



MASC 515 Basics of Machine Learning for Materials

Units: 4
Spring 2023

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

Instructor: Ken-ichi Nomura
Office: VHE 609
Office Hours: TBD
Contact Info: knomura@usc.edu

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 introduce 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

- *An Introduction to Statistical Learning* by G. James, D. Witten, T. Hastie, R. Tibshirani, ISBN-13: 978-1461471370
- *Deep Learning*, by I. Goodfellow, Y. Bengio, A. Courville ISBN-13: 978-0262035613
- *Effective Computation in Physics: Field Guide to Research with Python*, A. Scopatz & K. D. Huff, ISBN-13: 978-1491901533

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

Assignment	% of Grade
Homework	30%
Materials Modeling Projects	30%
Discussion	20%
Final Presentation	20%
TOTAL	100%

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else’s ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, “Behavior Violating University Standards” policy.usc.edu/scampus-part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, policy.usc.edu/scientific-misconduct.

Support Systems:

Counseling and Mental Health - (213) 740-9355 – 24/7 on call
studenthealth.usc.edu/counseling

Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

National Suicide Prevention Lifeline - 1 (800) 273-8255 – 24/7 on call
suicidepreventionlifeline.org

Free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week.

Relationship and Sexual Violence Prevention and Services (RSVP) - (213) 740-9355(WELL), press “0” after hours – 24/7 on call
studenthealth.usc.edu/sexual-assault

Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

Office of Equity and Diversity (OED)- (213) 740-5086 | Title IX – (213) 821-8298
equity.usc.edu, titleix.usc.edu

Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants. The university prohibits discrimination or harassment based on the following *protected characteristics*: race, color, national origin, ancestry, religion, sex, gender, gender identity, gender expression, sexual orientation, age, physical disability, medical condition, mental disability, marital status, pregnancy, veteran status, genetic information, and any other characteristic which may be specified in applicable laws and governmental regulations. The university also prohibits sexual assault, non-consensual sexual contact, sexual misconduct, intimate partner violence, stalking, malicious dissuasion, retaliation, and violation of interim measures.

Reporting Incidents of Bias or Harassment - (213) 740-5086 or (213) 821-8298
usc-advocate.symplicity.com/care_report

Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity | Title IX for appropriate investigation, supportive measures, and response.

The Office of Disability Services and Programs - (213) 740-0776

dsp.usc.edu

Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.

USC Support and Advocacy - (213) 821-4710

uscса.usc.edu

Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity at USC - (213) 740-2101

diversity.usc.edu

Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call

dps.usc.edu, emergency.usc.edu

Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-120 – 24/7 on call

dps.usc.edu

Non-emergency assistance or information.