Scientific Programming Practical 8

Introduction

Luca Bianco - Academic Year 2020-21
luca.bianco@fmach.it

Announcements

Two announcements:

Gabriele Masina is the new tutor for this course

Midterm: on Wednesday, November 4th - 11.30 - 13.30 online

(simulation of the midterm on Monday, November 2nd - 14.30 - 16.30 online)

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**!

```
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

Example: Given a list of 10 integers, 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**.

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, 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

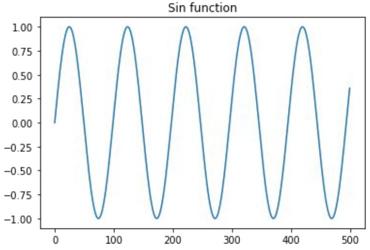
```
import pandas as pd
import random

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())
```

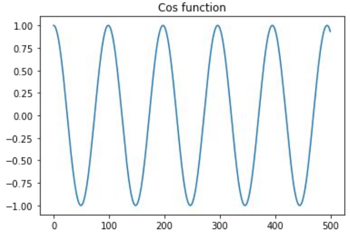
```
The data:
A     3
B    10
C     3
D     4
E     9
F     9
G     5
H     0
I    10
L     5
dtype: int64

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
```

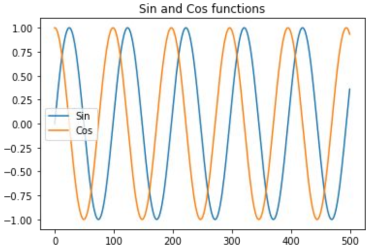
see notes for the complete results and other features like `Series.fillna(values)`

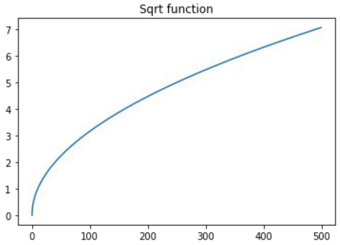
Plotting data

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



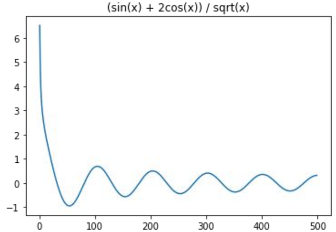






https://matplotlib.org/3.3.2/api/pyplot_summary.html

```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()
plt.title("Sin and Cos functions")
ySeries.plot()
ySeries1.plot()
plt.legend(["Sin", "Cos"])
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

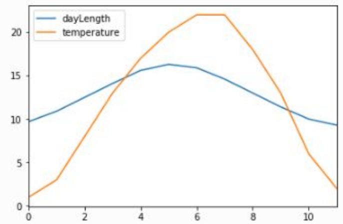
2D analogous of Series.
They have an **index** and several **columns**.

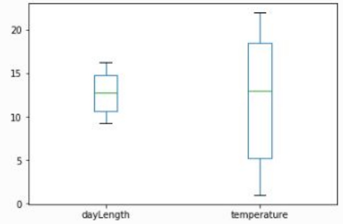
Data can be dishomogeneous.

Most of the the things seen for Series apply to DataFrames

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

myData = {
    "temperature" : pd.Series([1, 3, 8, 13, 17, 20,
                               22, 22,18 ,13,6,2]),
    "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])

}

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

DF.plot()
plt.show()
plt.close()
DF.plot(kind ="box")
plt.show()
```

```
     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

Load from file

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

```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")
```

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
```

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.

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

```
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
```

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

