings can span multiple lines. The line-feed character is retained in the last case.

```
>>> mydoc="""This is a doc string,
... spanning 2 lines."""
>>> mydoc
'This is a doc string,\nspanning 2 lines.'
```

Exercise 2.7. String methods

Find all methods of a string object.

They have a special the operator % (modulo) to format them. (remember Section 6.2.4).

2.4.4. Buffers

Buffers are sequence interfaces to a memory region that treats each byte as a 8-bit character. They can be created by the `buffer(obj [, offset] [, size])` function and share the same memory as the underlying object `obj`. This is an type for advanced use, so we will not say more about them.

2.5. Dictionaries

Dictionaries are collections of objects that are accessed by a key. They are created using a comma separated list of key-value pairs separated by colon enclosed in braces. Example 2.8 shows some examples of dictionary manipulation and Table 2.5 provides an overview of dictionary methods.

Example 2.8. Introduction to dictionaries

```
>>> code = {"GLY" : "G", "ALA" : "A", "LEU" : "L", "ILE" : "I",
...             "ARG" : "R", "LYS" : "K", "MET" : "M", "CYS" : "C",
...             "TYR" : "Y", "THR" : "T", "PRO" : "P", "SER" : "S",
...             "TRP" : "W", "ASP" : "D", "GLU" : "E", "ASN" : "N",
...             "GLN" : "Q", "PHE" : "F", "HIS" : "H", "VAL" : "V"}

>>> code['VAL']
'V'
>>> code.has_key('NNN')
0

>>> code.keys()
['CYS', 'ILE', 'SER', 'GLN', 'LYS', 'ASN', 'PRO', 'THR', 'PHE', 'ALA',
'HIS', 'GLY', 'ASP', 'LEU', 'ARG', 'TRP', 'VAL', 'GLU', 'TYR', 'MET']
```

```
>>> code.values()
['C', 'I', 'S', 'Q', 'K', 'N', 'P', 'T', 'F', 'A', 'H', 'G', 'D', 'L',
'R', 'W', 'V', 'E', 'Y', 'M']
>>> code.items()
[('CYS', 'C'), ('ILE', 'I'), ('SER', 'S'), ('GLN', 'Q'), ('LYS', 'K'),
('ASN', 'N'), ('PRO', 'P'), ('THR', 'T'), ('PHE', 'F'), ('ALA', 'A'),
('HIS', 'H'), ('GLY', 'G'), ('ASP', 'D'), ('LEU', 'L'), ('ARG', 'R'),
('TRP', 'W'), ('VAL', 'V'), ('GLU', 'E'), ('TYR', 'Y'), ('MET', 'M')]

>>> del code['CYS']
>>> del code['MET']
>>> code
{'ILE': 'I', 'SER': 'S', 'GLN': 'Q', 'LYS': 'K', 'ASN': 'N', 'PRO': 'P',
'THR': 'T', 'PHE': 'F', 'ALA': 'A', 'HIS': 'H', 'GLY': 'G', 'ASP': 'D',
'LEU': 'L', 'ARG': 'R', 'TRP': 'W', 'VAL': 'V', 'GLU': 'E', 'TYR': 'Y'}

>>> code.update({'CYS':'C', 'MET':'M', '?':'?'})
>>> code
{'CYS': 'C', 'ILE': 'I', 'SER': 'S', 'GLN': 'Q', 'LYS': 'K', 'TRP': 'W',
'PRO': 'P', '?': '?', 'THR': 'T', 'PHE': 'F', 'ALA': 'A', 'GLY': 'G',
'HIS': 'H', 'GLU': 'E', 'LEU': 'L', 'ARG': 'R', 'ASP': 'D', 'VAL': 'V',
'ASN': 'N', 'TYR': 'Y', 'MET': 'M'}

>>> one2three = {}
>>> for key,val in code.items():
...     one2three[val]= key
...
>>> one2three
{'A': 'ALA', 'C': 'CYS', 'E': 'GLU', 'D': 'ASP', 'G': 'GLY', 'F': 'PHE',
'I': 'ILE', 'H': 'HIS', 'K': 'LYS', 'M': 'MET', 'L': 'LEU', 'N': 'ASN',
'Q': 'GLN', 'P': 'PRO', 'S': 'SER', 'R': 'ARG', 'T': 'THR', 'W': 'TRP',
'V': 'VAL', 'Y': 'TYR', '?': '?'}
```

Table 2.5. Dictionary methods and operations

Method or Operation	Action
`d[key]`	get the value of the entry with key `key` in `d`
`d[key] = val`	set the value of entry with key `key` to `val`
`del d[key]`	delete entry with key `key`
`d.clear()`	removes all entries
`len(d)`	number of items
`d.copy()`	makes a shallow copy[a]
`d.has_key(key)`	returns 1 if `key` exists, 0 otherwise
`d.keys()`	gives a list of all keys
`d.values()`	gives a list of all values
`d.items()`	returns a list of all items as tuples (key,value)
`d.update(new)`	adds all entries of dictionary `new` to `d`
`d.get(key [, otherwise])`	returns value of the entry with key `key` if it exists otherwise returns `otherwise`

`d.setdefaults(key [, val])`	same as `d.get(key)`, but if `key` does not exists sets `d[key]` to `val`
`d.popitem()`	removes a random item and returns it as tuple

[a]

[a] **Important**
shallow copy (see Example 4.5)

Example 2.9. Protein 3-Letter-Code to 1-Letter-Code

```
def three2one(prot, sep=None):                                          ❶
    """ translate a protein sequence from 3 to 1 letter code
    sep - separator if not one of the whitespace characters
    """
    code = {"GLY" : "G", "ALA" : "A", "LEU" : "L", "ILE" : "I",
            "ARG" : "R", "LYS" : "K", "MET" : "M", "CYS" : "C",
            "TYR" : "Y", "THR" : "T", "PRO" : "P", "SER" : "S",
            "TRP" : "W", "ASP" : "D", "GLU" : "E", "ASN" : "N",
            "GLN" : "Q", "PHE" : "F", "HIS" : "H", "VAL" : "V"}

    newprot = ""
    for aa in prot.split(sep):
        newprot += code.get(aa, "?")

    return newprot
```

❶ This is an example of a default argument of a functional parameter.

It can be run as follow:

```
>>> prot ="""GLN ALA GLN ILE THR GLY ARG PRO GLU TRP ILE TRP LEU
... ALA LEU GLY THR ALA LEU MET GLY LEU GLY THR LEU TYR
... PHE LEU VAL LYS GLY MET GLY VAL SER ASP PRO ASP ALA
... LYS LYS PHE TYR ALA ILE THR THR LEU VAL PRO ALA ILE"""
>>> three2one(prot)
'QAQITGRPEWIWLALGTALMGLGTLYFLVKGMGVSDPDAKKFYAITTLVPAI'
```

Go to

See Section 6.5 to learn more about default values of functional parameters.

Exercise 2.8. Translate a DNA sequence

Write a function that takes a cDNA sequence and a genetic code and that returns the translated protein sequence. (Solution A.7)

Note

Local namespaces of objects, that contains their method and attribute definitions, are implemented as dictionaries (Section 4.3.1). Another internal use of dictionaries is the possibility to pass a variable list of parameters using keywords (Example 6.7).

Go to

Remember how to pass a variable number of arguments to a function (Section 6.6) and look how to do the same using keywords (Example 6.7).

2.6. Numbers

This section provides a short introduction to numbers in Python. Table 2.6 shows all built-in number types of Python and Example 2.10 shows an example of complex numbers which haves a built-in type in Python. Arithmetics in Python can be done as expected from pocket calculators.

Table 2.6. Number built-in types

Type	Example
integers	`10`
long integers (“unlimited size”)	`1000000000000000000L`
floating point numbers (64-bit precision)	`10.1`
complex numbers	`3+4j`

Example 2.10. Calculation with complex numbers

```
>>> (3+4j)
(3+4j)
>>> (3+4j) + (4+2j)
(7+6j)
>>> (3+4j).real
3.0
>>> (3+4j).imag
```

```
4.0
```

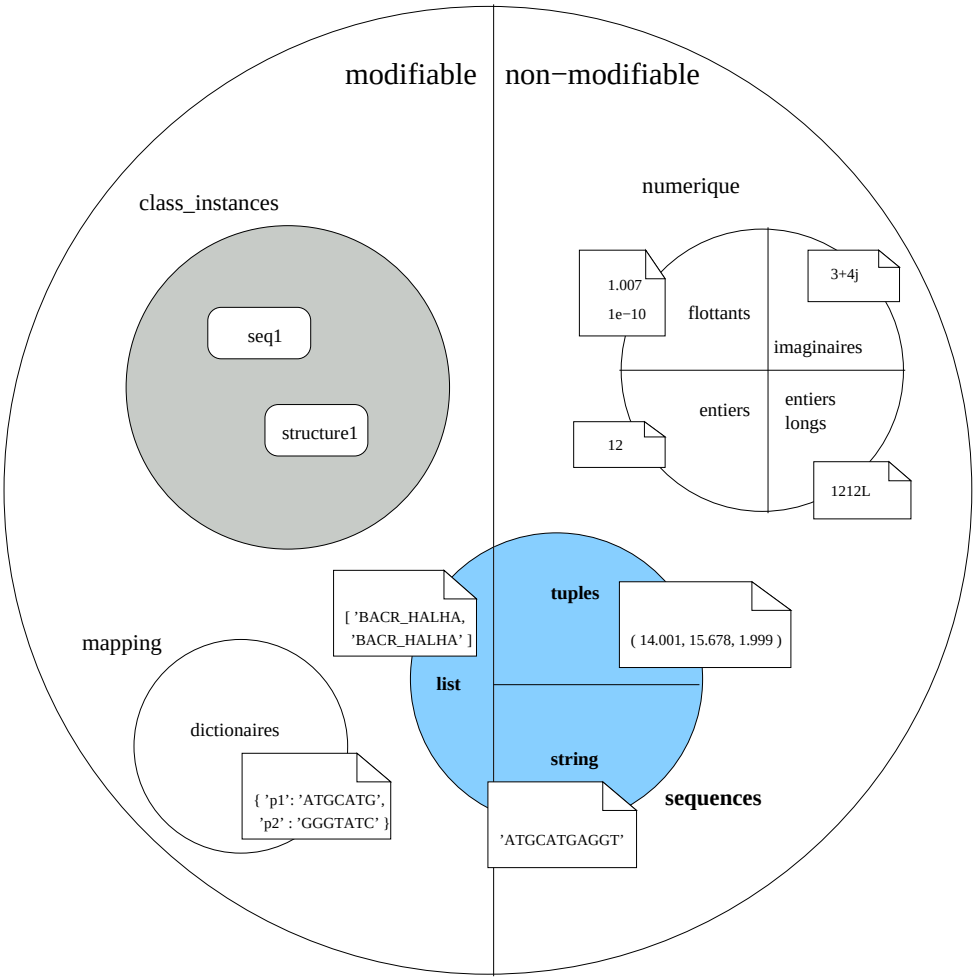
Exercise 2.9. Operators

Compare the behaviour of some operator application (see the operator list in Table 6.1) to numbers, strings and lists. Test at minimum:

- `a + b`
- `a * b`
- `a % b`

2.7. Type conversions

Figure 2.1. Diagram of some built-in types



It is sometimes necessary to convert variables from one type into another. For example, if you need to change some of the characters of a string, you will have to transform the string in a mutable list. Likewise, see Solution A.1 where it was necessary to convert integers into floating point numbers. Table 2.7 provides the list of all possible type conversions.

Table 2.7. Type conversion functions

Function	Description
`int(x [,base])`	converts `x` to an integer
`long(x [,base])`	converts `x` to a long integer
`float(x)`	converts `x` to a floating-point number
`complex(real [,imag])`	creates a complex number
`str(x)`	converts `x` to a string representation

`repr(x)`	converts `x` to an expression string
`eval(str)`	evaluates `str` and returns an object
`tuple(s)`	converts a sequence object to a tuple
`list(s)`	converts a sequence object to a list
`chr(x)`	converts an integer to a character
`unichr(x)`	converts an integer to a Unicode character
`ord(c)`	converts a character to its integer value
`hex(x)`	converts an integer to a hexadecimal string
`oct(x)`	converts an integer to an octal string

Go to

Read Section 4.3 to get a deeper inside into Python namespaces.

2.8. Files

The `open(<filename>, [<mode>])` function opens a file with the specified access rights (see Table 2.9) and returns a `FileType` object. Table 2.8 list some of the methods available for `FileType` objects.

Table 2.8. File methods

Method	Action
`read([n])`	reads at most `n` bytes; if no `n` is specified, reads the entire file
`readline([n])`	reads a line of input, if `n` is specified reads at most `n` bytes
`readlines()`	reads all lines and returns them in a list
`xreadlines()`	reads all lines but handles them as a `XRangeType`[a]
`write(s)`	writes strings `s`
`writelines(l)`	writes all strings in list `l` as lines
`close()`	closes the file
`seek(offset [, mode])`	changes to a new file `position=start + offset`. Start is specified by the mode argument: `mode=0` (default), start = start of the file, `mode=1`, start = current file position and `mode=2`, start = end of the file

[a] See Section 2.4.2 for more informations

Table 2.9. File modes

Mode	Description
r	read
w	write
a	append
[rwa]b	[reading,writing,append] as binary data (required on Windows)

r+	update+reading (output operations must flush their data before subsequent input operations)
w+	truncate to size zero followed by writing

Example 2.11. Reading Fasta

This example shows how to read sequence entries from a fasta file (data/seqs.fasta). You first have the format independent main loop of the program that reads the file sequence by sequence. The command line has to be replaced by instructions that do what should be done.

```
f = open("seq.fasta")                                    ❶

entry = get_fasta(f)                                     ❷
while entry:
    # ... do what you have to do
    entry = get_fasta(f)

f.close()                                                ❸
```

❶ Open the sequence file.
❷ Loop over the file reading entry by entry and doing what you want to do.
❸ Close the file.

The second part shows the code of the function `get_fasta` that reads one sequence from a fasta file.

Reading fasta files is not as simple as reading files in other sequence formats, because there is no explicit end of a sequence entry. You have to read the start of the following entry to know that your sequence is finished. The following shows two possibilities to handle this problem while reading the file line per line:

The first solution stores the line read too far:

```
_header = None
def get_fasta(fh):
    """ read a fasta entry from a file handle """
    global _header                                       ❶
    if _header:
        header, _header = _header, None
    else:
        header = fh.readline()
        # end of file detection
        if not header:
            return header

    if header[0] != '>':
        return None
```

```
    seq = ""
    line = fh.readline()
    while line and line[0] != '>':
        seq += line[:-1]
        line = fh.readline()
    _header = line

    return header[1:-1], seq
```

Go to

By default all variables are defined in the local namespace. Before looking at the second solution of the problem, read Section 4.1 for how to differentiate between local and global variables.

The second possibility seeks the current file position to the start of the new entry, before returning the sequence. So all but the first header lines are read twice:

```
def get_fasta(fh):
    """ read a fasta entry from a file handle """

    header = fh.readline()
    # eof detection
    if not header:
        return header
    # no fasta format
    if header[0] != '>':
        return None

    seq = ""
    line = fh.readline()
    while line:
        if line[0] == '>':
            # go back to the start of the header line
            fh.seek(-len(line), 1)
            break
        seq += line[:-1]
        line = fh.readline()

    return header[1:-1], seq
```

2.8.1. The print statement

All `FileType` objects have a `write` method to write strings to them. But sometimes the `print` statement can be more conveniently used.

By default `print` writes the given string to the standard output and adds a line-feed. If a comma separated list of strings is given, then all strings will be joined by a single whitespace before printing. The addition of a trailing comma prevents the line-feed, but in this case a final whitespace is added.

Example 2.12. Print statement

```
>>> renz = ['gaattc', 'ggatcc', 'aagctt']
>>> print renz
['gaattc', 'ggatcc', 'aagctt']
>>> print renz[0]
gaattc

>>> print "EcoRI pattern:", renz[0]
EcoRI pattern: gaattc
>>> print "EcoRI pattern: %s" % renz[0]
EcoRI pattern: gaattc

>>> for enz in renz:
...     print enz,
...

>>> log = open("log", "a")
>>> print >>log, "Handle restriction site:", renz[0]
>>> log.close()
```

The default destination can be redirected using the special `>>file` operator where *file* is the destination `FileType` object.

Exercise 2.10. Write a sequence in fasta format

Write a function that takes a `file` object (such as the one opened by the `open` function), a sequence, its ID and description as arguments, and write the sequence to the file (Solution A.8).

Tip

It is better to exclude the `open` and `close` functions to be able to write more than one sequence to a file.

Exercise 2.11. Header function

Write a function that takes the header line of a fasta entry and that returns the ID and description of the sequence (Solution A.9).

Chapter 3. Syntax rules

3.1. Indentation

3.1.1. Line structure

In Python you normally have one instruction per line. Long instructions can span several lines using the line-continuation character "\". Some instructions, as triple quoted strings, list, tuple and dictionary constructors or statements grouped by parentheses do not need a line-continuation character. It is possible to write several statements on the same line, provided they are separated by semi-colons.

```
>>> dna = dna + \
... 'aaagagagat'
>>> dna
'ataaaaaaaaagtatgcgggcgcgggcgcgaaagagagat'

>>> primers = [ 'aaaata',
... 'ggttgt' ]
>>> primers
['aaaata', 'ggttgt']

>>> dna += 'aaataggat'; primers += [ 'ttgtta' ]
>>> dna
'ataaaaaaaaagtatgcgggcgcgggcgcgaaagagagataaataggat'
>>> primers
['aaaata', 'ggttgt', 'ttgtta']

>>> dna = ( dna +
... 'tttat' ) * 2
>>> dna
'ataaaaaaaaagtatgcgggcgcgggcgcgaaagagagataaataggattttatataaaaaaaaagtat
gcgggcgcgggcgcgaaagagagataaataggattttat'
```

3.1.2. Block structure

Blocks of code, as function bodies, loops or conditions, are identified by indentation. The indentation length of the first statement of a block is arbitrary, but all instructions of a block have to be indented the same.

Caution

Do not mix tab and space characters. The indentation length is not the length you see in the buffer, but equal to the number of separation characters.

The *python-mode* of **emacs** deals with this issue: if you use tab characters, **emacs** will replace them by space characters.

A block of code is initiated by a colon character followed by the indented instructions of the block. A one line block can also be given one the same line as the colon character.

```
>>> dna = 'ataaaaaaaaagtatgcgggcgcgggcgcg'
>>> primer = 'tgctcgctc'
>>> if dna.find(primer):
...     'found'
... else:
...     'not found'
...
'found'

>>> if dna.find(primer): 'found'
... else: 'not found'
...
'found'

>>> if dna.find(primer):
...     found = 1
...     'found'
...
'found'
```

but:

```
>>> if dna.find(primer):
...     found = 1
...      'found'
  File "<string>", line 3
    'found'
    ^
SyntaxError: invalid syntax
```

3.2. Special objects

`None` is the empty or null object. It is always false and has its own type, the `NoneType`

Statements such as: `if`, `while` and `def` require a block of code containing at least one instruction. If there is nothing to do in the block, just use the `pass` statement.

Example 3.1. None and pass

```
>>> found = None

>>> if found:
...     pass
```

```
... else:
...     'not found'
...
'not found'

>>> if found:
... else:
   File "<string>", line 2
    else:
       ^
IndentationError: expected an indented block
```

Go back

Return to the function definition section (Section 6.3).

Chapter 4. Variables and namespaces

4.1. Variables

Variables have a type but are never declared in Python. They are instantiated when they are assigned for the first time. By default, variables are defined in the local namespace, or have to be declared explicitly as global variables, using the `global` statement.

Caution

The first assignment of a value stands for the variable declaration. If a value is assigned to a variable in a function body, the variable will be local, *even if there is a global variable with the same name, and this global variable has been used before the assignment.*

Example 4.1. Local variable definition

```
>>> enz = []
>>> def add_enz(*new):
...     enz = enz + list(new)
...
>>> add_enz('EcoRI')
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
  File "<stdin>", line 2, in add_enz
UnboundLocalError: local variable 'enz' referenced before assignment
```

This rule does not apply in the case of method calls. In the following example, the variable `enz` is only *used*, not *assigned*, even if `enz` is actually modified internally.

```
>>> def add_enz(*new):
...     enz.extend(list(new))
>>> add_enz('EcoRI')
>>> enz
['EcoRI']
```

The `global` statement has to be used to declare `enz` as a global variable

Example 4.2. Global statement

```
>>> def add_enz(*new):
...     global enz
...     enz = enz + list(new)
...
```

```
>>> add_enz('BamHI', 'HindIII')
>>> enz
[ 'EcoRI', 'BamHI', 'HindIII']
```

Go back

Return to the Fasta example (Example 2.11) and go on with the second solution.

4.1.1. Multiple assignments

The following example shows how to assign several variables in a single statement.

Example 4.3.

```
>>> (EcoRI, BamHI) = ('gaattc', 'ggatcc')

>>> EcoRI
'gaattc'
>>> BamHI
'ggatcc'
```

you can also omit the parentheses:

```
>>> EcoRI, BamHI = 'gaattc', 'ggatcc'
```

This is a convenient way to return multiple values from a function.

Go back

Return to the end of the introduction to tuples (Section 2.3).

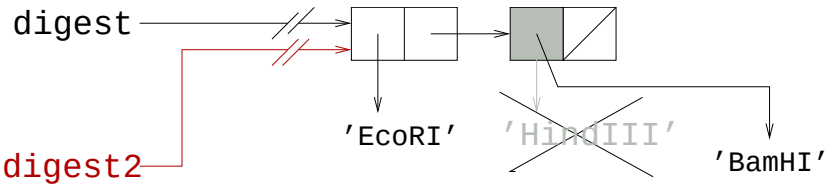
4.2. Assignments, references and copies of objects

Assignment *a = b* creates a new reference to the content of *b* and saves it in *a*. This means that *a* and *b* refer to the same object. If *b* is a mutable object and one of his items is modified, *a* will also change. Figure 4.1 illustrates Example 4.4 given below.

Example 4.4. Assignment by referencing

```
>>> digest = ['EcoRI', 'HindIII']

>>> digest2 = digest
>>> digest2
['EcoRI', 'HindIII']

>>> digest2[1] =  'BamHI'
>>> digest2
['EcoRI', 'BamHI']
>>> digest
['EcoRI', 'BamHI']
```

Figure 4.1. Assignment by referencing

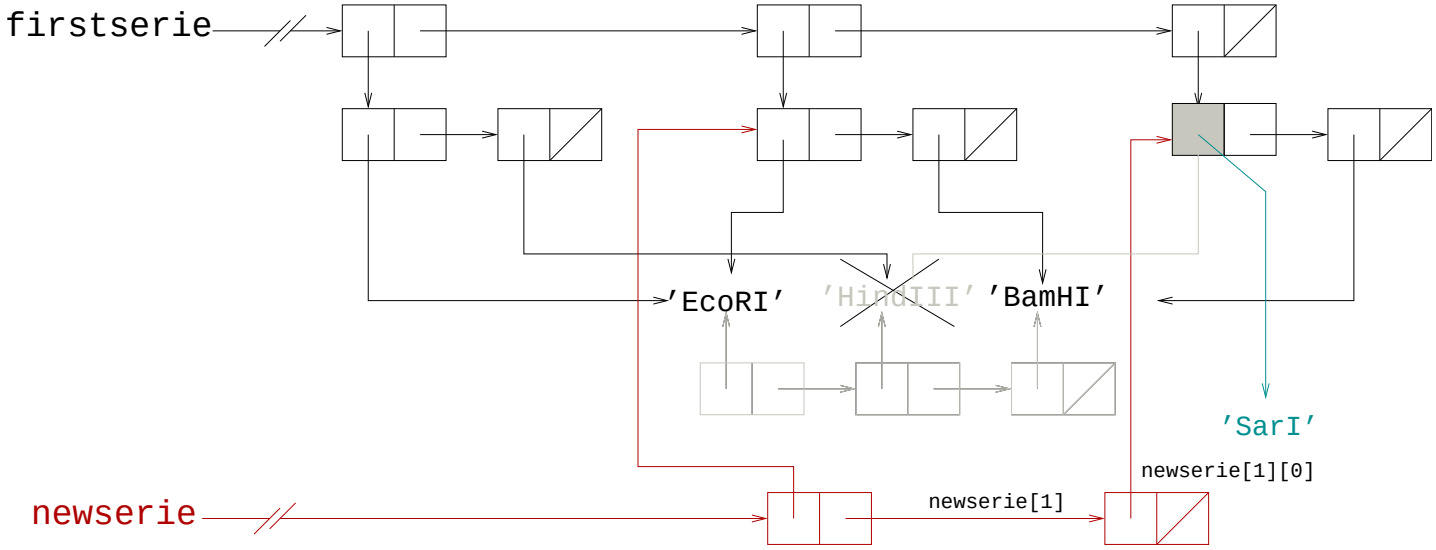


The same strategy is used for the copy of composed objects. A target object is created and populated by new references to the items of the source object. Figure 4.2 illustrates what happens in Example 4.5.

Example 4.5. Copy composed objects

```
>>> firstserie = all_2_digests(['EcoRI', 'HindIII', 'BamHI'])
>>> firstserie
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]

>>> newserie = firstserie[1:]
>>> newserie
[['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]

>>> newserie[1][0]='SarI'
>>> newserie
[['EcoRI', 'BamHI'], ['SarI', 'BamHI']]

>>> firstserie
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['SarI', 'BamHI']]
```

Figure 4.2. Reference copy



If an independent copy is needed, the `deepcopy` function of the `copy` module should be used.

