Scientific Programming Practical 8

Introduction

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Pandas

Pandas (**panel-data**) is a very efficient library to deal with **numerical tables** and time series

Two data structures:

Series: 1D tables
DataFrames: 2D tables

https://pandas.pydata.org/

Series

Series are 1-dimensional structures (like lists) containing data. Series are characterized by two types of information: the **values** and the **index** (a list of labels associated to the data). A bit like **list** and a bit like **dictionary**!

```python
import pandas as pd
import random

print("Values and index explicitly defined")
#values and index explicitely defined
S = pd.Series([random.randint(0,20) for x in range(0,10)],
              index = list("ABCDEFGHIL"))

print(S)
print("The index:", S.index)
print("The values:", S.values)

print("-----------------------\n")
print("From dictionary")
#from a dictionary
S1 = pd.Series({"one" : 1, "two" : 2, "ten": 10,
                "three" : 3, "four": 4, "forty" : 40})
print(S1)
print(S1.index)
print(S1.values)
```

```
Values and index explicitly defined
A    15
B     7
C    20
D     3
E    15
F     1
G     5
H    17
I    15
L    17
dtype: int64
The index: Index(['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I', 'L'], dtype='object')
The values: [15  7 20  3 15  1  5 17 15 17]
------------------------

From dictionary
forty    40
four      4
one       1
ten      10
three     3
two       2
dtype: int64
Index(['forty', 'four', 'one', 'ten', 'three', 'two'], dtype='object')
[40  4  1 10  3  2]
```

Series

Series are 1-dimensional structures (like lists) containing data. Series are characterized by two types of information: the **values** and the **index** (a list of labels associated to the data). A bit like **list** and a bit like **dictionary**!

```python
print("Default index")
#index added by default
myData = [random.randint(0,10) for x in range(10)]
S2 = pd.Series(myData)

print(S2)
print(S2.index)
print(S2.values)

print("-----------------------\n")
print("Same value repeated")
S3 = pd.Series(1.27, range(10))
print(S3)
print(S3.index)
print(S3.values)
```

```
Default index
0     8
1     2
2     8
3    10
4     1
5     5
6     3
7     8
8     9
9     5
dtype: int64
RangeIndex(start=0, stop=10, step=1)
[ 8  2  8 10  1  5  3  8  9  5]
-----------------------

Same value repeated
0    1.27
1    1.27
2    1.27
3    1.27
4    1.27
5    1.27
6    1.27
7    1.27
8    1.27
9    1.27
dtype: float64
RangeIndex(start=0, stop=10, step=1)
[1.27 1.27 1.27 1.27 1.27 1.27 1.27 1.27 1.27 1.27]
```

Series

Data in a series can be accessed by using the **label** (i.e. the index) as in a dictionary or through its **position** as in a list. Slicing is also allowed both by **position** and **index**.

In the latter case, `Series[S:E]` with **S and E indexes**, both **S and E are included**.

```python
import pandas as pd
import random

#values and index explicitely defined
S = pd.Series([random.randint(0,20) for x in range(0,10)],
              index = list("ABCDEFGHIL"))
print(S)
print("")

print("Value at label \"A\":", S["A"])
print("Value at index 1:", S[1])
print("")

print("Slicing from 1 to 3:") #note 3 excluded
print(S[1:3])
print("")
print("Slicing from C to H:") #note H included!
print(S["C":"H"])
print("")

print("Retrieving from list:")
print(S[[1,3,5,7,9]])
print(S[["A","C","E","G"]])
print("")

print("Top 3")
print(S.head(3))
print("")
print("Bottom 3")
print(S.tail(3))
```

```
A    15
B    11
C     4
D     7
E     1
F     4
G    15
H    14
I    14
L    17
dtype: int64

Value at label "A": 15
Value at index 1: 11

Slicing from 1 to 3:
B    11
C     4
dtype: int64

Slicing from C to H:
C     4
D     7
E     1
F     4
G    15
H    14
dtype: int64
```

Series

Data in a series can be accessed by using the **label** (i.e. the index) as in a dictionary or through its **position** as in a list. Slicing is also allowed both by **position** and **index**.

