Scientific Programming Practical 8

Introduction

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)



Exercise 1

>MDC020656.85

GAGGGGTTTAGTTCCTCATACTCGCAAAGCAAAGATACATAAATTTAGAAATTAAAACCC AAAGAAAGAAACACCTAGAAGNCTCCAACTTGGCAGCAAGATCATCAATGATTTCCCTT TCCTCCTTGCTGCNGCAGAGAGTTTAGAACAGGTTTTGGGTGGTATTTAGGGTGTAGAA TGGATGGGGAATGGTAGGGAAAGGTTTAGGGTTGATGGGGNTACGGCTAGGGATGATTT TGGGCAGAATTTTGGGACTTTGGTGATGGGAAGGTGCGGCNGAATGCAAGGGCAGATTTC ATAGGCATCCAAAACCCTAGGGTAATCAGATTAGGGTTTCTAGAAGCCCAAATCCACCAG AAATTAGGTTAAAACAATCAGATTTTTAGTGGGAATAAGGCCTAAGGTGNGGCTAGGGTT AGGGTTTAGAGATGGGCCTATGGTGCGGNAATGTCCAAGAATGTAAGGATGGGTCATCTA GAAGCCCAAAGCCAAGAATAGAAACTCTCACAAATGGAAACCTCCAAGAATAGAAACTTC CAACTTTAGAAACTTTGGNTTCTAATTCTGAATTCTTTGTTCTTCACTTTCATTTCTTCA TTTCTTAAGCTCCCTTTGACCTTCAACTCGTCCATTCCTTGTGCTCCATAAGTAAAAACG CCATTTTAGCTCAATTATGCTCCATTTTGCACTTCCTTGCATACTTTGTCTCTAAAACCT GAAAACACATAAAACTAGCTTAAAAGACTACGTTAACTAAGAAAACACCATGGAAATGCA NNNNNNNAAAAAGAAATTACACAATTAAATCATAAAACGAATTACACCTAGAA GTGGGTGAGTGTATGGATTGGGTTTTGGGGGTTATGGATGGTGTAGAAGGGTGGAATGGT GTTTAGGAAGGATGTATGGTGCGGCTAGGAGTGTTTTTTGGGCAGAAACTGTGGAGAATGG

Write a python program that reads two files. The first is a one column text file (contig_ids.txt) with the identifiers of some contigs that are present in the second file, which is a fasta formatted file (contigs82.fasta). The program will write on a third, fasta formatted file (e.g. filtered_contigs.fasta) only those entries in *contigs82.fasta* having identifier in *contig_ids.txt*.

```
"""exercises/filterFasta.py"""
import argparse
def readIDS(f):
    """reads a one column file in and stores
    the ids in a dictionary that is returned at the end"""
    ret = dict()
    with open(f, "r") as file:
        for line in file:
            line = line.strip()
            if(line not in ret):
                ret[line] = 1
    return ret
def filterFasta(inF. outF. ids2keep):
    oF = open(outF, "w")
    outputME = False
    with open(inF, "r") as file:
        for line in file:
            line = line.strip()
            if line.startswith(">"):
                #this is the header
                if ids2keep.get(line[1:],False):
                    oF.write(line +"\n")
                    outputME = True
                    print("Writing contig ", line[1:])
                else:
                    outputME = False
            else:
                if outputME:
                    oF.write(line +"\n")
    oF.close()
parser = argparse.ArgumentParser(description="Filters a fasta file")
parser.add argument("inputFasta", type = str, help = "The input fasta file")
parser.add argument("inputIDS", type = str, help = "The IDS to keep")
parser.add argument("outputFasta", type = str.
                    help = "The output fasta file with filtered entries")
args = parser.parse args()
idsFile = args.inputIDS
inFasta = args.inputFasta
outFasta = args.outputFasta
ids = readIDS(idsFile)
filterFasta(inFasta.outFasta, ids)
```

