

# Interact with files

September 6, 2017

```
In [1]: # The following is to know when this notebook has been run and with which python version
import time, sys
print(time.ctime())
print(sys.version.split('|')[0])
```

Wed Sep 6 13:58:31 2017  
3.6.1

## 1 C: How to read and write files (ASCII and FITS)

This is part of the Python lecture given by Veronica Gomez Llanos and Christophe Morisset at IA-UNAM.

Some informations are here: [http://www.tutorialspoint.com/python/python\\_files\\_io.htm](http://www.tutorialspoint.com/python/python_files_io.htm)

### 1.1 Reading a simple ascii file

```
In [2]: # numpy is needed in some part of the lecture
import numpy as np
```

First of all, we will have to have some files on the hard drive to read them The following notebook cell will write a file in the same directory where the notebook has been started.

```
In [3]: %%writefile data1.dat
1  2.3  6   8 star
2  3.5  7   9 galaxy
3 -4.2  5   7 cluster
```

Overwriting data1.dat

Now the goal is to read this file. The first way is to open the file, read it completely in a variable and close the file. Then we can play with the content of the file.

```
In [4]: datafile = open('data1.dat', 'r') # Open the file to read it
```

```
In [5]: data = datafile.readlines() # The variable data will receive the content of the file.
```

```
In [6]: datafile.close() # Not need anymore of the file.
```

```
In [7]: print(type(data)) # The data file is stored in the form of a list, each element of the l
<class 'list'>
```

```
In [8]: print(data) # Each row is a string and terminates with \n, symbol of END OF LINE.
['1  2.3  6   8 star\n', '2   3.5  7   9 galaxy\n', '3  -4.2  5   7 cluster']
```

```
In [9]: print(len(data)) # number of rows
3
```

```
In [10]: print(data[0], 'tralala')
1  2.3  6   8 star
tralala
```

```
In [11]: for row in data:
          print(row)
1  2.3  6   8 star
2   3.5  7   9 galaxy
3  -4.2  5   7 cluster
```

```
In [12]: # In python :
          for row in data:
              print(row),
1  2.3  6   8 star
2   3.5  7   9 galaxy
3  -4.2  5   7 cluster
```

```
In [13]: # In python 3:
          for row in data:
              print(row, end='')
1  2.3  6   8 star
2   3.5  7   9 galaxy
3  -4.2  5   7 cluster
```

```
In [14]: print(type(data[0])) # Each element is a string
<class 'str'>
```

Now it is easy to separate each field with the split command:

```
In [15]: for row in data:
          print(row.split())

['1', '2.3', '6', '8', 'star']
['2', '3.5', '7', '9', 'galaxy']
['3', '-4.2', '5', '7', 'cluster']
```

```
In [16]: # One can also transform the data if the type is known:
          for row in data:
              this_data = row.split()
              print('N = {0:2d} f = {1:5.2f} type = {2:>10s}'.format(int(this_data[0]),
                                                                      float(this_data[1]),
                                                                      this_data[4]))
```

```
N =  1 f =  2.30 type =      star
N =  2 f =  3.50 type =    galaxy
N =  3 f = -4.20 type =    cluster
```

```
In [17]: # One can even fill a list with the data, by column:
          N = []
          f = []
          type_ = [] # take care, type is a python command, you can erase it if you use it...
          for row in data:
              this_data = row.split()
              N.append(int(this_data[0]))
              f.append(float(this_data[1]))
              type_.append(this_data[4])
          print(N)
          print(f)
          print(type_)
          N = np.array(N)
          print(N)
```

```
[1, 2, 3]
[2.3, 3.5, -4.2]
['star', 'galaxy', 'cluster']
[1 2 3]
```

```
In [18]: # If the file number of rows is not too big, you can use list comprehension (and even s
N = np.array([int(row.split()[0]) for row in data])
f = np.array([float(row.split()[1]) for row in data])
# Each one of this command scans all the rows, don't use for huge files
print(N)
print(f)

[1 2 3]
[ 2.3  3.5 -4.2]
```

## 1.2 How to treat special rows (headers, comments)

```
In [19]: %%writefile data2.dat
# The following data are for test purpose
N      f      x      y type
1      2.3    6      8 star
2      3.5    7      9 galaxy
3     -4.2    5      7 cluster
#4    -10.5    5      7 test
```

Overwriting data2.dat

```
In [20]: !cat data2.dat # Just to check that the # comments are also in the file

# The following data are for test purpose
N      f      x      y type
1      2.3    6      8 star
2      3.5    7      9 galaxy
3     -4.2    5      7 cluster
#4    -10.5    5      7 test
```

The file has to be read row by row, to be sure that special cases are treated.

```
In [21]: datafile = open('data2.dat', 'r') # Open the file to read it

row = datafile.readline() # this reads only one line
first_comment = row
print(first_comment, end = '')

row = datafile.readline() # this reads only one line
header = row
print(header, end = '')

data = []
while True: # loops until exit by break command
    row = datafile.readline()
    if row == '':
```

```

        break
    if row[0] != '#' and row[0] != '\n': # comment lines are skipped
        data.append(row)
datafile.close()
print(data)

# The following data are for test purpose
N    f    x    y type
['1    2.3  6    8 star\n', '2    3.5  7    9 galaxy\n', '3   -4.2  5    7 cluster\n']

```

```

In [22]: datafile = open('data2.dat', 'r') # Open the file to read it
row = datafile.readline() # this reads only one line
first_comment = row
print(first_comment, end = '')
row = datafile.readline() # this reads only one line
header = row
print(header, end = '')
data = []
row = datafile.readline()
while row != '': # loops until exit by break command
    if row[0] != '#': # comment lines are skipped
        data.append(row)
    row = datafile.readline()
datafile.close()
print(data)

```

```

# The following data are for test purpose
N    f    x    y type
['1    2.3  6    8 star\n', '2    3.5  7    9 galaxy\n', '3   -4.2  5    7 cluster\n']

```

```

In [23]: # very shorter way to deal with the file. No need to look for the end of the file.
datafile = open('data2.dat', 'r') # Open the file to read it
data = []
for row in datafile:
    if row[0] != '#': # comment lines are skipped
        data.append(row)
datafile.close()
print(data)
# This way will include the header in the data... Not what we want

```

```

['N    f    x    y type\n', '1    2.3  6    8 star\n', '2    3.5  7    9 galaxy\n', '3   -4.2  5    7 cl

```

```

In [24]: # very shorter way to deal with the file:
# we know that the header is the first no-comment line in the file.
datafile = open('data2.dat', 'r') # Open the file to read it
data = []

```

```

comments = [] # we can keep the comments for some usage
header_read = False # We will turn it to True once the header is read
for row in datafile:
    if row[0] != '#': # comment lines are skipped
        if not header_read:
            header = row
            header_read = True # next time, data will be read
        else:
            data.append(row)
    else:
        comments.append(row)
datafile.close()
print(header, end='')
print(data)
print(comments)

```

```

N      f      x      y type
['1    2.3  6    8 star\n', '2    3.5  7    9 galaxy\n', '3   -4.2  5    7 cluster\n']
['# The following data are for test purpose\n', '#4   -10.5  5    7 test']