In the latter case, `Series[S:E]` with **S and E labels**, both **S and E are included**.

```
import pandas as pd
import random

#values and index explicitely defined
S = pd.Series([random.randint(0,20) for x in range(0,10)],
              index = list("ABCDEFGHIL"))
print(S)
print("")

print("Value at label \"A\":", S["A"])
print("Value at index 1:", S[1])
print("")

print("Slicing from 1 to 3:") #note 3 excluded
print(S[1:3])
print("")
print("Slicing from C to H:") #note H included!
print(S["C":"H"])
print("")

print("Retrieving from list:")
print(S[[1,3,5,7,9]])
print(S[["A","C","E","G"]])
print("")

print("Top 3")
print(S.head(3))
print("")
print("Bottom 3")
print(S.tail(3))
```

```
Retrieving from list:
B    11
D     7
F     4
H    14
L    17
dtype: int64
A    15
C     4
E     1
G    15
dtype: int64

Top 3
A    15
B    11
C     4
dtype: int64

Bottom 3
H    14
I    14
L    17
dtype: int64
```

Series

Important operations on series:

Operator broadcasting

Operations can automatically be broadcast to the entire Series. This is a quite cool feature and **saves us from looping through the elements of the Series**.

Example: Given a list of 10 integers and we want to divide them by 2.

Without pandas:

```
import random

listS = [random.randint(0,20) for x in range(0,10)]

print(listS)

for el in range(0,len(listS)):
    listS[el] /=2  #compact of X = X / 2

print(listS)
```

```
[6, 4, 5, 19, 14, 16, 9, 3, 13, 11]
[3.0, 2.0, 2.5, 9.5, 7.0, 8.0, 4.5, 1.5, 6.5, 5.5]
```

Series

Example: Given a list of 10 integers and we want to divide them by 2.

Important operations on series:

Operator broadcasting

Operations can automatically be broadcast to the entire Series. This is a quite cool feature and **saves us from looping through the elements of the Series**.

With pandas (operator broadcasting):

```python
import pandas as pd
import random

S = pd.Series([random.randint(0,20) for x in range(0,10)],
              index = list("ABCDEFGHIL"))

print(S)
print("")
S1 = S / 2
print(S1)
```

```
A     4
B    13
C    14
D     6
E    13
F     2
G    13
H    19
I    20
L     7
dtype: int64

A     2.0
B     6.5
C     7.0
D     3.0
E     6.5
F     1.0
G     6.5
H     9.5
I    10.0
L     3.5
dtype: float64
```

Series

Important operations on series:

Operator broadcasting

Filtering

We can also apply boolean operators to obtain only the **sub-Series** with all the values satisfying a specific condition. This allows us to **filter** the Series.

```python
import pandas as pd
import random

S = pd.Series([random.randint(0,20) for x in range(0,10)],
              index = list("ABCDEFGHIL"))

print(S)
print("")
S1 = S>10
print(S1)
print("")
S2 = S[S > 10]
print(S2)
```

```
A     3
B     3
C    18
D     1
E    12
F    11
G     4
H    11
I     5
L    14
dtype: int64

A    False
B    False
C     True
D    False
E     True
F     True
G    False
H     True
I    False
L     True
dtype: bool

C    18
E    12
F    11
H    11
L    14
dtype: int64
```

series of True and False where condition is/is not met

Series

Important operations on series:

Operator broadcasting

Filtering

Computing stats

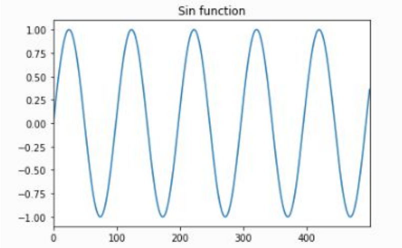
```python
import pandas as pd
import random

S = pd.Series([random.randint(0,10) for x in range(0,10)],
              index = list("ABCDEFGHIL"))
print("The data:")
print(S)
print("")
print("Its description")
print(S.describe())
print("")
print("Specifying different quantiles:")
print(S.quantile([0.1,0.2,0.8,0.9]))
print("")
print("Histogram:")
print(S.value_counts())
print("")
print("The type is a Series:")
print(type(S.value_counts()))
print("Summing the values:")
print(S.sum())
print("")
print("The cumulative sum:")
print(S.cumsum())
```

