CHEM 4930 — Chemical Applications of Machine Learning
Spring 2026

Updated: 1/13/2026

Instructor

- Dr. Omar Valsson
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Schedule

Lectures and hands-on computational labs: 11:00 am – 12:20 pm, Tuesday/Thursday in Chemistry Building, CCIL (CHEM 232).

All information given below is subject to change at the discretion of the instructor. All changes will be communicated to students via Canvas or email.

Office Hours

- Tuesday, 1:00 – 2:00 pm, or by appointment
- In-person at my office (Chem 205C)
- Can be online via Zoom if requested in advance
- A heads-up message if you are planning to come by would be appreciated

Description

The purpose of this course is to introduce the usage of machine learning (ML) method and artificial intelligence (AI) to study and model chemical systems and discuss the latest development within the field of ML/AI for chemical system. This course is intended for any undergraduate chemistry students interested in the usage of ML/AI for chemical applications, and it is also open to students from other majors, e.g., physics, biochemistry, biology, material science, and computer science.

The course will be heavily hands-on and project-based where the students will work on publicly available chemistry datasets and implement ML models, e.g., for predicting physical and molecular properties and chemical reactions. There will be a brief introduction to Python programing. The students will be introduced to ML frameworks such as pandas, sklearn, and PyTorch that they will use for their projects. Students will also be taught how to visualize data and results using python-based packages such as Matplotlib and Seaborn.

Prerequisite: C or better in CHEM 3520 (maybe taken concurrently) or consent of department.

Readings and Material

- No one single textbook covers the many aspects of applying machine learning to chemistry that will be discussed in this course.
- Main text: *Machine Learning for Physics and Astronomy*, Viviana Acquaviva (Princeton University Press, 2023).
- Other recommended and useful texts:
    - *Hands-On Machine Learning with Scikit-Learn and PyTorch: Concepts, Tools, and Techniques to Build Intelligent Systems*, Aurélien Géron (1st Edition, O'Reilly Media 2025)
    - *Deep Learning with Python, Third Edition,* Francois Chollet and Matthew Watson (Manning 2025)
    - *The Science of Deep Learning*, Iddo Drori (Cambridge University Press, 2022)
- Other reading material and handouts, including journal articles, will be made available on Canvas.
- All lecture slides and notes from my lectures will be made available on Canvas.

Course Objectives

At the completion of the course the students will understand the fundamentals of machine learning methods, including both supervised and non-supervised ML methods, and how linear and non-linear ML methods can be applied in chemistry, including modeling and prediction of physical and molecular properties and chemical reactivity. Students will learn the importance of feature selection and feature engineering for accurate description of chemical and molecular systems. Students will become familiar with the usage of python and ML frameworks to implement ML models. Students will learn about the latest developments in ML for chemistry, including generative AI models, such as large language models and diffusion models.

Course Outline/Schedule

The topics listed below is an estimate, and not all discussed topics might be listed. The order of topics is subject to change. Inevitably the pace of the lectures will adjust to the realities of the classroom, and we might not cover all the material.

- Introduction to python programming, python packages, working with datasets, visualization, and ML frameworks (NumPy, Pandas, Matplotlib, Seaborn, sklearn, PyTorch, RDKit) – **1/13, 1/15, 1/20, 1/22**
- Supervised machine learning methods – **1/27, 1/29, 2/3, 2/5**
- Features and descriptors used for chemical and molecular systems (SMILES, 0D, 1D, 2D, and 3D descriptors, fingerprints, SOAP) – **2/10, 2/12, 2/17, 2/19**
- Unsupervised machine learning methods (clustering, dimensionality reduction) – **2/24, 2/26, 3/3, 3/5**
- Deep learning (neural networks, autoencoders, variational autoencoders, graph neural networks, transformer) – **3/17, 3/19, 3/24, 3/26, 3/31, 4/2, 4/7**

- Exam **- 4/9**
- Generative AI models (diffusion models, large language models, ChatGPT) – **4/14, 4/16, 4/21, 4/23**

Course Grading

The course grades will be calculated as follows:

- Hands-on assignments – 50% (one worst graded assignment will be excluded from the final assignments)
- Exam – 20%
- Major final project – 30%

Note that there will be no final exam in the course.

Letter grades will be assigned based on the numerical scores: A = 90-100; B = 80-89; C = 70-79; D = 60-69.