Example 4.6. Independent copy

```
>>> firstserie =  all_2_digests(['EcoRI', 'HindIII', 'BamHI'])
>>> firstserie
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]

>>> import copy
>>> newserie = copy.deepcopy(firstserie)[1:]
>>> newserie
[['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]

>>> newserie[1][0]='SarI'
>>> newserie
[['EcoRI', 'BamHI'], ['SarI', 'BamHI']]

>>> firstserie
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]
```

Go back

Return to the end of the introduction to the list type (Section 2.3).

4.3. Namespaces

There are three different namespaces in Python: a local namespace, a module namespace and a global namespace. The latter contains all built-in functions. The module namespace contains all the function definitions and variables of a module. It can be accessed using the `.` (dot) operator. A local environment is created at function calls. It includes all the parameters and local variables of the function. Function definitions can be nested, and nested functions have their own local namespace.

Example 4.7. Function execution namespaces

```
>>> enz = []

>>> def add_enz(*new):
...     def verif():
...             print "enz: ", enz
...             print "new: ", new
...     verif()
...     enz.extend(list(new))

>>> add_enz('EcoRI')
enz:  []
new:  ('EcoRI',)

>>> enz
[ 'EcoRI' ]
```

Caution

This behaviour only exists in Python version 2.2. Previous versions have only one function execution namespace. In this case, the `new` variable in Example 4.7 is not accessible within the `verif` function.

4.3.1. Accessing namespaces

Variable names are resolved by searching the namespaces in the following order: local namespaces (function execution namespaces potentially nested), current module namespace and global namespace containing built-in definitions.

When object methods or attributes are addressed using the `.` (dot) operator, namespaces searching is different. Each object has its own local namespace implemented as a dictionary named `__dict__`. This dictionary is searched for the name following the `.` (dot) operator. If it is not found, the local namespace of its class, accessible via the `__class__` attribute, is searched for. If it is not found there, a lookup on the parent classes is performed. Since modules are objects, accessing the namespace of a module use the same mechanism.

```
>>> enz = ['EcoRI']

>>> enz.__dict__
```

```
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
AttributeError: 'list' object has no attribute '__dict__'
>>> enz.__class__.__dict__
<dict-proxy object at 0x815776c>

>>> print enz.__class__.__dict__
{'sort': <method 'sort' of 'list' objects>,
'__ne__': <slot wrapper '__ne__' of 'list' objects>,
'reverse': <method 'reverse' of 'list' objects>,
'__getslice__': <slot wrapper '__getslice__' of 'list' objects>,
'insert': <method 'insert' of 'list' objects>,
'__len__': <slot wrapper '__len__' of 'list' objects>,
'__getattribute__': <slot wrapper
'__getattribute__' of 'list' objects>,
'remove': <method 'remove' of 'list' objects>,
'append': <method 'append' of 'list' objects>,
'__setitem__': <slot wrapper '__setitem__' of 'list' objects>,
'pop': <method 'pop' of 'list' objects>,
'__add__': <slot wrapper '__add__' of 'list' objects>,
'__gt__': <slot wrapper '__gt__' of 'list' objects>,
'__rmul__': <slot wrapper '__rmul__' of 'list' objects>,
'__lt__': <slot wrapper '__lt__' of 'list' objects>,
'__eq__': <slot wrapper '__eq__' of 'list' objects>,
'__init__': <slot wrapper '__init__' of 'list' objects>,
'__imul__': <slot wrapper '__imul__' of 'list' objects>,
'extend': <method 'extend' of 'list' objects>,
'__delitem__': <slot wrapper '__delitem__' of 'list' objects>,
'__delslice__': <slot wrapper '__delslice__' of 'list' objects>,
'__getitem__': <slot wrapper '__getitem__' of 'list' objects>,
'__contains__': <slot wrapper '__contains__' of 'list' objects>,
'index': <method 'index' of 'list' objects>,
'__setslice__': <slot wrapper '__setslice__' of 'list' objects>,
'count': <method 'count' of 'list' objects>,
'__iadd__': <slot wrapper '__iadd__' of 'list' objects>,
'__le__': <slot wrapper '__le__' of 'list' objects>,
'__repr__': <slot wrapper '__repr__' of 'list' objects>,
'__hash__': <slot wrapper '__hash__' of 'list' objects>,
'__new__': <built-in method __new__ of type object at 0x80f1aa0>,
'__doc__': "list() -> new list\nlist(sequence) -> new list
initialized from sequence's items",
'__ge__': <slot wrapper '__ge__' of 'list' objects>,
'__mul__': <slot wrapper '__mul__' of 'list' objects>}

>>> dir (enz)
['__add__', '__class__', '__contains__', '__delattr__', '__delitem__',
'__delslice__', '__doc__', '__eq__', '__ge__', '__getattribute__',
'__getitem__', '__getslice__', '__gt__', '__hash__', '__iadd__',
'__imul__', '__init__', '__le__', '__len__', '__lt__', '__mul__',
'__ne__', '__new__', '__reduce__', '__repr__', '__rmul__', '__setattr__',
 '__setitem__', '__setslice__', '__str__', 'append', 'count', 'extend',
```

```
'index', 'insert', 'pop', 'remove', 'reverse', 'sort']
```

Go back

Return to Section 2.7.

Chapter 5. Control flow

5.1. Conditionals

The `if` statement and the optional `else` and `elif` statements perform tests.

Example 5.1. Test the character of a DNA base

```
>>> base = "e"

>>> if base in "atgc":
...     "exact"
...

>>> if base in "atgc":
...     "exact"
... elif base in "bdhkmnrsuvwxy":
...     "ambiguous"
... else:
...     "unknown"
...
'unknown'
```

More complex tests can be written with the `and`, `or` and `not` operators.

Example 5.2. More complex tests

```
>>> base in 'atgc'
0
>>> base not in 'atgc'
1
>>> not base in 'atgc'
1

>>> base.isalpha()                                          ❶
1

>>> base.isalpha() and base in 'atgc'
0
>>> base.isalpha() or base.isspace()                        ❷
1

>>> not None
1                                                           ❸
>>> not 0
1
>>> not ''
```

```
1

>>> base.isalpha() and base                                    ❹
'e'
>>> 1 or 1/0                                                   ❺
1
```

❶ Important

Here we ask for the `isalpha` method of the string object `base` (see Section 6.2.3).

❷ The object `None` is the special "empty" object. It is always false.

❸ Some expressions that are false.

❹ A logical expression returns 0 if it is `false` and the value of the last evaluation otherwise.

❺ Important

The components of the logical expression are evaluated until the value of the entire expression is known. Here the expression `1/0`is not executed because 1 is `true` and so the entire expression is `true`.

Go back

Return to Section 6.3 or go directly to Section 3.1.2.

5.2. Loops

The two statements `while` and `for` are used to write loops in Python.

5.2.1. while

The `while` construct executes a block of code while a condition is true.

Example 5.3. Find all occurrences of a restriction site

```
from string import *

def restrict(dna, enz):
    "print all start positions of a restriction site"
    site = find (dna, enz)
    while site != -1:
        print "restriction site %s at position %d" % (enz, site)
        site = find (dna, enz, site + 1)
```

```
>>> restrict(dna, EcoRI)
restriction site gaattc at position 188
restriction site gaattc at position 886
restriction site gaattc at position 1326
```

5.2.2. for

The loop construct `for` iterates over all members of a sequence.

Caution

This is equivalent to the `foreach` statement in some other programming languages. It is not the same as the `for` statement in most other programming languages.

Example 5.4. Remove whitespace characters from a string

```
>>> from string import *

>>> whitespace
'\t\n\x0b\x0c\r '
>>> dna = """
... aaattcctga gccctgggtg caaagtctca gttctctgaa atcctgacct aattcacaag
... ggttactgaa gatttttctt gtttccagga cctctacagt ggattaattg gccccctgat
... tgtttgtcga agaccttact tgaaagtatt caatcccaga aggaagctgg aatttgccct
... tctgtttcta gtttttgatg agaatgaatc ttggtactta gatgacaaca tcaaaacata
... ctctgatcac cccgagaaag taaacaaaga tgatgaggaa ttcatagaaa gcaataaaat
... gcatggtatg tcacattatt ctaaaacaa """

>>> for s in whitespace:
...     dna = replace(dna, s, "")
...
>>> dna
'aaattcctgagccctgggtgcaaagtctcagttctctgaaatcctgacctaattcacaagggttactga
agatttttcttgtttccaggacctctacagtggattaattggccccctgattgtttgtcgaagaccttac
ttgaaagtattcaatcccagaaggaagctggaatttgcccttctgtttctagtttttgatgagaatgaat
cttggtacttagatgacaacatcaaaacatactctgatcaccccgagaaagtaaacaaagatgatgagga
attcatagaaagcaataaaatgcatggtatgtcacattattctaaaacaa'
```

Exercise 5.1. Count ambiguous bases

Write a function returning the number of ambiguous bases in a DNA sequence (Solution A.10).

5.2.3. More about loops

Python provides the following advanced features while executing a loop:

- to quit a loop before the end condition is true by using `break`
- to go directly to the next iteration step by using `continue`
- to execute code only if the loop was not interrupted with `break` by using the `else` statement following the `while` clause

Caution

The `else` statement is also executed if the loop is not entered.

Example 5.5. Find a unique occurrence of a restriction site

```
def restrict_uni(dna, enz):
    """ find unique restriction sites """

    found = None
    site = dna.find(enz)

    while site != -1:
        if found:
            break
        found = site
        site = dna.find(enz, found+1)

    else:
        if found is not None:                                    ❶
            return found
```

❶ The test ensures that a restriction site occurrence at position 0 is also true.

Exercise 5.2. Check DNA alphabet

Write a loop to verify all bases in a DNA sequence. (Solution A.11).

Example 5.6. Find all possible start codons in a cds

```
def find_starts (cds):
    """ find start codons in a cds """

    start = -1
    while 1:
        start = cds.find("atg", start+1)

        if start == -1:
            break

        if start % 3:
            continue                                                    ❶

        print "possible start codon at position %d" % start
```

❶ The `continue` statement is used to skip all *atg* codons that are out of frame.

Go back

Return at the end of Section 2.1.

Chapter 6. Functions

6.1. Some definitions

Function — A function is a piece of code that performs a specific sub-task. It takes arguments that are passed to parameters (special place holders to customise the task) and returns a result.

Operator — An operator is a function that takes one or two arguments and that is invoked by the following syntax: *arg1 op arg2*.

Note

Operators are defined by special methods in Python:

```
>>> "atgacta" + "atgataga"
'atgactaatgataga'

>>> "atgacta".__add__("atgataga")
'atgactaatgataga'
```

Procedure — The terms "function" and "procedure" are often used as if they would be interchangeable. However, the role of a procedure is not to return a value, but to perform an action, such as printing something on the terminal or modifying data (i.e something which is sometimes called "doing side-effects" in functional programming parlance).
Strictly speaking, the definition of a function is the same as the mathematical definition: given the same arguments, the result will be identical, whereas the behaviour of a procedure can vary, even if the task is invoked with the same arguments.

In Python, as in most programming languages, there is no difference in function and procedure definitions or calls. But if no return value is specified or if the return value is empty, then the empty object `None` is returned. It is important to know if the called function returns a result.

Example 6.1. Differences between functions and procedures

```
>>> enznames = [ 'EcoRI', 'BamHI', 'HindIII' ]

>>> enznames.index('BamHI')
1

>>> enznames.reverse()                                    ❶

>>> enznames
['HindIII', 'BamHI', 'EcoRI']
```

❶ The `reverse()` method executes an inversion of the list `enzname`. It does it *inplace*, and does not construct a new list.

Method

A method is a function or procedure that is associated with an object. It executes a task an object can be asked for. In Python it is called via the `.` (dot) operator.

```
>>> dna='atgctcgctgc'
>>> dna.upper()
'ATGCTCGCTGC'
```

6.2. Operators

6.2.1. Order of evaluation

Table 6.1 provides the precedence of Python operators. They are listed from the highest to the lowest priority. Operators listed on the same row have equal priority.

Table 6.1. Order of operator evaluation (highest to lowest)

Operator	Name
`(..), [..], {..}, '..'`	Constructors
`s[i], s[i:j], s.attr, f(..)`	Indexing, slicing and function calls
`+x, -x, ~x`	Unary operators
`x ** y`	Power (right associative)
`x * y, x / y,x % y`	Multiplication, division, modulo
`x + y, x - y`	Addition, subtraction
`x << y, x >> y`	Bit shifting
`x & y`	Bitwise and
`x | y`	Bitwise or

`x < y, x <= y, x > y, x >= y, x == y, x != y, x <> y, x is y, x is not y, x in s, x not in s<`	Comparison, identity, sequence membership tests
`not x`	Logical negation
`x and y`	Logical and
`lambda args:  expr`	Anonymous function

6.2.2. Object comparisons

The `==` operator test the *equality* of objects, whereas the `is` operator test their *identity*. Two objects are identical if they refers to the same place in memory. For numbers and strings there is no difference in the result. List and tuples are equal if all their members are equal and dictionaries are equal if they have the same set of keys and the value of each key is also equal.

6.2.3. . (dot) operator

Everything in Python is an object, and the base types are implemented as classes. The `.` (dot) operator is used to ask an object to do something, or more formally to access its attributes and methods.

6.2.4. String formatting

The `%` (modulo) operator applied to strings formats them. Table 6.2 provides the characters that you can use in the formatting template and Table 6.3 gives the modifiers of the formatting character.

Table 6.2. String formatting: Conversion characters

Formatting character	Output	Example	Result
`d,i`	decimal or long integer	`"%d" % 10`	’10’
`o,x`	octal/hexadecimal integer	`"%o" % 10`	’12’
`f,e,E`	normal, ’E’ notation of floating point numbers	`"%e" % 10.0`	’1.000000e+01’
`s`	strings or any object that has a `str()` method	`"%s" % [1, 2, 3]`	’[1, 2, 3]’
`r`	string, use the `repr()` function of the object	`"%r" % [1, 2, 3]`	’[1, 2, 3]’
`%`	literal %		

Table 6.3. String formatting: Modifiers

Modifier	Action	Example	Result
name in parentheses	selects the key name in a mapping object	`"%(num)d %(str)s" % { ’num’:1, ’str’:’dna’}`	’1 dna’
`-,+`	left, right alignment	`"%-10s" % "dna"`	’dna_____’

`0`	zero filled string	`"%04i" % 10`	’0010’
number	minimum field width	`"%10s" % "dna"`	’_____dna’
`.` number	precision	`"%4.2f" % 10.1`	’10.10’

Go back

Return to Section 2.1 to continue the introduction to strings.

6.3. Defining functions

Functions are defined with the `def` statement followed by the name of the function, and the parameter list in parentheses. The result of the calculation is returned by the `return` statement.

Example 6.2. Defining functions

The following example transforms Exercise 2.1, that calculates the GC percentage of a DNA sequence, into a function:

```
>>> def gc(dna):
...     return (count(dna, 'c')+count(dna, 'g'))/float(len(dna))*100.0    ❶
...
>>> gc('atgtaatgatat')
16.666666666666664
>>> gc(dna)                                                               ❷
64.077669902912632
```

❶ The Python interpreter displays two different kinds of prompts. The first `>>>` is the normal one. The second `...` indicates the continuation of a block.

❷ 

Caution

Allthough the name of the argument (`dna`) is the same as the name of the parameter, their values are not the same.

Go to

Read also Section 3.1.2 to learn more about Python syntax. You might need to read Section 5.1 as well to understand the examples given in the syntax section.

Exercise 6.1. DNA complement function

Write a function to calculate the complement of a DNA sequence. (Solution A.12)

Go back

Return to Section 2.1 to carry on with the introduction to strings.

6.4. Passing arguments to parameters

6.4.1. Reference arguments

When a function is invoked, a reference to the value of the argument is passed to the parameter.

Example 6.3. Remove enzymes with ambiguous restriction patterns

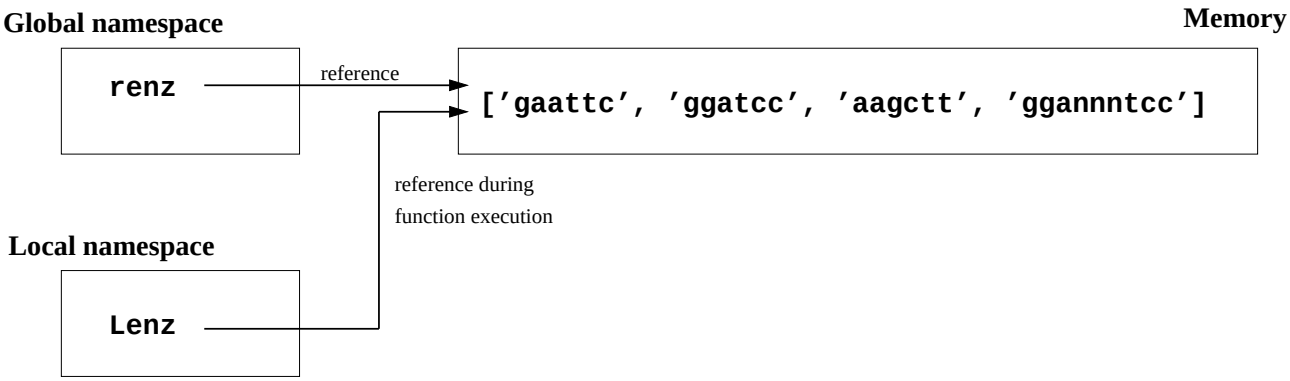
The following function removes all restriction enzyme patterns that contains ambiguous bases from a list.

```
def remove_ambigous_renz(Lenz):
    """ remove enzymes with ambiguous restriction patterns """
    for i in range(len(Lenz)):
        if not check_dna(Lenz[i]):
            del Lenz[i]
```

Figure 6.1 illustrates what happens when `remove_ambiguous_renz()` is invoked as follow:

```
>>> renz = ['gaattc', 'ggatcc', 'aagctt', 'ggannntcc']

>>> remove_ambiguous_renz(renz)
>>> renz
['gaattc', 'ggatcc', 'aagctt']
```

Figure 6.1. Referencing Arguments



During the execution of `remove_ambiguous_renz(renz)` the content of `Lenz` is modified. Figure 6.1 shows that `renz` and `Lenz` refers to the same object and explains why `renz` is also modified.

6.4.2. Passing arguments by keywords

When a function is invoked with a tuple of arguments, they will be associated to parameters according to their position in the tuple. But it is also possible to pass arguments by keywords. This means that the arguments are assigned to parameters by explicitly naming them.

Example 6.4. Passing arguments by keywords

The following function constructs the command line for the **blast** program:

```
def blast2(query, program, database):
    return "blastall -p %s -d %s -i %s" % (program, database, query)
```

The arguments can be passed by position:

```
>>> blast2("seq.fasta", "blastp", "swissprot")
'blastall -p blastp -d swissprot -i seq.fasta'
```

or by explicit naming:

```
>>> blast2(program='blastp', database='swissprot', query='seq.fasta')
'blastall -p blastp -d swissprot -i seq.fasta'
```

One advantage is that you do not have to know in what order parameters are declared in the function.

It is possible to mix the two mechanisms:

```
>>> blast2("seq.fasta", program='blastp', database='swissprot')
'blastall -p blastp -d swissprot -i seq.fasta'
```

But arguments passed by position must be provided first:

```
>>>  blast2("seq.fasta", program='blastp', 'swissprot')
  File "<string>", line 1
    blast2("seq.fasta", program='blastp', 'swissprot')
    ^
SyntaxError: invalid syntax
```

Go back

Return to the end of the introduction to the list type (Section 2.3).

6.5. Default values of parameters

Default values of parameters can be defined in the function definition.

Example 6.5. Default values of parameters

To use "blastp" and "swissprot" as default values for `program` and `database` parameters, the `blast2()` function can be redefined as follow:

```
def blast2(query, program='blastp', database='swissprot'):
    return "blastall -p %s -d %s -i %s" % (program, database, query)
```

So, you can now call it this way:

```
>>> blast2('seq.fasta')
'blastall -p blastp -d swissprot -i seq.fasta'

>>> blast2('seq.fasta', 'blastp', 'swissprot')
'blastall -p blastp -d swissprot -i seq.fasta'

>>> blast2('seq.fasta', database='nrprot')
'blastall -p blastp -d nrprot -i seq.fasta'
```

Default values are referenced when the function is defined.

Caution

Be careful if you pass mutable objects as default values. The content of the default value can be modified after function definition if there is a also a global reference to it.

Redefinition of `blast2()` when `params` is defined as:

```
params = { 'e': 1.0,
           'm': 8,
           'F': 'S 10 1.0 1.5' }

def blast2(query, program='blastp', database='swissprot', params=params):
    command = "blastall -p %s -d %s -i %s" % (program, database, query)

    if params:
        for para,value in params.items():
            command += " -%s '%s'" % (para, value)

    return command
```

creates the following behaviour:

```
>>> blast2('seq.fasta')
"blastall -p blastp -d swissprot -i seq.fasta -m '8' -e '1.0' -F 'S 10 1.0 1.5'"


>>> params['q']=-6

>>> blast2('seq.fasta')
"blastall -p blastp -d swissprot -i seq.fasta -q '-6' -m '8' -e '1.0' -F 'S 10 1.0 1.5'"
```

The default behaviour of the `blast2` function has been changed.

It's risky to keep global references to default values: when using global variables, rather make a deep copy of the object (see Example 4.6).

6.6. Variable number of parameters

A function can take additional optional arguments by prefixing the last parameter with an * (asterix). Optional arguments are then available in the tuple referenced by this parameter.

Example 6.6. Variable number of parameters

```
def multi_blast2 (query, program, database, *more_queries):
```

```
    for q in (query,) + more_queries:                                    ❶
        print blast2 (q, program, database)

>>> multi_blast2 ('seq.fasta', 'blastp', 'database', 'seq2.fasta')
blastall -p blastp -d database -i seq.fasta
blastall -p blastp -d database -i seq2.fasta
```

❶ `(query,)` is a tuple of one element. The comma is necessary because `(query)` is the syntax to indicate precedence.

Exercise 6.2. Variable number of arguments

Transform Example 2.6 such that it can be applied as follow: (Solution A.13)

```
>>> all_2_digests('EcoRI', 'HindIII', 'BamHI')
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]
```

instead of:

```
>>> all_2_digests(['EcoRI', 'HindIII', 'BamHI'])
[['EcoRI', 'HindIII'], ['EcoRI', 'BamHI'], ['HindIII', 'BamHI']]
```

Go back

Return to the end of the introduction to tuples (Section 2.3).

Optional variables can also by passed as keywords, if the last parameter is preceded by `**`. In this case, the optional variables are placed in a dictionary.

Example 6.7. Optional arguments as keywords

```
def blast2(query, program='blastp', database='swissprot', **params):
    command = "blastall -p %s -d %s -i %s" % (program, database, query)

    if params:
        for para,value in params.items():
            command += " -%s '%s'" % (para, value)

    return command
```

`blast2()` can now be invoked by:

```
>>> blast2('seq.fasta')
'blastall -p blastp -d swissprot -i seq.fasta'

>>> blast2('seq.fasta', m=8, e=1.0, F='S 10 1.0 1.5')
"blastall -p blastp -d swissprot -i seq.fasta -e '1.0' -m '8' -F 'S 10 1.0 1.5'"
```

You can also directly pass a dictionary as argument:

```
def blast2(query, program='blastp', database='swissprot', params=None):
    command = "blastall -p %s -d %s -i %s" % (program, database, query)

    if params:
        for para,value in params.items():
            command += " -%s '%s'" % (para, value)

    return command
```

Now pass the dictionary:

```
>>> params = { 'e': 1.0,
...            'm': 8,
...            'F': 'S 10 1.0 1.5' }

>>> blast2('seq.fasta', params=params)
"blastall -p blastp -d swissprot -i seq.fasta -q '-6' -m '8' -e '1.0' -F 'S 10 1.0 1.5'"
```

As for required arguments, you can mix positional and keyword based assignment for optional arguments.

```
def multi_blast2 (query, *more_queries, **params):

    database = params.get('database', 'swissprot')
    program = params.get('program', 'blastp')

    for q in (query,) + more_queries:
        print blast2(q, program, database, params)
```

Invoked as:

```
>>> multi_blast2 ('seq.fasta', 'seq2.fasta', m=8, e=1.0, F='')
"blastall -p blastp -d swissprot -i seq.fasta -m '8' -e '1.0' -F 'S 10 1.0 1.5'"
"blastall -p blastp -d swissprot -i seq2.fasta -m '8' -e '1.0' -F 'S 10 1.0 1.5'"
```

Go back

Return to the end of the introduction to dictionaries and carry on with the next section (Section 2.6).

Chapter 7. Functional programming or more about lists

Caution

This chapter is under construction.

