Course: Introduction to materials informatics



Tutorial 2

Title: Unsupervised machine learning

Questions

- 1. Write a code to calculate the volume fraction of the white phase for all 6 representative microstructures. Also calculate the average class-wise volume fraction of white phase from the autocorrelations data. Compare the volume fractions.
- 2. Perform Principal Component Analysis (PCA) on the autocorrelations data (components = 3). First take only 65025 features and then repeat for 130050 features. Comment on the results.
- 3. Perform Multi-Dimensional Scaling (MDS) on the autocorrelations data (components = 3). First take only 65025 features and then repeat for 130050 features. Comment on the results.
- 4. Calculate the preserved distances in reduced dimensions after PCA and MDS. Plot actual vs preserved distances.

Additional references:

PCA

https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html

MDS

https://scikit-learn.org/stable/modules/generated/sklearn.manifold.MDS.html

Euclidean distance

https://scikit-

learn.org/stable/modules/generated/sklearn.metrics.pairwise.euclidean_distances.html