```

```

In [25]: # Alternative way using "with". No need to close the file, done when the "with" block i
data = []
comments = []
header_read = False
def change_type(row_split):
    # This function change the type of the data read from the file from 5 strings into
    # It also return the result in form of a tuple
    return (int(row_split[0]),
            float(row_split[1]),
            float(row_split[2]),
            float(row_split[3]),
            row_split[4])
with open('data2.dat', 'r') as datafile:
    for row in datafile:
        if row[0] != '#' and row[0] != '\n': # comment lines are skipped
            if not header_read:
                header = row
                header_read = True
            else:
                data.append(change_type(row.split()))
        else:
            comments.append(row)
print(header)
print(data)
print(comments)

```

```

N      f      x      y type

```

```
[(1, 2.3, 6.0, 8.0, 'star'), (2, 3.5, 7.0, 9.0, 'galaxy'), (3, -4.2, 5.0, 7.0, 'cluster')]
['# The following data are for test purpose\n', '#4 -10.5 5 7 test']
```

```
In [26]: # We can define the result as a structured array
         # We use the header to define the field names.
         # data must be a list of tuples.
         a = np.array(data, dtype={'names':header.split(),
                                   'formats':['i4','f16', 'f16', 'f16', 'U10']})
```

```
In [27]: a
```

```
Out[27]: array([(1, 2.3, 6.0, 8.0, 'star'), (2, 3.5, 7.0, 9.0, 'galaxy'),
                (3, -4.2, 5.0, 7.0, 'cluster')],
              dtype=[('N', '<i4'), ('f', '<f16'), ('x', '<f16'), ('y', '<f16'), ('type', '<U10')])
```

```
In [28]: print(data[0])
```

```
(1, 2.3, 6.0, 8.0, 'star')
```

```
In [29]: print(a[0])
```

```
(1, 2.3, 6.0, 8.0, 'star')
```

```
In [30]: # Easy access to the columns, by their name
         print(a['N'])
```

```
[1 2 3]
```

```
In [31]: print(a['type'])
```

```
['star' 'galaxy' 'cluster']
```

```
In [32]: # Easy combine the values of columns
         print(np.sqrt(a['x']**2 + a['y']**2))
```

```
[ 10.0  11.401754  8.6023253]
```

### 1.2.1 Using numpy loadtxt

<http://docs.scipy.org/doc/numpy/reference/generated/numpy.loadtxt.html>

```
In [33]: # Fast way for reading the file
         # One has to tell to skip the 2 first rows
         # skiprows
         b = np.loadtxt('data2.dat', skiprows=2, dtype='i4,f, f, f, U10')
```

```
In [34]: print(b)
```

```
[(1, 2.29999995, 6., 8., "b'star'")
 (2, 3.5, 7., 9., "b'galaxy'")
 (3, -4.19999981, 5., 7., "b'cluster'")]
```

```
In [35]: type(b)
```

```
Out[35]: numpy.ndarray
```

```
In [36]: # The names of the columns are f0, f1, f2, etc
         b.dtype
```

```
Out[36]: dtype([('f0', '<i4'), ('f1', '<f4'), ('f2', '<f4'), ('f3', '<f4'), ('f4', '<U10')])
```

### 1.2.2 Using numpy genfromtxt

<http://docs.scipy.org/doc/numpy/reference/generated/numpy.genfromtxt.html>

```
In [37]: # Fast and versatile way to read the file
         # the names are taken from the file
         # The types are defined automatically when reading the columns
         c = np.genfromtxt('data2.dat', names=True, dtype=None, skip_header=1)
```

```
In [38]: print(c)
```

```
[(1, 2.3, 6, 8, b'star') (2, 3.5, 7, 9, b'galaxy')
 (3, -4.2, 5, 7, b'cluster')]
```

```
In [39]: type(c)
```

```
Out[39]: numpy.ndarray
```

```
In [40]: c.dtype
```

```
Out[40]: dtype([('N', '<i8'), ('f', '<f8'), ('x', '<i8'), ('y', '<i8'), ('type', 'S7')])
```

```
In [41]: c['f']
```

```
Out[41]: array([ 2.3,  3.5, -4.2])
```

Now a value of x is missing (not possible with space separator, so we use "," as separator):

```
In [42]: %%writefile data3.dat
         # The following data are for test purpose
         N, f, x, y, type
         1, 2.3, 6, 8, star
         2, 3000.5, , 9, galaxy
         3, -4.2, 5, 7, cluster
         #4, -10.5, 5, 7, test
```



Overwriting data3.dat

```
In [43]: d = np.genfromtxt('data3.dat', names=True, dtype=None, skip_header=1,
                        delimiter=',')
```

```
In [44]: # The missing value has been changed to -1
d
```

```
Out[44]: array([(1,  2.30000000e+00,  6, 8, b' star'),
                (2,  3.00050000e+03, -1, 9, b' galaxy'),
                (3, -4.20000000e+00,  5, 7, b' cluster')],
              dtype=[('N', '<i8'), ('f', '<f8'), ('x', '<i8'), ('y', '<i8'), ('type', 'S8')])
```

```
In [45]: # The missing value can be set to whatever you want (but non a NaN here, as the type is float)
d = np.genfromtxt('data3.dat', names=True, dtype=None, skip_header=1, delimiter=',',
                  filling_values=0.0)
```

```
In [46]: d['x'][1]
```

```
Out[46]: 0
```

```
In [47]: # one can select the columns to be store
e = np.genfromtxt('data3.dat', names=True, dtype=None, skip_header=1,
                  delimiter=',', usecols=(0,1,4))
```

```
In [48]: print(e)
```

```
[(1,  2.30000000e+00, b' star') (2,  3.00050000e+03, b' galaxy')
 (3, -4.20000000e+00, b' cluster')]
```

```
In [49]: # one can select the columns to be store
N, f, typ = np.genfromtxt('data3.dat', skip_header=2,
                          delimiter=',', usecols=(0,1,4), unpack=True, dtype = None)
```

```
In [50]: # The resulting array now contains only the given columns
print(N)
print(f)
print(typ)
```

```
(1,  2.3, b' star')
(2, 3000.5, b' galaxy')
(3, -4.2, b' cluster')
```

### 1.2.3 Using recfrom to obtain a record array

```
In [51]: # Uses the same keywords than genfromtxt
```

```
f = np.recfromtxt('data3.dat', names=True, dtype=None, skip_header=1,  
                  delimiter=',', usecols=("N", "f", "type"))
```

```
In [52]: f
```

```
Out[52]: rec.array([(1,  2.30000000e+00, b' star'), (2,  3.00050000e+03, b' galaxy'),  
                   (3, -4.20000000e+00, b' cluster')],  
                  dtype=[('N', '<i8'), ('f', '<f8'), ('type', 'S8')])
```

```
In [53]: f.N
```

```
Out[53]: array([1, 2, 3])
```

```
In [54]: f.f
```

```
Out[54]: array([ 2.30000000e+00,  3.00050000e+03, -4.20000000e+00])
```

### 1.2.4 Using pandas to read a file

```
In [55]: import pandas as pd
```

```
In [56]: g = pd.read_csv('data3.dat', skiprows = 2, usecols = (0,1,4), comment = '#', names = ['
```

```
In [57]: print(g)
```

	N	f	type
0	1	2.3	star
1	2	3000.5	galaxy
2	3	-4.2	cluster

```
In [58]: print(g['f'])
```

```
0      2.3  
1    3000.5  
2      -4.2  
Name: f, dtype: float64
```

```
In [59]: print(g['type'])
```

```
0      star  
1    galaxy  
2    cluster  
Name: type, dtype: object
```