Hands-on Assignments

- There will around 7-8 hands-on assignments throughout the semester, depending on the pace at which the material is covered.
- All assignments will be posted and collected via the internet.
- You must access your assignment online on the course website on Canvas, work the assignment, and submit your solutions by the due date indicated online.
- In general, no late assignments will be accepted. Deadline extensions may be given on a case-by-case basis for exceptional cases or for religious observance. Excused extensions should be arranged prior to the due date.
- Assignments will be graded, and the grades returned around two weeks after the due date. All questions concerning the grading of homework assignments must be directed to the instructor in writing within two weeks after the grades are returned to the class.
- The one worst assignment will be excluded from the final grade calculation of the assignments. All other assignments will carry equal weight towards the grade, unless otherwise instructed.

Exam

- There will be one exam during the semester.
- The exam is provisionally planned on April 9.
- The exact format of the exam will be detailed later.
- The exams questions will be based on lecture material, material contained in the texts and in the assignments.
- Any student caught cheating will be given a grade of zero for the midterm exam.
- All questions concerning the grading of the midterm exam must be directed to the instructor in writing within two weeks after the grades are returned to the class.

Major Final Project

- There will be a major final project where you will apply machine learning to a chemistry research problem.
- You can work on this project as a group, with a maximum of three group members per project.
- There will be a presentation on the final project in last week of class, provisionally planned on April 28.
- Further information will be given later.

AI Usage Policy

- You are fully allowed and even encouraged to use AI tools such as large language models (LLM) (e.g., ChatGPT, Gemini, Copilot) to aid with writing code and code blocks.
- Such tools are powerful and often give you code that runs but might not do what you want it to do. Thus, use such tools with care. You are expected to understand any code in the work that you submit.
- Final responsibility for the correctness of your work and code rests with you.
- In any submission, you must state which parts of the work you employed AI tools to assist you.

Class Policy

- Connect with me through email and/or by attending office hours. During busy times, my inbox becomes rather full, so if you contact me and do not receive a response within two business days, please send a follow up email. A gentle nudge is always appreciated.
- Research has shown that students who attend class are more likely to be successful. Therefore, attendance to the lectures is, in principle, mandatory and you should attend every class. Acceptable exceptions will be approved on a case-by-case basis. Acceptable university excused absence include active military service, a religious holy day, or an official university function as stated in the Student Attendance and Authorized Absences Policy (PDF). If you cannot attend a class due to an emergency, please let me know. Your safety and well-being are important to me.
- It is important for all of us to be mindful of the health and safety of everyone in our community. Please contact the instructor if you are unable to attend class because you are ill, or unable to attend class due to a health related issue. Acceptable exceptions will be approved on a case-by-case basis.
- I value the many perspectives students bring to our campus. Please work with me to create a classroom culture of open communication, mutual respect, and inclusion. All discussions should be respectful and civil. Although disagreements and debates are encouraged, personal attacks are unacceptable. Together, we can ensure a safe and welcoming classroom for all. If you ever feel like this is not the case, please stop by my office and let me know. We are all learning together.
- Being punctual indicates our respect for others. Please arrive before class begins to find a seat, prepare your materials, and connect with your peers. The beginning of class is

especially critical—just like the beginning of a movie or book. Being late to class is sometimes inevitable. If you are late, know that you are welcome to join the class, but please do so without distracting others. More than two instances of tardiness will result in an absence from class.

- Silence mobile phones prior to attending class. Put mobile phones away.
- Learning is a two–way street, therefore, I will ask you for feedback throughout the course. I will take your feedback seriously, and work hard to incorporate your ideas on how to improve the course.
- My policy in this class is to not communicate any details regarding your grade through email. I will only discuss these details in private in-person meetings or through private online meetings.

Ancillary Information

Succeed at UNT

UNT endeavors to offer you a high-quality education and to provide a supportive environment to help you learn and grown. And, as a faculty member, I am committed to helping you be successful as a student. Here's how to succeed at UNT: Show up. Find Support. Get advised. Be prepared. Get involved. Stay focused. To learn more about campus resources and information on how you can achieve success, go to http://success.unt.edu/.

Legal Notice Regarding Lecture Notes

My lectures and notes are protected by state common law and federal copyright law. You are authorized to take notes in class thereby creating a derivative work from my lecture, but the authorization extends only to making one set of notes for your own personal use and no other use. You are not authorized to record my lectures, to provide your notes to anyone else (hard copy or electronic), or to make any other use of those notes without express prior written permission from me.

