External libraries

BB1000 Programming in Python KTH

Essential Python libraries

- NumPy: 'Numerical python' package for scientific computing in Python. Ment primarily to sort, reshape, and index array types...
- pandas: data structures and functions to work with structured data. The main object in pandas is the DataFrame, which is a two-dimentional tabular.
- matplotlib: producing plots; the basic functions handled in this course are all in the matplotlib.pyplot module.

```
>>> import pandas as pd
>>> import numpy as np
>>> import matplotlib.pyplot as plt
```

NumPy

One of the key fatures of NumPy is its N-dimensional array object: ndarray. They enable to perform mathematical operations on blocks of data.

NumPy - Default arrays

```
>>> print(np.zeros(10))
[ 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

>>> print(np.zeros((3,6)))
[[ 0. 0. 0. 0. 0. 0.]
[ 0. 0. 0. 0. 0. 0.]
[ 0. 0. 0. 0. 0. 0.]]

>>> print(np.arange(15))
[ 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14]
```

Remark that for higher dimensional arrays, we have used tuples.

NumPy - Default arrays

empty creates an array without initializing its values to any particular value. It does the ideal recipe to return garbage...

NumPy - Operations between arrays and scalars

```
>>> arr = np.array([[1., 2., 3.], [4., 5., 6.]])
>>> print(arr*arr)
[[1. 4. 9.]
[ 16. 25. 36.]]
>>> print(arr-arr)
[[ 0. 0. 0.]
[ 0. 0. 0.]]
>>> print(1/arr)
[[ 1.
                         0.33333333]
0.25
              0.2
                         0.16666667]]
>>> print(arr**0.5)
              1.41421356 1.73205081]
[[ 1.
              2.23606798 2.44948974
  2.
```

NumPy - Basic indexing and slicing

```
>>> arr= np.arange(10)
>>> print(arr[5])
5
>>> print(arr[5:8])
[5 6 7]
>>> arr[5:8] = 12
>>> print(arr)
[ 0  1  2  3  4  12  12  12  8  9]

>>> arr_slice = arr[5:8]
>>> arr_slice[:] = 64
>>> print(arr)
[ 0  1  2  3  4  64  64  64  8  9]
```

NumPy - Basic indexing and slicing

```
>>> arr2d = np.array([[1, 2, 3], [4, 5, 6], [7, 8, 9]])
>>> print(arr2d[2])
[7 8 9]
>>> print(arr2d[0][2])
3
```

```
>>> print(arr2d[:2, 1:])
[[2 3]
[5 6]]
```

Entries up till (but not including) the second row are kept, as well as the column starting from (and including) the first one.

NumPy - Boolean indexing

NumPy - Boolean indexing

Those rows in data indexed with 'True' can be selected:

And also slicing is possible:

For negation != can be used as wel as -

NumPy - Boolean indexing

To select two of the three names to combine multiple boolean conditions, use boolean arithmetic operators like & (and) and | (or):

```
>>> mask = (names == 'Asterix') | (names == 'Idefix')
>>> mask
array([ True, False, True, True, False, False], dtype=bool)
```

In this way, it is possible to set data to whole rows:

NumPy - Transposing arrays

Arrays have the transpose method and also the special T attribute:

The method is very interesting in linear algebra, as the inner matrix product 'X^TX' can be easily calculated:

NumPy - Unary and binary universal functions

A universal function ('ufunction') is a function that performs elementwise operations on data in ndarrays. A unary one only focusses upon one array, while binary ones require 2 arrays.

Examples of unary ufunctions are sqrt, exp, abs, log, sign, floor (largest integer less than or equal to the element), ceil (analogon for floor but then higher or equal to the element), cos,...

Examples of binary ufunctions are add, subtract, multiply, divide, power, max, min, mod (remainder of division), greater, less, less equal, ...

NumPy - Unary and binary universal functions

A few examples...