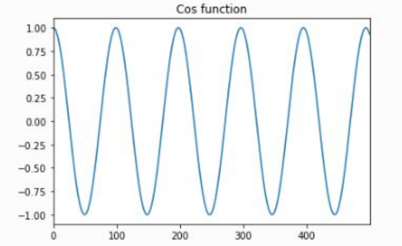
```
The data:
A     3
B    10
C     3
D     4
E     9
F     9
G     5
H     0
I    10
L     5
dtype: int64

Its description
count    10.000000
mean      5.800000
std       3.489667
min       0.000000
25%       3.250000
50%       5.000000
75%       9.000000
max      10.000000
dtype: float64

Specifying different quantiles:
0.1     2.7
0.2     3.0
0.8     9.2
0.9    10.0
dtype: float64

Histogram:
10    2
9     2
5     2
3     2
4     1
0     1
dtype: int64
```

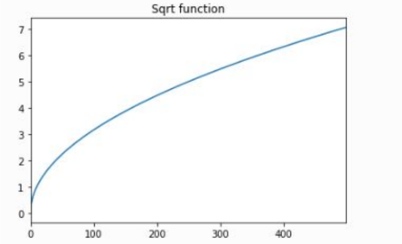
see notes for the complete results and other features like `Series.fillna(values)`

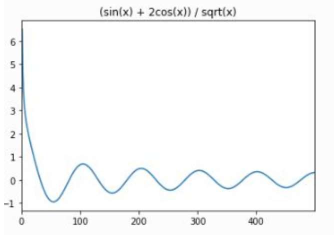
Plotting data

It is quite easy to plot data in Series and DataFrames thanks to matplotlib










```python
import math
import matplotlib.pyplot as plt
import pandas as pd

x = [i/10 for i in range(0,500)]


y =  [math.sin(2*i/3.14 ) for i in x]
y1 = [math.cos(2*i/3.14 ) for i in x]
y2 = [math.sqrt(i) for i in x]
#print(x)

ySeries = pd.Series(y)
ySeries1 = pd.Series(y1)
ySeries2 = pd.Series(y2)

ySeries.plot()
plt.title("Sin function")
plt.show()
plt.close()
ySeries1.plot()
plt.title("Cos function")
plt.show()
plt.close()
ySeries2.plot()
plt.title("Sqrt function")
plt.show()
plt.close()
ySeries2 = (ySeries + 2*ySeries1)/ySeries2
ySeries2.plot()
plt.title("(sin(x) + 2cos(x)) / sqrt(x)")
plt.show()
```

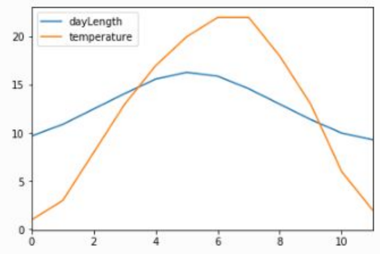
DataFrames

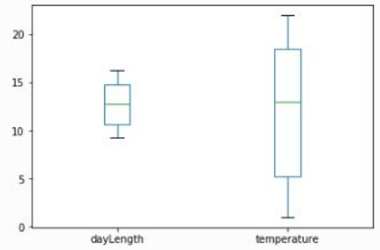
2D analogous of Series.
They have an **index** and several **columns**.

Data can be dishomogeneous.

Most of the the things seen for Series apply to DataFrames

```python
import pandas as pd

myData = {
    "temperature" : pd.Series([1, 3, 8, 13, 17, 20, 22, 22,18 ,13,6,2],
                         index = ["Jan","Feb", "Mar","Apr","May","Jun",
                                  "Jul","Aug","Sep","Oct","Nov","Dec"]
                          ),
    "dayLength" : pd.Series([9.7, 10.9, 12.5, 14.1, 15.6, 16.3, 15.9,
                          14.6,13,11.4,10,9.3],
                         index = ["Jan","Feb", "Mar","Apr","May","Jun",
                                  "Jul","Aug","Sep","Oct","Nov","Dec"]
                          )

}

DF = pd.DataFrame(myData)
print(DF)

print(DF.columns)
print(DF.index)
```






```
     dayLength  temperature
Jan        9.7            1
Feb       10.9            3
Mar       12.5            8
Apr       14.1           13
May       15.6           17
Jun       16.3           20
Jul       15.9           22
Aug       14.6           22
Sep       13.0           18
Oct       11.4           13
Nov       10.0            6
Dec        9.3            2
Index(['dayLength', 'temperature'], dtype='object')
Index(['Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul', 'Aug', 'Sep', 'Oct',
       'Nov', 'Dec'],
      dtype='object')
```

DataFrames

We can **load external files**, extract info and apply operators, broadcasting and filtering...

