

Course Syllabus

December 11, 2024

Course Title Applications of Chemometrics

Course Code CHM1157H

Instructor Michael DM Dryden <mk.dryden@utoronto.ca>

Office Hours 13:00–14:00 Wednesdays, MY820

Semester Winter 2025

Class Schedule Tuesdays and Thursdays, 13:00–14:00

Location SS1080 (Tuesdays) & SS2125 (Thursdays)

Hybrid option Classes will be provided live over Zoom or Teams, particularly for UTM/UTSC students, but in person attendance is preferred. Online participants are expected to keep their webcams on at all times.

Course Description

This course provides a comprehensive introduction to chemometrics, emphasizing statistical and machine learning methods applied to chemical data. Students will learn the fundamentals of key topics in chemometrics, be introduced to modern chemometric tools, and understand the integration of AI/ML techniques in chemometric analysis. The course will also cover essential statistical concepts, introductory image analysis, and the practical applications of chemometrics in scientific research.

Course Objectives

- To understand the fundamental principles and applications of chemometrics.
- To develop the skills to understand and select chemometric techniques to solve different types of problems.
- To explore AI and machine learning methodologies as applied to chemical data.

Course Outline

Topics and order are subject to change.

Week 1–2 Introduction to Chemometrics

- Fundamental concepts of chemometrics

- Overview of applications in chemistry and related fields
- Information theory

Week 3–4 Review of Basic Statistical Concepts

- Gaussian error model
- Fitting & residuals
- Correlation
- Non-parametric methods
- Sampling

Week 5 Data Acquisition

- Digital signals
- Frequency-domain analysis

Week 6 Multivariate Data Analysis

- Dimensionality reduction
- Cluster analysis
- Factor analysis

Week 7 Experimental Design and Optimization

- Design patterns
- Optimization techniques

Week 8 Introduction to Image Analysis

- Image acquisition and processing
- Image analysis techniques in chemometrics
- Applications of image analysis in chemistry

Week 9–10 AI and ML Methods in Chemometrics

- Machine learning basics
- Supervised and unsupervised learning
- Neural networks and deep learning in chemometrics

Week 11–12 Presentations

- Student presentations and group discussions

Assessment Methods

Participation 20%

- Grade will be based on attendance and participation in class discussions and peer review for the written report (see below)

Presentation 40%

- Each student will present a 40 minute (+ questions) lecture on a chemometrics related topic of their choice
- Presentation should be styled to give the other students an introduction to this topic, a basic explanation of the implementation of related methods, and examples showing how problems are solved conceptually within the topic
 - For example, for the topic “Image preprocessing”, the presentation could introduce the concept of preprocessing and when/why it is needed, examine some specific areas of preprocessing and the techniques used, and present detailed examples (e.g., demonstrate a few raw images with varying brightness and show a couple of methods for normalizing them, explaining the differences between them and when to use each one)
- Tentatively Weeks 11–12
- Topics should be selected by Week 6 to avoid any duplicated topics
- Presentation grade based upon the quality and ease of understanding of the presentation

Written Review or Project 40%

- Each student will select one of two options:
 1. A short (20–30 pages) written review of a topic in chemometrics, including a literature review, explanation of the topic, and examples of its applications
 2. A project applying chemometric techniques to real data, delivering the raw analysis program/script and a 2–3 page summary of the methods and results. To select this option, students **must** discuss their proposed project with the instructor by Week 6.
- A draft of the written review or project summary is due by Week 10 for peer review, and the final version is due by the end of the semester. (Exact dates TBA)
- Written reports or project summaries will be peer-reviewed by another student in the class, and comments will be submitted to the instructor and author by the end of Week 11.
- *Note: since no term work is to be submitted before the final date to withdraw from the course without academic penalty (Feb 28), no grades will be available before this date.*

Course Policies

- Each member of this course is expected to maintain a:
 1. professional and respectful attitude during all course activities, including classes, laboratories, tutorials, and other online activities.
 2. personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
 3. collection of notes recorded independently based on concepts covered in course activities (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation)
 4. familiarity with the university policy on Academic Integrity
- The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another’s differences. The CHM1157H Teaching team will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and

we wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment, and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our [Equity Offices](#).

- Students may use artificial intelligence tools (including generative AI) in this course as learning aids or to help produce assignments. This use must be documented in an appendix for each assignment.
 - The documentation should include what tool(s) were used, how they were used, and how the results from the AI were incorporated into the submitted work.
 - Students are ultimately accountable for the work they submit (make sure citations are real!)
- Late submissions of assignments incur a penalty of 5% per day.

Institutional Policies and Support

Academic Integrity

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The [University of Toronto's Code of Behaviour on Academic Matters](#) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see www.academicintegrity.utoronto.ca/).

Copyright

If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited. More information regarding this is available [here](#).

Accessibility Needs

Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact [Accessibility Services](#) as soon as possible.

Accommodations for Religious Observances

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor before the session/assignment date to arrange accommodations.

Additional Services & Support

The following are some important links to help you with academic and/or technical service and support:

- School of Graduate Studies' [Policies and Guidelines](#)
- Full library service and resources on conducting online research through University of Toronto Libraries [University Libraries Research](#)
- Resources on academic support from the [Academic Success Centre](#)
- Learner support at the [Writing Centre](#)
- Information for [Technical Support/Quercus Support](#)

Acknowledgement of Traditional Lands

We wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.