NumPy - Conditions and arrays

The numpy.where(condition, firstargument, secondargument) function reduces the expression x if condition else y for arrays: if the condition is true, then the firstargument is executed, else the secondargument is done.

```
>>> xarr = np.array([1.1, 1.2, 1.3 , 1.4, 1.5])
>>> yarr = np.array([2.1, 2.2, 2.3 , 2.4, 2.5])
>>> cond = np.array([True, False, True, True, False])
>>> result = np.where(cond, xarr, yarr)
>>> result
array([ 1.1, 2.2, 1.3, 1.4, 2.5])
```

For boolean arrays, any tests whether one or more values in an array is True, while all checks if every value is True.

```
>>> bools = np.array([False, False, True, False])
>>> np.any(bools)
True
>>> np.all(bools)
False
```

NumPy - Sorting and Unique

NumPy - Storing array, saving and loading

np.save and np.load allow to save and load data on disk. It will be in raw binary format and have file extension .npy.

```
>>> arr = np.arange(10)
>>> np.save('some_array', arr)
>>> np.load('some_array.npy')
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

Heroix finds a paper with the service numbers of the roman soldiers which attacked his village yesterday. How can he manipulate this using arrays?

When Heroix wants to write the service numbers of his Celtic warriors on a file, he uses np.savetxt:

```
>>> arr2=np.random.randn(8)
>>> np.savetxt('CelticWarr.txt',arr2)
```

NumPy - Linear algebra

Attention has to be paid at * which is an element-wsie product instead of a matrix dot product. The function dot is used in numpy (see 'Transposing arrays').

To do calculations on matrices, numpy.linalg has a standard set of functions, like diag (return the diagonal elements of a square matrix), trace, det (matrix determinant), eig (eigenvalues and eigenvectors of a square matrix), inv (inverse),...

```
>>> X = np.random.randn(2,2)

>>> mat = X.T.dot(X)

>>> np.linalg.inv(mat)

array([[ 1.70182387,  3.91458018],

       [ 3.91458018,  10.22597796]])
```

Pandas - Series

A Series is a one-dimensional object containing an array of data and an associated array of data labels, called its index.

```
>>> obj = pd.Series([4, 7, -5, 3])
>>> obj
0     4
1     7
2     -5
3     3
dtype: int64
>>> obj.values
array([ 4,  7, -5,  3])
>>> obj.index
RangeIndex(start=0, stop=4, step=1)
>>> for j in obj.index : print j
0
1
2
3
```

Pandas - Series

It is also possible to define the index.

Single values can be selected and assigned.

```
>>> obj2['a']
-5
>>> obj2['d'] = 6
```

Numpy array operations are possible - the index value does not change.

```
>>> np.exp(obj2)
d 403.428793
b 1096.633158
a 0.006738
c 20.085537
dtype: float64
```

A DataFrame represents a tabular, spreadsheet-like data structure which contains an ordered collection of columns, which can have a different value type (numeric, boolean,...). A DataFrame has both a row and a column index.

```
>>> data = {'Celt': ['Asterix', 'Asterix', 'Obelix', 'Obelix'], 'age' [18, 19, 20, 19, 20], 'numberofromans': [1.5, 1.7, 3.6, 2.4, 2.9]}
>>> frame = pd.DataFrame(data)
>>> frame
      Celt age numberofromans
0 Asterix 18
                                 1.5
1 Asterix 19
                                 1.7
2 Asterix
               20
                                 3.6
    Obelix
               19
                                 2.4
    Obelix
               20
                                 2.9
```

The sequence of columns can be specified and the index can be redefined.

```
>>> frame2 = pd.DataFrame(data, columns=['numberofromans','Celt'], index=['one',
'two', 'three', 'four', 'five'1)
>>> frame2
      numberofromans
                         Celt
                 1.5 Asterix
one
two
                 1.7 Asterix
three
                 3.6
                      Asterix
                       Obelix
four
                 2.4
five
                 2.9
                       Obelix
```

In order to write out the DataFrame, to_csv is used.

```
>>> frame2.to_csv('out_frame2.csv')
```

Columns can be retrieved in two different ways.

