ME 793 - Assignment 3

Department of Mechanical Engineering, IIT Bombay

Spring 2022

Due Date: 10:30 AM, Feb 10, 2022, Marks 10

Assignment Date: 9:30 AM, Wednesday, Feb 03, 2022

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. Make a table of elements from periodic table as following:

- Collect letter symbols of elements in column1
- Collect atomic numbers in column2
- Collect electronegativity in column3
- Collect atomic radii in column4 (you can use this link: https://en.wikipedia.org/wiki/Atomic_radii_of_the_elements_(data_page))
- Collect thermal conductivity in column5
- Collect density in column6
- Collect crystal system in column7. If crystal system is not available for any element, delete this element from your dataset.

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

- Plot these values on the Y-axis vs. elements on the X-axis. You can do 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.

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.

Q 2. If you were to apply PCA 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.

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