1. Select by column `DataFrame[col]` returns a Series
2. Select by row label `DataFrame.loc[row_label]` returns a Series
3. Select row by integer location `DataFrame.iloc[row_position]` returns a Series
4. Slice rows `DataFrame[S:E]` (S and E are labels, both included) returns a DataFrame
5. Select rows by boolean vector `DataFrame[bool_vect]` returns a DataFrame

Row ID	Sales	Profit	Product Category
1	261.5400	-213.25	Office Supplies
49	10123.0200	457.81	Office Supplies
50	244.5700	46.71	Office Supplies
80	4965.7595	1198.97	Technology
85	394.2700	30.94	Office Supplies
86	146.6900	4.43	Furniture
97	93.5400	-54.04	Office Supplies

Load from file

```python
import pandas as pd

orders = pd.read_csv("file_samples/sampledata_orders.csv", sep=",",
index_col =0, header=0)

print("The Order Quantity column (top 5)")
print(orders["Order Quantity"].head(5))
print("")
print("The Sales column (top 10)")
print(orders.Sales.head(10))
print("")
print("The row with ID:50")
r50 = orders.loc[50]
print(r50)
print("")
print("The third row:")
print(orders.iloc[3])

print("The Order Quantity, Sales, Discount and Profit of the 2nd,
4th, 6th and 8th row:")
print(orders[1:8:2][["Order Quantity", "Sales","Discount", "Profit"]])
print("The Order Quantity, Sales, Discount and  Profit of orders with
discount > 10%:")
print(orders[orders["Discount"] > 0.1][["Order Quantity", "Sales",
"Discount", "Profit"]])
```

see notes for results

Merging DataFrames

```
pandas.merge(DataFrame1, DataFrame2, on="col_name", how="inner/outer/left/right")
```

1. how = inner : non-matching entries are discarded;
2. how = left : ids are taken from the first DataFrame;
3. how = right : ids are taken from the second DataFrame;
4. how = outer : ids from both are retained.

DFs1

	id	type
0	SNP_FB_0411211	SNP
1	SNP_FB_0412425	SNP
2	SNP_FB_0942385	SNP
3	CH01f09	SSR
4	Hi05f12x	SSR
5	SNP_FB_0942712	SNP

DFs2

	chr	id
0	1	SNP_FB_0411211
1	15	SNP_FB_0412425
2	7	SNP_FB_0942385
3	9	CH01f09
4	1	SNP_FB_0428218

```python
inJ = pd.merge(DFs1,DFs2, on = "id", how = "inner")
print(inJ)
```

```python
leftJ = pd.merge(DFs1,DFs2, on = "id", how = "left")
print(leftJ)
```

Inner merge (only common in both)

	id	type	chr
0	SNP_FB_0411211	SNP	1
1	SNP_FB_0412425	SNP	15
2	SNP_FB_0942385	SNP	7
3	CH01f09	SSR	9

Left merge (IDS from DFs1)

	id	type	chr
0	SNP_FB_0411211	SNP	1
1	SNP_FB_0412425	SNP	15
2	SNP_FB_0942385	SNP	7
3	CH01f09	SSR	9
4	Hi05f12x	SSR	NaN
5	SNP_FB_0942712	SNP	NaN

Right merge (IDS from DFs2)