```
>>> frame2['Celt']
one
          Asterix
          Asterix
two
three
          Asterix
four
           Obelix
five
           Obelix
Name: Celt, dtype: object >>> frame2.numberofromans
one
          1.5
          1.7
two
          3.6
three
four
          2.4
five
          2.9
Name: numberofromans, dtype: float64
```

Rows can be retrieved by using ix and the index.

```
>>> frame2.ix['three']
numberofromans 3.6
Celt Asterix
Name: three, dtype: object
```

Assigning a column that doesn't exist will create a new column.

```
>>> frame2['thick'] = frame2.Celt == 'Obelix'
>>> frame2
             numberofromans
                                Celt thick
                        1.5 Asterix False
      one
                        1.7
                             Asterix False
      two
                        3.6 Asterix False
      three
                              Obelix
      four
                        2.4
                                       True
      five
                              Obelix
                        2.9
                                       True
```

del removes columns

```
>>> del frame2['thick']
>>> frame2
       numberofromans
                         Celt
                        1.5 Asterix
       one
                        1.7 Asterix
       two
       three
                        3.6 Asterix
       four
                        2.4
                              Obelix
       five
                         2.9
                              Obelix
```

Use can be made of nested structures:

... and it can be transposed

Pandas - Data alignment

```
>>> A = pd.Series([7.3, -2.5, 3.4, 1.5], index = ['a', 'c', 'd', 'e'])
>>> B = pd.Series([-2.1, 3.6, -1.5, 4, 3.1], index = ['a', 'c', 'e', 'f', 'g'])
>>> A+B
a     5.2
c     1.1
d     NaN
e     0.0
f     NaN
g     NaN
dtype: float64
```

Remark that d is missing in B, while f and g are absent in A.

Pandas - Data alignment

```
>>> df1 = pd.DataFrame(np.arange(9.).reshape((3, 3)), columns=list('bcd'),
index=['Asterix', 'Obelix', 'Kanalltix'])
>>> df2 = pd.DataFrame(np.arange(12.).reshape((4,3)), columns=list('bde'),
index=['Miraculix', 'Asterix', 'Obelix', 'Kaningentix'])
>>> df1
           Ь
                     d
                C
         0.0 1.0 2.0
Asterix
Obelix
         3.0
              4.0 5.0
Kanalltix 6.0 7.0 8.0
>>> df2
              Ь
                    d
                          e
Miraculix
            0.0
                  1.0 2.0
Asterix
            3.0
                  4.0
                        5.0
Obelix
            6.0 7.0
                        8.0
Kaningentix 9.0 10.0 11.0
>>> df1+df2
              Ь
                        d e
                 C
Asterix
            3.0 NaN
                      6.0 NaN
Kanaltix
                      NaN NaN
            NaN NaN
Kaningentix NaN NaN
                      NaN NaN
Miraculix
            NaN NaN
                      NaN NaN
Obelix
            9.0 NaN 12.0 NaN
```

Pandas - Sorting

Pandas - Sorting

When Kanalltix wants to sort the values by a specified column, however, he cannot use sort_index, but has to revert to sort_values(by=).

```
>>> frame = pd.DataFrame({'b': [4, 7, -3], 'a': [0, 1, 0]})
>>> frame.sort_values(by='b')
    a    b
2    0 -3
0    0    4
1    1    7
```

Pandas - Baby names 1880-2015

On http://www.ssa.gov/oact/babynames/limits.html the total number of births for each gender/name combination is given as a raw archive.

```
Mary,F,7065
Anna,F,2604
Emma,F,2003
Elizabeth,F,1939
Minnie,F,1746
```

Since this is a comma-separated form, use is made of pandas.read_csv to load the data

```
import pandas as pd
names1880 = pd.read_csv('names/yob1880.txt', names=['name', 'sex', 'births'])
```

The data are printed as

```
Mary
                   7065
0
        Anna
                   2604
2
3
4
                   2003
        Emma
        Elizabeth
                       1939
        Minnie
                     1746
                F
1996
        Worthy
                       5
5
5
5
1997
        Wright
1998
          York
                Μ
1999 Zachariah
                Μ
[2000 rows x 3 columns]
```

To get an overview over all births, we can use the sum of the births by sex:

```
>>> names1880.groupby('sex')['births'].sum()
sex
F     90992
M     110490
Name: births, dtype: int64
```

Pandas - Excel

On the internet, Kaningentix finds an excel sheet containing all herbs, grasses and vegetables which can be found in the forest. The list contains not only the names and the subsequent characterizations, but also where these are found and the time of the medicinal effect.

It is advisable to use pandas, making use of the ExcelFile class.

