CVL867: Atomistic and multiscale modelling

Assignment – 01

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[Note: All the code is available in Assignment1_AmanPawar.ipynb]

Answer 01)

Part a)

The dataset is read using the periodic-table package, the first 20 elements, and the corresponding data, it was selected from it and returned in the form of a dictionary. After that, the dataset was converted into a pandas data frame for better representation purposes and clarity. The necessary cleaning of the data frame was done to remove the strings, None type data, duplicate columns, and other low-level data pre-processing was done on the data frame and it was put into the standard normal form. The data type of the data frame was corrected to float64. Two algorithms are written in python to find the max values of the respective properties

i) Exhaustive Search: computational complexity O(n)
ii) Recursive Search: computational complexity O(N log N)

Results from the 1st Algorithm implementation:

Outputs:

The maximum value of Atomic Number: is 20.0 corresponding to Calcium Maximum value of Atomic Mass: is 40.078 corresponding to the Calcium's Maximum value of the Melting point (K): is 3823.0 corresponding to the Carbon Maximum value of the Boiling point (K): 5100.0 corresponding to Carbon Maximum value of Density g/cm^3: 2.7 corresponding to Aluminium

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Part b)

3 Sorting algorithms were written in python that return the sorted order and the index value of the input data series/list.

i) Bubble Sort: Computational complexity $O(n^2)$
ii) Insertion Sort: Computational complexity $O(n^2)$
iii) Selection Sort: Computational complexity $O(n^2)$

Results from all the algorithms were similar further discussion over the effectiveness of the algorithms is discussed further in the last section.

Outputs:

Sorted List of Melting points of elements using sort1

Melting point 0.95: Helium -->>

Melting point 13.99: Hydrogen -->>

Melting point 24.56: Neon -->>

Melting point 53.48: Fluorine -->>

Melting point 54.36: Oxygen -->>

Melting point 63.23: Nitrogen -->>

Melting point 83.81: Argon -->>

Melting point 171.6: Chlorine -->>

Melting point 317.3: Phosphorus -->>

Melting point 336.7: Potassium -->>

Melting point 370.944: Sodium -->>

Melting point 388.36: Sulphur -->>

Melting point 453.65: Lithium -->>

Melting point 923.0: Magnesium -->>

Melting point 933.47: Aluminium -->>

Melting point 1115.0: Calcium -->>

Melting point 1414.0: Silicon -->>

Melting point 1560.0: Beryllium -->>

Melting point 2349.0: Boron -->>

Melting point 3823.0: Carbon -->>

Sorted List of Boiling points of elements using sort1

Boiling point 4.222: Helium -->>

Boiling point 20.271: Hydrogen -->>

Boiling point 27.104: Neon -->>

Boiling point 77.355: Nitrogen -->>

Boiling point 85.03: Fluorine -->>

Boiling point 87.302: Argon -->>

Boiling point 90.188: Oxygen -->>

Boiling point 239.11: Chlorine -->>

Boiling point 553.7: Phosphorus -->>

Boiling point 717.8: Sulphur -->>

Boiling point 1032.0: Potassium -->>

Boiling point 1156.09: Sodium -->>

Boiling point 1363.0: Magnesium -->>

Boiling point 1603.0: Lithium -->>

Boiling point 1757.0: Calcium -->>

Boiling point 2742.0: Beryllium -->>

Boiling point 2743.0: Aluminium -->>

Boiling point 3538.0: Silicon -->>

Boiling point 4200.0: Boron -->>

Boiling point 5100.0: Carbon -->>

Answer 02)

Functions for Pearson’s correlation coefficient and spearman’s correlation coefficient are made

Part i)

The Pearson’s correlation value between mass and density is 0.16

The Spearman's correlation value between mass and density is 0.27

Part ii)

The Pearson’s correlation value between melting point and boiling point is 0.94

The Spearman's correlation value between melting point and boiling point is 0.9

Part iii)

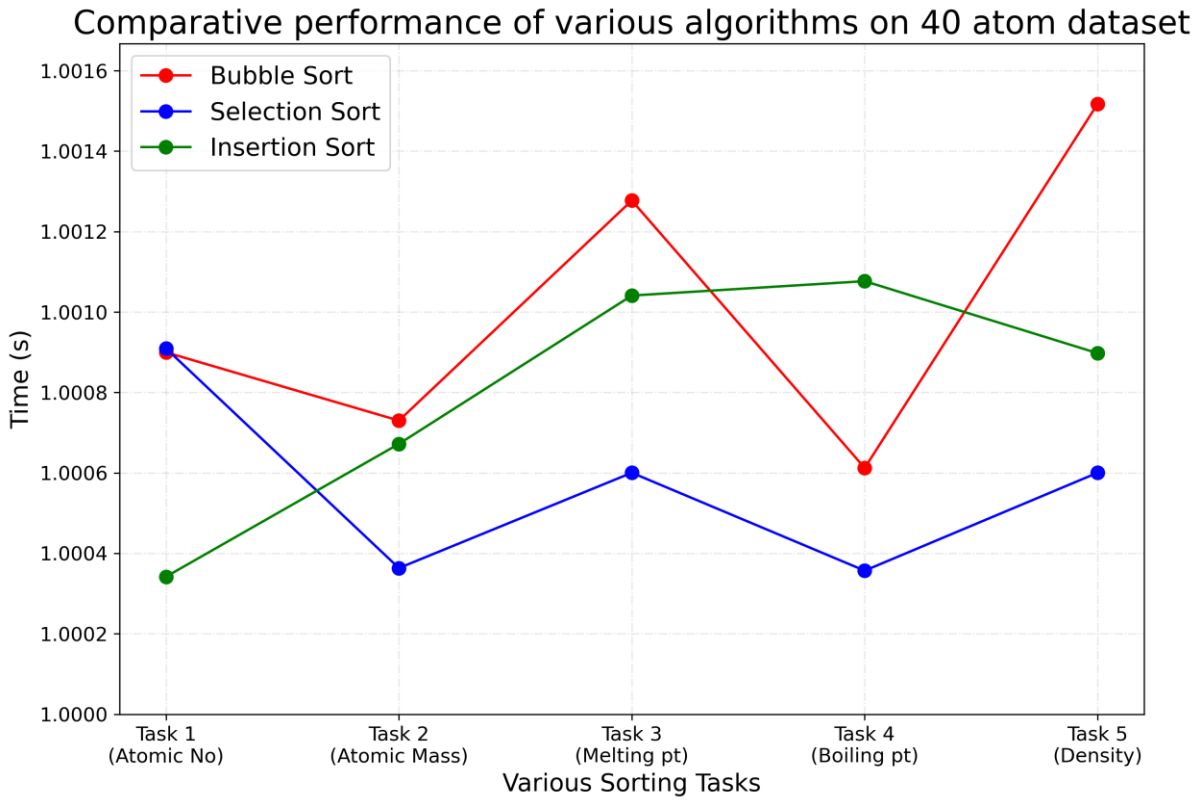
The Pearson’s correlation value between density and melting point is 0.70