Chapter 8. Exceptions

8.1. General Mechanism

Exceptions are a mechanism to handle errors during the execution of a program. An exception is *raised* whenever an error occurs:

Example 8.1. Filename error

```
>>> f = open('my_fil')
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
IOError: [Errno 2] No such file or directory: 'my_fil'
```

An exception can be *caught* by the code where the error occured:

```
try:
   f = open('my_fil')
except IOError, e:
   print e
```

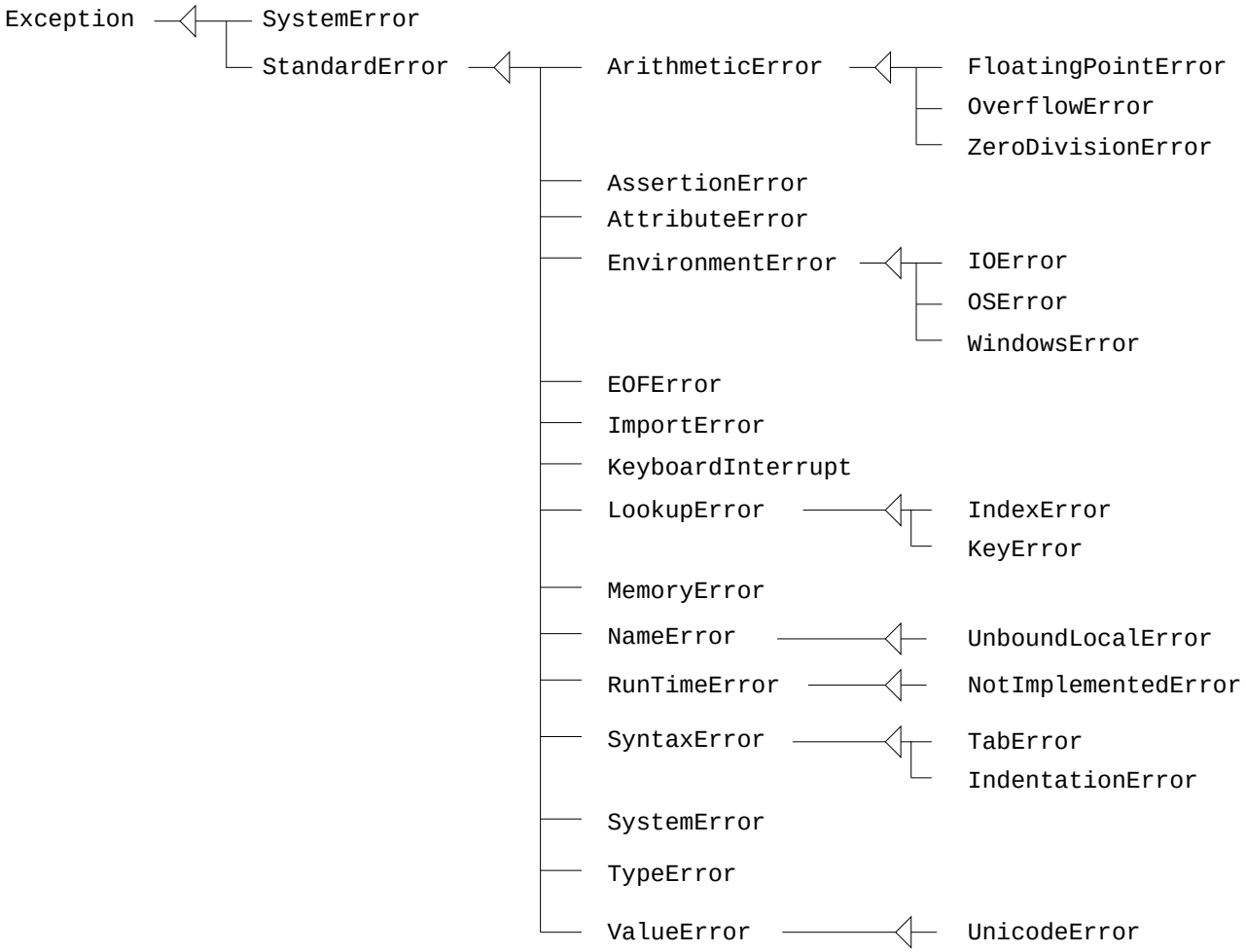
Variable e contains the cause of the error:

```
[Errno 2] No such file or directory: 'my_fil'
```

8.2. Python built-in exceptions

Python predefines several exceptions (Figure 8.1).

Figure 8.1. Exceptions class hierarchy



- `AttributeError`: when you attempt to access a non-existing attribute (method or variable) of an object.
- `NameError`: failure to find a global name (module, ...)
- `IndexError`, `KeyError`: occurs when attempting to access either an out-of-range index in a list or a non-existing key in a dictionary
- `TypeError`: passing an inappropiate value to an operation
- `TabError`, `IndentationError`: two kinds of `SyntaxError`

8.3. Raising exceptions

You can also *raise* an exception in your code, if you consider that the program should be interrupted:

```
   if something_wrong:
             raise Exception
```

You can associate a message to the `raise` statement:

```
   if something_wrong:
             raise Exception, " something went wrong"
```

Example 8.2. Raising an exception in case of a wrong DNA character

```
def check_dna(dna, alphabet='atgc'):
    """ using exceptions """

    for base in dna:
        if base not in alphabet:
            raise ValueError, "%s not in %s" % (base, alphabet)

    return 1
```

8.4. Defining exceptions

Python provides a set of pre-defined exception classes that you can specialize by sub-classing to define specific exceptions for your application (Figure 8.1).

Go to

Since exceptions are defined as classes and by inheritance, you will need some knowledge about classes in order to fully understand this section (see Chapter 12).

Example 8.3. Raising your own exception in case of a wrong DNA character

In the following code, you define an exception `AlphabetError` that can be used when the sequence passed to the function does not correspond to the `alphabet`.

```
class AlphabetError(ValueError):                                    ❶
    pass
```

```
def check_dna(dna, alphabet='atgc'):
    """ using exceptions """

    for base in dna:
        if base not in alphabet:
            raise AlphabetError, "%s not in %s" % (base, alphabet)

    return 1
```

❶ Definition of a new exception in category `ValueError`: `AlphabetError` is a class, that is a subclass of class `ValueError`. The only statement present in class `AlphabetError` is `pass` since `AlphabetError` does not define any new behaviour: is just a new class name.

Example 8.4. Exceptions defined in Biopython

Some Biopython modules define their own exceptions, such as:

- `ParserFailureError` (`GenBank` package)
- `BadMatrix` (`SubsMat` package)

Chapter 9. Modules and packages

9.1. Modules

A module is a piece of code contained in a file. For instance, if the file `ValSeq.py` contains the following code (adapted from Biopython module `NBRF.ValSeq`):

Example 9.1. A module

```
# file Valseq.py

valid_sequence_dict = { "P1": "complete protein", \
 "F1": "protein fragment", "DL": "linear DNA", "DC": "circular DNA", \
 "RL": "linear RNA", "RC":"circular RNA", "N3": "transfer RNA", \
 "N1": "other"   }

def find_valid_key(e):
   for key,value in valid_sequence_dict.items():
             if value == e:
                 return key
```

you can use it by loading it:

```
import ValSeq
```

where `ValSeq` is the module name, and then access to its components, which may be variables, functions, classes, etc...:

```
>>> print ValSeq.valid_sequence_dict['RL']
linear RNA
>>> ValSeq.find_valid_key("linear RNA")
       RL
```

 **Exercise 9.1. Loading and using modules**

Write the code needed to print the command line arguments of a program, by using the `sys` module and its `argv` variable (Solution A.14).

9.1.1. Where are the modules?

Modules are mainly stored in files that are searched:

- in `PYTHONHOME`, where Python has been installed (at Pasteur it is currently `/local/lib/python2.2/`),
- in a path, i.e a colon (':') separated list of file pathes, stored in the environment variable `PYTHONPATH`.

Files may be:

- Python files, suffixed by `.py` (when loaded for the first time, compiled version of the file is stored in the corresponding `.pyc` file),
- defined as C extensions,
- built-in modules linked to the Python interpreter.

Exercise 9.2. Creating a module for DNA utilities

Create a module `dna` containing the functions defined on DNA in previous exercises: `complement` (Exercise 6.1), `ambiguous` (Exercise 5.1), `check_dna` (Exercise 5.2), `restrict` (Exercise 2.3), `digest` and `frag_len` (Exercise 2.4), `revcomp` (Exercise 2.6), `dna_translate` and the standard genetic code (Exercise 2.8). (Solution A.15)

Exercise 9.3. Locating modules

Sometimes, it is not enough to use **pydoc** or `help`. Looking at the source code can brings a better understanding, *even if you should of course never use undocumented features*.

Browse the directory tree `PYTHONHOME`/site-packages/Bio/.

9.1.2. Loading

When importing a module, for example the `dna` module you have just created (Exercise 9.2), you "open" its namespace, which becomes available to your program:

```
>>> import dna
>>> dna.complement('aattttt')
'ttaaaaa'
>>> dna.revcomp('aattttt')
'aaaaatt'
>>> dna.dna_translate('atggacaatttttccgggacgtag')
'MASPNFSGT*'
```

You may also select specific components from the module as "opened" (Figure 9.1):

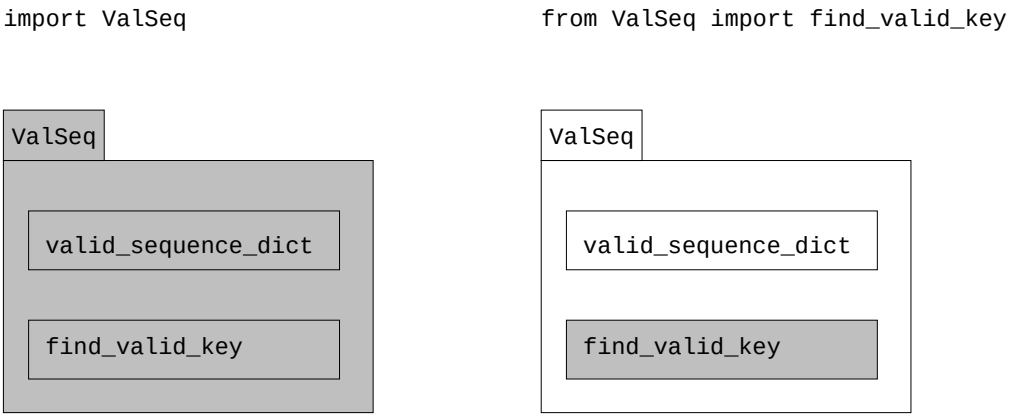
Example 9.2. Loading a module's components

```
>>> from ValSeq import find_valid_key
>>> find_valid_key("linear RNA")
RL
```

In such cases, other components stay hidden, and the namespace is not the one of the module, e.g:

```
>>> print valid_sequence_dict['RL']
NameError: name 'valid_sequence_dict' is not defined
>>> print ValSeq.valid_sequence_dict['RL']
NameError: name 'ValSeq' is not defined
```

Figure 9.1. Loading specific components



You can also load "all" the components from a module, which makes them available *directly* into your code:

```
>>> from ValSeq import *
>>> find_valid_key("linear RNA")
```

Caution

You can restrict the components being imported by an `import *` statement. The `__all__` variable, also used for packages (Section 9.2), can explicitly list the components to be directly accessible (see Exercise 9.8).

A module is loaded only once, i.e, a second **import** statement will not re-execute the code inside the module (see Python **reload** statement in the reference guides).

When loaded from the command line:

```
% python dna.py
```

the module is executed within the `__main__` module (i.e not the `dna` module):

```
% python -i dna.py
>>> dna.complement('aattttt')
NameError: name 'dna' is not defined
>>> complement('aattttt')
'ttaaaaa'
>>> revcomp('aattttt')
'aaaaatt'
>>> dna_translate('atggacaatttttccgggacgtag')
'MASPNFSGT*'
```

For this reason, the code executed at module loading time can be made dependent of the current module name:

```
if __name__ == '__main__':
   # statements that you want to be executed only when the
   # module is executed from the command line
   # (not when importing the code by an import statement)
```

Exercise 9.4. Locating components in modules

What are the components of the Bio.utils module? of the Bio.Prosite.Pattern module? See also the **pydoc** and **help** commands.

Exercise 9.5. Bio.Seq module

Write the `import` statement required to import the `Seq` class from module `Bio.Seq`, in order to create a sequence:

```
> seq=Seq("actttgccatatg")                                    ❶
```

❶ `Seq()` is a function call that creates an instance of the class `Seq`, so you need to be able to access to this component of the `Bio.Seq` module.

Go to

This is not required, but you can see Chapter 10 for more explanations.

Solution A.16

9.2. Packages

A package is a set of modules or sub-packages. A package is actually a directory containing either `.py` files or sub-directories defining other packages.

The dot (.) operator is used to describe a hierarchy of packages and modules. For instance, the module `Bio.WWW.ExPASy` is located in the file `PYTHONHOME/site-packages/Bio/WWW/ExPASy.py`. This module belongs to the Bio.WWW package located into the `PYTHONHOME/site-packages/Bio/WWW/` directory.

9.2.1. Loading

When loading a package, the `__init__.py` file is executed. If the `__init__.py` defines classes, functions, etc... they become available at once, as shown in the following example:

Example 9.3. Using the Bio.Fasta package

```
>>> import Bio.Fasta
>>> handle = open("data/ceru_human.fasta")
>>> it = Bio.Fasta.Iterator(pin, Bio.Fasta.SequenceParser())
>>> seq = it.next()
>>> print seq.seq
>>> it.close()
```

However, loading a package does not automatically load the inner modules. For instance, even though the `Bio.Fasta` package directory contains the following files:

```
% ls Bio/Fasta
       FastaAlign.py   FastaAlign.pyc  __init__.py     __init__.pyc
```

this does not imply that importing the `Bio.Fasta` package loads the `Bio.Fasta.FastaAlign` module:

```
>>> import Bio.Fasta
>>> Bio.Fasta.FastaAlign.parse_file("data/ceru_human.fasta")
AttributeError: 'module' object has no attribute 'FastaAlign'
```

Issuing:

```
>>> from Bio.Fasta import *
```

will however load the `Bio.Fasta.FastaAlign`, because this module is mentioned in the `__all__` attribute in the `Bio/Fasta/__init__.py` file:

```
__all__ = [
   'FastaAlign',
]
```

Other attributes of interest for packages and modules:

- `__name__`
- `__path__`
- `__file__`

Exercise 9.6. Bio.SwissProt package

Which import statements are necessary to make the following code work?

```
expasy = ExPASy.get_sprot_raw('CERU_HUMAN')
sp = SProt.Iterator(expasy, SProt.RecordParser())
record = sp.next()
print record.keywords
```

Solution A.17

Exercise 9.7. Using a class from a module

Why does the following code issue an error?

```
from Bio.SubsMat import FreqTable
dict = ...  # whatever
f = FreqTable(dict, 'COUNT')
TypeError: 'module' object is not callable
```

Solution A.18

Exercise 9.8. Import from Bio.Clustalw

Why does the following code not work?

```
from Bio.Clustalw import *
a=ClustalAlignment()
NameError: name 'ClustalAlignment' is not defined
```

Solution A.19

Chapter 10. Classes: Using classes

The presentation of classes is divided in two parts. The first part (present chapter) explains how to use classes, while the second part (Chapter 12), put after the introduction to Biopython, introduces the definition of new classes.

10.1. Creating instances

You have actually already used classes, or rather objects, i.e *instances of classes*, throughout this tutorial: : strings, lists, etc... However, most of the time the objects you have manipulated were not directly created by your own code, but rather by other components: for instance the “[]” operator creates a list, the “"""” operator creates a string, the `open` function creates a file handle, etc...

The actual direct syntax to *instantiate* a class, i.e to create an instance of class, is by calling a function with the same name as the class. For instance, the `random` Python module defines a class `Random`. In order to create an instance of this class, i.e an object which generates random numbers, you do:

```
>>> from random import Random
>>> generator = Random()
```

This creates the object and makes it available from the `generator` variable. You can now use this object to call Random class methods:

```
>>> generator.randrange(100)
 75
```

Sometimes, the instanciation needs arguments, depending on the definition of the class. For instance, there is a class `Netscape` defined in the `webbrowser` Python module. In order to create an instance of this class, i.e a browser that is able to browse Web documents, you need to pass the path of the **netscape** program on your computer:

```
from webbrowser import Netscape
browser = Netscape('/local/bin/netscape')
```

Now, you can use the browser and open a Web document by:

```
browser.open('http://www.biopython.org/')
```

Or, if we want to directly create an instance of class `Seq`, one of the class defined in Biopython to create sequence objects (see Section 11.3), we do:

```
from Bio.Seq import Seq
```

```
seq = Seq('gcatgacgttattacgactctgtcacgccgcggtgcgacgcgtctgctggg')
```

The call to perform the instanciation (i.e: `Random()`, `Netscape('/local/bin/netscape')`, etc...) actually calls the `__init__` method defined in the class. Thus, passing arguments to parameters for the instanciation call (i.e `__init__` method call) follows exactly the same rules as for usual functions (see Section 6.4). So, passing the alphabet as a parameter to the `Seq()` call for creating a protein sequence, would be written as:

```
seq = Seq('MKILILGIFLFLCSTPAWAKEKHYYIGIIETTWDYASDHGEKKLISVDTE',
                  alphabet=Alphabet.ProteinAlphabet()
      )
```

10.2. Getting information on a class

It is important to know what classes are available, what methods are defined for a class, and what arguments can be passed to them. First, classes are generally defined in modules, and the modules you want to use should have some documentation to explain how to use them. Then, you have the **pydoc** command that lists the methods of the class, and describes their parameters. The following command displays information on the `Netscape` class:

```
pydoc webbrowser.Netscape
```

See also the embedding module, which might bring additional documentation about related components:

```
pydoc webbrowser
```

Attributes of a class also include variables. The variables defined for the instances can however not be listed by pydoc, since they belong to the instances, not to the class. That is why they should be described in the documentation string of the class. If they are not, which sometimes happens..., run the Python interpretor and create an instance, then ask for its dictionary:

```
>>> seq = Seq('gcatgacgttattacgactctgtcacgccgcggtgcgacgcgtctgctggg')
>>> dir(seq)
['__add__', '__doc__', '__getitem__', '__getslice__',
'__init__', '__len__', '__module__', '__radd__', '__repr__',
'__str__', 'alphabet', 'count', 'data', 'tomutable',
'tostring']
```

So now, we know that the seq object has a `data` attribute:

```
>>> seq.data
```

```
'gcatgacgttattacgactctgtcacgccgcggtgcgacgcgtctgctggg'
```

When you consult the documentation of a class with the **pydoc** command, you get most of the time a list a strange method names, such as `__add__` or `__getitem__`. These methods are special methods to redefine operators, and will be explained in the next chapter on classes (Chapter 12, Section 12.2).

Chapter 11. Biopython: Introduction

11.1. Introduction

Biopython is a set of modules and packages for biology, including sequence analysis, database access, etc... or parsers components. Since it is very well described by the documentation (see Section 11.2), we are not going here to describe it extensively. Rather, we provide several exercises, since we think that the best way to understand and master Biopython is by practice.

The course about Biopython is divided in two parts, separated by a chapter explaining how to define new classes in Python (Chapter 12). The first part (present chapter), attempts to cover the use of central components such as components for sequences (Seq, SeqRecord, SeqFeature), alignments (Blast, Clustalw) and database access (SwissProt, GenBank). Then, the second part (Chapter 13) presents the main concepts of parsing in Biopython, associated with exercises to build parsing classes for Enzyme entries. The last part of the Biopython presentation summarizes several of the exercises provided in this course by the study of disulfid bonds in Human Ferroxidase 3D structure and alignments (see Section 13.2).

11.2. Documentation

- http://www.biopython.org/
- Biopython tutorial (PDF [http://www.bioinformatics.org/bradstuff/bp/tut/Tutorial.pdf], HTML [http://www.bioinformatics.org/bradstuff/bp/tut/Tutorial.html]) [1]
- Biopython examples [http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/examples/] from the Biopython distribution.
- API documentation [http://www.bioinformatics.org/bradstuff/bp/api/]

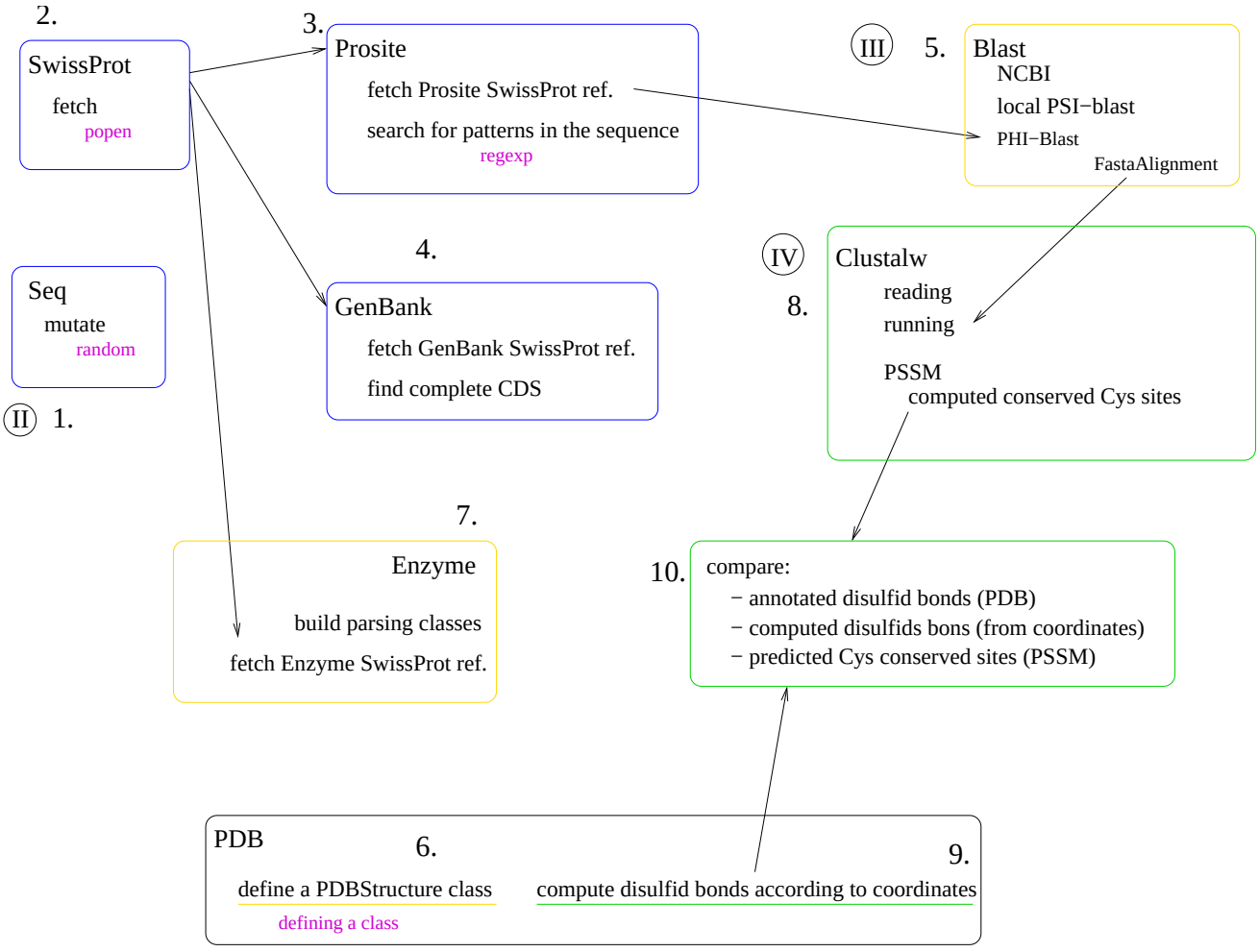
See also:

- Python Scripting in Computational Biology [http://smi.stanford.edu/projects/helix/bmi214/python_mis214_000331.pdf] (PDF)
- Tutorial at PSB 2001: Python for Structural Bioinformatics [http://www.scripps.edu/pub/olson-web/people/sanner/html/talks/PSB2001talk.html]
- Software development - Python [http://www.scripps.edu/pub/olson-web/people/sanner/home.html], by Michel Sanner at Molecular Graphics Lab (MGL), Scripps, including ViPEr, a great visual environment for molecular visualization (see [http://www.scripps.edu/~sanner/python/index.html] for details).

[1] Mirror copy of PDF [http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/Tutorial.pdf].

- All Sites > BioInformatics [http://www.pythonandzope.com/BioInformatics/index_html] directory in the Python and Zope directory.
- Using Python to solve problems in bioinformatics [http://bonsai.ims.u-tokyo.ac.jp/~mdehoon/software/software.html], by Michiel de Hoon.
- Object-oriented parsing of biological databases with Python [http://bioinformatics.oupjournals.org/cgi/content/abstract/16/7/628] (paper about PySAT [http://www.embl-heidelberg.de/~chenna/PySAT/]).
- Python for Science [http://starship.python.net/crew/hinsen/], by Konrad Hinsen.
- SciPy - Scientific tools for Python [http://www.scipy.org/].

Figure 11.1. Overview of the Biopython course



11.3. Bio.Seq and Bio.SeqRecord modules

Look at chapter 2 in Biopython tutorial (PDF [http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/Tutorial.pdf]) (the following of this section actually assumes that you have read it).

11.3.1. Using Seq class

The `Seq` class is defined in the `Bio.Seq` module.

Example 11.1. Building Seq sequences from strings

```
from Bio.Seq import Seq
seq = Seq('gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg')
print seq
```

Most of string manipulations seen in Section 2.1 are available on `Seq` objects.