```
>>> import pandas as pd
>>> xls_file = pd.ExcelFile('data.xls')
```

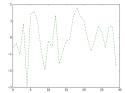
Data stored in a sheet can then be read into DataFrame using parse:

```
>>> table = xls_file.parse('sheet1')
```

Matplotlib

Basic syntax for a plot

```
>>> plt.plot(np.random.randn(30), linestyle='--', color='g')
```



Other styles and colors are available and can easily be searched.

```
>>> plt.plot(np.random.randn(30).cumsum(), color='k', linestyle='solid', marker='*
```



The cumsum() function gives out the cumulative sum of the numbers in the array.

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Matplotlib - Figures and subplots

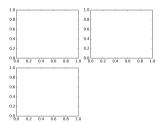
To manipulate figures, use is made of a Figure 'object'.

```
>>> fig = plt.figure()
```

Subplots are made using add_subplot.

```
>>> ax1 = fig.add_subplot(2,2,1)
>>> ax2 = fig.add_subplot(2,2,2)
>>> ax3 = fig.add_subplot(2,2,3)
```

The first two arguments of subplot point at the amount of pictures in one row and in one column. The last argument counts: left above is picture 1, right above is picture 2, left down is 3 etc.

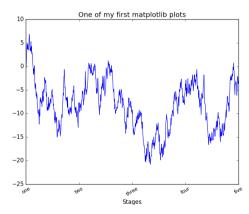


Techniques to fill these plots will be given in the following slides.

Matplotlib - title, axis labels, ticks, and ticklabels

To adjust the axes, it is a good idea to use add_subplot - even when there is only one plot in the figure.

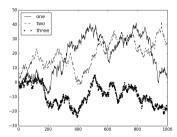
```
>>> fig= plt.figure(); ax = fig.add_subplot(1, 1, 1)
>>> ax.plot(np.random.randn(1000).cumsum())
[<matplotlib.lines.Line2D at 0x2ab9f8ee0fd0>]
>>> ticks = ax.set_xticks([0, 250, 500, 750, 1000])
>>> labels = ax.set_xticklabels(['one', 'two', 'three', 'four', 'five'],
rotation=30, fontsize='small')
>>> ax.set_title('One of my first matplotlib plots')
<matplotlib.text.Text at 0x2ab9f9648c50>
>>> ax.set_xlabel('Stages')
```



Matplotlib - adding legends

Adding a legend is only possible when more than one plot is included in the graphic.

```
>>> fig = plt.figure(); ax = fig.add_subplot(1, 1, 1)
>>> ax.plot(np.random.randn(1000).cumsum(), 'k', label='one')
[<matplotlib.lines.Line2D at 0x2ab9f9aaae50>]
>>> ax.plot(np.random.randn(1000).cumsum(), 'k--', label='two')
[<matplotlib.lines.Line2D at 0x2ab9f9dbd150>]
>>> ax.plot(np.random.randn(1000).cumsum(), 'k.', label='three')
[<matplotlib.lines.Line2D at 0x2ab9f9aa96d0>]
>>> ax.legend(loc='best')
```



Matplotlib - Saving plots to a file

To save the figure on the last figure, savefig can be used. Pay attention to the extension - .png, .jpg and .pdf give the respective format of the pictures. The resolution can be indicated using dpi.

>>> plt.savefig('myfavouritelastpic.png', dpi=400)

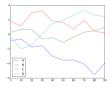
Matplotlib - Plotting functions in Pandas

Line plots