Academic Dishonesty

Students caught cheating or plagiarizing will receive a "0" for that particular assignment or exam. Additionally, the incident will be reported to the Dean of Students, who may impose further penalty. According to the UNT catalog, the term "cheating" includes, but is not limited to: (a) use of any unauthorized assistance in taking quizzes, tests, or examinations; (b) dependence upon the aid of sources beyond those authorized by the instructor in writing papers, preparing reports, solving problems, or carrying out other assignments; (c) the acquisition, without permission, of tests or other academic material belonging to a faculty or staff member of the university; (d) dual submission of a paper or project, or resubmission of a paper or project to a different class without express permission from the instructor(s); or (e) any other act designed to give a student an unfair advantage. The term "plagiarism" includes, but is not limited to: (a) the knowing or negligent use by paraphrase or direct quotation of the published or unpublished work of another person without full and clear acknowledgment; and

(b) the knowing or negligent unacknowledged use of materials prepared by another person or agency engaged in the selling of term papers or other academic materials. Further information on UNT's policy on ***Academic Dishonesty*** can be found at: http://www.vpaa.unt.edu/academic-integrity

Acceptable Student Behavior

Student behavior that interferes with an instructor's ability to conduct a class or other students' opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UNT. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student's conduct violated the Code of Student Conduct. The university's expectations for student conduct apply to all instructional forums, including university and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct can be found at http://deanofstudents.unt.edu.

Withdrawal from Class

The administration of this institution has set deadlines for withdrawal of any college-level courses. These dates and times are published in that semester's course catalog. Administration procedures must be followed. It is the student's responsibility to handle withdrawal requirements from any class. In other words, I cannot drop or withdraw any student. You must do the proper paperwork to ensure that you will not receive a final grade of "F" in a course if you choose not to attend the class once you are enrolled.

ADA Policy

The University of North Texas makes reasonable academic accommodation for students with disabilities. Students seeking reasonable accommodation must first register with the Office of Disability Access (ODA) to verify their eligibility. If a disability is verified, the ODA will provide you with a reasonable accommodation letter to be delivered to faculty to begin a private discussion regarding your specific needs in a course. You may request reasonable accommodations at any time; however, ODA notices of reasonable accommodation should be provided as early as possible in the semester to avoid any delay in implementation. Note that students must obtain a new letter of reasonable accommodation for every semester and must meet with each faculty member prior to implementation in each class. Students are strongly encouraged to deliver letters of reasonable accommodation during faculty office hours or by appointment. Faculty members have the authority to ask students to discuss such letters during their designated office hours to protect the privacy of the student. For additional information, refer to the Office of Disability Access website (http://www.unt.edu/oda). You may also contact ODA by phone at (940) 565-4323.

Canvas

Canvas will be used to post course materials and your grades. To get to this resource, go to https://unt.instructure.com/login/canvas and follow the UNT link to log on. (You will log on using your UNT EUID and password.) Once logged on, select this course.

Course Evaluation - Student Perceptions On Teaching (SPOT)

Student feedback is important and an essential part of participation in this course. The Student Perceptions On Teaching (SPOT) is a requirement for all organized classes at UNT. This short survey will be made available at the end of the semester to provide you with an opportunity to evaluate how this course is taught.

Retention of Student Records

Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Canvas online system, including grading information and comments, is also stored in a safe electronic environment for one year. You have a right to view your individual record; however, information about your records will not be divulged to other individuals without the proper written consent. You are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the university's policy in accordance with those mandates at the following link: http://essc.unt.edu/registrar/ferpa.html

Emergency Notification and Procedures

UNT uses a system called Eagle Alert to quickly notify you with critical information in the event of an emergency (i.e., severe weather, campus closing, and health and public safety emergencies like chemical spills, fires, or violence). The system sends voice messages (and text messages upon permission) to the phones of all active faculty staff, and students. Please make certain to update your phone numbers at http://www.my.unt.edu. Some helpful emergency preparedness actions include: 1) know the evacuation routes and severe weather shelter areas in the buildings where your classes are held, 2) determine how you will contact family and friends if phones are temporarily unavailable, and 3) identify where you will go if you need to evacuate the Denton area suddenly. In the event of a university closure, please refer to Canvas for contingency plans for covering course materials.

Sexual Assault Prevention

UNT is committed to providing a safe learning environment free of all forms of sexual misconduct, including sexual harassment sexual assault, domestic violence, dating violence, and stalking. Federal laws (Title IX and the Violence Against Women Act) and UNT policies prohibit discrimination on the basis of sex, and therefore prohibit sexual misconduct. If you or someone you know is experiencing sexual harassment, relationship violence, stalking, and/or sexual assault, there are campus resources available to provide support and assistance. UNT's Survivor Advocates can assist a student who has been impacted by violence by filing protective orders, completing crime victim's compensation applications, contacting professors for absences related to an assault, working with housing to facilitate a room change where appropriate, and connecting students to other resources available both on and off campus. The Survivor Advocates can be reached at SurvivorAdvocate@unt.edu or by calling the Dean of Students

Office at 940-565- 2648. Additionally, alleged sexual misconduct can be non-confidentially reported to the Title IX Coordinator at oeo@unt.edu or at (940) 565 2759.