Exercise 11.1. Length of a Seq sequence

Display the length of a sequence, and count the number of occurrences of 'a'.
Solution A.20

Exercise 11.2. GC content of a Seq sequence

Adapt Exercise 2.1 (display GC content) to `Bio.Seq.Seq`.
Solution A.21

11.3.2. Sequences reading and writing

There are several ways in Biopython to handle sequence files. The Fasta formatted sequences might be read either through the `Bio.Fasta Iterator` (an iterator is an object that sequentially return successive records from a data input, see Section 13.1.3 for explanations), or with the `FastaReader` from the `Bio.Seqio.FASTA` module. There are also specialized modules to read flat format files (e.g SwissProt or GenBank formatted files) (see Section 11.4 and Section 11.5).

Example 11.2. Reading a FASTA sequence with the Bio.Fasta package

```
import Bio.Fasta
import sys

handle = open(sys.argv[1])
it = Bio.Fasta.Iterator(handle, Bio.Fasta.SequenceParser())
seq = it.next()
```

```
while seq:
  print seq.name
  print seq.seq
  seq = it.next()
handle.close()
```

Example 11.3. Reading a FASTA sequence with the Bio.Seqio.FASTA module

```
from Bio.SeqIO import FASTA
import sys

handle = open(sys.argv[1])
it = FASTA.FastaReader(handle)
seq = it.next()
while seq:
    print seq.name
    print seq.seq
    seq = it.next()

handle.close()
```

 Exercise 11.3. Write a sequence in FASTA format

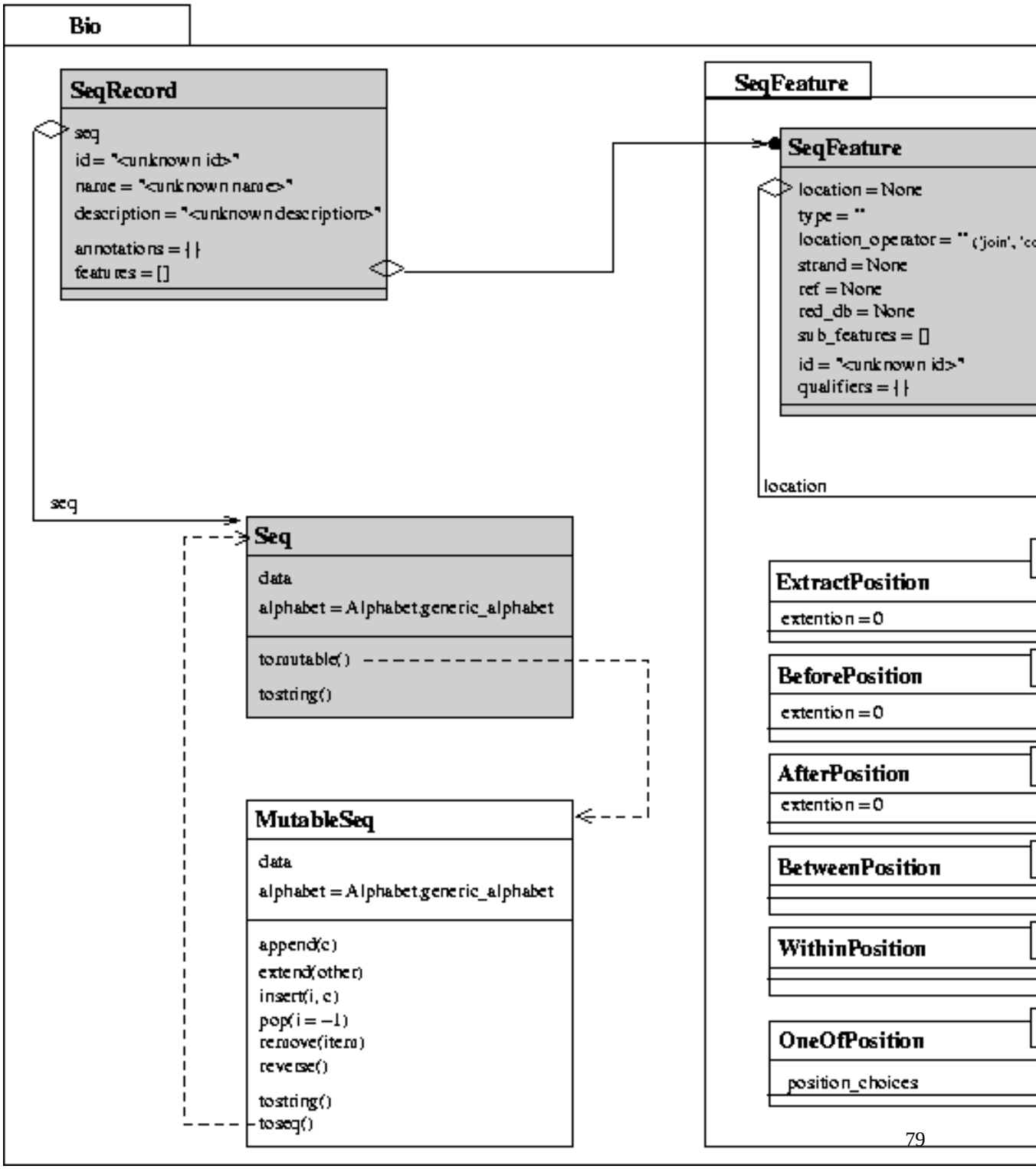
Write a sequence in FASTA format using the `Bio.Seqio.FASTA` module. Initialize the sequence from a string as shown in example Example 11.1.
Solution A.22

 Exercise 11.4. Code reading: Bio.sequtils

11.3.3. Bio classes for sequences

Figure 11.2 describes the classes to handle sequences. A `SeqRecord` is composed of `Seq` and `SeqFeatures`.

Figure 11.2. Seq, SeqRecord and SeqFeatures modules and classes hierarchies

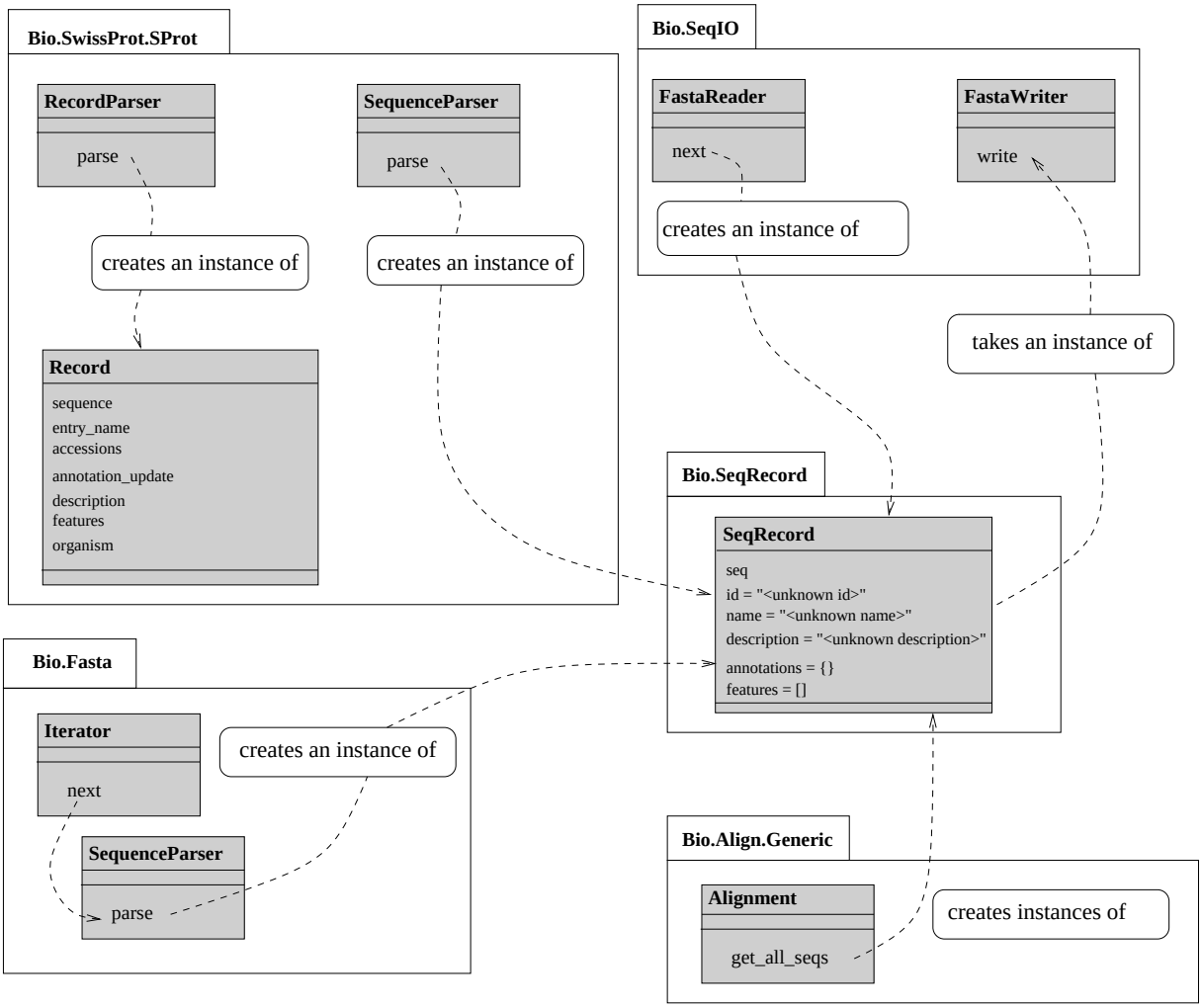


11.3.3.1. SeqRecord objects

`SeqRecord` is central in Biopython. `SeqRecord` objects are created by various Biopython components (most of them not covered yet) Figure 11.3:

- `FastaReader` class in `Bio.SeqIO.FASTA` module (as shown above in Example 11.3)
- `SequenceParser` class in `Bio.Fasta` module (used as argument for creating and `Iterator` in Example 11.2).
- `SequenceParser` class in `Bio.SwissProt.Sprot` module (see Section 11.4)
- `get_all_seqs` method of `Alignment` class in `Bio.Align.Generic` module (see Section 11.6.2)
- `Bio.GenBank` parser (not tested and thus not represented in Figure 11.3) (see Section 11.5)

Figure 11.3. SeqRecord links to other classes



11.3.3.2. MutableSeq objects

A `MutableSeq` differs from a `Seq` by being modifiable.

Exercise 11.5. Random mutation of a sequence

Write a function `mutateseq` that randomly mutate a sequence. This function could take the following parameters, (with appropriate default values): sequence, random seed, span and probability:

```
mutateseq(seq,span=1000,p=0.01)
```

Solution A.23

Exercise 11.6. Random mutation of a sequence: count codons frequency

With the `mutateseq` function from the previous exercise (Exercise 11.5) and the `codons` function (Exercise 2.5), write a program that displays the frequencies of each codon, before and after the mutation of the sequence.
Solution A.24

Example 11.4. Plotting codon frequency

The following code use a `tkplot` module written by Michiel Jan Laurens de Hoon [http://bonsai.ims.u-tokyo.ac.jp/~mdehoon/], that we have a little modified, to plot a bar chart of each codon frequency.

```
#-------------------------------------------------------
# bar charts of codons frequencies
#   - for legibility, 2 charts are built

from tkplot import *
from Numeric import *

def codon_sort(a,b):
 if a < b:
  return -1
 elif a > b:
  return 1
 else:
  return 0

labels=count.keys()
labels.sort(codon_sort)

w1=window(plot_title='Count codons',width=1000)
y=array(count.values())[:len(count)/2]
x=arange(len(y)+1)
w1.bar(y,x,label=labels[:len(count)/2])

w2=window(plot_title='Count codons(2)',width=1000)
y=array(count.values())[(len(count)/2)+1:]
x=arange(len(y)+1)
w2.bar(y,x,label=labels[(len(count)/2)+1:])
```

(original Tk plot module [http://bonsai.ims.u-tokyo.ac.jp/~mdehoon/software/software.html] - Python code [http://bonsai.ims.u-tokyo.ac.jp/~mdehoon/software/tkplot/tkplot.py]), modified module [modules/tkplot.py] - the one that you need to get the example work [2])

 **Exercise 11.7. Random mutation of a sequence: plot codons frequency**

Use the code of Example 11.4 to plot both the normal and mutated codon counts of (Exercise 11.6).
Solution A.25

11.4. Bio.SwissProt.SProt and Bio.WWW.ExPASy

11.4.1. Reading entries

You can read SwissProt entries by using the SProt.Iterator [http://www.bioinformatics.org/bradstuff/bp/api/Bio/SwissProt/SProt_
(an iterator is an object that sequentially return successive records from a data input, see Section 13.1.3 for explanations). This iterator takes 2 arguments: the handle from where to read the entry, which may be an open file or the data fetched from an url, and a parser, which actually builds the objects returned by the iterator. For this purpose, you either use the `SProt.RecordParser` and get a `SProt.Record`, or use the `SProt.SequenceParser` and get a `Bio.Seq.Seq` sequence (see Section 13.1 for more information on parsing in Biopython).

In the following example, the entry is fetched from a local file, provided on the command line:

Example 11.5. Fetching a SwissProt entry from a file

```
# reading a SwissProt entry from a file

from Bio.SwissProt import SProt
from sys import *

handle = open(argv[1])
sp = SProt.Iterator(handle, SProt.RecordParser())
record = sp.next()
print record.entry_name
print record.sequence
```

(you can try it on data/ceru_human.sp)

[2] See also Chapter 14 on Graphics.

Exercise 11.8. Code reading: connecting with ExPASy and parsing SwissProt records

A second example is given by the script swissprot.py [http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/examples/swissprot.py] provided within the Biopython distribution.

Exercise 11.9. SwissProt to FASTA

Write a function `sp_fasta` which converts a SwissProt file in FASTA format and use the `FastaWriter` defined in module `Bio.SeqIO.FASTA`. The function defined could be called this way:

```
convert_sp_fasta('data/ceru_human.sp', stdout)
```

You can store this function in a `sprot` module (`sprot.py`).

Tip

Look again at Example 11.3 which uses the `Bio.SeqIO.FASTA` module.

Tip

To read the SwissProt entry, you will need to use another parser than in Example 11.5, since the record you need must be compatable with the `FastaWriter` class (see Figure 11.3).

Look at Figure 11.3 to understand how to use the `FastaWriter` class in conjunction with a SwissProt parser.
Solution A.26

Exercise 11.10. Fetch an entry from a local SwissProt database

Changes Example 11.5 to fetch the entry from a local SwissProt database via the **golden** program (available from ftp://ftp.pasteur.fr/pub/GenSoft/unix/db_soft/golden/). Write this as a function `get_sprot_entry_local` that you can add in the `sprot` module (`sprot.py`).
Solution A.27

Tip

Use the Python **os.popen** function.

11.4.2. Regular expressions in Python

An detailed presentation of Python regular expressions is available here: Regular Expression HOWTO [http://py-howto.sourceforge.net/regex/regex.html].

In Python, regular expressions are handled by a module: `re`:

```
>>> import re
```

Before searching for a pattern, you must first *compile* it:

```
>>> expression = '[AP]{1,2}D'
>>> p = re.compile(expression)
```

You then issue a *search*, for instance in the small sequence `seq`, by:

```
>>> seq = "RPAD"
>>> result = p.search(seq)
```

To get the occurrences, you can ask for the start and end of the match in the searched text:

```
>>> print result.start(), result.end(), seq[result.start():result.end()]
1 4 PAD
```

Example 11.6. Searching for the occurrence of PS00079 and PS00080 Prosite patterns in the Human Ferroxidase protein

```
import sys
import re
from Bio.SwissProt import SProt

sp = open(sys.argv[1])
iterator = SProt.Iterator(sp, SProt.SequenceParser())
seq = iterator.next().seq
sp.close()

PS00079 = 'G.[FYW].[LIVMFYW].[CST].{8,8}G[LM]...[LIVMFYW]'                ❶
p = re.compile(PS00079)                                                   ❷
result = p.search(seq.tostring())                                         ❸
print PS00079
print result.start(), result.end(), seq[result.start():result.end()]      ❹
```

❶ The regular expression is stored in a string.
❷ The regular expression is compiled in a pattern.
❸ The compiled pattern is searched in the sequence.
❹ The result of the search is printed.

A convenient feature enables to associate a name to sub-parts of the matched text:

```
import sys
import re
from Bio.SwissProt import SProt

sp = open(sys.argv[1])
iterator = SProt.Iterator(sp, SProt.SequenceParser())
seq = iterator.next().seq
sp.close()

PS00080 = '(?P<copper3>H)CH...H...[AG](?P<copper1>[LM])'                    ❶
p = re.compile(PS00080)
result = p.search(seq.tostring())
print PS00080
print result.start(), result.end(), seq[result.start():result.end()]

print 'copper type 3 binding residue: ', result.group('copper3')            ❷
print 'copper type 1 binding residue: ', result.group('copper1')
```

❶ The regular expression now contains 2 identifiers: `copper1` and `copper3`.
❷ You can print the sub-parts of the result identified by variables: `copper1` and `copper3`.

To get information about the `re` module, see pydoc, but also the `sre` module (Support for regular expressions), for which `re` is a wrapper.

Exercise 11.11. Enzymes referenced in a SwissProt entry

Write a function `get_enzyme_ref` which extracts the enzyme reference from SwissProt entry (you find it in the SwissProt description field). You can add this function in your `sprot` module (`sprot.py`). (Solution A.28)

11.4.3. Prosite

11.4.3.1. Prosite Dictionary

Biopython defines several dictionaries to access biological databases. Having a dictionary means that you can fetch an entry by:

```
entry = prosite['PS00079']
```

For this to work, you first need to create the dictionary:

```
prosite = Bio.Prosite.ExPASyDictionary()
```

As you can guess by the name of the module, you actually fetch the Prosite entry on the Web. You could also fetch the Prosite entry from a local database with the golden program (see Exercise 11.10). The entry fetched above is actually a string. In order to have the dictionary return a record, you must rather create it like this:

```
prosite = Bio.Prosite.ExPASyDictionary(parser=Bio.Prosite.RecordParser())
```

11.4.3.2. Prosite patterns

Exercise 11.12. Print the pattern of a Prosite entry

Write a function `get_prosite_pattern` that returns a string containing the pattern of a Prosite entry (provided as an id):

```
get_prosite_pattern('PS00079')
```

Solution A.29

Exercise 11.13. Display the Prosite references of a SwissProt protein.

The SwissProt entry contains references to databases, including potential references to the Prosite [http://www.expasy.ch/prosite/] database (see `SProt.Record` class documentation).

Write a function `get_prosite_refs` that extracts the references to Prosite from a SwissProt entry (provided as a handle) (data [data/ceru_human.sp]).

The functions `get_prosite_pattern`, defined in Solution A.29 and the function `get_prosite_refs` can be used combined to display the patterns of the Prosite references given in a SwissProt entry. Write the statements to achieve this task.

You can also add these functions in the `sprot` module (`sprot.py`).
Solution A.30

The `Bio.Prosite` package defines a `Pattern` class that enables to create patterns which may be searched for in sequences objects, as in the `re` Python module for regular expressions. The result of a search is a `PrositeMatch`, that behaves in a way similar to a regular expression match.

Exercise 11.14. Search for occurrences of a protein PROSITE patterns in the sequence

Now, you know how to fetch a Prosite entry, how to extract a Prosite reference from a SwissProt entry, and how to search for pattern occurrences in a sequence. Search for the occurrences of the `prosite_refs` patterns in the sequence `seq`. Display:

- the pattern itself
- the start and end position in the sequence
- the corresponding sub-sequence.

Solution A.31

11.5. Bio.GenBank

11.5.1. Reading entries

11.5.1.1. NCBIDictionary

Example 11.7. Using a NCBIDictionary

You can use the `GenBank.NCBIDictionary` to access a GenBank entry by its genbank ID (accession numbers do not work yet):

```
from Bio import GenBank
ncbi_dict = GenBank.NCBIDictionary()
gb_entry = ncbi_dict[id]
```

where `gb_entry` is a string.

The `GenBank.NCBIDictionary` may also be combined with a parser, producing either (there is a bug in the current Biopython release that disables this feature):

- a `GenBank.Record` instance:

```
from Bio import GenBank
record_parser = GenBank.RecordParser()
ncbi_dict = GenBank.NCBIDictionary(record_parser)
gb_record = ncbi_dict[id]
```

- or a `SeqRecord` instance:

```
from Bio import GenBank
feature_parser = GenBank.FeatureParser()
ncbi_dict = GenBank.NCBIDictionary(feature_parser)
seqrecord = ncbi_dict[id]
```

11.5.1.2. Iterator

Example 11.8. GenBank Iterator class

You can also use the `GenBank.Iterator` class to browse a file containing several GenBank entries:

```
from Bio import GenBank

gb_file = argv[1]
gb_handle = open(gb_file, 'r')
feature_parser = GenBank.FeatureParser()
gb_iterator = GenBank.Iterator(gb_handle, feature_parser)
while 1:
   cur_record = gb_iterator.next()
   if cur_record is None:
       break
   print cur_record.seq
```

 **Exercise 11.15. Extracting the complete CDS from a GenBank entry**

Write a function `get_complete_cds`:

```
cds = get_complete_cds(seqrecord)
```

that returns the DNA sequence of the complete CDS.
Solution A.32

11.6. Running Blast and Clustalw

11.6.1. Blast

Look at chapter 3 in Biopython tutorial [http://www.bioinformatics.org/bradstuff/bp/tut/Tutorial.html] (the following of this section actually assumes that you have read it).

Exercise 11.16. Remote Blast, run and save results

Run a remote Blast on the SwissProt databank, with Blast parameter E set to 1, number of descriptions and alignments set to 100, and save the result in a file (query [data/ceru_human.fasta]).
Solution A.33

Exercise 11.17. Remote Blast, parse results

Parse the Blast result saved in previous exercise (Exercise 11.16). Only display hits (not HSP) having and Expect value equal to 0.0. (NCBI Blast report [data/ceru_human.fasta.blast])
Solution A.34

Tip

There is a class which stores the description of the hit, including the Expect value (which is not necessarily the same as the Expect value of each HSP).

Exercise 11.18. Local PSI-Blast

Run a blastpgp locally on the SwissProt databank. Display only HSPs which expect value is above a given threshold.
Solution A.35

Exercise 11.19. Search Prosite patterns with PHI-blast

Use the patterns associated to the Prosite references found in a SwissProt entry with PHI-blast.

Start from `get_prosite_refs` and `get_prosite_pattern` (Exercise 11.13) to get the patterns (these functions should have been saved in module sprot.py [exercises/sprot.py]). You will then have to provide the patterns to PHI-Blast in a "hitfile" (-k parameter) to run a PHI-Blast (see Solution A.35).
Solution A.36

Exercise 11.20. Running FASTA

How would write a `run_fasta` function to run a FASTA search:

```
result=run_fasta(query_file, 'gbmam')
```

Write the `run_fasta`, knowing that the appropriate fasta command line to search a protein database is for instance: **fasta_t -q data/ceru_human.fasta /local/databases/fasta/gpmam**
Result can be provided as text (i.e not as Python classes). Solution A.37

Tip

Use the Python **os.popen** function.

11.6.2. Clustalw

11.6.2.1. Loading a Clustalw file

Example 11.9. Loading a Clustalw file

```
import Bio.Clustalw
from Bio.Alphabet import IUPAC
from sys import *

align = Bio.Clustalw.parse_file(argv[1], alphabet=IUPAC.protein)          ❶

for seq in align.get_all_seqs():
    print seq.description
```

❶ The default alphabet seems to be nucleic.

11.6.2.2. Running Clustalw

Exercise 11.21. Doing a Clustalw alignmnent

Run the following code (completing the statements for loading the appropriate components).

```
cline = MultipleAlignCL(argv[1])                                          ❶
cline.set_output('data/test.aln')
print "Command line: ", cline

align = do_alignment(cline)                                               ❷
for seq in align.get_all_seqs():                                          ❸
    print seq.description
    print seq.seq
```

❶ Construction of the command line to run Clustalw.

❷ Construction of a `ClustalAlignment` object (`Bio.Clustalw` package). `ClustalAlignment` is a sub-class of the `Alignment` class, defined in the `Bio.Align.Generic` module.
❸ The `get_all_seqs` method returns `SeqRecord` objects (defined in the `Bio.SeqRecord` module).

Solution A.38

Exercise 11.22. Align Blast HSPs

Create a Fasta formatted sequences file from the HSPs of a Blast report and align these sequences. Starting from the Blast parsing in Exercise 11.18, create a `Bio.Fasta.FastaAlign.FastaAlignment` from the HSPs, remove the gaps, and align the sequences. Only keep the 10 first hits.
Solution A.39

11.6.2.3. Extracting information from alignments

Example 11.10. Get the consensus sequence of an alignment

```
import Bio.Clustalw
import Bio.Align.AlignInfo
from Bio.Alphabet import IUPAC
from sys import *

align = Bio.Clustalw.parse_file(argv[1], alphabet=IUPAC.protein)
align_info = Bio.Align.AlignInfo.SummaryInfo(align)
consensus = align_info.dumb_consensus()
print "Consensus: ", consensus.tostring()
```

(alignment [data/ceru_human.blastp-edit.aln])

Exercise 11.23. Get the PSSM from an alignment

First get the PSSM (Position Specic Score Matrices - you should look at the section 3.5.4 in Biopython tutorial [http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/Tutorial.html] for explanations) from an alignment (loaded from a Clustalw format as in Example 11.9):

```
align = Bio.Clustalw.parse_file(sys.argv[1], alphabet=IUPAC.protein)
ref_seq = align.get_seq_by_num(0)                                    ❶
pssm = align_info.pos_specific_score_matrix(ref_seq, chars_to_ignore = ['X'])
```

❶ A PSSM is related to one the the sequence in the alignment (here the first one)

Using this PSSM, then display the positions in the alignment that have a percent identity above a given threshold. Notice positions with conserved cysteins (Cys).
Solution A.40

Exercise 11.24. Plotting Cys conserved positions

You can use Tkinter to display various plots [3]. The following code shows how to create a plot widget, given 2 tuples (`vector_x` and `vector_y`, containing the x and y axes values.

