Prediction of Lattice Structure of Perovskites from physical properties using ML

- Group 22: Sunil S Raja (SPS, Batch 20), Kaling Vikram Singh (SPS, Batch 20).
Guide: Dr Subhankar Mishra

IDEA: Perovskite are crystals with ABX3 configurations. This project tends to find the lattice structure of such crystals using physical properties such as radius, electronegativity, valence, tolerance factor, etc using machine learning. These predictions can help in finding out new Perovskites materials by providing behaviors of lattices with different physical properties.

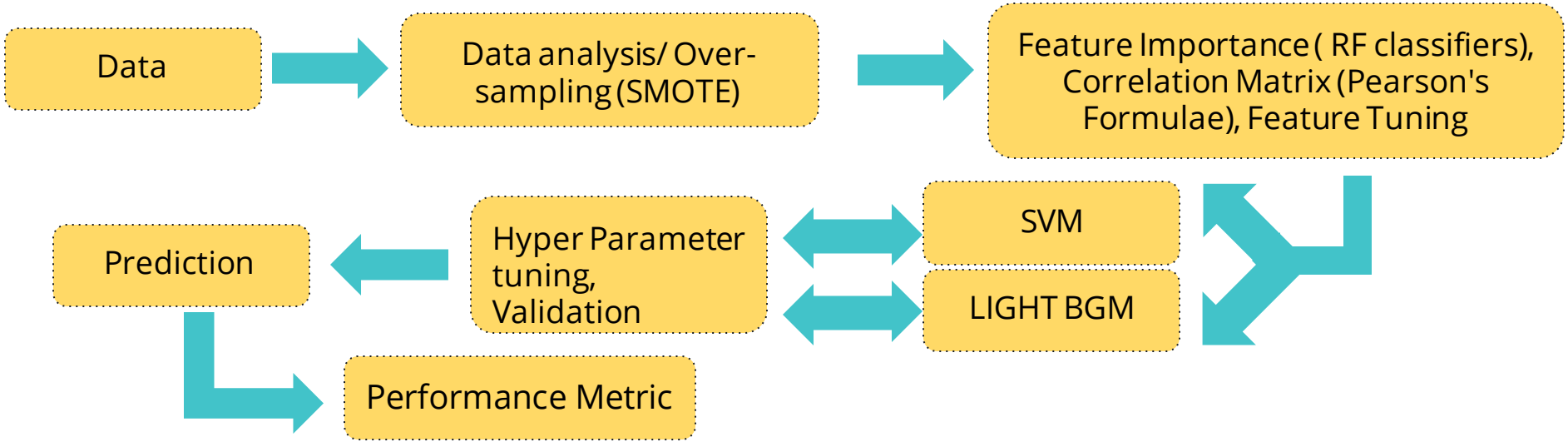
DATA SET: https://figshare.com/articles/dataset/Wolverton_Oxides_Data/7250417?file=13354619

GOALS/Expected results:

- We wish to achieve at least 80% accuracy in correctly predicting crystal structure of different Perovskites.
- We wish to implement multiple models and compare them in order to achieve best maximum accuracy.

RELEVANT PAPERS: (I): Santosh Behara et . al . Crystal structure classification in ABO3 Perovskites via machine learning, Computational Materials Science, Volume 188, 2021. https://doi.org/10.1016/j.commatsci.2020.110191.
(II): Jarin S et.al. . Predicting the Crystal Structure and Lattice Parameters of the Perovskite Materials via Different Machine Learning Models Based on Basic Atom Properties. Crystals. 2022; 12(11):1570. https://doi.org/10.3390/cryst12111570

BASELINES AND WORK DIVISION



Work Division:

- Sunil would work and code on SVM.
- Kaling will work and code on Light GBM.
- The models would be merged together with contribution from both.
- Reports and Slides would be prepared together.