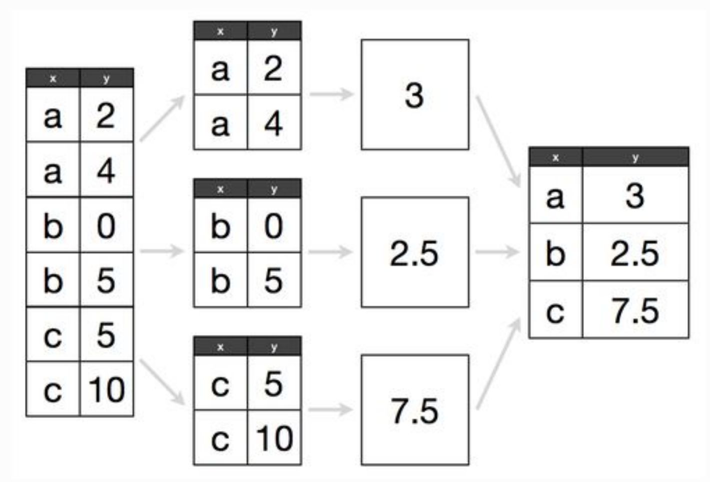
	id	type	chr
0	SNP_FB_0411211	SNP	1
1	SNP_FB_0412425	SNP	15
2	SNP_FB_0942385	SNP	7
3	CH01f09	SSR	9
4	SNP_FB_0428218	NaN	1

Outer merge (IDS from both)

	id	type	chr
0	SNP_FB_0411211	SNP	1
1	SNP_FB_0412425	SNP	15
2	SNP_FB_0942385	SNP	7
3	CH01f09	SSR	9
4	Hi05f12x	SSR	NaN
5	SNP_FB_0942712	SNP	NaN
6	SNP_FB_0428218	NaN	1

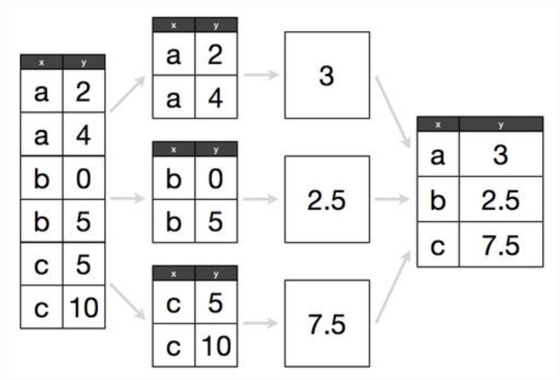
Grouping DataFrames

The split-apply-aggregate paradigm



Grouping DataFrames

The split-apply-aggregate paradigm




```python
import pandas as pd

test = {"x": ["a","a", "b", "b", "c", "c" ],
        "y" : [2,4,0,5,5,10]
       }

DF = pd.DataFrame(test)
print(DF)
print("")
gDF = DF.groupby("x")
for i,g in gDF:
    print("Group: ", i)
    print(g)
    print(type(g))

aggDF = gDF.aggregate(pd.DataFrame.mean)
print(aggDF)
```

```
   x   y
0  a   2
1  a   4
2  b   0
3  b   5
4  c   5
5  c  10

Group:   a
   x  y
0  a  2
1  a  4
<class 'pandas.core.frame.DataFrame'>
Group:   b
   x  y
2  b  0
3  b  5
<class 'pandas.core.frame.DataFrame'>
Group:   c
   x   y
4  c   5
5  c  10
<class 'pandas.core.frame.DataFrame'>
     y
x
a  3.0
b  2.5
c  7.5
```