```
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
```

Merging DataFrames

The columns we merge on do not necessarily need to be the same, we can specify a correspondence between the row of the first dataframe (the one on the left) and the second dataframe (the one on the right) specifying which columns must have the same values to perform the merge.

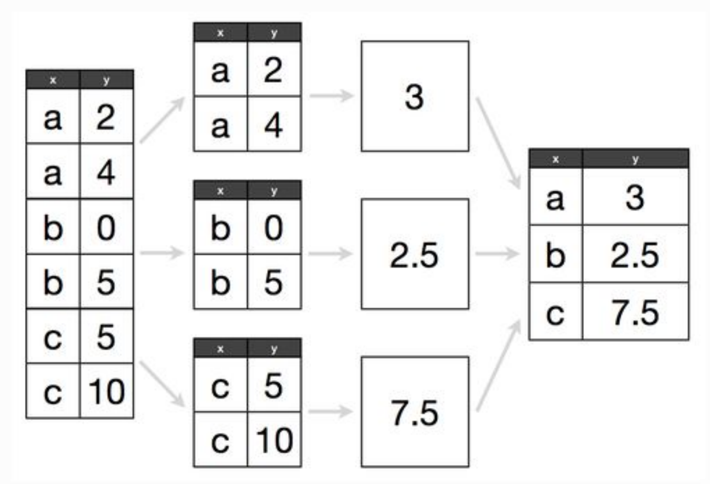
This can be done by using the parameters right_on = column_name and left_on = column_name

```python
import pandas as pd

d = dict({"A" : [1,2,3,4], "B" : [3,4,73,13]})
d2 = dict({"E" : [1,4,3,13], "F" : [3,1,71,1]})

DF = pd.DataFrame(d)
DF2 = pd.DataFrame(d2)

merged_onBE = DF.merge(DF2, left_on = 'B', right_on = 'E', how = "inner")
merged_onAF = DF.merge(DF2, right_on = "F", left_on = "A", how = "outer")
print("DF:")
print(DF)
print("DF2:")
print(DF2)
print("\ninner merge on BE")
print(merged_onBE)
print("\nouter merge on AF:")
print(merged_onAF)
```

```
DF:
   A   B
0  1   3
1  2   4
2  3  73
3  4  13
DF2:
    E   F
0   1   3
1   4   1
2   3  71
3  13   1

inner merge on BE
   A   B   E   F
0  1   3   3  71
1  2   4   4   1
2  4  13  13   1

outer merge on AF:
     A     B     E     F
0  1.0   3.0   4.0   1.0
1  1.0   3.0  13.0   1.0
2  2.0   4.0   NaN   NaN
3  3.0  73.0   1.0   3.0
4  4.0  13.0   NaN   NaN
5  NaN   NaN   3.0  71.0
```

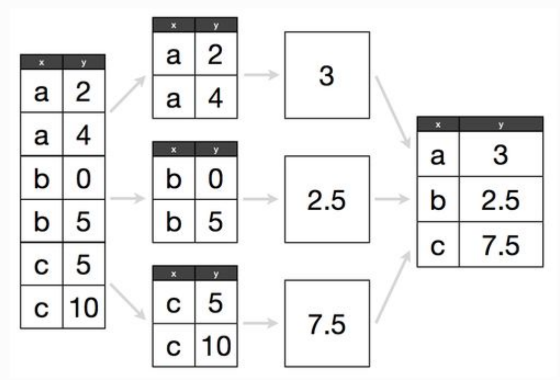
Grouping DataFrames

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]))
```

https://pandas.pydata.org/pandas-docs/stable/reference/index.html

Search the docs ...

Input/output
General functions
Series
DataFrame
pandas arrays
Panel
Index objects
Date offsets
Window
GroupBy
Resampling
Style
Plotting
General utility functions
Extensions

API reference

This page gives an overview of all public pandas objects, functions and methods. All classes and functions exposed in `pandas.*` namespace are public.

Some subpackages are public which include `pandas.errors`, `pandas.plotting`, and `pandas.testing`. Public functions in `pandas.io` and `pandas.tseries` submodules are mentioned in the documentation. `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 PRIVATE. Stable functionality in such modules is not guaranteed.

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://qcbsciprolab2020.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"}
```