



## **MASC 515 – Basics of Machine Learning for Materials**

**Units: 4**

**Spring, 2024 M/W 12-1:50 pm**

**Location: DMC 101**

**Instructor: Paulo Branicio**

**Office: VHE 602**

**Office Hours: In-person/Online Wed 4-5pm. Email to book a time slot or request another time.**

**Contact Info: [branicio@usc.edu](mailto:branicio@usc.edu). Emails are replied within 24 hours.**

**Teaching Assistant: TBD**

**Office: TBD**

**Office Hours: TBD**

**Contact Info: TBD**

### **Course Description**

Artificial Intelligence (AI) and Machine Learning (ML) are at the forefront of the fourth paradigm in scientific discovery, evolving from empirical observation and experimentation, theoretical models, and computational science and simulations. This shift underscores their importance for future workforce competitiveness. The development of new materials, once a time-intensive process, is revolutionized by AI and ML, offering new predictive capabilities, and harmonizing with data science advancements for innovative material design. This graduate-level course introduces AI and ML fundamentals to students in materials science and related engineering fields. It offers practical tutorials in Python programming, Object-Oriented Programming, and data science tools such as Jupyter Notebooks and PyTorch. The course is accessible to those without prior programming or computer science background.

### **Learning Objectives**

Students will gain foundational knowledge in AI/ML and Python programming, enabling them to:

- Acquire a data-driven problem-solving mindset and apply Python to bring their innovative ideas to fruition.
- Execute a comprehensive ML workflow to predict material properties, utilizing data science tools and online databases.
- Understand various deep learning architectures, including MLP, CNN, RNN, and GNN, and carry out materials modeling and characterization through cloud-based simulations.

**Prerequisite(s):** 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 with Applications in Python*, Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani, Jonathan Taylor, ISBN-13 978-3031387463
- *Effective Computation in Physics: Field Guide to Research with Python*, A. Scopatz & K. D. Huff, ISBN-13: 978-1491901533
- *Deep Learning*, by I. Goodfellow, Y. Bengio, A. Courville ISBN-13: 978-0262035613

## 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%
Discussion	20%
Materials Modeling Project	30%
Final Presentation	20%
<b>TOTAL</b>	<b>100%</b>

## Academic Integrity:

The University of Southern California is a learning community committed to developing successful scholars and researchers dedicated to the pursuit of knowledge and the dissemination of ideas. Academic misconduct, which includes any act of dishonesty in the production or submission of academic work, compromises the integrity of the person who commits the act and can impugn the perceived integrity of the entire university community. It stands in opposition to the university's mission to research, educate, and contribute productively to our community and the world.

All students are expected to submit assignments that represent their own original work, and that have been prepared specifically for the course or section for which they have been submitted. You may not submit work written by others or "recycle" work prepared for other courses without obtaining written permission from the instructor(s).

Other violations of academic integrity include, but are not limited to, cheating, plagiarism, fabrication (e.g., falsifying data), collusion, knowingly assisting others in acts of academic dishonesty, and any act that gains or is intended to gain an unfair academic advantage.

The impact of academic dishonesty is far-reaching and is considered a serious offense against the university. All incidences of academic misconduct will be reported to the Office of Academic Integrity and could result in outcomes such as failure on the assignment, failure in the course, suspension, or even expulsion from the university.

For more information about academic integrity see [the student handbook](#) or the [Office of Academic Integrity's website](#), and university policies on [Research and Scholarship Misconduct](#).

Please ask your instructor if you are unsure what constitutes unauthorized assistance on an exam or assignment, or what information requires citation and/or attribution.

### **Course Content Distribution and Synchronous Session Recordings Policies**

USC has policies that prohibit recording and distribution of any synchronous and asynchronous course content outside of the learning environment.

Recording a university class without the express permission of the instructor and announcement to the class, or unless conducted pursuant to an Office of Student Accessibility Services (OSAS) accommodation. Recording can inhibit free discussion in the future, and thus infringe on the academic freedom of other students as well as the instructor. ([Living our Unifying Values: The USC Student Handbook](#), page 13).

Distribution or use of notes, recordings, exams, or other intellectual property, based on university classes or lectures without the express permission of the instructor for purposes other than individual or group study. This includes but is not limited to providing materials for distribution by services publishing course materials. This restriction on unauthorized use also applies to all information, which had been distributed to students or in any way had been displayed for use in relationship to the class, whether obtained in class, via email, on the internet, or via any other media. ([Living our Unifying Values: The USC Student Handbook](#), page 13).

### **Students and Disability Accommodations:**

USC welcomes students with disabilities into all of the University's educational programs. [The Office of Student Accessibility Services](#) (OSAS) is responsible for the determination of appropriate accommodations for students who encounter disability-related barriers. Once a student has completed the OSAS process (registration, initial appointment, and submitted documentation) and accommodations are determined to be reasonable and appropriate, a Letter of Accommodation (LOA) will be available to generate for each course. The LOA must be given to each course instructor by the student and followed up with a discussion. This should be done as early in the semester as possible as accommodations are not retroactive. More information can be found at [osas.usc.edu](https://osas.usc.edu). You may contact OSAS at (213) 740-0776 or via email at [osasfrontdesk@usc.edu](mailto:osasfrontdesk@usc.edu).

### **Support Systems:**

[Counseling and Mental Health](#) - (213) 740-9355 – 24/7 on call

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

[988 Suicide and Crisis Lifeline](#) - 988 for both calls and text messages – 24/7 on call

The 988 Suicide and Crisis Lifeline (formerly known as the National Suicide Prevention Lifeline) provides free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week, across the United States. The Lifeline is comprised of a national network of over 200 local crisis centers, combining custom local care and resources with national standards and best practices. The new, shorter phone number makes it easier for people to remember and access mental health crisis services (though the previous 1 (800) 273-8255 number will continue to function indefinitely) and represents a continued commitment to those in crisis.

[Relationship and Sexual Violence Prevention Services \(RSVP\)](#) - (213) 740-9355(WELL) – 24/7 on call

Free and confidential therapy services, workshops, and training for situations related to gender- and power-based harm (including sexual assault, intimate partner violence, and stalking).

[Office for Equity, Equal Opportunity, and Title IX \(EEO-TIX\)](#) - (213) 740-5086

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.

[Reporting Incidents of Bias or Harassment](#) - (213) 740-5086 or (213) 821-8298

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

[The Office of Student Accessibility Services \(OSAS\)](#) - (213) 740-0776

OSAS ensures equal access for students with disabilities through providing academic accommodations and auxiliary aids in accordance with federal laws and university policy.

[USC Campus Support and Intervention](#) - (213) 740-0411

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

[Diversity, Equity and Inclusion](#) - (213) 740-2101

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

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) 442-1200 – 24/7 on call

Non-emergency assistance or information.

[Office of the Ombuds](#) - (213) 821-9556 (UPC) / (323-442-0382 (HSC)

A safe and confidential place to share your USC-related issues with a University Ombuds who will work with you to explore options or paths to manage your concern.

[Occupational Therapy Faculty Practice](#) - (323) 442-2850 or [otfp@med.usc.edu](mailto:otfp@med.usc.edu)

Confidential Lifestyle Redesign services for USC students to support health promoting habits and routines that enhance quality of life and academic performance.