

ME 793 - Assignment 3

Department of Mechanical Engineering, IIT Bombay

Spring 2022

Due Date: 11:30 AM, Feb 13, 2023, Marks 20

Assignment Date: 10:30 AM, Tuesday, Feb 06, 2023

Objective and Instructions

1. The objective is to understand the distribution of certain features in your data. Seek application of PCA on materials data.
2. This needs to be performed using Jupyter Notebook or Google Colab Notebook or only.
3. Submit Jupyter Notebook, Jupyter Notebook pdf, and your data file to Moodle.

Q 1. A material dataset "assignment3.txt" has been provided with this assignment. The columns are in the following order: element symbol, atomic numbers, electronegativity, atomic radii, thermal conductivity, density, crystal system, If crystal system is not available for any element, delete this element from your dataset.

For electronegativity, radii, thermal conductivity and density, do the following analysis:

- Plot these values on the Y-axis vs. elements on the X-axis. You can make a separate plot for each of these *features*.
- Arrange in increasing order, divide the span of the values of each of these into 10 equal size bins, count the number of elements in each bin and plot number of elements on the Y-axis vs. bins on the X-axis. If you know another method of making bar chart for number distribution, you can use that. Is there any similarity between distributions of two features?

Q 2. Make bins of crystal systems, count the number of elements falling in each crystal system and plot the number of elements in each bin on Y-axis vs. bin on the X-axis. Analyze and describe your observations in the context of probability distributions. Do you observe a specific type of probability distribution? Mark each plot with mean?

Q 3. For this dataset, what can you say based on the concept of co-variance?

Q 4. If you were to apply PCA or SVD on your master data set collected in Q. 1, what could you find? Any interesting trends / observation?

You are welcome to use any existing function or library if you are aware of.

—end—