Grouping DataFrames

Questions:
How many Product categories?
Total sales and profits per category?
What is the most profitable category?

```
              Sales   Profit Product Category
Row ID
1          261.5400  -213.25   Office Supplies
49       10123.0200   457.81   Office Supplies
50         244.5700    46.71   Office Supplies
80        4965.7595  1198.97        Technology
85         394.2700    30.94   Office Supplies
```

```
Group:  Furniture
Group:  Office Supplies
Group:  Technology

Count elements per category:
Office Supplies    4610
Technology         2065
Furniture          1724
Name: Product Category, dtype: int64

Total values:
                       Sales     Profit
Product Category
Furniture        5178590.542  117433.03
Office Supplies  3752762.100  518021.42
Technology       5984248.182  886313.52
Mean values (sorted by profit):
                       Sales      Profit
Product Category
Furniture        3003.822820   68.116607
Office Supplies   814.048178  112.369072
Technology       2897.941008  429.207516

The most profitable is Technology
```

```python
import pandas as pd
import matplotlib.pyplot as plt

orders = pd.read_csv("file_samples/sampledata_orders.csv", sep=",",
                     index_col =0, header=0)

SPC = orders[["Sales","Profit", "Product Category"]]
print(SPC.head())

SPC.plot(kind = "hist", bins = 10)
plt.show()

print("")
grouped = SPC.groupby("Product Category")
for i,g in grouped:
    print("Group: ", i)

print("")
print("Count elements per category:") #get the series corresponding to the column
                                      #and apply the value_counts() method
print(orders["Product Category"].value_counts())
print("")
print("Total values:")
print(grouped.aggregate(pd.DataFrame.sum))

print("Mean values (sorted by profit):")
mv_sorted = grouped.aggregate(pd.DataFrame.mean).sort_values(by="Profit")
print(mv_sorted)
print("")
print("The most profitable is {}".format(mv_sorted.index[-1]))
```

http://pandas.pydata.org/pandas-docs/stable/api.html

pandas 0.20.3 documentation »

Table Of Contents

API Reference

This page gives an overview of all public pandas objects, functions and methods. In general, all classes and functions exposed in the top-level `pandas.*` namespace are regarded as public.

Further some of the subpackages are public, including `pandas.errors`, `pandas.plotting`, and `pandas.testing`. Certain functions in the the `pandas.io` and `pandas.tseries` submodules are public as well (those mentioned in the documentation). Further, the `pandas.api.types` subpackage holds some public functions related to data types in pandas.

Warning: The `pandas.core`, `pandas.compat`, and `pandas.util` top-level modules are considered to be PRIVATE. Stability of functionality in those modules in not guaranteed.

Input/Output

Pickling

read_pickle(path[, compression])	Load pickled pandas object (or any other pickled object) from the specified

Flat File

read_table(filepath_or_buffer[, sep, ...])	Read general delimited file into DataFrame
read_csv(filepath_or_buffer[, sep, ...])	Read CSV (comma-separated) file into DataFrame
read_fwf(filepath_or_buffer[, colspecs, widths])	Read a table of fixed-width formatted lines into DataFrame
read_msgpack(path_or_buf[, encoding, iterator])	Load msgpack pandas object from the specified

Clipboard

read_clipboard([sep])	Read text from clipboard and pass to read_table.

Excel

First things first

We are going to need some libraries

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

In **Linux** you can install the libraries by typing in a terminal `sudo pip3 install matplotlib`, `sudo pip3 install pandas` and `sudo pip3 install numpy` (or `sudo python3.X -m pip install matplotlib`, `sudo python3.X -m pip install pandas` and `sudo python3.6 -m pip install numpy`), where X is your python version.

In **Windows** you can install the libraries by typing in the command prompt (to open it type `cmd` in the search) `pip3 install matplotlib`, `pip3 install pandas` and `pip3 install numpy`.

http://qcbsciprolab2019.readthedocs.io/en/latest/practical8.html

Exercises

1. The file top_3000_words.txt is a one-column file representing the top 3000 English words. Read the file and for each letter, count how many words start with that letter. Store this information in a dictionary. Create a pandas series from the dictionary and plot an histogram of all initials counting more than 100 words starting with them.

Show/Hide Solution

2. The file filt_aligns.tsv is a tab separated value file representing alignments of paired-end reads on some apple chromosomes. Paired end reads have the property of being X bases apart from each other as they have been sequenced from the two ends of some size-selected DNA molecules.

Each line of the file has the following information `readID\tChrPE1\tAlignmentPosition1\tChrPE2\tAlignmentPosition2`. The two ends of the same pair have the same readID. Load the read pairs aligning on the same chromosome into two dictionaries. The first (`inserts`) having readID as keys and the insert size (i.e. the absolute value of AlignmentPosition1 - AlignmentPosition2) as value. The second dictionary (`chrs`)will have readID as key and chromosome ID as value. Example:

```
readID Chr11 31120 Chr11 31472
readID1 Chr7 12000 Chr11 11680
```

will result in:

```
inserts = {"readID" : 352, "readID1" : 320}
chrs = {"readID" : "Chr11", "readID1" : "Chr7"}
```