### 1.3 Fixed size ascii files

```
In [60]: %%writefile data4.dat
# Line      Iobs      lambda  relat_error Obs_code
H 1 4861A 1.00000      4861. 0.08000  Anabel
H 1 6563A 2.8667      6563. 0.19467  Anabel
H 1 4340A 0.4933      4340. 0.03307  Anabel
H 1 4102A 0.2907      4102. 0.02229  Anabel
H 1 3970A 0.1800      3970. 0.01253  Anabel
N 2 6584A 2.1681      6584. 0.08686  Anabel
N 2 121.7m 0.0044621217000. 0.20000  Liu
O 1 6300A 0.0147      6300. 0.00325  Anabel
TOTL 2326A 0.07900      2326. 0.20000  Adams
C 2 157.6m 0.00856 1576000. 0.20000  Liu
O 1 63.17m 0.13647 631700. 0.10000  Liu
O 1 145.5m 0.00446 1455000. 0.200  Liu
TOTL 3727A 0.77609      3727. 0.200  Torres-Peimbert
S II 4070A 0.06174      4070. 0.200  Torres-Peimbert
S II 4078A 0.06174      4078. 0.200  Torres-Peimbert
```

Overwriting data4.dat

```
In [61]: # Here we cannot use SPACE as a separator, as some strings contains spaces.
# "delimiter" is used to specify the size (in characters in the file) of each variables
# The types must be clearly defined too.
obs = np.genfromtxt('data4.dat',
                    dtype=["U11","float","float","float","U2"],
                    delimiter=[11,7,10,10,2],
                    names = True
                    )
```

```
In [62]: obs # The same delimiter (fixed sizes) is applied to the names. May not be what you want
```

```
Out[62]: array([('H 1 4861A', 1. , nan, 0.08 , 'An'),
                ('H 1 6563A', 2.8667, 6.563000000e+03, 0.19467, 'An'),
                ('H 1 4340A', 0.4933, 4.340000000e+03, 0.03307, 'An'),
                ('H 1 4102A', 0.2907, 4.102000000e+03, 0.02229, 'An'),
                ('H 1 3970A', 0.18 , 3.970000000e+03, 0.01253, 'An'),
                ('N 2 6584A', 2.1681, 6.584000000e+03, 0.08686, 'An'),
                ('N 2 121.7m', 0.0044, 6.212170000e+08, 0.2 , 'Li'),
                ('O 1 6300A', 0.0147, 6.300000000e+03, 0.00325, 'An'),
                ('TOTL 2326A', 0.079 , nan, 0.2 , 'Ad'),
                ('C 2 157.6m', 0.0085, nan, 0.2 , 'Li'),
                ('O 1 63.17m', 0.1364, nan, 0.1 , 'Li'),
                ('O 1 145.5m', 0.0044, nan, 0.2 , 'Li'),
                ('TOTL 3727A', 0.776 , nan, 0.2 , 'To'),
                ('S II 4070A', 0.0617, nan, 0.2 , 'To'),
                ('S II 4078A', 0.0617, nan, 0.2 , 'To')],
            dtype=[('Line', '<U11'), ('Iobs', '<f8'), ('lambda', '<f8'), ('relat_erro', '<f8')])
```

```

In [63]: # Defining the names:
obs2 = np.genfromtxt('data4.dat', skip_header=1,
                    dtype=None,
                    delimiter=[11,7,10,10,2],
                    names = ['label', 'i_obs', 'lambda', 'e_obs', 'observer']
                    )

In [64]: obs2

Out[64]: array([(b'H 1 4861A', 1.0, b'0 4861.', 0.08, b'An'),
                (b'H 1 6563A', 2.8667, b' 6563.', 0.19467, b'An'),
                (b'H 1 4340A', 0.4933, b' 4340.', 0.03307, b'An'),
                (b'H 1 4102A', 0.2907, b' 4102.', 0.02229, b'An'),
                (b'H 1 3970A', 0.18, b' 3970.', 0.01253, b'An'),
                (b'N 2 6584A', 2.1681, b' 6584.', 0.08686, b'An'),
                (b'N 2 121.7m', 0.0044, b'621217000.', 0.2, b'Li'),
                (b'O 1 6300A', 0.0147, b' 6300.', 0.00325, b'An'),
                (b'TOTL 2326A', 0.079, b'0 2326.', 0.2, b'Ad'),
                (b'C 2 157.6m', 0.0085, b'6 1576000.', 0.2, b'Li'),
                (b'O 1 63.17m', 0.1364, b'7 631700.', 0.1, b'Li'),
                (b'O 1 145.5m', 0.0044, b'6 1455000.', 0.2, b'Li'),
                (b'TOTL 3727A', 0.776, b'9 3727.', 0.2, b'To'),
                (b'S II 4070A', 0.0617, b'4 4070.', 0.2, b'To'),
                (b'S II 4078A', 0.0617, b'4 4078.', 0.2, b'To')],
            dtype=[('label', 'S11'), ('i_obs', '<f8'), ('lambda', 'S10'), ('e_obs', '<f8'), ('observer', 'S10')])

In [65]: %%writefile data5.dat
# Line      Iobs      lambda      relat_error      Obs_code
H 1 4861A 1.00000      4861. 0.08000 x Anabel
H 1 6563A 2.8667      6563. 0.19467 x Anabel
H 1 4340A 0.4933      4340. 0.03307 x Anabel
H 1 4102A 0.2907      4102. 0.02229 x Anabel
H 1 3970A 0.1800      3970. 0.01253 t Anabel
N 2 6584A 2.1681      0.08686 x Anabel
N 2 121.7m 0.00446 1217000. 0.20000 g Liu
O 1 6300A 0.0147      6300. 0.00325 t Anabel
TOTL 2326A 0.07900      2326. 0.20000 g Adams
C 2 157.6m 0.00856 1576000. 0.20000 t Liu
O 1 63.17m 0.13647 631700. 0.10000 g Liu
O 1 145.5m 0.00446 1455000. 0.200 g Liu
TOTL 3727A 0.77609      3727. 0.200 g Torres-Peimbert
S II 4070A 0.06174      4070. 0.200 g Torres-Peimbert
S II 4078A 0.06174      4078. 0.200 g Torres-Peimbert

```

Overwriting data5.dat

```

In [66]: # Here we want to skip one column:
obs3 = np.genfromtxt('data5.dat', skip_header=1,

```

```

dtype=None,
delimiter=[11, 8, 9, 9, 2, 2],
names = ['label', 'i_obs', 'lambda', 'e_obs', 'na', 'observer'],
usecols = (0, 1, 2, 3, 5)
)

