MSE-242 Machine Learning in Materials Engineering

Credit Hours: 2-1

Pre-requisites: CS-117

Course Description

In recent years, machine learning has revolutionized the way materials are designed, discovered, characterized, and optimized. In this course, students will learn how machine learning techniques can be applied to materials engineering such as predicting material properties, analyzing materials data, and designing materials.

Course Contents

Introduction to machine learning in metallurgical and materials engineering: Materials discovery, property prediction, structure-property relationships, materials design, and materials informatics Basic Math: Review of Linear Algebra, Statistics, and Probability Programming and Data Science Tool: Introduction to Python (scikit-learn, pytorch, Jupyter notebook), Materials Databases (Materials Project, Citrination) Linear Regression: Univariate, Multivariate, Polynomial Regressions Clustering data/classification: K-means/db-scan, classification trees/forests Computer vision: applying concepts from clustering data, training models and Evaluating results with validation methods(e.g. Cross-validation) Deep Neural Network: Basic architecture of neural networks, different types of neural networks, Retraining hyper parameter modification Excursion: Big data in Materials science, Inverse design of materials, DFT Ml Potentials, Integrations of machine learning, simulations, and experiments.

Weekly Plan

Week	Topics
1	Introduction to machine learning in metallurgical and materials engineering
2	Materials discovery, property prediction, structure-property relationships, materials design, and materials
3	Informatics Basic Math: Review of Linear Algebra, Statistics, and Probability Programming and Data Science Tool:
4	
5	Introduction to Python (scikit-learn, pytorch, Jupyter notebook),
6	Materials Databases (Materials Project, Citrination) Linear Regression
7	Univariate, Multivariate, Polynomial Regressions Clustering data/classification
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9	**Mid-Semester Exams**
10	K-means/db-scan, classification trees/forests Computer vision: applying

11	concepts from clustering data
12	Training models and Evaluating results with validation methods(e.g. Cross-validation) Deep Neural Network: Basic architecture of neural networks, different types of neural networks
13	
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15	Retraining hyper parameter modification Excursion: Big data in Materials science, Inverse design of materials, DFT Ml Potentials, Integrations of machine learning, simulations, and experiments
16	
17-18	**End Semester Exams**

Course Outcomes

At the end of the course, students will be able to:

- Use regression and classification algorithms to predict structure-property relationship for different materials.
- Compare and analyze the performance of different machine learning models.
- Apply different machine learning methods to solve a given materials engineering problem. Select an optimum characterization technique for a given material under different circumstances.

Suggested Books

- Deep learning by I. Goodfellow, Y. Bengio, A. Courville. MIT Press (2016).
- Hands-on machine learning with Scikit-Learn, Keras, and TensorFlow by A. Geron. 2nd ed., O'Reilly Media (2019).
- Machine Learning in Materials Science by K. T. Butler, F. Oviedo, P. Canepa. American Chemical Society (2022).
- Artificial Intelligence for Materials Science by Y. Cheng, T. Wang, G. Zhang, 1st ed., Springer (2021).