Use this code and Exercise 11.23 to plot the Cys conserved positions of the alignment.

```
# ------------------------------------------------
#    plot of Cys positions
#

from Numeric import *
from Tkinter import *
import Pmw

# vector_y must be a tuple
vector_y =                                                    ❶
vector_x =

root = Tk()
frame = Frame(root)
frame.pack()
g = Pmw.Blt.Graph(frame)
g.pack( expand=1, fill='both' )
g.line_create( "percent of identity", xdata=vector_x, ydata=vector_y )
g.configure(width=1000)
g.configure(height=500)
g.element_configure('percent of identity', symbol='none')
g.axis_configure('x', stepsize=100)
```

❶ Fill this with the code necessary to get tuples containing the plot values (percent of Cys).

Solution A.41

11.6.3. Running other bioinformatics programs under Pise

You can run several other programs interfaced under the Pise [http://www.pasteur.fr/recherche/unites/sis/Pise/] system, by using this API [http://www.pasteur.fr/recherche/unites/sis/Pise/#pisepython].

Example 11.11. Running the EMBOSS cusp program

The following example shows how to run the EMBOSS [http://www.hgmp.mrc.ac.uk/Software/EMBOSS/] cusp [http://bioweb.pasteur.fr/seqanal/interfaces/cusp.html] program to create a codon usage table:

[3] See also Chapter 14 on Graphics.

```
from Pise import PiseFactory
from Bio.SeqIO import FASTA
import sys

handle = open(sys.argv[1])
it = FASTA.FastaReader(handle)
seq = it.next()
handle.close()

factory = PiseFactory(email='user@domain')   # you have to put your email here

cusp = factory.program('cusp')
cusp.sequence(seq)

job = cusp.run()
if job.error():
    print "Error: " + job.error_message()
else:
    print "Output:\n", job.content(".out")
```

Chapter 12. Classes: Defining a new class

12.1. Basic class definition

Up to now, you have *used* many objects, and even directly done some classes instanciations (explained in (Chapter 10). The next question is: how do you *define* new kinds of ojects? In Python, you do this by defining a *class*, which describes of how the corresponding class of objects will behave and what operations, or *methods*, or more generally what *attributes* will be available on them.

You define a class by:

- the **class classname** statement
- describing its attributes, e.g methods and variables

Example 12.1. A sequence class

The following example defines a sequence class (simplified from Biopython `Seq` class). It defines several methods:

- `__init__`, called at instance creation
- `tostring`
- `tomutable`
- `count`

```
class Seq:                                                          ❶

    def __init__(self, data, alphabet = Alphabet.generic_alphabet):
        self.data = data
        self.alphabet = alphabet

    def tostring(self):                                             ❷
        return self.data                                            ❸

    def tomutable(self):
        return MutableSeq(self.data, self.alphabet)

    def count(self, item):
        return len([x for x in self.data if x == item])
```

❶ This method is always called when creating a new instance of class `Seq`. It's the constructor.

❷ The first argument passed to a class method call is always the object itself. Thus, the first parameter of a class method must be a variable pointing to the object itself, thus enabling to access to its attributes from inside the body of the method. `self` is just a naming convention.
❸ Use of the `self` variable and the '.' (dot) operator to access the `data` attribute.

Exercise 12.1. A class to store PDB residues

Define a class to store PDB residues. A residue has: a name, a position in the sequence, and a list of atoms. An atom has a name and coordinates. Define 2 methods: `add_residue` and `add_atom` that you will use as follows:

```
struct = PDBStructure()
residue = struct.add_residue(name = "ILE", posseq = 1 )
struct.add_atom(residue, name = "N",
                coord = (23.46800041, -8.01799965, -15.26200008))
struct.add_atom(residue, name = "CZ",
                coord = (125.50499725, 4.50500011, -19.14800072))
residue = struct.add_residue(name = "LYS", posseq = 2 )
struct.add_atom(residue, name = "OE1",
                coord = (126.12000275, -1.78199995, -15.04199982))

print struct.residues
```

You also might need an `__init__` method to initialize the data structures.

Tip

The print statement should return:

```
[{'name': 'ILE', 'posseq': 1, 'atoms': [ \
{'name': 'N', 'coord': (23.468000409999998, -8.0179996500000001, -15.26200008)}, \

{'name': 'CZ', 'coord': (125.50499725, 4.5050001100000001, -19.148000719999999)}]}, \

{'name': 'LYS', 'posseq': 2, 'atoms': [ \
{'name': 'OE1', 'coord': (126.12000275, -1.7819999500000001, -15.041999819999999)}]}]
```

To which kind of data structures does it correspond?
(Solution A.42)

Exercise 12.2. A class to store PDB residues (cont)

- Add 2 variables `model_id` `chain_id` to the residue, in order to store the model ID (a PDB entry may have more than one model) and the chains.
- Add fields in the atom: `tempfactor` to store the factor of temperature, `occupancy`, `altloc`, for an alternate location, and `element`, which is the chemical name, e.g “C” (while name, e.g “CG2”, is the chemical name plus the position).

```
struct = PDBStructure()
residue = struct.add_residue(model_id="1", chain_id="A",
                             name = "ILE", posseq = 1 )
struct.add_atom(residue, name = "N",
                coord = (23.46800041, -8.01799965, -15.26200008),
                tempfactor=169.09, occupancy = 1.0,
                element = "N")
```

(Solution A.43)

Exercise 12.3. A class to store PDB residues (cont)

Add to your class definition the code required:

- to retrieve the residues by their name (method `get_residues_by_name`)
- to retrieve the model and chain a residue belongs to (methods `residue_model` and `residue_chain`)
- to list the residues of given chain (method `get_residues_of_chain`)

```
print "residues of name ILE:"
for residue in struct.get_residues_by_name("ILE"):
   print residue
   print "model: ", struct.residue_model(residue)
          print "chain: ", struct.residue_chain(residue)

print "residues of chain B:"
for residue in struct.get_residues_of_chain("B"):
  print residue
```

(Solution A.44)

12.2. Defining operators for classes

Standard methods enable to define the behaviour of standard operators:

- `__add__`: defines +
- `__sub__`: defines -
- `__str__`: defines how to convert the instance to a string representation (for e.g **print** statement)
- `__getitem__`: defines the access by key (object['key'])
- etc...

Example 12.2. Seq operators

For instance, the `Seq` class defines a method `__str__` which returns a string informally representing the sequence, that will be used in **print** statement, as well as several other operators:

- `__add__` to concatenate sub-sequences by the `+` operator
- `__len__` for computing the length
- `__getitem__` for indexed access to a position in the sequence, etc....
- `__getslice__` for ranges in the sequence
- etc...

```
class Seq:

    def __repr__(self):
        return "%s(%s, %s)" % (self.__class__.__name__,
                               repr(self.data),
                               repr(self.alphabet))
    def __str__(self):
        if len(self.data) > 60:
            s = repr(self.data[:60] + " ...")
        else:
            s = repr(self.data)
        return "%s(%s, %s)" % (self.__class__.__name__, s,
                               repr(self.alphabet))
    def __len__(self): return len(self.data)

    def __getitem__(self, i): return self.data[i]

    def __getslice__(self, i, j):
        i = max(i, 0); j = max(j, 0)
        return Seq(self.data[i:j], self.alphabet)

    def __add__(self, other):
        if type(other) == type(' '):
            return self.__class__(self.data + other, self.alphabet)
        elif self.alphabet.contains(other.alphabet):
            return self.__class__(self.data + other.data, self.alphabet)
        elif other.alphabet.contains(self.alphabet):
            return self.__class__(self.data + other.data, other.alphabet)
        else:
            raise TypeError, ("incompatable alphabets", str(self.alphabet),
                              str(other.alphabet))
```

Exercise 12.4. Code reading: Bio.GenBank.Dictionary class

Look at the source code of class `Bio.GenBank.Dictionary` in order to understand how the following code works:

```
from Bio import GenBank
gb_dict = GenBank.NCBIDictionary()
gb_rec = gb_dict['1617401']                                    ❶
print gb_rec
```

❶ What happens here?

12.3. Inheritance

Example 12.3. biopython FastaAlignment class

The following code shows the definition of the class `FastaAlignment` in module `Bio.Fasta.FastaAlign`. This class inherits from class `Bio.Align.Generic.Alignment`, which defines generic methods for alignments.

```
from Bio.Align.Generic import Alignment

class FastaAlignment(Alignment):                               ❶
    def __init__(self, alphabet = Alphabet.Gapped(IUPAC.ambiguous_dna)):
        Alignment.__init__(self, alphabet)                     ❷

    def __str__(self):
        """Print out a fasta version of the alignment info."""
        return_string = ''
        for item in self._records:
            new_f_record = Fasta.Record()
            new_f_record.title = item.description
            new_f_record.sequence = item.seq.data

            return_string = return_string + str(new_f_record) + "\n\n"

        # have a extra newline, so strip two off and add one before returning
        return string.rstrip(return_string) + "\n"
```

❶ This class is a sub-class of class `Bio.Align.Generic.Alignment`
❷ Call the super-class `__init__` method. There is no special statement in Python to perform this (such as `super`).

See also class `Bio.Clustal.ClustalAlignment`.

Exercise 12.5. Biopython Alphabet class hierachy

Look at the `Bio.Alphabet` module and draw the `Bio.Alphabet` class hierarchy.
Solution A.45

Example 12.4. Exceptions class hierarchy

Exceptions are defined by inheritance (see Chapter 8 and Figure 8.1).

12.4. Classes variables

Example 12.5. Bio.Data.CodonTable class variables

The class Bio.Data.CodonTable [http://www.bioinformatics.org/bradstuff/bp/api/Bio/Data/CodonTable.py.html] relies on several variables, some of them being instances variables, other being *class variables*. Since they belong to the class namespace, class variables are shared by all the instances of the class.

```
class CodonTable:
    nucleotide_alphabet = Alphabet.generic_nucleotide                    ❶
    protein_alphabet = Alphabet.generic_protein

    forward_table = {}    # only includes codons which actually code
    back_table = {}       # for back translations
    start_codons = []
    stop_codons = []
    # Not always called from derived classes!
    def __init__(self, nucleotide_alphabet = nucleotide_alphabet,
                 protein_alphabet = protein_alphabet,
                 forward_table = forward_table, back_table = back_table,
                 start_codons = start_codons, stop_codons = stop_codons):
        self.nucleotide_alphabet = nucleotide_alphabet                   ❷
        self.protein_alphabet = protein_alphabet
        self.forward_table = forward_table
        self.back_table = back_table
        self.start_codons = start_codons
        self.stop_codons = stop_codons
```

❶ Class variables definition (notice that they are declared outside of the methods). Notice that these definitions also use `Alphabet` `generic_nucleotide` and `generic_protein` class variables.
❷ Instance variables definition (initialized at `__init()__`). Instance variables are initialized with default values that are provided either by the class variables, or by the parameters.

Exercise 12.6. A class to store PDB residues (cont')

Add a verbose functionality in the class that you can change by a switch:

```
struct = PDBStructure()
self.verbose(1)
```

You can then add some verbose code into the methods of the class, such as:

```
def add_atom(self, residue, name, coord, tempfactor, occupancy, element):
    if self.verbose():
   print "add_atom: "," residue: ", residue['name'],
   residue['posseq'],  " name: ", name, " coord: ",
   coord, " tempfactor: ", tempfactor, " occupancy: ",
   occupancy, " element: ", element
```

If you have some time left, you can try to use the Python Numeric [http://www.python.org/topics/scicomp/numpy.html] module for computing with multi-dimensionals arrays - see also "Python for Scientific Computing" (PPT [http://www.python9.org/p9-jones.ppt]) for a presentation at Python 9 Conference [http://www.python9.org/].

```
from Numeric import array, Float0
coord=array((x, y, z), Float0)
```

Solution A.46

Chapter 13. Biopython, continued

13.1. Parsers

13.1.1. Introduction

In Bioinformatics, parsing is very important, since it enables to extract informations from data files or to extract results produced by various analysis programs, and to make them available in your programs. For instance, a Blast parser will transform a text output into `Bio.Blast.Record` objects, directly available to the program. There are already several parsers in Biopython: Clustalw and Blast (standalone and NCBI) parsers, parsers for databases records (SwissProt, GenBank, Medline, SCOP, NBRF, Prosite, InterPro, Rebase, Kabat, ...). One of the reasons there are so many parsers available is that Biopython relies on Martel [http://www.dalkescientific.com/Martel/] (by Andrew Dalke), a scanner generator.

The aim of this section is not to describe all these tools, but rather to explain how they work, in order for you to be able to build one for your own programs or databases, or for programs not having their parser, yet (see also Parser.txt [http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/Parser.txt] from the Biopython documentation for a design overview of parsers). For this purpose, we will build a simple parser for the Enzyme [http://www.expasy.ch/enzyme/] database, that is only able to store the enzyme ID and the references of an entry to other databases. There is already a `Bio.Enzyme` package in Biopython, which defines a `_Scanner` class, that we are going to use, but no parser (yet).

In Biopython, parsing is often organized according to an event/callback model, one component, often called the *scanner*, generating parsing events when encountering a tag, and another component, often called the *consumer*, receiving and handling these events. Generally, you feed data to scan to the scanner through a handle, which can be an open file or an http stream.

```
scanner.feed(handle)
```

The scanner has to know about which consumer to call, which can be achieved by having a standard consumer for a given type of data. You can also provide a consumer as a parameter to the scanner:

```
scanner.feed(handle, consumer)
```

This architecture has the advantage of dividing the tasks of scanning the text and deciding what to do with the recognized text elements. Writing your own consumer enables you to build your own data structures.

At a higher level, a *parser* component may wrap the two other components in one class, providing a simpler component to the programmer, since he or she just has to call the parser:

```
    parser.parse(handle)
```

to process the text. Such a parser might be implemented like this:

```
class Parser(AbstractParser):                                    ❶
    def __init__(self):
        self._scanner = _Scanner()                               ❷
        self._consumer = _Consumer()

    def parse(self, handle):
        self._scanner.feed(handle, self._consumer)
        return self._consumer.data
```

❶ `AbstractParser`: see below for explanation about Biopython classes to support parsing.
❷ Wrapped scanner and consumer.

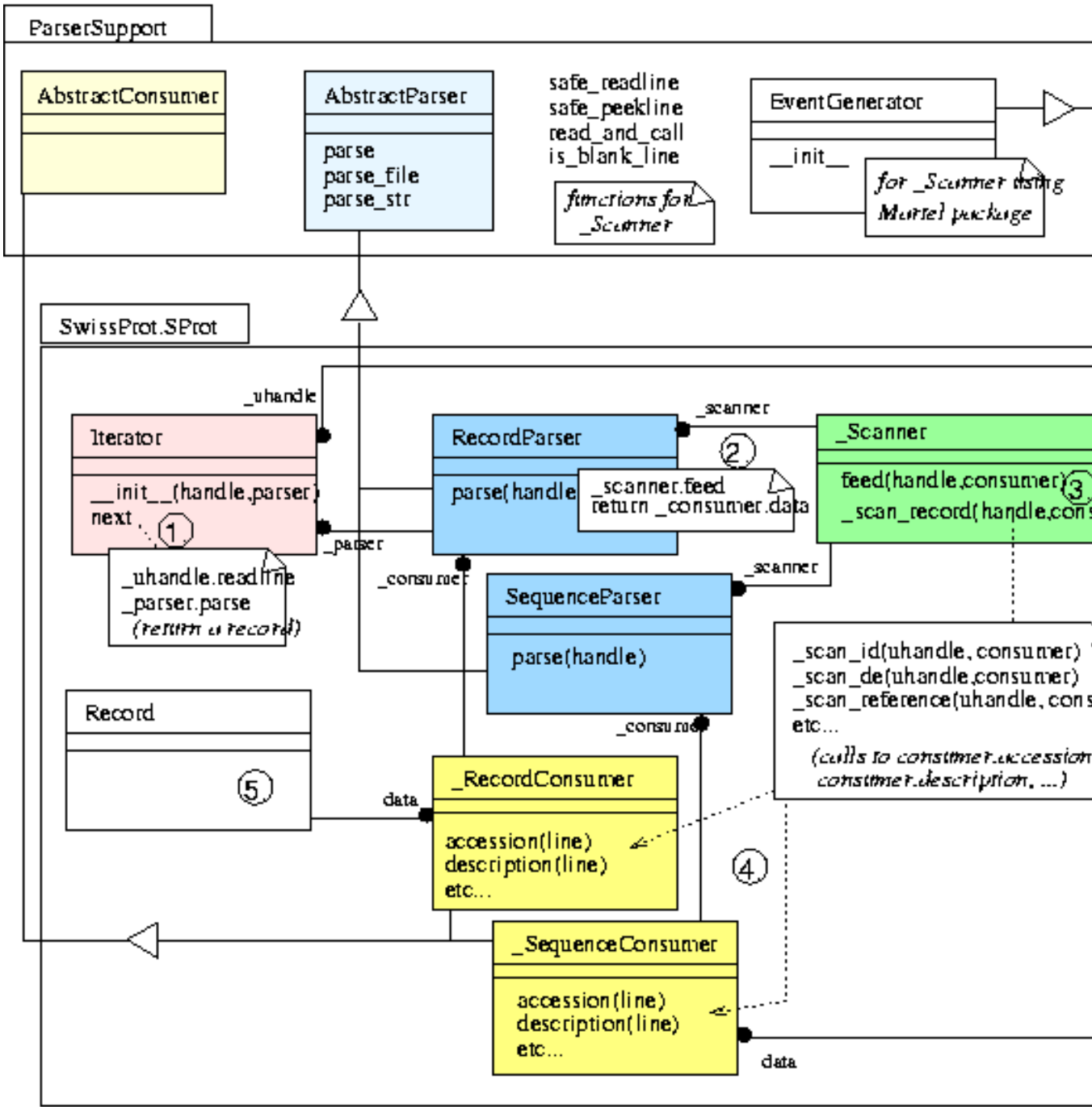
Biopython provides a support for defining new parsers and consumers classes through the `Bio.ParserSupport` module (`AbstractParser`and `AbstractConsumer` classes).

Example 13.1. Using SProt.RecordParser and SProt.SequenceParser

For instance, the `Bio.Swissprot.Sprot` module defines (Figure 13.1):

- a scanner: class `Bio.Swissprot.Sprot._Scanner`
- 2 consumers:
  - class `Bio.Swissprot.Sprot._RecordConsumer`
  - and `Bio.Swissprot.Sprot._SequenceConsumer`
- 2 parsers: classes `Bio.Swissprot.Sprot.RecordParser` and `Bio.Swissprot.Sprot.SequenceParser`, that we have already used in several occasions (Section 11.4.1).

Figure 13.1. Parsers class hierarchy



Using the `SequenceParser`, you get `Seq` objects, while using the `RecordParser`, you get `SeqRecord` objects.

```
from Bio.SwissProt import SProt
from sys import *

fh = open(argv[1])
sp = SProt.Iterator(fh, SProt.RecordParser())                    ❶
record = sp.next()
for feat in record.features:
    if feat[0] == 'DOMAIN':
       print "domain:", record.sequence[feat[1]:feat[2]+1]
fh.close()

fh = open(argv[1])
sp = SProt.Iterator(fh, SProt.SequenceParser())                  ❷
sequence = sp.next()
print "sequence: ", sequence.seq
fh.close()
```

❶ Reading the file with `SProt.RecordParser`. This enables to access to the annotations and features.
❷ Re-reading the file with `SProt.SequenceParser`.

13.1.2. Exercises: building parsing classes for Enzyme

We start by defining a simple consumer to receive the scanner events, first for only one entry (Exercise 13.1), then for a file containing several entries (Exercise 13.2). After this, we will wrap this consumer and the scanner in a parser class (Exercise 13.3). The next step is an iterator, which sequentially return "records" (Exercise 13.5). In order to be able to do a search in a enzyme database, we will then add a `lookup` method to the iterator (Exercise 13.6), then define a proper dictionary class, such as the one that we have seen in Example 11.7 (Exercise 13.7). The last step will be to pack all this classes into a module (Exercise 13.8), and to use it to fetch the enzyme entry referenced in a SwissProt record, and display all the related proteins (Exercise 13.9).

To build a consumer, you need to know which events the scanner will generate. Biopython distribution contains documentation on this topic. See for instance a copy at: http://bioweb.pasteur.fr/docs/doc-gensoft/biopython/Doc/.

Exercise 13.1. EnzymeConsumer, reading one entry from a file

Define a class `EnzymeConsumer` storing the references of the enzyme entry. Use the class `Enzyme._Scanner` for reading the entry from a file (data [data/enzyme.1.16.3.1]). `EnzymeConsumer` should be a sub-class of `AbstractConsumer` from module `Bio.ParserSupport`. Thanks to this, you will not have to provide all the callback methods called by the scanner, but only the methods that are of interest for you.

```
handle = open(argv[1])
```

```
scanner  = Enzyme._Scanner()
consumer = EnzymeConsumer()
scanner.feed(handle, consumer)
print "results: ", consumer._references
```

(Solution A.47)

Exercise 13.2. EnzymeConsumer, reading n entries from a file

Define the same class as in Exercise 13.1, but stores the references for several enzyme entries (data [data/enzymes]).

```
for id in consumer._references.keys():
    print id, consumer._references[id]
```

(Solution A.48)

Exercise 13.3. EnzymeParser

Define a parser to wrap the scanner and the consumer previously defined (Exercise 13.2).

```
handle = open(argv[1])
parser = EnzymeParser()
references = parser.parse(handle)

for id in references.keys():
    print id, references[id]
```

(Solution A.49)

13.1.3. Iterator

An iterator is an object that sequentially return successive records from a data input:

```
iterator = Iterator(handle)
record = iterator.next()
while record:
    print record
    record = iterator.next()
```

From with this data input, the iterator `next` method provides a parser with the lines corresponding to a record, from which the parser will build a record, e.g (simplified):

```
    def next(self):
 # 1) read the appropriate lines (until end of record)
 # 2) call the parser
        return self._parser.parse(lines)
```

You might need to convert the lines back into a handle before passing them to the parser, since the parser rather takes a handle. You can use the `Bio.File.StringHandle` class for this purpose.

Exercise 13.4. Code reading: Bio.Swissprot.SProt.Iterator class

Read the definition of the `Bio.Swissprot.SProt.Iterator`

13.1.4. Exercises: building parsing classes for Enzyme (cont)

Exercise 13.5. EnzymeIterator

Define a class `EnzymeIterator` based on the parser previously defined (Exercise 13.3). The parser just return a dictionary as a "record", with an 'id' and a 'references' keys.

```
handle = open(argv[1])
iterator = EnzymeIterator(handle)
record = iterator.next()
while record:
    print record['id'], record['references']
    record = iterator.next()
handle.close()
```

The 'references' value could be look this:

```
[{'ac': 'P00450,', 'id': 'CERU_HUMAN;'},
 {'ac': 'Q61147,', 'id': 'CERU_MOUSE;'},
 {'ac': 'P13635,', 'id': 'CERU_RAT'}]
```

(Solution A.50)

Exercise 13.6. EnzymeIterator with lookup

Add to the class `EnzymeIterator` previously defined (Exercise 13.5) a `lookup` method, that goes through the file looking for an entry of a given ID. Try on the real enzyme database (at Pasteur: `/local/databases/release/Enzyme/enzyme.dat`). You can use the getopt module to pass the database and id from the command line.

```
database = open(db)
iterator = EnzymeIterator(database)
record = iterator.lookup(id)
if record:
    print record['id'], join(record['references'],"")
else:
    print "id not found in database ", db
database.close()
```

(Solution A.51)

13.1.5. Dictionary

In Section 12.2, we have seen how to define operators for a class. Namely, the `__getitem__` method is a way to define an operator to provide an indexed acces to data.