```

In [67]: obs3

```

Out[67]: array([(b'H 1 4861A', 1.      ,      4861., 0.08      , b'An'),
                (b'H 1 6563A', 2.8667 ,      6563., 0.19467, b'An'),
                (b'H 1 4340A', 0.4933 ,      4340., 0.03307, b'An'),
                (b'H 1 4102A', 0.2907 ,      4102., 0.02229, b'An'),
                (b'H 1 3970A', 0.18    ,      3970., 0.01253, b'An'),
                (b'N 2 6584A', 2.1681 ,      nan, 0.08686, b'An'),
                (b'N 2 121.7m', 0.00446, 1217000., 0.2      , b'Li'),
                (b'O 1 6300A', 0.0147 ,      6300., 0.00325, b'An'),
                (b'TOTL 2326A', 0.079  ,      2326., 0.2      , b'Ad'),
                (b'C 2 157.6m', 0.00856, 1576000., 0.2      , b'Li'),
                (b'O 1 63.17m', 0.13647, 631700., 0.1      , b'Li'),
                (b'O 1 145.5m', 0.00446, 1455000., 0.2      , b'Li'),
                (b'TOTL 3727A', 0.77609, 3727., 0.2      , b'To'),
                (b'S II 4070A', 0.06174, 4070., 0.2      , b'To'),
                (b'S II 4078A', 0.06174, 4078., 0.2      , b'To')],
            dtype=[('label', 'S11'), ('i_obs', '<f8'), ('lambda', '<f8'), ('e_obs', '<f8'), ('na', '<f8'), ('observer', '<f8')])

```

In [68]: obs3['lambda']

```

Out[68]: array([ 4861.,  6563.,  4340.,  4102.,  3970.,      nan,
                1217000.,  6300.,  2326., 1576000.,  631700., 1455000.,
                3727.,  4070.,  4078.])

```

In [69]: new\_obs3 = obs3.view(np.recarray)

In [70]: new\_obs3.label

```

Out[70]: array([b'H 1 4861A', b'H 1 6563A', b'H 1 4340A', b'H 1 4102A',
                b'H 1 3970A', b'N 2 6584A', b'N 2 121.7m', b'O 1 6300A',
                b'TOTL 2326A', b'C 2 157.6m', b'O 1 63.17m', b'O 1 145.5m',
                b'TOTL 3727A', b'S II 4070A', b'S II 4078A'],
            dtype='|S11')

```

In [71]: new\_obs3.lambda # lambda is reserved!!!

```

File "<ipython-input-71-a5c3f73ef51d>", line 1
new_obs3.lambda # lambda is reserved!!!
    ^

```

SyntaxError: invalid syntax

```
In [72]: new_obs3['lambda']
```

```
Out[72]: array([ 4861.,  6563.,  4340.,  4102.,  3970.,    nan,
                1217000.,  6300.,  2326., 1576000.,  631700., 1455000.,
                3727.,  4070.,  4078.]
```

Using masks on the structured array.

```
In [73]: mask_observer = (obs3['observer'] == b'An') & (np.isfinite(obs3['lambda']))
         print(obs3[mask_observer])
```

```
[(b'H 1 4861A', 1., 4861., 0.08, b'An')
 (b'H 1 6563A', 2.8667, 6563., 0.19467, b'An')
 (b'H 1 4340A', 0.4933, 4340., 0.03307, b'An')
 (b'H 1 4102A', 0.2907, 4102., 0.02229, b'An')
 (b'H 1 3970A', 0.18, 3970., 0.01253, b'An')
 (b'O 1 6300A', 0.0147, 6300., 0.00325, b'An')]
```

```
In [74]: for o in obs3[mask_observer]:
         print('line {}, wavelength={}A Intensity={:.3f}+/-{:4.1f}%').format(o['label'], o['
```

```
line b'H 1 4861A', wavelength=4861.0A Intensity=1.000+/- 8.0%)
line b'H 1 6563A', wavelength=6563.0A Intensity=2.867+/-19.5%)
line b'H 1 4340A', wavelength=4340.0A Intensity=0.493+/- 3.3%)
line b'H 1 4102A', wavelength=4102.0A Intensity=0.291+/- 2.2%)
line b'H 1 3970A', wavelength=3970.0A Intensity=0.180+/- 1.3%)
line b'O 1 6300A', wavelength=6300.0A Intensity=0.015+/- 0.3%)
```

## 1.4 Writing files

### 1.4.1 Simple "write" method from "open" class

```
In [75]: f = open('data10.dat', 'w')
```

```
In [76]: f.write('tralala')
         f.write('trololo')
```

```
Out[76]: 7
```

```
In [77]: f.close()
```

```
In [78]: !cat 'data10.dat' # the writing method put everything together.
```

```
tralalatrololo
```

```
In [79]: f = open('data11.dat', 'w')
         f.write('tralala\n') # \n to indicate end of line
         f.write('trololo\n')
         f.close()
         !cat 'data11.dat'
```

```
tralala
trololo
```

```
In [80]: f = open('data11.dat', 'a') # Append to the end of the file
         f.write('trilili\n') # \n to indicate end of line
         f.write('trululu\n')
         f.close()
         !cat 'data11.dat'
```

```
tralala
trololo
trilili
trululu
```

```
In [81]: a = 'Gato'
         b = 3
         with open('data12.dat', 'w') as datafile:
             datafile.write("""Hola Sr. {0}
This is a file
with a lot of lines.
It is easy to write it.
The value of your data is {1}.
""".format(a, b))
         !cat "data12.dat"
```

```
Hola Sr. Gato
This is a file
with a lot of lines.
It is easy to write it.
The value of your data is 3.
```

```
In [82]: #Using the for command one can add to a text file lines containing the values of variables
         c = np.linspace(0.5,15,11)
         d = np.log10(c)+5
         with open('data13.dat', 'w') as f:
             f.write('#This is a file containing the log(x) + 5 for x between 0.5 and 15\n')
             f.write('x y\n')
             for i,j in zip(c,d):
                 f.write('{:.2f} {:.3f}\n'.format(i,j))
         !cat 'data13.dat'
```

```
#This is a file containing the log(x) + 5 for x between 0.5 and 15
x y
0.50 4.699
1.95 5.290
3.40 5.531
```

```
4.85 5.686
6.30 5.799
7.75 5.889
9.20 5.964
10.65 6.027
12.10 6.083
13.55 6.132
15.00 6.176
```

## 1.4.2 Using pickle (and cpickle) python specific format

```
In [83]: # Let's define some stuffs we want to keep in a file (data and variable names)
```

```
    a = 5
    b = 'Hola'
    c = np.array([1,2,3,4,5])
    def d(x):
        """ Function mia"""
        return x**2
```

```
In [84]: import pickle # The module we will use for this
```

```
In [85]: pickle.dump((a,b,c,d), open('Demo.pickle','wb')) # Writing the variables
```

```
In [86]: res = pickle.load(open('Demo.pickle', 'rb'))
```

```
In [87]: type(res)
```

```
Out[87]: tuple
```

```
In [88]: print(res[0])
          print(res[1])
          print(res[2])
```

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

```
In [89]: print(res[3](5))
```

```
25
```

```
In [90]: a2,b2,c2,d2 = pickle.load(open('Demo.pickle', 'rb'))
```

```
In [91]: a2
```

```
Out[91]: 5
```



```
In [92]: d2(10)
```

```
Out[92]: 100
```

```
In [93]: help(d2)
```

```
Help on function d in module __main__:
```

```
d(x)
    Function mia
```

```
In [94]: %timeit res = pickle.load(open('Demo.pickle', 'rb'))
```

The slowest run took 33.79 times longer than the fastest. This could mean that an intermediate result was not cached.  
100000 loops, best of 3: 17.3  $\mu$ s per loop

```
In [95]: import gzip
         pickle.dump((a,b,c,d), gzip.open('Demo.pklz', 'wb')) # Writing the variables
```

```
In [96]: f = gzip.open('Demo.pklz', 'rb')
         a, b, c, d = pickle.load(f)
         f.close()
```

### 1.4.3 FITS files

What is the FITS format? The FITS format is the most popular way to save and interchange astronomical data. The files are organized in units each of which contains a human readable header and a data. This structure is refereed as HDUs (Header/DATA Unit).

