USC Viterbi
School of Engineering

MASC 515 Basics of Machine Learning for Materials
Section 32129

Units: 4
Fall 2021

Time: 12-1:50pm, MW
Location: GFS111

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Teaching Assistant: TBD
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Course Description

This course introduces basics of materials modeling using machine learning (ML) and data science techniques. Discovery of novel materials has been a long and time-consuming process because of the inherently large materials design spaces. Recent progresses in theory and experiment have enabled unprecedented predictive capability of novel materials and their functionalities. Combined with rapidly advancing data science methodologies and database infrastructures, data-centric materials modeling has become a promising approach to accelerate the design and discovery of novel materials, resulting in many applications in the materials science and engineering fields.

This is a graduate-level course to introduces basics of ML for students with materials science and related engineering backgrounds. This course also offers Python hands-on programming exercises and basic math to understand ML models, but no prior experience of programming nor computer science background is needed.

Learning Objectives

Students will learn basic knowledge and hands-on experience in order to:

1. Understand basics of ML algorithms, theories, and their applications for materials.
2. Develop suitable ML model to predict materials properties using data science tools.
3. Perform ML-assisted materials modeling and carry out simulation on cloud computer.

Prerequisite(s): None

Recommended Preparation: Basic Python programming, Calculus, Linear Algebra, and Probability.

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 class projects.

Recommended Readings

- *Effective Computation in Physics: Field Guide to Research with Python,* A. Scopatz & K. D. Huff, ISBN-13: 978-1491901533
- *Deep Learning*, I. Goodfellow, Y. Bengio, A. Courville ISBN-13: 978-0262035613

Grading Breakdown

Assignment	Points	% of Grade
Homework	100	40%
Midterm	100	30%
Projects	100	30%
TOTAL	300	100%

Course Breakdown:

- Basic calculus, statistics, and probabilities
- Linear model: regression and classification
- Loss function, regularization, generalization
- Logistic regression, decision tree, random forest, support vector machine
- Unsupervised learning (clustering, dimensionality reduction)
- Deep learning (MLP, CNN, RNN)
- Python programming (scikit-learn, pytorch, Jupyter notebook)
- Materials database (Materials Project, Citrination)

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
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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.

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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

uscsa.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.