Exercise 13.7. EnzymeDictionary

Define a class `EnzymeDictionary` based on the iterator previously defined (Exercise 13.5) (now, it is not anymore the `EnzymeIterator` class which handles the lookup). The way to use the dictionary is as following (db is the database filename, e.g `/local/databases/release/Enzyme/enzyme.dat`, id the enzyme id, e.g 1.16.3.1):

```
enzyme = EnzymeDictionary(db)
record = enzyme[id]
print record['references']
```

You may improve the code above by handling the `KeyError` exception.
(Solution A.52)

13.1.6. Using the parsers classes

Exercise 13.8. EnzymeParsing module

Define an `EnzymeParsing` module. (Solution A.53)

Exercise 13.9. Fetching enzymes referenced in a SwissProt entry and display related proteins

Re-using Exercise 11.11 to find the enzyme number from the description text of a SwissProt entry, fetch the corresponding enzyme data. Return the list of SwissProt records referenced by the enzyme entry, and display their entry name and description. (Solution A.54)

13.2. Practical: studying disulfid bonds in Human Ferroxidase 3D structure and alignments

13.2.1. Working with PDB

Exercise 13.10. Fetch a PDB entry from the RCSB Web server

Look at the code of the `Bio.WWW.ExPASy` module, e.g function `get_sprot_raw` and define a function `get_pdb_entry_remote` that returns a handle (something that can be opened by **open()** on a given PDB entry.
The url that you need is: http://www.rcsb.org/pdb/cgi/export.cgi/%s.pdb?format=PDB&compression=None&pdbId=%s.
Try your code with the 1KCW [http://www.rcsb.org/pdb/cgi/export.cgi/1KCW.pdb?format=PDB&compression=None&pdbId=1KCW] ident, which is the PDB entry corresponding to the CERU_HUMAN protein we are studying.
Solution A.55

Exercise 13.11. Define a PDBStructure class

You can start from Exercise 12.3. In summary, this class should define the following methods (constructors):

- `__init__`
- `__str__`
- `set_id`
- `set_pdb_ident`
- `add_dbref`
- `add_ssbond`
- `add_residue`
- `add_atom`

and (selectors):

- `get_residues`
- `get_atoms`
- `get_ssbonds`
- `get_residues_by_name`
- `get_residues_of_chain`
- `residue_model`
- `residue_chain`

Solution A.56

Exercise 13.12. Define a PDBConsumer class

In Exercise 12.3, the structure was build "by hand". Indeed, we had to write all the statements to add residues and atoms in our program:

```
residue = struct.add_residue(model_id, chain_id, name = "ILE",
                             posseq = 1 )
struct.add_atom(residue, name = "N",
                coord = (23.46800041, -8.01799965, -15.26200008) ,
                tempfactor=169.09, occupancy = 1.0, element = "N")
```

We don't really want to do this for real data. Instead, we now want to load the structure from a PDB file.

The `PDBConsumer` class we would like to build for this purpose roughly follows the scanner/consumer scheme that we have seen previously (Section 13.1). Our consumer's job is to build a `PDBStructure` object as it receives parsing events. As a "scanner", you can actually use this PDBParser [modules/PDBParser.py] provided by Thomas Hamelryck (thamelry@vub.ac.be).
Solution A.57

Tip

The methods the `PDBConsumer` class will contains thus should correspond to the "events" (or callbacks) of the `PDBParser` class. For instance, the statement in `PDBParser`:

```
self.structure_builder.set_ssbond(_from,_to)
```

calls the `set_ssbond` method of the consumer (here `structure_builder` is an equivalent of our "consumer").

Tip

When using this `PDBParser` class, the actual structure is returned to the program as follows:

```
parser=PDBParser(PDBConsumer())                                    ❶
struct = parser.get(id, file)                                      ❷
```

❶ Parser instanciation: the consumer is passed as an argument to the `__init__` of the parser.
❷ Structure creation: the `get` method in the parser takes an `id` and a filename as arguments.

Tip

You also have to know that the `get` method in the `PDBParser` needs to call a `get` method in the consumer, whose only task is to actually return the `PDBStructure` just built.

13.2.2. Study of disulfid bonds

Exercise 13.13. Compute disulfid bonds in 1KCW

Add a method in the `PDBStructure` called `disulfid_bridges`. Then write a program using the parser and checking for corresponding annotations in the PDB entry. (data [data/pdb1kcw.ent])
Solution A.58

Exercise 13.14. Compare 3D disulfid bonds with Cys positions in the alignment (take #1).

Compare annotated and computed disulfid bonds in 1KCW with cystein positions in the alignment. Take the code written in Exercise 11.23 to get position with a high-level of cysteins and check if they correspond to the bonds in the 3D structure.
Solution A.59

Exercise 13.15. Compare 3D disulfid bonds with Cys positions in the alignment (take #2).

The positions in the alignment and in the structure are somewhat different. Write a method `pdb2seq_pos` which use the DBREF lines of the PDB entry (see method `add_dbref`). Then, use can use this `pdb2seq_pos` method to display the actual positions in the alignment.
Solution A.60

Chapter 14. Graphics in Python

Note

Graphical programming is not the main purpose of this course. We just list here some resources (both tutorials and software) related to graphics, mainly:

- -dimensional graphics, chart/graph generation and scientific plots,
- GUI toolkits.

14.1. Tutorials

- An Introduction to Tkinter [http://www.pythonware.com/library/tkinter/introduction/], by Fredrik Lundh.
- The Python Short Course [http://www.wag.caltech.edu/home/rpm/python_course/] has a section about Tkinter (Python GUIs with Tkinter [http://www.wag.caltech.edu/home/rpm/python_course/Lecture_6.htm]).
- Python and Tkinter Programming [http://www.manning.com/Grayson/], John E. Grayson (book). The chapter "Graphs and charts" is available online [http://www.manning.com/grayson/chapt11.pdf], together with the source code [http://www.manning.com/getpage.html?project=grayson&filename=Source.html] of the examples.
- Tkinter reference: A GUI for Python [http://www.nmt.edu/tcc/help/lang/python/tkinter.pdf] (PDF).
- Tkinter help [http://www.isd197.org/sibley/cs/icp/tips/tkinter_html]: links to resources.
- Handbook of the Physics Computing Course [http://users.ox.ac.uk/~sann1276/handbook/handbook.html] (by Michael Williams) with a section on graphical programming (on `Gnuplot`).

Exercise 14.1. Code reading: Drawing by Numbers

Read the code and comments provided in Chapter Graphs and Charts [http://www.manning.com/grayson/chapt11.pdf] of the book cited above, Python and Tkinter Programming.

14.2. Software

- Python Tkinter Resources [http://www.python.org/topics/tkinter/]
- Gnuplot.py [http://gnuplot-py.sourceforge.net/]
- Vaults of Parnassus [http://www.vex.net/parnassus/]: see the "Graphics" section, which has a "GUI" (Graphical User Interfaces) section.
- debian python-graphics [http://packages.debian.org/stable/graphics/python-graphics.html]
- Plot-resources [http://starship.python.net/crew/jhauser/plot-res.html], a collection of links to plotting resources for Python on Python Starship [http://starship.python.net/] site.
- Pmw [http://pmw.sourceforge.net/]: Python megawidgets.
- PyQwt [http://gerard.vermeulen.free.fr]: data plotting with Python and Numerical Python.
- wxPython [http://wxpython.org/]: maybe a futur standard.
- Biggles [http://sourceforge.net/projects/biggles/]: a 2D scientific plotting package for Python, geared toward the production of publication-quality plots.
- Piddle [http://piddle.sourceforge.net/]: module for creating two-dimensional graphics in a manner that is both cross-pla tform and cross-media
- PLplot [http://plplot.sourceforge.net]: scientific graphics package
- GGobi [http://www.ggobi.org/] Data Visualization System
- GDChart [http://www.fred.net/brv/chart/]: chart/graph generation in GIF format
- Using Python to solve problems in bioinformatics [http://bonsai.ims.u-tokyo.ac.jp/~mdehoon/software/software.html] (plotting with PyGist, Tk plot).
- PyGist [http://w3.pppl.gov/~hammett/comp/python/koer.ioc.ee/man/pygraph/PyGist/PyGist_Title.mkr.html] (PDF manual [http://w3.pppl.gov/~hammett/comp/python/PyGraphics/pygist.pdf] and presentation [http://www.python.org/workshops/1996-06/papers/l.busby-gist.html]).

14.3. Summary of examples and exercises with some graphics in this course

- Plotting codon frequency (Example 11.4). This example uses a Tkinter canvas to draw a bar chart. A documentation on the Tkinter canvas can be found here [http://www.pythonware.com/library/tkinter/introduction/canvas.htm].
- Plotting Cys conserved positions (Exercise 11.24). This example uses the Pmw.Blt [http://pmw.sourceforge.net/doc/Blt.html] package to draw a plot representing Cys conservation at each position of an alignment.

Appendix A. Solutions

A.1. Introduction to basic types in Python

Solution A.1. GC content ()

```
>>>(count(dna, 'c') + count(dna, 'g')) / len(dna)                    ❶
0

>>>(count(dna, 'c') + count(dna, 'g')) / float(len(dna))
0.64077669902912626

>>> (count(dna, 'c') + count(dna, 'g')) * 100.0 / len(dna)
64.077669902912618

>>> (count(dna, 'c') + count(dna, 'g')) / len(dna) * 100.0           ❶
0.0

>>> gc = (count(dna, 'c') + count(dna, 'g')) / float(len(dna)) * 100  ❷
>>> "%.2f" % gc
'64.08'
```

❶ Why does this solution not work? (Section 2.7)
❷ This is an example of the % string formating operator (for more explanation see Section 6.2.4).

Solution A.2. DNA complement ()

```
>>> replace(replace(replace(replace(replace(replace(dna, 'a', 'x'),  ❶
't', 'a'),  'x', 't'), 'c', 'x'), 'g', 'c'), 'x', 'g')
'cgtactgcaataatgctgagacagtgcggcgccacgctgactccgcaccgcagacgacccggaaatgaa
gcggaggcgcgggacgtaaggcaaggaccggagc'

>>> t=maketrans("AGCTagct", "TCGAtcga")                              ❷
>>> t

>>> translate(dna, t)
'cgtactgcaataatgctgagacagtgcggcgccacgctgactccgcaccgcagacgacccggaaatgaa
gcggaggcgcgggacgtaaggcaaggaccggagc'
```

❶ This is a simple version using `replace`.
❷ This version use a translation table.

Solution A.3. Restriction site occurrences as a list ()

```
def restrict(dna, enz):
    "find all start positions of a restriction site"

    res = []

    site = dna.find(enz)
    while site != -1:
        res.append(site)
        site = dna.find(enz, site + 1)

    return res
```

Solution A.4. Restriction digest ()

```
def digest(dna, enzlist):
    """
    returns a list containing the cut positions
    when cutting dna with all enzymes in enzlist
    """

    Lcuts = []
    # get all cut positions
    for enz,pcut in (enzlist):
        print enz, pcut
        start = 0
        stop = dna.find(enz)
        while stop != -1:
            Lcuts.append(stop + pcut)
            stop = dna.find(enz, stop+1)

    # sort
    Lcuts.sort()

    return Lcuts

def frag_len(Lcuts):
    """
    get fragment lengths from  a list containing the cutting positions
    of an restriction digest sorted by order
    + start(=0) and end(=dna length) of the dna sequence
    """

    Lres = []
    start = Lcuts[0]
    for end in Lcuts[1:]:
        Lres.append(end-start)
        start = end
```

```
    return Lres
```

Solution A.5. Get the codon list from a DNA sequence ()

```
def codons(s,frame=0):
 codons=[]
 end=len(s[frame:]) - (len(s[frame:]) % 3) - 1
 for i in range(frame,end,3):
  codons.append(s[i:i+3])
 return codons
```

Solution A.6. Reverse Complement of DNA ()

```
from string import *

def revcomp(dna):
    """ reverse complement of a DNA sequence """

    comp = dna.translate(maketrans("AGCTagct", "TCGAtcga"))
    lcomp = list(comp)
    lcomp.reverse()

    return join(lcomp, "")
```

Solution A.7. Translate a DNA sequence ()

```
standard = { 'ttt': 'F', 'tct': 'S', 'tat': 'Y', 'tgt': 'C',
             'ttc': 'F', 'tcc': 'S', 'tac': 'Y', 'tgc': 'C',
             'tta': 'L', 'tca': 'S', 'taa': '*' , 'tca': '*',
             'ttg': 'L', 'tcg': 'S', 'tag': '*', 'tcg': 'W',

             'ctt': 'L', 'cct': 'P', 'cat': 'H', 'cgt': 'R',
             'ctc': 'L', 'ccc': 'P', 'cac': 'H', 'cgc': 'R',
             'cta': 'L', 'cca': 'P', 'caa': 'Q', 'cga': 'R',
             'ctg': 'L', 'ccg': 'P', 'cag': 'Q', 'cgg': 'R',

             'att': 'I', 'act': 'T', 'aat': 'N', 'agt': 'S',
             'atc': 'I', 'acc': 'T', 'aac': 'N', 'agc': 'S',
             'ata': 'I', 'aca': 'T', 'aaa': 'K', 'aga': 'R',
             'atg': 'M', 'acg': 'T', 'aag': 'K', 'agg': 'R',
```

```
            'gtt': 'V', 'gct': 'A', 'gat': 'D', 'ggt': 'G',
            'gtc': 'V', 'gcc': 'A', 'gac': 'D', 'ggc': 'G',
            'gta': 'V', 'gca': 'A', 'gaa': 'E', 'gga': 'G',
            'gtg': 'V', 'gcg': 'A', 'gag': 'E', 'ggg': 'G'
    }

def dna_translate(cdna, code=standard):
    """ translate a cDNA sequence to a protein """

    prot = ""
    for i in xrange(0,len(cdna),3):
        prot += code.get(cdna[i:i+3], "?")
    return prot

def dna_translate2(cdna, code=standard):
    """ translate a cDNA sequence to a protein """

    return "".join([ code.get(cdna[i:i+3], "?")
                     for i in xrange(0,len(cdna),3) ])
```

❶ This is a special syntax named list comprehension. It creates a list and populates it with the results of the first expression by replacing `i` with all values of the `for` loop (see also Chapter 7).

Solution A.8. Write a sequence in fasta format ()

```
def write_fasta(fh, seq, id="", desc="", width=60):
    """ write a sequence in fasta format.
    The following parameters can be specified:
      fh    - file descriptor
      seq   - sequence as a string
      id    - sequence id (default is no id)
      desc  - sequence description (default is no description)
      width - number of characters per sequence line (default 60)"""

    print >>fh, ">%s %s" % (id, desc)
    for i in xrange(0, len(seq), width):
        print >>fh, "%s" % seq[i:i+width]
```

Solution A.9. Header function ()

```
import string

def header(title):
    """splits a fasta header in ID and description of a sequence
    if one of the two is not given None is returned instead"""

    id = desc = None
```

```
    res = title.split(None,1)

    if len(res) == 0:
        pass
    elif len(res) == 2:
        id, desc = res[0][1:], res[1]
    elif title[0] in string.whitespace:
        desc = res[0]
    else:
        id = res[0][1:]

    return id, desc
```

A.2. Control Flow

Solution A.10. Count ambiguous bases ()

```
def ambiguous(dna):
    "returns the number of ambiguous characters in a dna sequence"

    nb = 0
    for i in dna:
        if i not in 'atgc':
            nb += 1

    return nb
```

Solution A.11. Verify DNA bases ()

```
# first version

def check_dna(dna, alphabet='atgc'):
    """ using break and continue """

    for base in dna:
        if base not in alphabet:
            break

    else:
        return "dna ok"


# second version

def check_dna2(dna, alphabet='atgcATGC'):
```

```
    """ loop without break or continue """

    ok = 1
    for base in dna:
        if base in alphabet:
            pass                                                    ❶
        else:
            ok = 0

    if ok:
        return "dna ok"
```

❶ `pass` is the empty statement.

A.3. Functions

Solution A.12. DNA complement function ()

```
from string import *

def complement(dna):
    "function to calculate the complement of a DNA sequence"              ❶

    tab = maketrans("AGCTagct", "TCGAtcga")
    return translate(dna, tab)
```

❶ If the first statement of a function is a string this string is the documentation of the function. It can be accessed by `func.func_doc`.

```
>>> complement.func_doc
'function to calculate the complement of a DNA sequence'
```

Solution A.13. Variable number of arguments ()

```
def all_2_digests(*enzymes):
    """ generate all possible digests with 2 enzymes """

    digests = []
    for i in range(len(enzymes)):
        for k in range(i+1, len(enzymes)):
            digests.append( [enzymes[i], enzymes[k]] )
    return digests
```

A.4. Modules and packages

Solution A.14. Loading and using a module: print the command line arguments

Exercise 9.1

```
import sys
print sys.argv
```

Solution A.15. Creating a module

Exercise 9.2

In order to create a module called `dna`, just put the your functions definitions in a file called `dna.py` (dna.py [exercises/dna.py]).

Do a:

```
pydoc dna
```

Solution A.16. Bio.Seq module

Exercise 9.5

```
from Bio.Seq import Seq

seq=Seq("actttgccatatg")
```

Solution A.17. Bio.SwissProt package

Exercise 9.6

Which import statements are necessary to make the following code work?

```
from Bio.WWW import *                                                    ❶
from Bio.SwissProt import SProt

expasy = ExPASy.get_sprot_raw('CERU_HUMAN')
sp = SProt.Iterator(expasy, SProt.RecordParser())
record = sp.next()
print record.keywords
```

❶ This statement import "all" components from the `Bio.WWW` package, including the `ExPASy` module (see: pydoc Bio.WWW and pydoc Bio.WWW.ExPASy, and llok at the `__all__` and `__path__` in the DATA section).

Solution A.18. Using a class from a module

Exercise 9.7

Why does the following code issue an error?

```
from Bio.SubsMat import FreqTable
dict = ...  # whatever
f = FreqTable(dict, 'COUNT')
TypeError: 'module' object is not callable
```

The reason is that `Bio.SubsMat.FreqTable` is the *module* containing `FreqTable`, not the class (see pydoc Bio.SubsMat.FreqTable). The `FreqTable` class is available as `Bio.SubsMat.FreqTable.FreqTable`. The import statement should be:

```
from Bio.SubsMat.FreqTable import FreqTable
```

(see also: Exercise 9.5).

Solution A.19. Import from Bio.Clustalw

Exercise 9.8

Why does the following code not work?

```
from Bio.Clustalw import *
```

```
a=ClustalAlignment()
NameError: name 'ClustalAlignment' is not defined
```

Look at the `__all__` variable in the `__init__.py` module file (or with pydoc Bio.Clustalw). It is not empty, but it does not contain `ClustalAlignment`. The import statement should be (see Example 9.2):

```
from Bio.Clustalw import ClustalAlignment
```

A.5. Biopython: Introduction

A.5.1. Bio.Seq package

Solution A.20. Using a Bio.Seq.Seq sequence

Exercise 11.1

Display the length of a sequence, and count the number of occurrences of 'a'.

```
from Bio.Seq import Seq

seq = Seq('gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg')
print len(seq)
print seq.count('a')
```

Solution A.21. Using a Bio.Seq.Seq sequence (cont)

Exercise 11.2

Display GC content.

```
from Bio.Seq import Seq

seq = Seq('gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg')
gc = seq.count('c') + seq.count('g') / float(len(seq)) * 100
print gc
```

Solution A.22. Write a sequence in FASTA format

Exercise 11.3

Write a sequence in FASTA format using the `Bio.Seqio.FASTA` module.

```
from Bio.SeqIO import FASTA
from Bio.Seq import Seq
from Bio.SeqRecord import SeqRecord
from sys import *

dna = Seq('gcatgacgttattacgactctgtcacgccgcggtgcgactgaggcgtggcgtctgctggg') ❶
seq = SeqRecord(dna, id = 'my_seq', description= 'a random sequence')     ❷
out = FASTA.FastaWriter(stdout)
out.write(seq)
```

❶ Creation of the `Seq` object required to create a `SeqRecord` object.
❷ Creation of the `SeqRecord` object.

Solution A.23. Random mutation of a sequence

Exercise 11.5

```
from random import *

def mutateseq(seq, rseed=0, span=10, p=0.1, verbose=0):
 if seed == 0:
  seed()
 else:
  seed(rseed)
 for t in range(0,span):
  r=randrange(0,1/p)                                                    ❶
  if r == 0:
   newbase = choice(['a', 'c', 't', 'g'])
   position = randrange(0,len(seq)-1)
   oldbase = seq[position]
   seq[position] = newbase                                              ❷
   if verbose:
    print t, seq.toseq().tostring(), position, "(%s => %s)" % (oldbase, newbase)
```

❶ Pick one value (here 0) among the possible integer values (which should be equally distributed during the span given).
❷ The sequence must be from class `MutableSeq`, of course.

Solution A.24. Random mutation of a sequence: count codons frequency

Exercise 11.6

```
import Bio.Fasta
from sys import *
from string import *
from dna import codons
from mutateseq import mutateseq

file = argv[1]
handle = open(file)
it = Bio.Fasta.Iterator(handle, Bio.Fasta.SequenceParser())
count = {}                                                          ❶
count_random = {}
seq = it.next()
while seq:
 for codon in codons(seq.seq.tostring()):                           ❷
  if count.has_key(codon):
   count[codon] += 1
  else:
   count[codon] = 0
 mutableseq = seq.seq.tomutable()
 mutateseq(mutableseq,span=1000,p=0.1)
 for codon in codons(mutableseq.tostring()):
  if count_random.has_key(codon):
   count_random[codon] += 1
  else:
   count_random[codon] = 0

 seq = it.next()

handle.close()

l=count.items()
l.sort()
print "count: ", l
l=count_random.items()
l.sort()
print "random: ", l
```

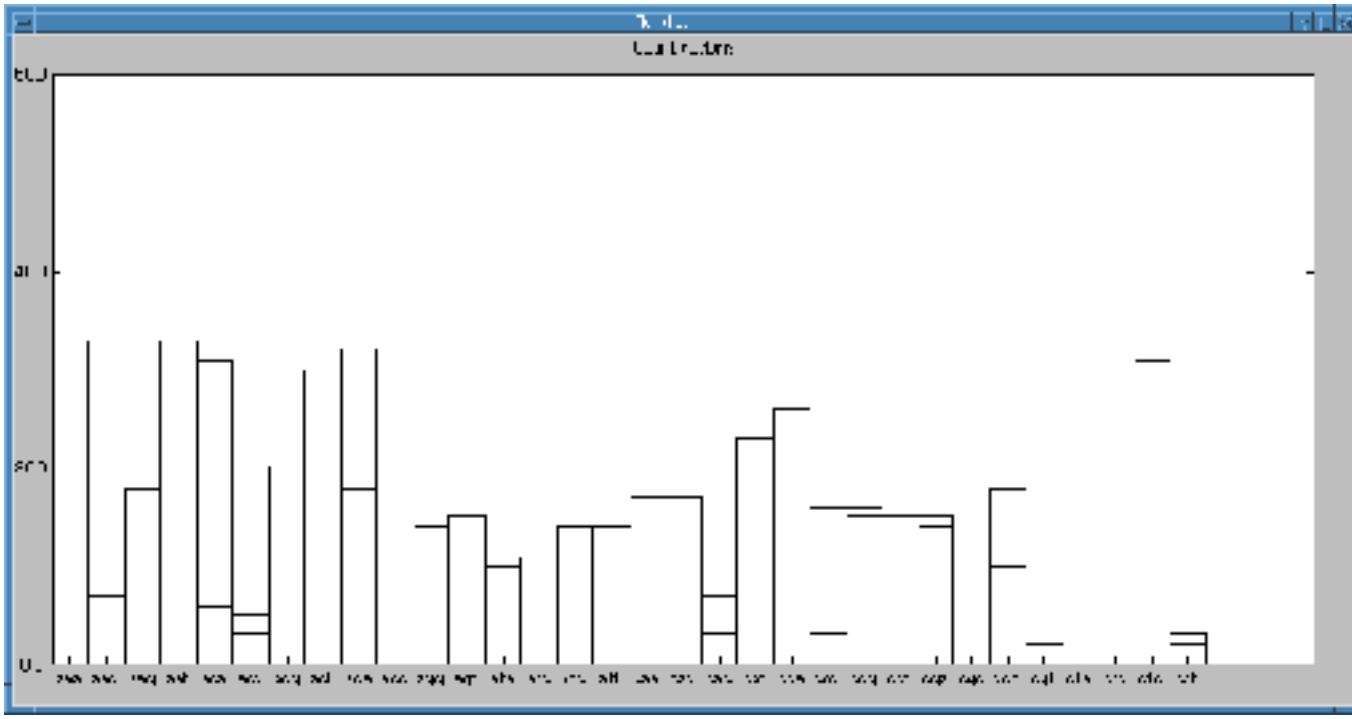
❶ Initialization of the dictionaries `count` and `count_random`.
❷ Test of the existence of a dictionary key.

Solution A.25. Random mutation of a sequence: plot codons frequency

Exercise 11.7

```
#-------------------------------------------------------
# bar charts of codons frequencies
#   - for legibility, 2 charts are built
#   - both random and normal frequencies are dsplayed

from tkplot import *
from Numeric import *

def codon_sort(a,b):
 if a < b:
  return -1
 elif a > b:
  return 1
 else:
  return 0

for codon in count.keys():
 if not count_random.has_key(codon):
  count_random[codon] = 0

for codon in count_random.keys():
 if not count.has_key(codon):
  count[codon] = 0

labels=count.keys()
labels.sort(codon_sort)

w1=window(plot_title='Count codons',width=1000)
y=array(count.values())[:len(count)/2]
x=arange(len(y)+1)
w1.bar(y,x,label=labels[:len(count)/2])

w2=window(plot_title='Count codons(2)',width=1000)
y=array(count.values())[(len(count)/2)+1:]
x=arange(len(y)+1)
w2.bar(y,x,label=labels[(len(count)/2)+1:])

y=array(count_random.values())[:len(count_random)/2]
x=arange(len(y)+1)
w1.bar(y,x,label=labels[:len(count_random)/2])

y=array(count_random.values())[(len(count_random)/2)+1:]
x=arange(len(y)+1)
w2.bar(y,x,label=labels[(len(count_random)/2)+1:])
```

Figure A.1. Plotting codons frequencies



(full code [exercises/seqrandom_count_codons_plot.py])

A.5.2. Bio.SwissProt.SProt and Bio.WWW.ExPASy

Solution A.26. SwissProt to FASTA

Exercise 11.9

```
from Bio.SeqIO import FASTA
from Bio.SwissProt import SProt
from sys import *

def convert_sp_fasta(infile,outfile):
    """
    convert a SwissProt file into a Fasta formatted file
    """
    in_h = open(infile)
    sp = SProt.Iterator(in_h, SProt.SequenceParser())
    out_h = FASTA.FastaWriter(outfile)
    sequence = sp.next()
    out_h.write(sequence)
```

```
    in_h.close()
    out_h.close()
```

Solution A.27. Fetch an entry from a local SwissProt database

Exercise 11.10

```
from Bio.SwissProt import SProt
from os import *

def get_sprot_entry_local (sprot_id):
    cmd="golden sp:" + sprot_id
    golden = popen(cmd, 'r')
    iterator = SProt.Iterator(golden, SProt.RecordParser())
    entry = iterator.next()
    golden.close()
    return entry
```

Solution A.28. Enzymes referenced in a SwissProt entry

Exercise 11.11

```
import re

def get_enzyme_ref(record):
    description = record.description
    enzyme_re = re.compile(r'\(EC\s+(?P<id>([\w\.]+))\).*')
    m=enzyme_re.search(record.description)
    return m.group('id')
```

Solution A.29. Print the pattern of a Prosite entry.