A FITS file can contain one or more HDUs, the first of which is called "primary" and the rest are called "extensions". The primary HDU usually contains 1D spectrum, 2D image or 3D data cube, although any dimension from 0 to 999 are possible. The data are 1, 2 or 4 bytes integers or 4 or 8 bytes real numbers.

The extensions can contain arrays as in the primary HDU or ascii tables or binary tables. If a FITS file contains only tables, the primary HDU does not contain data, but only header.

Both headers and data in a FITS file are organized in blocs of 2880 bytes. The header contains 80 bytes lines each of which consists of a keyword of 8 bytes followed in most of the cases by '=' in the position 9 and 10 and then the value of the keyword. The rest of the line is a comment string beginning with '/'. Each header begins with the following lines

```
SIMPLE = T / file conforms to FITS standard BITPIX = 16 / number of bits per data pixel
NAXIS = 2 / number of data axes NAXIS1 = 440 / length of data axis 1 NAXIS2 = 300 / length of
data axis 2
```

which defines the format of the file as standard FITS, the data format and the dimensions of the stored data.

One block of 2880 bytes contains 36 lines of 80 characters per line. The header can have several blocks of 36 lines. The last block is identified by the presence of the keyword 'END'. The next 2880 bytes block contains the first part of the data. The empty lines after 'END' keyword are filled with blanks and the unused bytes from the end of the data to the end of the 2880 bytes block are filled with NULLs.

```
In [97]: import astropy
        print(astropy.__version__)
```

1.3.2

```
In [98]: from astropy.io import fits
```

```
In [99]: # All of the functionality of PyFITS is now available in Astropy
        # from astropy.io import fits as pyfits
```

Manual here: <https://pythonhosted.org/pyfits/>

We will use one FITS files from San Pedro Martir echelle spectrograph. The file can be downloaded from: <https://github.com/Morisset/Python-lectures-Notebooks/raw/master/Notebooks/n10017o.fits>

```
In [100]: hdulist = fits.open('n10017o.fits')
```

```
In [101]: # The result hdulist is a list of HDU objects.
        # In the case of a simple file, there is only one primary HDU so the list contains only one
        len(hdulist)
```

```
Out[101]: 1
```

```
In [102]: # The information on what the file contains can be obtained by calling the info() method
        hdulist.info()
        # The table said that there is only a primary HDU which contains 2154 X 2048 image with
```

Filename: n10017o.fits

No.	Name	Type	Cards	Dimensions	Format
0	PRIMARY	PrimaryHDU	62	(2154, 2048)	int16 (rescales to uint16)

```
In [103]: # As described above, the HDU (header/data unit) contains header and data. The header
        # To see what keywords were used in the header one can do:
        list(hdulist[0].header.keys())
```

```
Out[103]: ['SIMPLE',
          'BITPIX',
          'NAXIS',
          'NAXIS1',
          'NAXIS2',
          'EXTEND',
          'COMMENT',
          'COMMENT',
          'BZERO',
          'BSCALE',
          'EXPTIME',
          'DETECTOR',
          'ORIGIN',
```

'OBSERVAT',  
'TELESCOP',  
'LATITUDE',  
'LONGITUD',  
'ALTITUD',  
'SECONDAR',  
'TIMEZONE',  
'OBSERVER',  
'OBJECT',  
'INSTRUME',  
'GAINMODE',  
'FILTER',  
'IMGTYPE',  
'EQUINOX',  
'ST',  
'UT',  
'JD',  
'DATE-OBS',  
'CCDSUM',  
'RA',  
'DEC',  
'AH',  
'AIRMASS',  
'TMMIRROR',  
'TSMIRROR',  
'TAIR',  
'XTEMP',  
'HUMIDITY',  
'ATMOSBAR',  
'WIND',  
'WDATE',  
'DATE',  
'NAMPS',  
'CCDNAMPS',  
'AMPNAME',  
'CREATOR',  
'VERSION',  
'COMMENT',  
'COMMENT',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',  
'HISTORY',

```
'HISTORY']
```

```
In [104]: # and to get the value of a given keyword :  
          hdulist[0].header['OBJECT']
```

```
Out[104]: '107 Psc'
```

```
In [105]: hh = hdulist[0].header  
          hh?
```

```
In [106]: hdulist[0].header
```

```
Out[106]: SIMPLE = T / conforms to FITS standard  
          BITPIX = 16 / array data type  
          NAXIS = 2 / number of array dimensions  
          NAXIS1 = 2154 / length of data axis 1  
          NAXIS2 = 2048 / length of data axis 2  
          EXTEND = T  
          COMMENT FITS (Flexible Image Transport System) format is defined in 'Astronomy  
          COMMENT and Astrophysics', volume 376, page 359; bibcode: 2001A&A...376..359H  
          BZERO = 32768 / BZERO  
          BSCALE = 1 / BSCALE  
          EXPTIME = 600.0 / Integration Time, sec.  
          DETECTOR= 'e2vm2 E2V-4240' / CCD Type  
          ORIGIN = 'UNAM ' / OAN SPM, IA-UNAM  
          OBSERVAT= 'SPM ' / Observatory  
          TELESCOP= '2.12m ' / Telescope  
          LATITUDE= '+31:02:39' / Latitude  
          LONGITUD= '115:27:49' / Longitud  
          ALTITUD = 2800 / altitud  
          SECONDAR= -1 / F/ Secondary type  
          TIMEZONE= 8 / Time Zone  
          OBSERVER= 'Leonid ' / Observer's Name  
          OBJECT = '107 Psc ' / Object  
          INSTRUME= 'Echelle ' / Instrument  
          GAINMODE= 1 / Gain factor in the CCD  
          FILTER = 'None ' / Filter  
          IMGTYPE = 'object ' / Image Type  
          EQUINOX = 2011.7 / Equinox  
          ST = '01:25:41.3' / Sideral Time  
          UT = '10:34:27' / Universal Time  
          JD = 2455803.5 / Julian Date  
          DATE-OBS= '2011-08-30' / Observation Date UTM  
          CCDSUM = '1 1 ' / Binning [ Cols:Rows ]  
          RA = ' 01:43:10.8' / Right Ascension  
          DEC = ' 20''19''43.0' / Declination  
          AH = ' -00:17:29.1' / Hour Angle  
          AIRMASS = 1.02 / Airmass  
          TMMIRROR= 0 / Primary Mirror Temperature (celsius degree)
```

```

TSMIRROR=                0 / Secondary Mirror Temperature (celsius degree)
TAIR    =                0 / Internal Telescope Air Temperature (celsius deg
XTEMP   =                14.7 / Exterior Temperature (celsius degree)
HUMIDITY=                46.0 / % external Humidity
ATMOSBAR=              731.9 / Atmospheric Pressure in mb
WIND     = 'S at 30.6 km/h' / Wind Direction
WDATE    = '10:34:10, 08/30/11' / Weather Acquisition Date (Local time)
DATE     = '2011-08-30T10:34:29' / file creation date (YYYY-MM-DDThh:mm:ss UT)
NAMPS    =                1 / Number of Amplifiers
CCDNAMPS=                1 / Number of amplifiers used
AMPNAME  = '1 Channel' / Amplifier name
CREATOR  = 'Python Oan ccds' / Name of the software task that created the file
VERSION  = '4.12D ' / Application Software Version
COMMENT  Visit our weather site http://www.astrossp.unam.mx/weather15
COMMENT  for complete meteorological data of your observation night
HISTORY  bin2fits V1.0
HISTORY  Programmer: Enrique Colorado [ colorado@astrosen.unam.mx ]
HISTORY  Observatorio Astronomico Nacional -UNAM
HISTORY  V1.00 By Arturo Nunez and Colorado >Ported to Python using pyfits
HISTORY  V0.50 By E. Colorado >Added interior mirrors temperatures
HISTORY  V0.49 By E. Colorado >Added BIASSEC parameter
HISTORY  V0.48 By E. Colorado >Additional info for autofocus calculations
HISTORY  V0.4 By E. Colorado >Now we include timezone, and remove lat. sign
HISTORY  V0.3 By E. Colorado >Now we include weather data
HISTORY  V0.2 By E. Colorado >General OAN Working Release