The Spearman's correlation value between density and melting point is 0.90

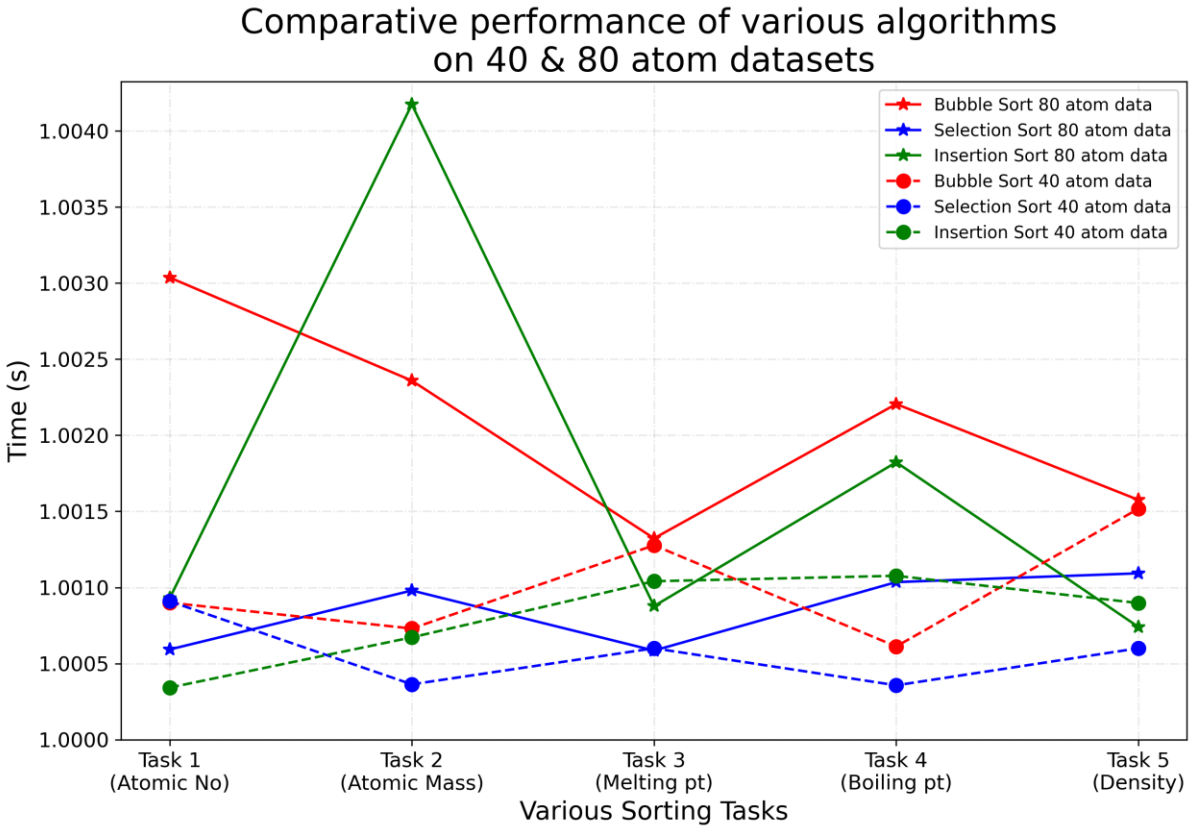
Answer 03)

Datasets are prepared for 40 atom points and 80 data points and algorithms were run to find how the computational performance of various algorithms.

Part a)



Part b)


Comparative performance of various algorithms
on 40 & 80 atom datasets
Bubble Sort 80 atom data
Selection Sort 80 atom data
Insertion Sort 80 atom data
Bubble Sort 40 atom data
Selection Sort 40 atom data
Insertion Sort 40 atom data
Time (s)
1.0040
1.0035
1.0030
1.0025
1.0020
1.0015
1.0010
1.0005
1.0000
Task 1
(Atomic No)
Task 2
(Atomic Mass)
Task 3
(Melting pt)
Task 4
(Boiling pt)
Task 5
(Density)
Various Sorting Tasks