BB1000 Programming in Python
Computer Exercise 11-12:
External libraries
(2017-05-05, RB33, 9:00-12:00)
(2017-05-08, RB33, 9:00-12:00)

(1) Consider the out_top1000.csv list of most popular names per year since 1880 (the file can be pulled from our repository). [E,C,A]

(a) Make a plot of the total sum of births through the years.

(b) Extract all the entries with 'Donald' from the list and plot the propensity through the years. (The fast fluctuations back to zero between 1920 and 1945 are due to mistakes in the basis data)

(2) Solve exercise 4 ('standard deviation') of "Filehandling" using numpy. [E,C,A]

(3) Extend exercise 9 ('analyses files in pdb format and write out atoms') of "Filehandling" using pandas: use dataframes to add an extra column to the information which is already available in file HETATOMS.out - call the file HETATOMS_extra.out. The extra column should say 'True' when the atom Oxygen is. [E,C,A]

(4) Extend exercise 10 ('shift HETATOMS') of "Filehandling" by a few lines. Save the coordinates of the atoms-to-be-written-out in a list of Series, save the coordinates of the translation vector also in a Series. Write finally the difference of the coordinates out in a file "_shifted_negatively.xyz". [A]