```

```

In [107]: # The header can be printed as it appears in the file by
          print(hdulist[0].header.cards)

```

```

('SIMPLE', True, 'conforms to FITS standard')
('BITPIX', 16, 'array data type')
('NAXIS', 2, 'number of array dimensions')
('NAXIS1', 2154, 'length of data axis 1')
('NAXIS2', 2048, 'length of data axis 2')
('EXTEND', True, '')
('COMMENT', "FITS (Flexible Image Transport System) format is defined in 'Astronomy", '')
('COMMENT', "and Astrophysics", volume 376, page 359; bibcode: 2001A&A...376..359H", '')
('BZERO', 32768, 'BZERO')
('BSCALE', 1, 'BSCALE')
('EXPTIME', 600.0, 'Integration Time, sec.')
('DETECTOR', 'e2vm2 E2V-4240', 'CCD Type')
('ORIGIN', 'UNAM', 'OAN SPM, IA-UNAM')
('OBSERVAT', 'SPM', 'Observatory')
('TELESCOP', '2.12m', 'Telescope')
('LATITUDE', '+31:02:39', 'Latitude')
('LONGITUD', '115:27:49', 'Longitud')
('ALTITUD', 2800, 'altitud')
('SECONDAR', -1, 'F/ Secondary type')

```

```

('TIMEZONE', 8, 'Time Zone')
('OBSERVER', 'Leonid', "Observer's Name")
('OBJECT', '107 Psc', 'Object')
('INSTRUME', 'Echelle', 'Instrument')
('GAINMODE', 1, 'Gain factor in the CCD')
('FILTER', 'None', 'Filter')
('IMGTYPE', 'object', 'Image Type')
('EQUINOX', 2011.7, 'Equinox')
('ST', '01:25:41.3', 'Sideral Time')
('UT', '10:34:27', 'Universal Time')
('JD', 2455803.5, 'Julian Date')
('DATE-OBS', '2011-08-30', 'Observation Date UTM')
('CCDSUM', '1 1', 'Binning [ Cols:Rows ]')
('RA', ' 01:43:10.8', 'Right Ascension')
('DEC', ' " 20'19'43.0", 'Declination')
('AH', ' -00:17:29.1', 'Hour Angle')
('AIRMASS', 1.02, 'Airmass')
('TMMIRROR', 0, 'Primary Mirror Temperature (celsius degree)')
('TSMIRROR', 0, 'Secondary Mirror Temperature (celsius degree)')
('TAIR', 0, 'Internal Telescope Air Temperature (celsius deg)')
('XTEMP', 14.7, 'Exterior Temperature (celsius degree)')
('HUMIDITY', 46.0, '% external Humidity')
('ATMOSBAR', 731.9, 'Atmosferic Presure in mb')
('WIND', 'S at 30.6 km/h', 'Wind Direction')
('WDATE', '10:34:10, 08/30/11', 'Weather Acquisition Date (Local time)')
('DATE', '2011-08-30T10:34:29', 'file creation date (YYYY-MM-DDThh:mm:ss UT)')
('NAMPS', 1, 'Number of Amplifiers')
('CCDNAMPS', 1, 'Number of amplifiers used')
('AMPNAME', '1 Channel', 'Amplifier name')
('CREATOR', 'Python Oan ccds', 'Name of the software task that created the file')
('VERSION', '4.12D', 'Application Software Version')
('COMMENT', 'Visit our weather site http://www.astrossp.unam.mx/weather15', '')
('COMMENT', 'for complete meteorological data of your observation night', '')
('HISTORY', 'bin2fits V1.0', '')
('HISTORY', 'Programmer: Enrique Colorado [ colorado@astrosen.unam.mx ]', '')
('HISTORY', 'Observatorio Astronomico Nacional -UNAM', '')
('HISTORY', 'V1.00 By Arturo Nunez and Colorado >Ported to Python using pyfits', '')
('HISTORY', 'V0.50 By E. Colorado >Added interior mirrors temperatures', '')
('HISTORY', 'V0.49 By E. Colorado >Added BIASSEC parameter', '')
('HISTORY', 'V0.48 By E. Colorado >Additional info for autofocus calculations', '')
('HISTORY', 'V0.4 By E. Colorado >Now we include timezone, and remove lat. sign', '')
('HISTORY', 'V0.3 By E. Colorado >Now we include weather data', '')
('HISTORY', 'V0.2 By E. Colorado >General OAN Working Release', '')

```

```

In [108]: # The data in the file are accessible with
          data = hdulist[0].data