Exercise 11.12

```
import Bio.Prosite
```

```
prosite=Bio.Prosite.ExPASyDictionary(parser=Bio.Prosite.RecordParser())

def get_prosite_pattern(id):
    record=prosite[id]
    return record.pattern
```

You can also use a local Prosite database, and use the golden program to fetch entries:

```
from Bio.Prosite import Iterator, RecordParser
from os import popen

def get_prosite_pattern_local(id):
    cmd="golden prosite:" + id
    handle=popen(cmd, 'r')
    iterator=Iterator(handle,RecordParser())
    record=iterator.next()
    handle.close()
    return record.pattern
```

Solution A.30. Display the Prosite patterns of a SwissProt protein.

Exercise 11.13

The function is defined as follows:

```
from Bio.SwissProt import SProt

def get_prosite_refs(handle):
    sp = SProt.Iterator(handle, SProt.RecordParser())
    refs=[]
    record = sp.next()
    for ref in record.cross_references:
        if ref[0] == 'PROSITE':
            refs.append(ref[1])
    return refs
```

To display the patterns of the Prosite references given in a SwissProt entry, you can do like this:

```
import sys
from Bio.SwissProt import SProt
from sprot import get_prosite_refs, get_prosite_pattern

sp = open(sys.argv[1])
prosite_refs = get_prosite_refs(sp)
sp.close()

for id in prosite_refs:
    print id
    pattern=get_prosite_pattern(id)
    print pattern
```

Solution A.31. Search for occurrences of a protein PROSITE patterns in the sequence

Exercise 11.14

```
import sys
from Bio.Prosite import Pattern
from Bio.SwissProt import SProt
from sprot import get_prosite_refs, get_prosite_pattern

# prosite refs
sp = open(sys.argv[1])
prosite_refs = get_prosite_refs(sp)
sp.close()

# sequence
sp = open(sys.argv[1])
iterator = SProt.Iterator(sp, SProt.SequenceParser())
seq = iterator.next().seq
sp.close()

for id in prosite_refs:
    print id
    pattern=get_prosite_pattern(id)
    print pattern
    p = Pattern.compile(pattern)
    m = p.search(seq)
    print "[", m.start(), ":", m.end(), "]", seq[m.start():m.end()]
```

A.5.3. GenBank

Solution A.32. Extracting the complete CDS from a GenBank entry

Exercise 11.15

(not tested, due to a bug in the parser)

```
import string

def get_complete_cds(seqrecord):
    """
    This code has not been tested.
    """
    if string.find(seqrecord.description, 'complete cds') == -1:
        return None
    for feature in seqrecord.features:
        if feature.key == 'CDS':
            for qualifier in feature.qualifiers:
                if qualifier == 'location':
                    location = qualifier.value
                    break
            break

    seq = seqrecord.seq
    return seq[location.start-1:location.end+1]
```

A.5.4. Blast

Solution A.33. Remote Blast: save results

Exercise 11.16

```
from Bio.Blast import NCBIWWW
from Bio import Fasta
from sys import *

query_file = open(argv[1])
```

```
fasta = Fasta.Iterator(query_file)
query = fasta.next()
result_file = argv[1] + '.blast'
save_file = open(result_file, 'w')
results_handle = NCBIWWW.blast('blastp', 'swissprot',
                               query, expect=1,
                               descriptions = 100, alignments = 100)
blast_results = results_handle.read()
save_file.write(blast_results)
save_file.close()

print "Results saved in : ", result_file
```

Solution A.34. Remote Blast: parse results

Exercise 11.17

```
from Bio.Blast import NCBIWWW
from sys import *

blast_results = open(argv[1])
blast_parser = NCBIWWW.BlastParser()
record = blast_parser.parse(blast_results)

for (description,alignment) in zip(record.descriptions,record.alignments):❶
    if description.e == 0.0:
        for hsp in alignment.hsps:
            print '\n****Alignment****'
            print 'sequence:', alignment.title
            print 'length:', alignment.length
            print 'e value:', hsp.expect
            print hsp.query[0:75] + '...'
            print hsp.match[0:75] + '...'
            print hsp.sbjct[0:75] + '...'
```

❶ The `zip` Python function merge 2 lists with one item from each list every 2 items. So, in the code above, you get a list with a description, an alignment, the next description, the next alignment, etc...

Solution A.35. Local PSI-Blast

Exercise 11.18

```
from Bio.Blast import *
from sys import *

file = argv[1]

E_VALUE_THRESH = 0.04

blast_out, error_info = NCBIStandalone.blastpgp(
 blastcmd='/local/gensoft/bin/scripts/blastpgp',
 database='swissprot',
 infile=file,
 npasses=2)

b_parser = NCBIStandalone.PSIBlastParser()

# this creates a Bio.Blast.Record.PSIBlast
b_record = b_parser.parse(blast_out)

for round in b_record.rounds:
    for alignment in round.alignments:
        for hsp in alignment.hsps:
            if hsp.expect < E_VALUE_THRESH:
                print '****Alignment****'
                print 'sequence:', alignment.title
                print 'length:', alignment.length
                print 'e value:', hsp.expect
                print hsp.query[0:75] + '...'
                print hsp.match[0:75] + '...'
                print hsp.sbjct[0:75] + '...'
```

Just adding a pattern file to this query makes it a PHI-Blast:

```
blast_out, error_info = NCBIStandalone.blastpgp(
   blastcmd=blastcmd,
   database='swissprot',
   infile=queryfile,
   hit_infile=patternfile)
```

where `patternfile` contains a Prosite entry (pattern file [data/ceru_human-pattern1.dat]).

Solution A.36. Search Prosite patterns with PHI-blast

Exercise 11.19

```
from Bio.Blast import *
from Bio.WWW import *
from Bio.SwissProt import SProt
from Bio.SeqIO import FASTA
import Bio.Prosite
from Bio import File
from sys import *
import os
import tempfile
import sprot

# blast config
blast_parser = NCBIStandalone.PSIBlastParser()
E_VALUE_THRESH = 0.04
blastcmd='/local/gensoft/bin/scripts/blastpgp'

# utilities to build files for PHI-blast
def write_query(id):
    expasy = ExPASy.get_sprot_raw(id)
    sp = SProt.Iterator(expasy, SProt.SequenceParser())
    sequence = sp.next()
    fasta_file = tempfile.mktemp()
    fasta_handle=open(fasta_file,'w')
    fasta_out = FASTA.FastaWriter(fasta_handle)
    fasta_out.write(sequence)
    fasta_handle.close
    return fasta_file

def write_pattern(ref, pattern):
    patternfile = tempfile.mktemp()
    f=open(patternfile,'w')
    f.write("ID " + ref)
    f.write("\n")
    f.write("PA " + pattern)
    f.close
    return patternfile

#-----------------------------------------------------------------
# get SP entry and PROSITE references
sp_id = argv[1]
print >>stderr, "Fetching ", sp_id, " from ExPASy..."
expasy = ExPASy.get_sprot_raw(sp_id)
prosite_refs = sprot.get_prosite_refs(expasy)
expasy.close()
queryfile = write_query(sp_id)
```

```
#-----------------------------------------------------------------
# actual phi-blasting of each PROSITE pattern
for ref in prosite_refs:

    pattern = sprot.get_prosite_pattern(ref)
    print >>stderr, "Doing ", ref, " ...."
    print >>stderr, pattern
    patternfile = write_pattern(ref, pattern)

    print >>stderr, "+--------------------------------\nRunning blastpgp..."
    blast_out, error_info = NCBIStandalone.blastpgp(
 blastcmd=blastcmd,
 database='swissprot',
 infile=queryfile,
 hit_infile=patternfile)

    blast_record = blast_parser.parse(blast_out)
    for round in blast_record.rounds:
        for alignment in round.alignments:
            for hsp in alignment.hsps:
                if hsp.expect < E_VALUE_THRESH:
                    print '****Alignment****'
                    print 'sequence:', alignment.title
                    print 'length:', alignment.length
                    print 'e value:', hsp.expect
                    print hsp.query[0:75] + '...'
                    print hsp.match[0:75] + '...'
                    print hsp.sbjct[0:75] + '...'

    os.unlink(patternfile)

os.unlink(queryfile)
```

Solution A.37. Run FASTA

Exercise 11.20

```
from os import *
import string

DB_ROOT = '/local/databases/fasta'

def run_fasta(query, db):
    cmd="fasta_t -q %s %s/%s" % (query,DB_ROOT,db)
    fasta = popen(cmd, 'r')
    lines = fasta.readlines()
    fasta.close()
```

```
    if not lines:
        return None
    result = string.join(lines, ”)
    return result
```

You can use it this way:

```
result=run_fasta(’data/ceru_human.fasta’, ’gpmam’)
```

A.5.5. Clustalw

Solution A.38. Doing a Clustalw alignemnent

Exercise 11.21

```
import os
from Bio.Clustalw import MultipleAlignCL
from Bio.Clustalw import do_alignment
from sys import *

cline = MultipleAlignCL(argv[1])
cline.set_output(’data/test.aln’)
print "Command line: ", cline

align = do_alignment(cline)
for seq in align.get_all_seqs():
    print seq.description
    print seq.seq
```

Solution A.39. Align Blast HSPs

Exercise 11.22

```
from Bio.Blast import *
from Bio.Fasta.FastaAlign import FastaAlignment
from Bio import Alphabet
from Bio.Alphabet import IUPAC
from Bio.Clustalw import MultipleAlignCL
from Bio.Clustalw import do_alignment
from Bio.SeqIO import FASTA
import sys
```

```
import os

fasta_seqs = FastaAlignment(alphabet=IUPAC.protein)

# first, put the entire query sequence in the fasta set of sequences
handle = open(sys.argv[1])
seq = FASTA.FastaReader(handle).next()
handle.close()
fasta_seqs.add_sequence(descriptor=seq.description,
                        sequence=seq.seq.tostring())

# blast
E_VALUE_THRESH=0
done={}
blast_parser = NCBIStandalone.BlastParser()
blastcmd='/local/gensoft/bin/scripts/blastall'
blast_out, error_info = NCBIStandalone.blastall(blastcmd=blastcmd,
                                                program='blastp',
                                                database='swissprot',
                                                infile=sys.argv[1],
                                                expectation=1,
                                                descriptions=10,
                                                alignments=10)

blast_record = blast_parser.parse(blast_out)
for (description,alignment) in zip(blast_record.descriptions,blast_record.alignments):

    hsp_nb = 0
    for hsp in alignment.hsps:
        hsp_nb = hsp_nb + 1
        if hsp.expect <= E_VALUE_THRESH:
            sbjct=hsp.sbjct.replace('-',")
            title = description.title
            if done.has_key(title):
                continue
            else:
                done[title] = 1
            print "%s HSP %d " % (title, hsp_nb)
            fasta_seqs.add_sequence(descriptor="%s HSP %d " % (title, hsp_nb),
                                    sequence=sbjct)

# save fasta sequences
alig_f = sys.argv[1] + '.seqs'
out=open(alig_f,'w')
print >>out, fasta_seqs
out.close()

# alignment
cline = MultipleAlignCL(alig_f)
clustalw_out = sys.argv[1] + '.aln'
cline.set_output(clustalw_out)
```

```
clustalw_align = do_alignment(cline)
os.unlink(alig_f)

print "Clustalw output written in: ", clustalw_out
```

Solution A.40. Get a PSSM from an alignment

Exercise 11.23

```
import Bio.Clustalw
import Bio.Align.AlignInfo
from Bio.Alphabet import IUPAC
from sys import *

if len(argv) == 2:
    threshold=40.0
else:
    threshold=argv[2]

align = Bio.Clustalw.parse_file(argv[1], alphabet=IUPAC.protein)
alig_len = align.get_alignment_length()
align_info = Bio.Align.AlignInfo.SummaryInfo(align)
ref_seq = align.get_seq_by_num(0)
pssm = align_info.pos_specific_score_matrix(ref_seq, chars_to_ignore = ['X'])
max = len(align_info.get_column(0))

# ----------------------
print "Conservation above %d: " % threshold
for pos in xrange(alig_len):
    for letter in pssm[pos].keys():
        percent = (pssm[pos][letter] / max) * 100.0
        if percent > threshold:
            print "%d %s %3.2f%s" % (pos, letter, percent, '%')
```

Solution A.41. Plotting Cys conserved position

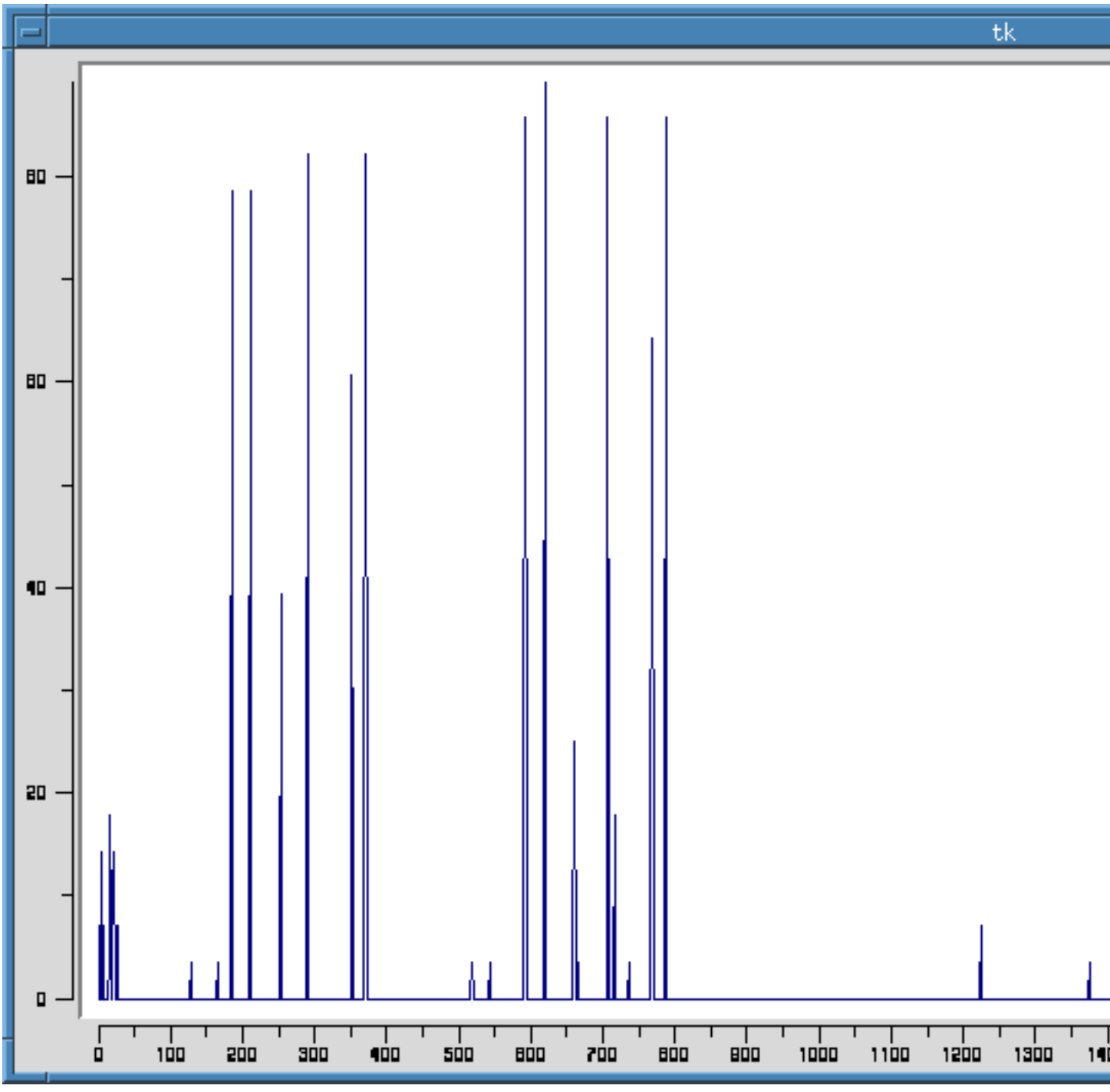
Exercise 11.24

Change the loop of Exercise 11.23 like this:

```
y = []
```

```
for pos in xrange(alig_len):
    max_percent = 0
    for letter in pssm[pos].keys():
        percent = (pssm[pos][letter] / max) * 100.0
        if letter == 'C' and percent > max_percent:
            max_percent = percent
    y.append(max_percent)
```

Figure A.2. Cys conserved positions



(full code [exercises/clustalw_plot_cys.py])

A.6. Classes

Solution A.42. Define a PDB structure class

Exercise 12.1

```
class PDBStructure:

    def __init__(self):
        self._residues=[]

    def add_residue(self, name, posseq):
        residue = {'name': resname,                                    ❶
                   'posseq': posseq,
                   'atoms': []}
        self._residues.append(residue)
        return residue

    def add_atom(self, residue, name, coord):
        atom = {'residue': residue,
                'name': name,
                'coord': coord
                }
        residue['atoms'].append(atom)                                  ❷
        return atom
```

❶ The residue is an anonymous dictionary being returned as a result to the method call, in order for the user of the class to pass it as an argument to the next `add_atom` method call.
❷ Is is the residue structure passed as argument that is actually changed, not a copy of it.

Solution A.43. Define a PDB structure class (cont)

Exercise 12.2

```
class PDBStructure:

    def __init__(self):
        self.residues=[]
        self._ssbonds = []
        self.dbrefs = ""

    def add_residue(self, model_id, chain_id, name, posseq):
        residue = {'model_id': model_id,
                   'chain_id': chain_id,
                   'name': name,
                   'posseq': posseq,
                   'atoms': []}
        self.residues.append(residue)
        return residue

    def add_atom(self, residue, name, coord, tempfactor, occupancy, altloc, element):

        atom = {'residue': residue,
                'name': name,
                'coord': coord,
                'tempfactor': tempfactor,
                'occupancy': occupancy,
                'altloc': altloc,
                'element': element
                }
        residue['atoms'].append(atom)
        return atom
```

(complete code for testing [exercises/PDBStructure_start.py])

Solution A.44. Define a PDB structure class (cont)

Exercise 12.3

Additional methods definitions:

```
    def get_residues(self):
        return self.residues

    def get_residues_by_name(self, name):
        result = []
        for residue in self.residues:
            if residue['name'] == name:
```

```
                result.append(residue)
        return result

    def get_residues_of_chain(self, chain_id):
        result = []
        for residue in self.residues:
            if residue['chain_id'] == chain_id:
                result.append(residue)
        return result

    def residue_model(self, residue):
        return residue['model_id']

    def residue_chain(self, residue):
        return residue['chain_id']
```

You can use them like this:

```
if __name__ == '__main__':
    print "--------------testing my class--------------------"
    struct = PDBStructure()

    model_id = 0
    chain_id = "A"

    residue = struct.add_residue(model_id, chain_id, name = "ILE",
                                 posseq = 1 )
    struct.add_atom(residue, name = "N",
                    coord = (23.46800041, -8.01799965, -15.26200008) ,
                    tempfactor=169.09, occupancy = 1.0, altloc = 0,
                    element = "N")
    struct.add_atom(residue, name = "CZ",
                    coord = (125.50499725, 4.50500011, -19.14800072),
                    tempfactor=169.09, occupancy = 1.0, altloc = 0,
                    element = "C")

    residue = struct.add_residue(model_id, chain_id, name = "LYS",
                                 posseq = 2 )
    struct.add_atom(residue, name = "OE1",
                    coord = (126.12000275, -1.78199995, -15.04199982),
                    tempfactor= 83.69, occupancy = 1.0, altloc = 0,
                    element = "O")

    chain_id = "B"

    residue = struct.add_residue(model_id, chain_id, name = "HIS",
                                 posseq = 1 )
    struct.add_atom(residue, name = "N",
                    coord = (23.46800041, -8.01799965, -15.26200008) ,
```

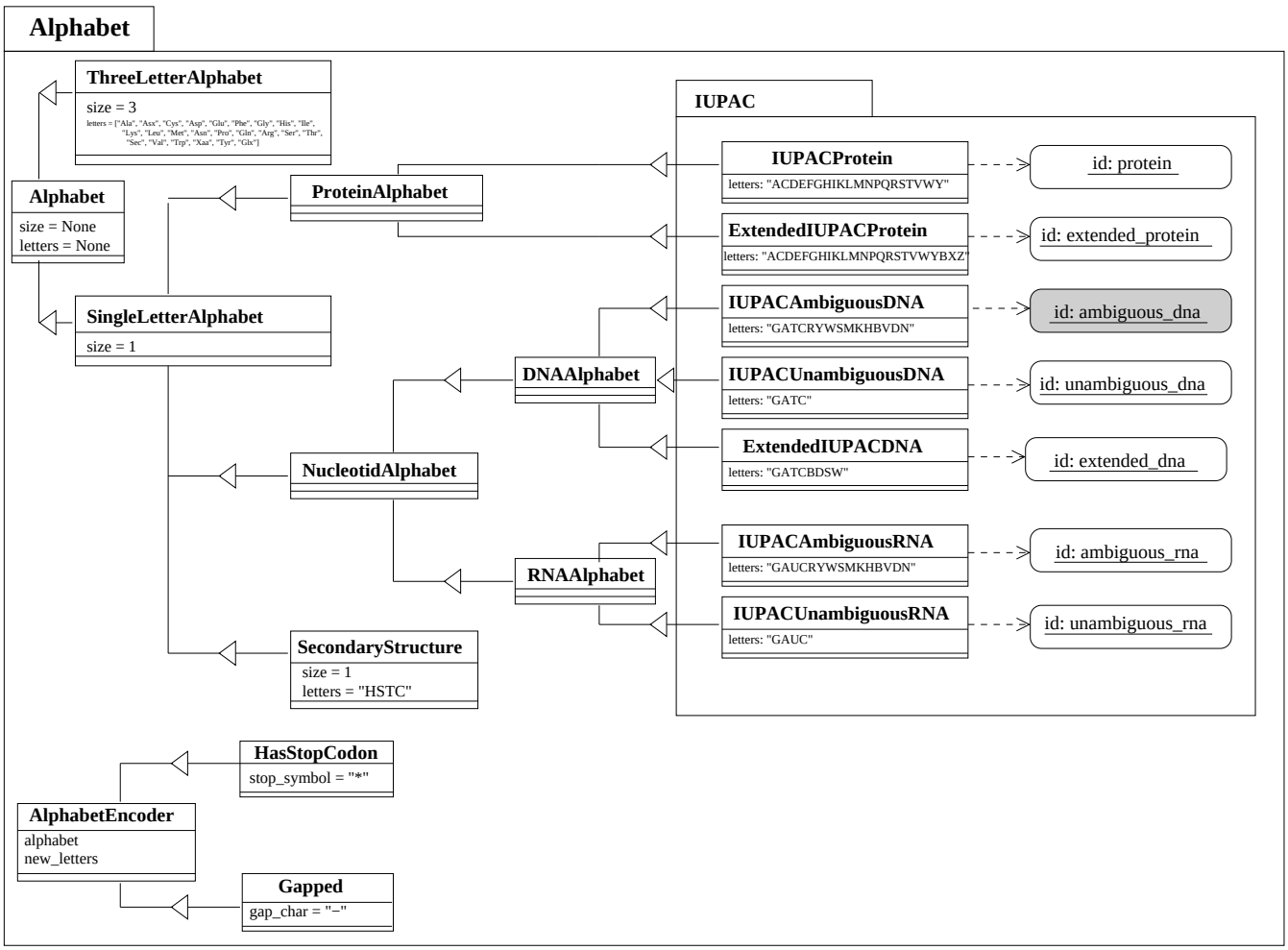
```
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "N")
struct.add_atom(residue, name = "CB",
                coord = (125.50499725, 4.50500011, -19.14800072),
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "C")

residue = struct.add_residue(model_id, chain_id, name = "ILE",
                             posseq = 2 )
struct.add_atom(residue, name = "N",
                coord = (23.46800041, -8.01799965, -15.26200008),
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "N")
struct.add_atom(residue, name = "CZ",
                coord = (125.50499725, 4.50500011, -19.14800072),
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "C")

print "residues of name ILE:"

for residue in struct.get_residues_by_name("ILE"):
    print residue
    print "model: ", struct.residue_model(residue)
    print "chain: ", struct.residue_chain(residue)

print "residues of chain B:"
for residue in struct.get_residues_of_chain("B"):
    print residue
```

(complete code for testing [exercises/PDBStructure_next.py])

