

10744 - Machine Learning for Science

Fall 2025, Syllabus

August 26, 2025

Instructor Leila Wehbe. Office hours are by appointment or right after class.

Day, time, location: Tuesdays and Thursdays at 12:30pm-1:50pm, HH B131.

This course will cover important topics that surround the use of Machine Learning to create scientific models and make scientific inferences. This includes methodological domains such as robustness and reproducibility, statistical testing, model interpretability, post-selection inference, tradeoff of simplicity and predictivity, learning from scratch vs. implementing domain knowledge, the increasing use of deep learning to make scientific breakthroughs, etc. We will evaluate these topics in general as well as applied to specific scientific fields. We will also interact with a wide array of scientists from different disciplines on campus to understand how Machine Learning is currently applied in different domains of science (genomics, physics, chemistry, neuroscience, epidemiology, etc).

The course will include readings, discussions, interviews, weekly short quizzes and two midterm exams.

Topics Here is a list of the weeks of the class, with each one more or less focusing on a topic. Many of them will include a lecture by an invited speaker.

- **Week 1:** Introduction to Machine Learning and Scientific Modeling: Overview of ML in scientific discovery, prediction vs. explanation, types of models, and the role of ML in the scientific method.
- **Week 2:** Interpretability and Explainability in Scientific ML: Techniques for model interpretation, explainability tools, and scientific trust in model outputs.
- **Week 3:** Post-selection Inference and Statistical Testing: Challenges of inference after model selection, multiple comparisons, selective inference, and causal interpretations.
- **Week 4:** Robustness and Reproducibility in Scientific ML: Sensitivity analysis, reproducibility crisis, pre-registration, and robust experimental design.
- **Week 5:** Domain Knowledge vs. Learning from Scratch: Incorporating scientific priors, physics-informed ML, inductive biases, and theory-guided data science.
- **Week 6:** Causal inference: correlation vs. causation, mediation, causality in AI.
- **Week 7:** Extra topics, review & Midterm 1.
- **Week of October 13:** *Fall Break – No Class*
- **Week 8:** Deep Learning for Neuroscience and Cognitive Science.
- **Week 9:** Deep Learning for Epidemiology.
- **Week 10:** Deep Learning for Computational Biology.
- **Week 11:** Deep Learning for Physics and Chemistry.
- **Week 12:** Deep Learning for Environmental and Earth Sciences: ML for climate modeling, remote sensing, and ecological forecasting.
- **Week 13:** AI Driven Science: hypotheses generation, using AI for predictions along with data (e.g., prediction powered inference).
- **Week 14:** Extra topics, review and Midterm 2.

Learning Objectives: The aim of this class is to enable students to:

- develop an understanding of the methodological and procedural considerations related to applying machine learning for scientific inquiry,
- develop critical thinking in analyzing and interpreting machine learning results,
- survey recent breakthroughs in science that rely on machine learning and AI,
- connect with researchers on campus.

Prerequisites Any version of intro to machine learning or similar class (10301, 10315, 10405, 10601, 10605, 10701, 10715). If you believe your background from other coursework or experience is equivalent, please contact the instructor.

Credits and assessment structure The course is a 12 unit class. The graded components are as follows:

- 50% lecture quizzes. Each lecture, a very short quiz will be administered on the materials from the last lecture, with open handwritten notes allowed (the 20 best scores will be counted towards the grade).
- 30% Midterms. Two in-class exams (one in the middle and one at the end of the semester. No final scheduled after the end of classes)
- 20% Participation in class discussion and in discussions with invited speakers.

Course policies

Screens Most of the work in this class will happen in class. You are discouraged from trying to do other work in class. Laptops and other screens are also discouraged. They can really interfere with your focus and learning. If you must use a laptop, I ask you to sit in the back or sides of the class to avoid distracting others.

Attendance This course is a discussion-based course and therefore attendance is essential for benefiting from it and contributing to it. Attendance will not be directly graded but every lecture there will be a quiz, and participation will be recorded. We understand that some events such as conferences will lead to absence. Please communicate your absence in advance to the course staff.

Collaboration Discussion of class material is heavily encouraged. Obviously, collaboration in quizzes and exams is not allowed.

Academic Integrity We have a zero tolerance policy for violation of class policies. If you are in any doubt in regards to the policy, please clarify with the course staff before proceeding.

- Any deviation from the rules will be dealt with according to the severity of the case.
- In line with university policy, all instances of cheating will be reported to your academic advisor and the dean of student affairs. See the university policy on academic integrity.

Additional information

Accommodations for Students with Disabilities

If you have a disability and are registered with the Office of Disability Resources, I encourage you to use their online system to notify me of your accommodations and discuss your needs with me as early in the semester as possible. I will work with you to ensure that accommodations are provided as appropriate. If you suspect that you may have a disability and would benefit from accommodations but are not yet registered with the Office of Disability Resources, I encourage you to contact them at access@andrew.cmu.edu.

Statement of Support for Students' Health & Well-being

Take care of yourself. Do your best to maintain a healthy lifestyle this semester by eating well, exercising, avoiding drugs and alcohol, getting enough sleep and taking some time to relax. This will help you achieve your goals and cope with stress.

If you or anyone you know experiences any academic stress, difficult life events, or feelings like anxiety or depression, we strongly encourage you to seek support. Counseling and Psychological Services (CaPS) is here to help: call 412-268-2922 and visit <http://www.cmu.edu/counseling/>. Consider reaching out to a friend, faculty or family member you trust for help getting connected to the support that can help.

If you or someone you know is feeling suicidal or in danger of self-harm, call someone immediately, day or night (CaPS: 412-268-2922, Resolve Crisis Network: 888-796-8226). If the situation is life threatening, call the police (On-campus CMU Police: 412-268-2323, Off-campus Police: 911).