```

```

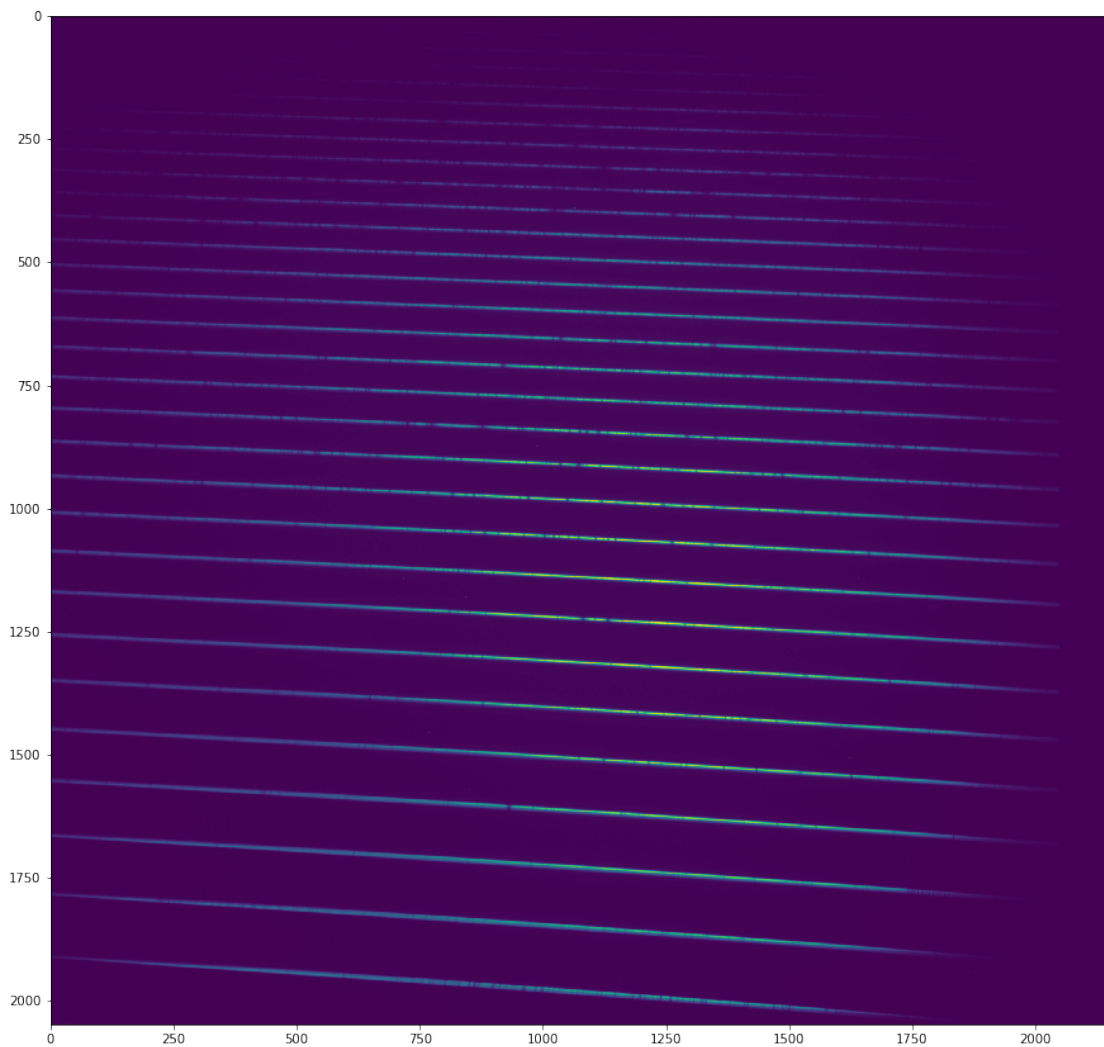
In [109]: data

```

```
Out[109]: array([[873, 875, 872, ..., 870, 865, 867],
                 [874, 878, 874, ..., 869, 871, 867],
                 [877, 875, 879, ..., 865, 867, 865],
                 ...,
                 [965, 946, 988, ..., 868, 872, 869],
                 [954, 922, 965, ..., 872, 870, 871],
                 [922, 919, 930, ..., 870, 870, 871]], dtype=uint16)
```

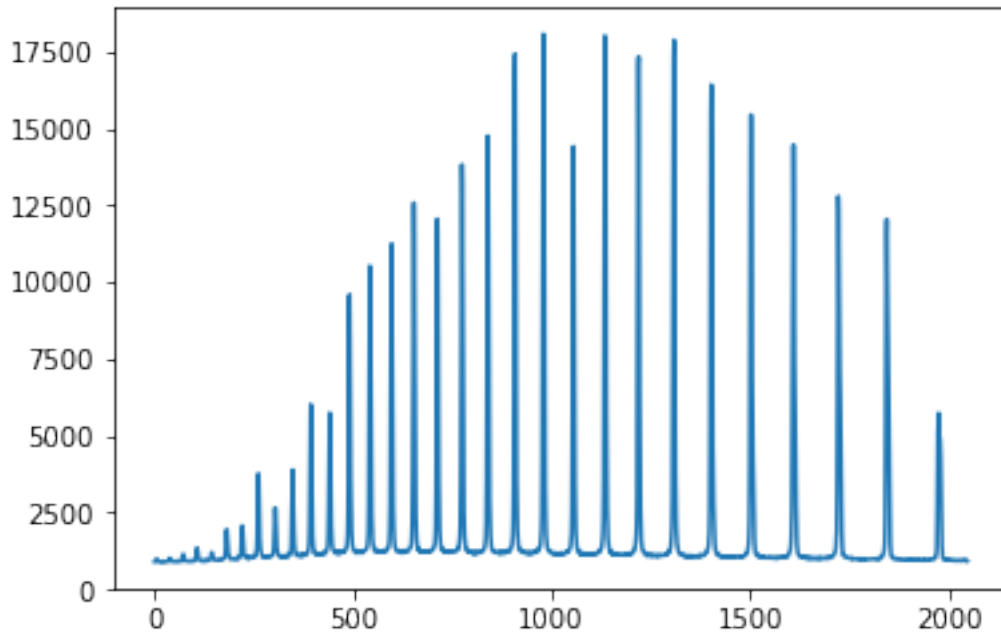
```
In [110]: # and can be seen with [we need to import matplotlib.pyplot as plt before running this]
          %matplotlib inline
          import matplotlib.pyplot as plt
          f, ax = plt.subplots(figsize=(15,15))
          ax.imshow(data)
```

```
Out[110]: <matplotlib.image.AxesImage at 0x7f02a1082080>
```



```
In [111]: # A column from the data can be plotted with  
plt.plot(data[:,1000])  
# where I am plotting the column number 1000.
```

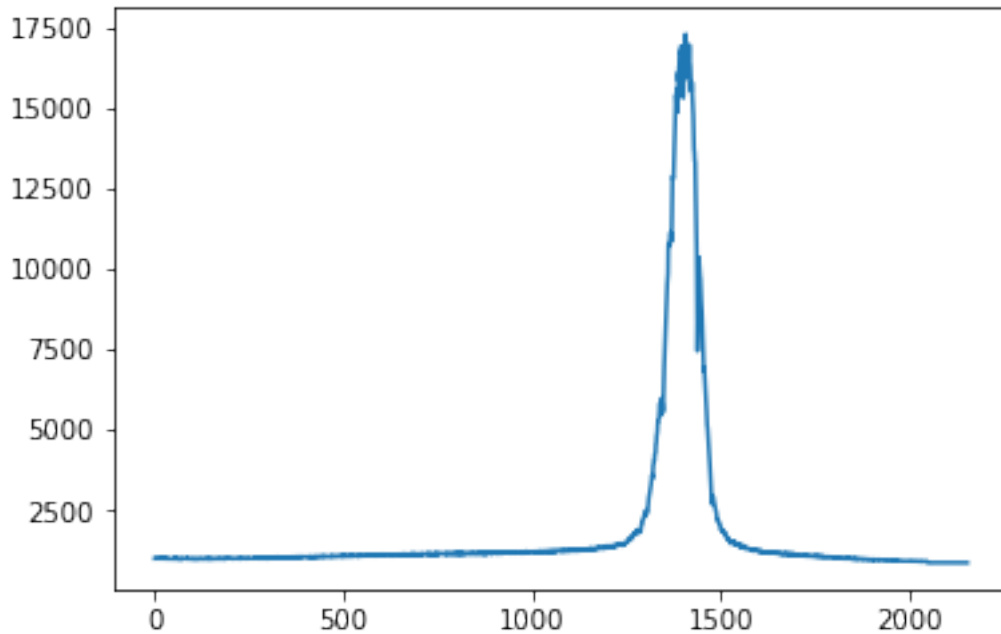
```
Out[111]: [<matplotlib.lines.Line2D at 0x7f029d16cc50>]
```



```
In [112]: # In the same way a line from the data is plotted with:  
plt.plot(data[1000,:])
```

```
Out[112]: [<matplotlib.lines.Line2D at 0x7f029d086710>]
```





```
In [113]: # For this example I'll use a spectrum obtain with the high dispersion camera on board
# The file is opened as usual:
hdulist = fits.open('swp04345.mxhi')
```