MDC001115.177 MDC013284.379 MDC018185.243 MDC018185.241 MDC004527.213 MDC012176.157 MDC001204.810

Exercise 1

```
biancol@bludell:~/work/courses/QCBsciprolab2020$ python3 exercises/filterFasta.py --help
usage: filterFasta.py [-h] inputFasta inputIDS outputFasta
Filters a fasta file
positional arguments:
 inputFasta The input fasta file
  inputIDS The IDS to keep
 outputFasta The output fasta file with filtered entries
optional arguments:
 -h, --help show this help message and exit
biancol@bludell:~/work/courses/QCBsciprolab2020$ python3 exercises/filterFasta.py file samples/contigs82.fasta file samples/contig ids.txt file samples/filtered contigs.fasta
Writing contig MDC001115.177
Writing contig MDC013284.379
Writing contig MDC018185.243
Writing contig MDC018185.241
Writing contig MDC004527.213
Writing contig MDC012176.157
Writing contig MDC001204.810
Writing contig MDC004389.256
Writing contig MDC018297.229
Writing contig MDC001802.364
```

```
biancol@bludell:~/work/courses/QCBsciprolab2020$ cat file_samples/filtered_contigs.fasta | grep ">"
>MDC001115.177
>MDC013284.379
>MDC018185.243
>MDC018185.241
>MDC004527.213
>MDC001276.157
>MDC001204.810
>MDC001204.810
>MDC0018297.229
>MDC001802.364
>MDC001807.243
>MDC0011015.302
>MDC017187.314
>MDC012865.410
```

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 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("From dictionary")
                                    #from a dictionary
Values and index explicitly defined
   15
   7
    20
                                    print(S1)
    15
                                    print(S1.index)
                                    print(S1.values)
   17
  15
   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
       40
forty
four
one
ten
       10
three
dtvpe: int64
Index(['forty', 'four', 'one', 'ten', 'three', 'two'], dtype='object')
[40 4 1 10 3 2]
```

```
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")
S1 = pd.Series({"one" : 1, "two" : 2, "ten": 10,
               "three": 3, "four": 4, "forty": 40})
```

dictionary!

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

If not specified, the index is added by default

print("Default index")

RangeIndex(start=0, stop=10, step=1)
[8 2 8 10 1 5 3 8 9 5]

Default index

2

10

dtype: int64

1

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.

```
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))
```

```
15
     11
     15
     14
     14
     17
dtype: int64
Value at label "A": 15
Value at index 1: 11
Slicing from 1 to 3:
    11
dtype: int64
Slicing from C to H:
D
     15
     14
dtype: int64
```

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:
     11
     14
     17
dtype: int64
     15
     15
dtype: int64
Top 3
    15
В
     11
dtype: int64
Bottom 3
     14
     14
     17
dtype: int64
```

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, 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]
```

```
[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]
```

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):

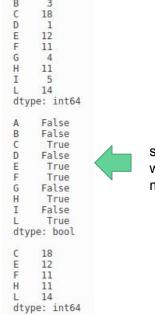
```
import pandas as pd
               import random
ABCDEF
     13
               S = pd.Series([random.randint(0,20) for x in range(0,10)],
     14
                              index = list("ABCDEFGHIL"))
      6
     13
               print(S)
               print("")
     13
               S1 = S / 2
     19
               print(S1)
     20
dtype: int64
      2.0
      6.5
      7.0
      3.0
      6.5
      1.0
      6.5
      9.5
     10.0
      3.5
dtype: float64
```

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.



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

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())
```

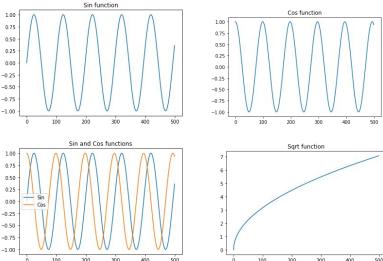
see notes for the complete results and other features

```
like Series.fillna(values)
```

```
The data:
      3
     10
     10
dtype: int64
Its description
         10.000000
count
mean
          5.800000
          3.489667
std
          0.000000
          3.250000
          5.000000
50%
75%
          9.000000
         10.000000
max
dtype: float64
Specifying different quantiles:
        2.7
0.2
        3.0
0.8
        9.2
0.9
       10.0
dtype: float64
Histogram:
10
dtype: int64
```

Plotting data

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

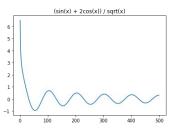


```
x = [i/10 \text{ for } i \text{ in } range(0,500)]
     [math.sin(2*i/3.14 ) for i in x]
v1 = [math.cos(2*i/3.14) for i in x]
y2 = [math.sqrt(i) for i in x]
#print(x)
vSeries = pd.Series(v)
ySeries1 = pd.Series(y1)
ySeries2 = pd.Series(y2)
ySeries.plot()
plt.title("Sin function")
plt.show()
plt.close()
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()
```

import math

import pandas as pd

import matplotlib.pyplot as plt



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

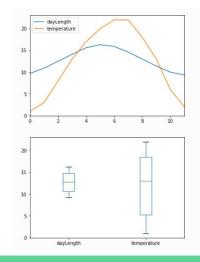
DataFrames

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

```
dayLength temperature
Jan
           9.7
          10.9
Feb
         12.5
Mar
         14.1
Apr
                         17
         15.6
May
         16.3
                         20
Jun
Jul
         15.9
Aug
          14.6
          13.0
                         18
Sep
                         13
0ct
          11.4
Nov
          10.0
           9.3
Dec
Index(['dayLength', 'temperature'], dtype='object')
Index(['Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul', 'Aug', 'Sep', 'Oct',
       'Nov', 'Dec'l,
      dtype='object')
```