Solution A.45. Bio.Alphabet class hierarchy

Exercise 12.5

Figure A.3. Biopython Alphabet class hierachy



Solution A.46. Define a PDB structure class (cont')

Exercise 12.6

With an instance variable:

```
class PDBStructure:
```

```
    def verbose(self, state=None):
        if state == None:
            return self._verbose
        else:
            self._verbose = state

    def __init__(self):
        self.residues=[]
        self._verbose = 0

    def add_residue(self, model_id, chain_id, name, posseq):
        if self.verbose():
            print "add_residue: ", " model_id: ",
            model_id, " chain_id: ", chain_id, " name: ",
            name, " posseq: ", posseq

        residue = {'model_id': model_id,
                   'chain_id': chain_id,
                   'name': name,
                   'posseq': posseq,
                   'atoms': []}
        self.residues.append(residue)
        return residue
```

With a class variable:

```
class PDBStructure:

    _verbose = 0

    def verbose(self, state=None):
        if state == None:
            return PDBStructure._verbose
        else:
            PDBStructure._verbose = state

    def __init__(self):
        self.residues=[]

    def add_residue(self, model_id, chain_id, name, posseq):
        if self.verbose():
            print "add_residue: ", " model_id: ",
            model_id, " chain_id: ", chain_id, " name: ",
            name, " posseq: ", posseq

        residue = {'model_id': model_id,
                   'chain_id': chain_id,
                   'name': name,
```

```
                'posseq': posseq,
                'atoms': []}
        self.residues.append(residue)
        return residue
```

You can use it with:

```
if __name__ == '__main__':
    print "--------------testing my class--------------------"
    struct = PDBStructure()

    print "verbose on"
    struct.verbose(1)

    model_id = 0
    chain_id = "A"

    residue = struct.add_residue(model_id, chain_id, name = "ILE",
                                 posseq = 1 )
    struct.add_atom(residue, name = "N",
                    coord = (23.46800041, -8.01799965, -15.26200008) ,
                    tempfactor=169.09, occupancy = 1.0, altloc = 0,
                    element = "N")
    struct.add_atom(residue, name = "CZ",
                    coord = (125.50499725, 4.50500011, -19.14800072),
                    tempfactor=169.09, occupancy = 1.0, altloc = 0,
                    element = "C")

    residue = struct.add_residue(model_id, chain_id, name = "LYS",
                                 posseq = 2)
    struct.add_atom(residue, name = "OE1",
                    coord = (126.12000275, -1.78199995, -15.04199982),
                    tempfactor= 83.69, occupancy = 1.0, altloc = 0,
                    element = "O")

    print "verbose off"
    struct.verbose(0)

    chain_id = "B"

    residue = struct.add_residue(model_id, chain_id, name = "HIS",
                                 posseq = 1)
    struct.add_atom(residue, name = "N",
                    coord = (23.46800041, -8.01799965, -15.26200008) ,
                    tempfactor=169.09, occupancy = 1.0, altloc = 0,
                    element = "N")
    struct.add_atom(residue, name = "CB",
                    coord = (125.50499725, 4.50500011, -19.14800072),
```

```
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "C")

    residue = struct.add_residue(model_id, chain_id, name = "ILE",
                                 posseq = 2)
    struct.add_atom(residue, name = "N",
                coord = (23.46800041, -8.01799965, -15.26200008),
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "N")
    struct.add_atom(residue, name = "CZ",
                coord = (125.50499725, 4.50500011, -19.14800072),
                tempfactor=169.09, occupancy = 1.0, altloc = 0,
                element = "C")

    print "\n-----------------Structure:--------------------\n", struct
```

A.7. Biopython, continued

A.7.1. Enzyme

Solution A.47. EnzymeConsumer, reading one entry from a file

Exercise 13.1

```
from Bio.ParserSupport import *

class EnzymeConsumer(AbstractConsumer):

    def __init__(self):
        self._references = ""

    def databank_reference(self, line):
        self._references += line
```

Which can be used this way:

```
handle = open(argv[1])
scanner  = Enzyme._Scanner()
consumer = EnzymeConsumer()
scanner.feed(handle, consumer)
print "results: ", consumer._references
```

Solution A.48. EnzymeConsumer, reading n entries from a file

Exercise 13.2

```
from Bio.ParserSupport import *

class EnzymeConsumer(AbstractConsumer):

    def __init__(self):
        self._references = {}

    def end_record(self):
        self._references[self._id] = self._refs

    def databank_reference(self, line):
        self._refs += line

    def identification(self, line):
        self._id = line
        self._refs = ""
```

Which can be used this way:

```
handle = open(argv[1])
scanner  = Enzyme._Scanner()
consumer = EnzymeConsumer()
scanner.feed(handle, consumer)

for id in consumer._references.keys():
    print id, consumer._references[id]
```

Solution A.49. EnzymeParser

Exercise 13.3

```
from Bio import Enzyme
from Bio.ParserSupport import *

class EnzymeParser(AbstractParser):
    def __init__(self):
        self._scanner  = Enzyme._Scanner()
        self._consumer = EnzymeConsumer()

    def parse(self, handle):
        self._scanner.feed(handle, self._consumer)
```

```
        return self._consumer._references
```

This can be used like this:

```
from sys import *
from EnzymeParser import EnzymeParser

handle = open(argv[1])
parser = EnzymeParser()
references = parser.parse(handle)

for id in references.keys():
    print id, references[id]
```

(complete classes definition [exercises/EnzymeParser.py])

Solution A.50. EnzymeIterator

Exercise 13.5

The iterator might be defined like this:

```
import re
import string

class EnzymeIterator:

    blank = re.compile(r'^\s*$')

    def __init__(self, handle, parser=EnzymeParser()):
        self._parser = parser
        self._uhandle = File.UndoHandle(handle)

    def next(self):

        lines = ""
        while 1:
            line = self._uhandle.readline()
            if not line:
                break
            if EnzymeIterator.blank.match(line):
                break
            lines += line
            if line[:2] == '//':
                break
        if not lines:
```

```
            return None

        if self._parser is not None:
            return self._parser.parse(File.StringHandle(lines))
        return lines
```

(complete classes definition [exercises/enzyme_iterator.py])

The code to use the iterator may be:

```
from enzyme_iterator import EnzymeIterator
from sys import *

handle = open(argv[1])
iterator = EnzymeIterator(handle)
record = iterator.next()
while record:
    print record['id'], record['references']
    record = iterator.next()


handle.close()
```

The consumer and the parsers may be the same as before (Exercise 13.3). However, in order to get this output:

```
[{'ac': 'P00450,', 'id': 'CERU_HUMAN;'},
 {'ac': 'Q61147,', 'id': 'CERU_MOUSE;'},
 {'ac': 'P13635,', 'id': 'CERU_RAT'}]
```

we need to change the `databank_reference` method:

```
    def databank_reference(self, line):
        items = line.split()[1:]
        for i in range(0,len(items)):
            if (i % 2) == 0:
                ac=items[i]
                if ac[:-1] == ',' or ac[:-1] == ';':
                    ac=ac[:-1]
            else:
                id=items[i]
                if id[:-1] == ',' or id[:-1] == ';':
                    id=id[:-1]
                self._references.append( {'ac': ac, 'id': id  } )
```

(complete classes definition [exercises/enzyme_iterator.py])

Solution A.51. EnzymeIterator with lookup

Exercise 13.6

The consumer and the parser are the same than in Exercise 13.5. The iterator defines an additional method, `lookup`, to search in the database:

```
import re
import string

class EnzymeIterator:

    def __init__(self, handle, parser=EnzymeParser()):
        self._parser = parser
        self._uhandle = File.UndoHandle(handle)

    def lookup(self,id):
        ID = re.compile(r'ID\s*(?P<id>([\w\.]+))\s*')
        while 1:
            record = self.next()
            if not record:
                break
            m=ID.match(record['id'])
            if m.group('id') == id:
                return record

        return None

    def next(self):
        blank = re.compile(r'^\s*$')
        lines = []

        start=1
        while(1):
            line = self._uhandle.readline()
            if start:
                while line[:2] == 'CC':
                    line = self._uhandle.readline()
            if start:
                while line[:2] == '//':
                    line = self._uhandle.readline()
                start=0

            if not line:
                break
            if blank.match(line):
                break
            lines.append(line)
            if line[:2] == '//':
                break
```

```
        if not lines:
            return None

        data = string.join(lines, ”)
        if self._parser is not None:
            return self._parser.parse(File.StringHandle(data))
        return data
```

The code to use the iterator may be:

```
from enzyme_iterator_db import EnzymeIterator
import getopt
from sys import *
from string import *

ENZYMEDB = ’/local/databases/release/Enzyme/enzyme.dat’

o, id = getopt.getopt(argv[1:], ’d:’)
opts = {}
for k,v in o:
    opts[k] = v
if  opts.has_key(’-d’):
    db = opts[’-d’]
else:
    db = ENZYMEDB
if len(id) < 1:
    usage(); sys.exit("provide an id to search")
else:
    id=id[0]

database = open(db)
iterator = EnzymeIterator(database)
record = iterator.lookup(id)
if record:
    print record[’id’], join(record[’references’],"")
else:
    print "id: ", id, " not found in database ’", db, "’"

database.close()
```

(complete classes definition [exercises/enzyme_iterator_db.py])

Solution A.52. EnzymeDictionary

Exercise 13.7

The iterator is the same than in Exercise 13.6.

```
from enzyme_iterator_db import EnzymeIterator
import re

class EnzymeDictionary:

    #_ID = re.compile(r'ID\s*(?P<id>([\w\.]+))\s*')

    def __init__(self, db):
        self._index = {}
        self._db = db
        self._handle = open(self._db)
        self._iterator = EnzymeIterator(self._handle)
        self._index = {}

    def __getitem__(self, id):
        if self._index.has_key(id):
            return self._index[id]
        while 1:
            record = self._iterator.next()
            if not record:
                self._handle.close()
                break
            self._index[record['id']] = record
            if id == record['id']:
                break
        return self._index[id]
```

The code to use the dictionary may be:

```
from enzyme_dictionary import EnzymeDictionary
import getopt
from sys import *
from string import *

ENZYMEDB = '/local/databases/release/Enzyme/enzyme.dat'

o, id = getopt.getopt(argv[1:], 'd:')
opts = {}
for k,v in o:
    opts[k] = v
if  opts.has_key('-d'):
    db = opts['-d']
else:
```

```
    db = ENZYMEDB
if len(id) < 1:
    usage(); sys.exit("provide an id to search")
else:
    id=id[0]

enzyme = EnzymeDictionary(db)

try:
    record = enzyme[id]
    print record['id'], join(record['references'],"")
except KeyError, e:
    print "key not found: ", e

print "end of lookup for ", enzyme[id]['id']
```

Solution A.53. EnzymeParsing module

Exercise 13.8

Create an `EnzymeParsing.py` file containing the required classes (the one used in Exercise 13.7 preferably).

The code to use the dictionary may be for instance:

```
>>> from EnzymeParsing import EnzymeDictionary
>>> enzyme = EnzymeDictionary('/local/databases/release/Enzyme/enzyme.dat')
>>> print enzyme['1.1.1.5']
{'references': [{'ac': 'Q48436,', 'id': 'BUDC_KLEPN;'}, {'ac': 'Q04520,', 'id': 'BUDC_KLETE;'}
```

(complete module definition [exercises/EnzymeParsing.py])

Solution A.54. Fetching enzymes referenced in a SwissProt entry and related proteins

Exercise 13.9

Fetch the enzyme entry and the corresponding SwissProt references.

```
from EnzymeParsing import EnzymeDictionary
import sprot
from sys import *
```

```
sp_record = sprot.get_sprot_entry_local(argv[1])
enzyme_id = sprot.get_enzyme_ref(sp_record)

enzyme = EnzymeDictionary('/local/databases/release/Enzyme/enzyme.dat')
enzyme_record = enzyme[enzyme_id]
for ref in enzyme_record['references']:
    sp_id = ref['id']
    sp_r = sprot.get_sprot_entry_local(sp_id)
    print sp_r.entry_name, sp_r.description
```

A.7.2. PDB

Solution A.55. Get a PDB entry from RCSB Web server

Exercise 13.10

```
import urllib
import string
from Bio import File

def get_pdb_entry_remote(id):
    #http://www.rcsb.org/pdb/cgi/export.cgi/1KCW.pdb?format=PDB&pdbId=1KCW&compression=None


    fullcgi = "http://www.rcsb.org/pdb/cgi/export.cgi/%s.pdb?format=PDB&compression=None&pdbId=%s" %

    #print fullcgi
    handle = urllib.urlopen(fullcgi)

    uhandle = File.UndoHandle(handle)

    if not uhandle.peekline():
        raise IOError, "no results"

    return uhandle

def get_pdb_entry_local(id):
    id = string.lower(id)
    filename = "data/pdb" + id + ".pdb"
    try:
        print "trying to open " , filename
        handle = open(filename)
    except IOError, e:
        print e
```

```
        filename = "data/" + id + ".pdb"
        try:
            print "trying to open " , filename
            handle = open(filename)
        except IOError, e:
            print e
            filename = "data/pdb" + id + ".ent"
            try:
                print "trying to open " , filename
                handle = open(filename)
            except IOError, e:
                print e
                return None

    return handle
```

Solution A.56. Define a PDBStructure class

Exercise 13.11

Add the following code to the code already written in Exercise 12.6:

```
    def __str__(self):
        for residue in self._residues:
            print residue
        return ""

    def set_id(self, structure_id):
        self._structure_id = structure_id

    def set_pdb_ident(self, pdb_ident):
        self.pdb_ident = pdb_ident

    def add_dbref(self, dbref):
        self.dbrefs += dbref

    def add_ssbond(self, _from, _to):
        self._ssbonds.append({'from': _from, 'to': _to})
```

(complete class definition [exercises/PDBStructure1.py]).

Solution A.57. Define a PDBConsumer class

Exercise 13.12

```
#
# PDBConsumer creates instances of PDBStructure
#

from Bio.ParserSupport import *
from PDBParser import PDBParser
from PDBStructure import PDBStructure
import sys

class PDBConsumer(AbstractConsumer):

    _verbose = 0

    def __init__(self):
        self._current_struct = None

    def set_id(self, structure_id):
        # start a new structure
        if self._verbose:
            print "set_id: ",structure_id
        self._current_struct = PDBStructure()
        self._current_struct.set_id(structure_id)

    def set_pdb_ident(self, pdb_ident):
        if self._verbose:
            print "set_pdb_ident: ", pdb_ident
        self._current_struct.set_pdb_ident(pdb_ident)

    def set_symmetry(self, spacegroup, cell):
        pass

    def init_model(self, model_id):
        if self._verbose:
            print "init_model: ", model_id
        self._current_model_id = model_id

    def init_chain(self, chain_id):
        if self._verbose:
            print "init_chain: ", chain_id
        self._current_chain_id = chain_id

    def set_anisou(self, anisou):
        pass

    def set_sigatm(self, sigatm):
        pass

    def set_siguij(self, siguij):
        pass
```

```
    def set_ssbond(self, _from, _to):
        self._current_struct.add_ssbond(_from, _to)

    def set_dbref(self, line):
        self._current_struct.add_dbref(line)

    def init_residue(self, name, field, posseq, icode):
        if self._verbose:
            print "init_residue: name: ", name, " field: ", field, " posseq: ", posseq, " icod

        residue = self._current_struct.add_residue(self._current_model_id,
                                                   self._current_chain_id,
                                                   name, field, posseq, icode)
        self._current_residue = residue

    def init_atom(self, name, coord, tempfactor, occupancy, altloc, element):
        if self._verbose:
            print "init_atom: name: ", name, " coord: ", coord, " tempfactor: ",tempfactor, "

        self._current_struct.add_atom(self._current_residue,
                                      name, coord, tempfactor,
                                      occupancy, altloc, element)

    def get(self):
        return self._current_struct
```

Solution A.58. Compute disulfid bonds in 1KCW

Exercise 13.13 You first need to complete the `PDBStructure` class by adding a `disulfid_bridges` method:

```
    BRIDGE_DIST=8.0

    def dist(self, a1, a2):
        dx = a1[0] - a2[0]
        dy = a1[1] - a2[1]
        dz = a1[2] - a2[2]
        return math.sqrt(dx*dx + dy*dy + dz*dz)

    def disulfid_bridges(self):
        sulfurs=[]
        for cys_residue in self.get_residues_by_name('CYS'):
            #print "cys: ",cys_residue['name'], cys_residue['posseq']
```

```
            for atom in cys_residue['atoms']:
                if atom['name'] == 'SG':
                    sulfurs.append({'posseq': cys_residue['posseq'],
                                    'atom': atom})

        result=[]
        nb = len(sulfurs)
        for i in xrange(nb):
            for j in xrange(i+1, nb):
                d = self.dist(sulfurs[i]['atom']['coord'], sulfurs[j]['atom']['coord'])

                if d < self.BRIDGE_DIST:
                    print "residue %d in contact with residue %d (distance:%.3f)." % (sulfurs[i]['pos

                    print "\t", sulfurs[i]['atom']['coord'], "\n\t", sulfurs[j]['atom']['coord']

                    result.append({'from': sulfurs[i]['posseq'],
                                   'to': sulfurs[j]['posseq'],
                                   'dist': d
                                   })
        return result
```

Then, you can use the class from:

```
#
# Compute disulfide bonds.
#
#  - search for sulfur (S) atoms in Cys residues of the structure
#  - compute distance between all of them
#  - displays residue pairs (position) where distance < BRIDGE_DIST
#
#

from PDBParser import PDBParser
from PDBConsumer import PDBConsumer
from PDBStructure import PDBStructure
import sys


if __name__ == '__main__':
    p=PDBParser(PDBConsumer())
    struct = p.get("scratch", sys.argv[1])

    detected = struct.disulfid_bridges()
    for annot in struct._ssbonds:
        found=0
        for detect in detected:
            if annot['from'] == detect['from'] and annot['to'] == detect['to']:
```

```
                print annot, " also detected: ", detect['dist']
                found=1
                break
        if not found:
            print annot, " not found"
```

(complete class definition [exercises/PDBStructure2.py])

Solution A.59. Compare 3D disulfid bonds with Cys positions in the alignment (take #1).

Exercise 13.14

```
import Bio.Clustalw
from Bio.Seq import Seq
import Bio.Align.AlignInfo
from Bio.WWW import *
from Bio.Alphabet import IUPAC
from Bio.SwissProt import SProt
import sys
from os import *
import string
from WWWPDB import *
from PDBParser import PDBParser
from PDBConsumer import PDBConsumer

def get_pdb_entries(sprot):
    refs=[]
    for ref in sprot.cross_references:
        if ref[0] == 'PDB':
            refs.append(ref[1])
    return refs


def get_sprot_entry_remote (sprot_id):
    expasy = ExPASy.get_sprot_raw(sprot_id)
    iterator = SProt.Iterator(expasy, SProt.RecordParser())
    entry = iterator.next()
    expasy.close()
    return entry

def get_sprot_entry_local (sprot_id):
    cmd="golden sprot:" + sprot_id
    print "Fetching entry by ",cmd
```

```
    golden = popen(cmd, 'r')
    iterator = SProt.Iterator(golden, SProt.RecordParser())
    entry = iterator.next()
    golden.close()
    return entry

def align2seqpos(seq,col):
    "returns the original sequence position from a gapped sequence position"
    s=list(seq.tostring())
    gaps = 0
    for i in xrange(len(s)):
        if i >= col:
            break
        if s[i] == '-':
            gaps = gaps + 1
    #print "gaps: ", gaps
    result = col - gaps
    return result


def get_seq_description(alignment,seq_nb):
    return alignment._records[seq_nb].description

"""
  open alignement and create pssm
"""

align = Bio.Clustalw.parse_file(sys.argv[1], alphabet=IUPAC.protein)
align_info = Bio.Align.AlignInfo.SummaryInfo(align)
ref_seq = align.get_seq_by_num(0)
pssm = align_info.pos_specific_score_matrix(ref_seq, chars_to_ignore = ['X'])
max = len(align_info.get_column(0))
alig_len = align.get_alignment_length()

"""
fetch PDB entry from swissprot references
"""
seq_id = get_seq_description(align,0)
print "Swissprot ID: ", seq_id
try:
    seq_record = get_sprot_entry_remote(seq_id)
except IOError, e:
    #print "Remote acces not available: ", e
    seq_record = get_sprot_entry_local(seq_id)

refs = get_pdb_entries(seq_record)
print "PDB reference: ", refs

try:
    pdb_handle = get_pdb_entry_remote(refs[0])
except IOError, e:
```

```
    print e
    pdb_handle = get_pdb_entry_local(refs[0])

p=PDBParser(PDBConsumer())
struct = p.get_handle("scratch", pdb_handle)

# comparison

print "--- detected bonds from PDB coordinates:-------------"
detected = struct.disulfid_bridges()
for detect in detected:
    print detect

print "--- detected bonds from alignment: ----------"
for pos in xrange(alig_len):
    percent = (pssm[pos]['C'] / max) * 100.0
    if percent > 40.0:
        print "potential disulfid? ", pos + 1, " %: ",percent
```

Solution A.60. Compare 3D disulfid bonds with Cys positions in the alignment (take #2).

first add a method `pdb2seq_pos` into class `PDBStructure`:

```
    def pdb2seq_pos(self):
        """
        DBREF  1KCW      1   338  SWS    P00450   CERU_HUMAN      20    357
        DBREF  1KCW    347   474  SWS    P00450   CERU_HUMAN     366    493
        DBREF  1KCW    483   884  SWS    P00450   CERU_HUMAN     502    903
        DBREF  1KCW    892  1040  SWS    P00450   CERU_HUMAN     904   1059
        """
        lines = self.dbrefs.split("\n")
        items = lines[0].split()
        pos_pdb = string.atoi(items[7])
        pos_sws = string.atoi(items[2])
        if pos_sws < pos_pdb:
            return pos_pdb - pos_sws
        else:
            return pos_sws - pos_pdb
```

and use it as follows:

Exercise 13.15

```
#! /local/bin/python

import Bio.Clustalw
from Bio.Seq import Seq
import Bio.Align.AlignInfo
from Bio.WWW import *
from Bio.Alphabet import IUPAC
from Bio.SwissProt import SProt
import sys
from os import *
import string
from WWWPDB import *
from PDBParser import PDBParser
from PDBConsumer import PDBConsumer

def get_pdb_entries(sprot):
    refs=[]
    for ref in sprot.cross_references:
        if ref[0] == 'PDB':
            refs.append(ref[1])
    return refs


def get_sprot_entry_remote (sprot_id):
    expasy = ExPASy.get_sprot_raw(sprot_id)
    iterator = SProt.Iterator(expasy, SProt.RecordParser())
    entry = iterator.next()
    expasy.close()
    return entry

def get_sprot_entry_local (sprot_id):
    cmd="golden sprot:" + sprot_id
    print "Fetching entry by ",cmd
    golden = popen(cmd, 'r')
    iterator = SProt.Iterator(golden, SProt.RecordParser())
    entry = iterator.next()
    golden.close()
    return entry

def align2seqpos(seq,col):
    "returns the original sequence position from a gapped sequence position"
    s=list(seq.tostring())
    gaps = 0
    for i in xrange(len(s)):
        if i >= col:
            break
        if s[i] == '-':
            gaps = gaps + 1
```

```
    #print "gaps: ", gaps
    result = col - gaps
    return result


def get_seq_description(alignment,seq_nb):
    return alignment._records[seq_nb].description

"""
  open alignement and create pssm
"""

align = Bio.Clustalw.parse_file(sys.argv[1], alphabet=IUPAC.protein)
align_info = Bio.Align.AlignInfo.SummaryInfo(align)
ref_seq = align.get_seq_by_num(0)
pssm = align_info.pos_specific_score_matrix(ref_seq, chars_to_ignore = ['X'])
max = len(align_info.get_column(0))
alig_len = align.get_alignment_length()

"""
fetch PDB entry from swissprot references
"""
seq_id = get_seq_description(align,0)
print "Swissprot ID: ", seq_id
try:
    seq_record = get_sprot_entry_remote(seq_id)
except IOError, e:
    #print "Remote acces not available: ", e
    seq_record = get_sprot_entry_local(seq_id)

refs = get_pdb_entries(seq_record)
print "PDB reference: ", refs

try:
    pdb_handle = get_pdb_entry_remote(refs[0])
except IOError, e:
    print e
    pdb_handle = get_pdb_entry_local(refs[0])

p=PDBParser(PDBConsumer())
struct = p.get_handle("scratch", pdb_handle)

# comparison

print "--- detected bonds from PDB coordinates:-------------"
detected = struct.disulfid_bridges()
for detect in detected:
    print detect

diffpos = struct.pdb2seq_pos()
print "difference in PDB and sequence position: ", diffpos
```

```
print "--- detected bonds from alignment: ----------"
for pos in xrange(alig_len):
    percent = (pssm[pos]['C'] / max) * 100.0
    vector_y.append(percent)
    if percent > 40.0:
        print "potential disulfid? ", pos + 1, " %: ", \
 percent, " (seq: ", align2seqpos(ref_seq, pos) + 1, \
 " PDB seq: ", align2seqpos(ref_seq, pos) + 1 - diffpos, ")"
```

(complete PDBStructure class definition [exercises/PDBStructure.py])

Appendix B. Bibliography
Bibliography

[Beaz2001] David M. Beazley. *Python*. Essential Reference. 2. New Riders. 2001.

[Tis2001] James Tisdall. *Beginning Perl for Bioinformatics*. An introduction to Perl for Biologists. O'Reilly. 2001.