The file is there: <https://github.com/Morisset/Python-lectures-Notebooks/raw/master/Notebooks/swp04345.mxhi>

```
In [114]: #but now hdulist has 2 elements (2 header/data units):
len(hdulist)
```

```
Out[114]: 2
```

```
In [115]: # We can see that the primary header has dimension (), son does not contain any data.
# The data are in the extension.
hdulist.info()
```

Filename: swp04345.mxhi

No.	Name	Type	Cards	Dimensions	Format
0	PRIMARY	PrimaryHDU	421	()	
1	MEHI	BinTableHDU	61	60R x 17C	[1B, 1I, 1D, 1I, 1D, 1E, 1E, 768E, 768E, 768E,

```
In [116]: # The first header contains the minimal infirmation:
print(hdulist[0].header.cards[:5])
```

```
('SIMPLE', True, 'Standard FITS Format')
('BITPIX', 8, 'Binary data')
```

```

('NAXIS', 0, 'Two-dimensional image')
('EXTEND', True, 'Extensions are present')
('TELESCOP', 'IUE', 'International Ultraviolet Explorer')

```

```

In [117]: # The number of axis is 0 which means there is no data block in the primary HDU.
          # The header of the second HDU begins with the keyword XTENSION and with the specifica
          print(hdulist[1].header.cards[:5])

```

```

('XTENSION', 'BINTABLE', 'Binary table extension')
('BITPIX', 8, 'Binary data')
('NAXIS', 2, 'Two-dimensional table array')
('NAXIS1', 16961, 'Width of row in bytes')
('NAXIS2', 60, 'Number of orders')

```

```

In [118]: # To progress further we need to know what is in the table.
          # As usual, the columns have names and type of the stored data.
          # These information can be obtained using the column attribute of hdulist:
          cols = hdulist[1].columns

```

```

In [119]: # the cols.info returns the names of the columns and the information of their format a
          cols.info

```

```

Out[119]: <bound method ColDefs.info of ColDefs(
          name = 'ORDER'; format = '1B'
          name = 'NPOINTS'; format = '1I'
          name = 'WAVELENGTH'; format = '1D'; unit = 'ANGSTROM'
          name = 'STARTPIX'; format = '1I'; unit = 'PIXEL'
          name = 'DELTAW'; format = '1D'; unit = 'ANGSTROM'
          name = 'SLIT HEIGHT'; format = '1E'; unit = 'PIXEL'
          name = 'LINE_FOUND'; format = '1E'; unit = 'PIXEL'
          name = 'NET'; format = '768E'; unit = 'FN'
          name = 'BACKGROUND'; format = '768E'; unit = 'FN'
          name = 'NOISE'; format = '768E'; unit = 'FN'
          name = 'QUALITY'; format = '768I'
          name = 'RIPPLE'; format = '768E'; unit = 'FN'
          name = 'ABS_CAL'; format = '768E'; unit = 'ERG/CM2/S/A'
          name = 'START-BKG'; format = '1I'; unit = 'PIXEL'
          name = 'END-BKG'; format = '1I'; unit = 'PIXEL'
          name = 'SCALE_BKG'; format = '1E'
          name = 'COEFF'; format = '7E'
          )>

```

```

In [120]: # The data are available using (this example is NOT the right way of plotting the data
          # and don't forget to import numpy as np to have np.arange working):

```

```

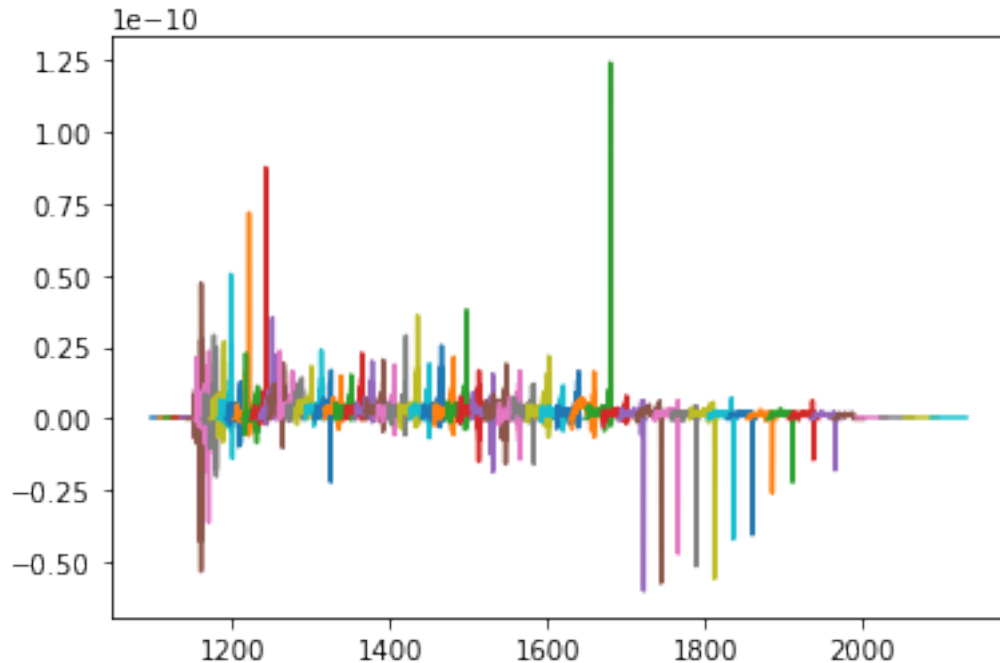
data1 = hdulist[1].data
DTs = data1.ABS_CAL

```

```

Wls = data1.WAVELENGTH
DWs = data1.DELTAW
for WL, DW, DT in zip(Wls, DWs, DTs):
    plt.plot(WL + np.arange(len(DT)) * DW, DT)

```



#### 1.4.4 Writing FITS files

```

In [121]: # Creation of numpy array with the data.
x = np.arange(100)

```

```

In [122]: # Creation of the HDU from the data.
hdu = fits.PrimaryHDU(x)
print(hdu.header.cards)

```

```

('SIMPLE', True, 'conforms to FITS standard')
('BITPIX', 64, 'array data type')
('NAXIS', 1, 'number of array dimensions')
('NAXIS1', 100, '')
('EXTEND', True, '')

```

```

In [123]: #Adding additional keywords to the header.
# The automatically created header contains only the required minimum of keywords.
# If additional keywords are needed they are added with:
hdu.header['testkey'] = (0.001, 'some test value')

```

```
In [124]: print(hdu.header.cards)

('SIMPLE', True, 'conforms to FITS standard')
('BITPIX', 64, 'array data type')
('NAXIS', 1, 'number of array dimensions')
('NAXIS1', 100, '')
('EXTEND', True, '')
('TESTKEY', 0.001, 'some test value')

In [125]: hdulist = fits.HDUList([hdu])
          hdulist.writeto('new.fits', overwrite=True)
          hdulist.close()
```

Another way to deal with FITS tables is to use the ATpy library, we'll see this later