MASC 515 Basics of Machine Learning for Materials

Units: 4
Spring 2023

Time: 12-1:50pm, MW
Location: WPH 101

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Teaching Assistant: TBD
Office Hours: TBD
Contact Info: TBD
Course Description

Artificial Intelligence (AI) and Machine Learning (ML), the fourth paradigm for data-driven scientific discovery, are an essential skillset to build competitive workforces for the future. Design and development of novel materials has been a long and time-consuming process because of the inherently large parameter space. Recent evaluations in AI and ML have enabled unprecedented predictive capability of novel materials and their functionalities. Combined with rapidly advancing data science tools and online database infrastructures, data-driven modeling has become a promising approach for material innovations.

This is a graduate-level course to introduces basics of AI and ML for students with materials science and related engineering backgrounds. The course also offers hands-on tutorials of Python programming, Object Oriented Programming, and data science tools (Jupyter notebook, Scikit-learn, Pandas and Pytorch). No prior experience of programming nor computer science background is needed.

Learning Objectives

Students will learn basics of AI/ML and Python programming in order to,

1. Familiarize data-driven problem-solving approach and learn how to implement your idea using Python.
2. Work on an end-to-end ML workflow to model materials properties using data science tools and online database.
3. Understand deep learning architectures (MLP, CNN, RNN, GNN) and carry out materials modeling and characterization simulations on cloud platforms.

Prerequisite(s): None

Recommended Preparation: None

Course Notes: Grading type: letter grade. All course notes will be provided on Blackboard.

Technological Proficiency and Hardware/Software Required: Personal laptop computer is necessary to work on hands-on tutorials.

Recommended Readings


Course Breakdown:

- Basic calculus, statistics, and probabilities
- Regression and Classification
- Supervised, Unsupervised and Reinforcement Learning
- Linear models, Logistic Regression, Decision Tree, Random Forest, Support Vector Machine
- Deep learning models (MLP, CNN, RNN, GNN)
- Python programming and ML/AL tools (scikit-learn, numpy, Pandas, pytorch, Jupyter notebook)
- Materials databases & Cloud computing
Grading Breakdown

<table>
<thead>
<tr>
<th>Assignment</th>
<th>% of Grade</th>
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<tbody>
<tr>
<td>Homework</td>
<td>30%</td>
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<tr>
<td>Materials Modeling Projects</td>
<td>30%</td>
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<tr>
<td>Discussion</td>
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<td>Final Presentation</td>
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<td>TOTAL</td>
<td>100%</td>
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