DataFrames

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

Select by column DataFrame[col] returns a Series
 Select by row label DataFrame.loc[row_label] returns a Series
 Select row by integer location DataFrame.iloc[row_position] returns a Series
 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

Profit Product Category Sales Row ID 261.5400 -213.25 Office Supplies 10123.0200 Office Supplies 49 50 244.5700 Office Supplies 4965.7595 1198.97 80 Technology 85 394,2700 30.94 Office Supplies 86 4.43 146,6900 Furniture 97 93.5400 -54.04 Office Supplies

```
import pandas as pd
Load from file
                  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"]])
```

Merging DataFrames

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

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

Inner merge (only common in both) id type chr SNP FB 0411211 SNP SNP FB 0412425 SNP FB 0942385 Left merge (IDS from DFs1) id type chr SNP FB 0411211 SNP SNP FB 0412425 SNP SNP FB 0942385 SNP CH01f09 SSR 9 Hi05f12x SSR

SNP FB 0942712

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
```

```
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 CH0169 SSR 9

4 Hi05f12x SSR NaN

5 SNP_FB_0942712 SNP NaN

6 SNP_FB_0428218 NaN 1
```

Merging DataFrames

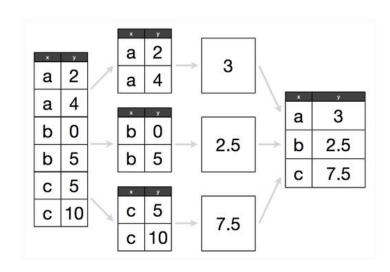
The columns we merge on do not necessarily need to be the same, we can specify a correspondence between the row of the first dataframe (the one on the left) and the second dataframe (the one on the right) specifying which columns must have the same values to perform the merge.

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

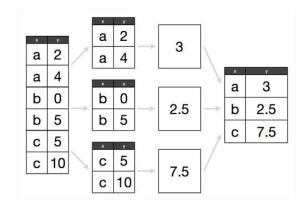
```
import pandas as pd
d = dict(\{"A" : [1,2,3,4], "B" : [3,4,73,13]\})

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:")
                                                    DF:
print(DF)
                                                           В
print("DF2:")
print(DF2)
print("\ninner merge on BE")
                                                          73
print(merged onBE)
print("\nouter merge on AF:")
                                                    DF2:
print(merged onAF)
                                                        3
                                                           71
                                                       13
                                                    inner merge on BE
                                                    outer merge on AF:
                                                                   13.0
                                                                          1.0
                                                             4.0
                                                                    NaN
                                                                          NaN
                                                            73.0
                                                                    1.0
                                                                          3.0
                                                                    NaN
                                                                          NaN
                                                              NaN
                                                                    3.0
                                                                         71.0
```

The split-apply-aggregate paradigm



The split-apply-aggregate paradigm



```
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,q in qDF:
                    print("Group: ", i)
                    print(g)
  b
                    print(type(g))
                aggDF = gDF.aggregate(pd.DataFrame.mean)
                print(aggDF)
Group: a
<class 'pandas.core.frame.DataFrame'>
Group: b
  x y
  b
     0
<class 'pandas.core.frame.DataFrame'>
Group: c
<class 'pandas.core.frame.DataFrame'>
a 3.0
 2.5
c 7.5
```

The split-apply-aggregate paradigm

	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
                  1724
Furniture
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
```

Questions:

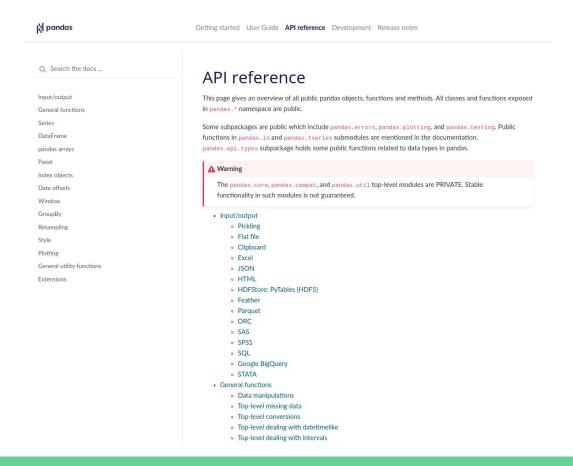
How many Product categories? Total sales and profits per category? What is the most profitable category?

```
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,q 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(my sorted)
print("")
print("The most profitable is {}".format(mv sorted.index[-1]))
```





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



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"}
```