```
>>> s= pd.Series(np.random.randn(10).cumsum(), index=np.arange(0, 100, 10))
>>> s.plot()
```



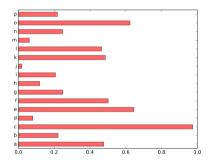
```
>>> df = DataFrame(np.random.randn(10, 4).cumsum(0),
columns = ['A', 'B', 'C', 'D'], index=np.arange(0, 100, 10))
>>> df.plot()
```



Matplotlib - Plotting functions in Pandas

Bar plots

```
>>> data = pd.Series(np.random.rand(16), index=list('abcdefghijklmnop'))
>>> data.plot(kind='barh', color='r', alpha=0.5)
```

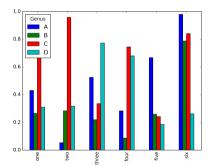


alpha points at the intensity of the red color.

Matplotlib - Plotting functions in Pandas

Bar plots

```
>>> df = pd.DataFrame(np.random.rand(6,4), index= ['one', 'two', 'three', 'four',
>>> df
Genus
             Α
      0.430194
                0.264419
                          0.863249 0.309548
one
two
      0.053039 0.283306
                          0.958429
                                    0.317259
      0.525248 0.218834
                          0.334936
three
                                    0.772332
      0.282869
                0.086094
four
                          0.745032
                                    0.680265
five
      0.667275 0.258653
                          0.241644
                                    0.185485
six
      0.979554 0.787525
                          0.840468 0.261518
>>> df.plot(kind='bar')
```

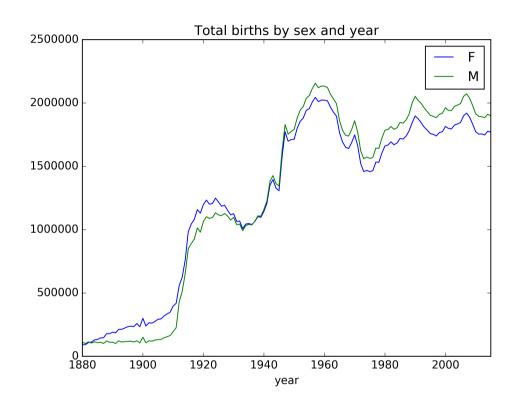


Matplotlib - Total births by gender and year

From 1880 to 2015, a file is available containing the year of birth, together with the amount of born females and males.

```
>>> tb=pd.read_csv('out_total_births.csv')
>>> tb
     year
                          Μ
                     110490
    1880
             90992
                     100743
    1881
             91953
    1882
            107848
                     113686
3
     1883
            112318
                     104627
133
    2013
          1747544
                    1883945
     2014
           1777242
                    1910876
    2015 1769325
                    1898858
[136 rows x 3 columns]
>>> tb.plot(title='Total births by sex and year', x='year',y=['F','M'])
```

Matplotlib - Total births by gender and year



PIP

Pip is a package management system used to install and manage software packages written in Python, taken from the `Python Package Index' (PyPI).

Use:

```
>>> pip install package-name
>>> pip uninstall package-name
```

Virtual environments

Miraculix has been coding a lot throughout his life. He has programs made from the early days of Python - and he has ones which he made yesterday. To avoid compatibility issues ("program Herbs1.py needs the module ColorGrass-1.0.2, while program IdefixIllness.py needs the module ColorGrass-12.1.15b"), Miraculix uses virtual environments in which he can load the exact packages he needs.

```
$ which python3
/usr/bin/python3
$ python3 -m venv ./venv
$ source venv/bin/activate
(venv)$ which python3
.../venv/bin/python3
(venv)$ which pip3
.../venv/bin/pip3
(venv)$ pip3 install ColorGrass-1.0.2
```

... and Miraculix makes sure he is aware of the employed packages:

```
(venv)$ pip3 freeze > requirements.txt
```

References

"Python for Data Analysis", Wes McKinney, O'Reilly Media, Sebastopol, CA: 2013

https://docs.python.org/3/