Chemometrics Syllabus

Department of Chemistry

Chemistry 4205B/5205B Winter 2026

Dalhousie University acknowledges that we are in Mi'kma'ki, the ancestral and unceded territory of the Mi'kmaq People and pays respect to the Indigenous knowledges held by the Mi'kmaq People, and to the wisdom of their Elders past and present. The Mi'kmaq People signed Peace and Friendship Treaties with the Crown, and section 35 of the Constitution Act, 1982 recognizes and affirms Aboriginal and Treaty rights. We are all Treaty people.

Dalhousie University also acknowledges the histories, contributions, and legacies of African Nova Scotians, who have been here for over 400 years.

Course Instructor(s)

Name	Email	Office Hours
Dr. Michael Freund	michael.freund@dal.ca	By appointment

Course Description

The application of statistical tools to univariate and multivariate chemical measurements is explored. Topics include descriptive statistics, probability and probability distributions, propagation of errors, hypothesis testing, analysis of variance, experimental design, univariate and multivariate calibration, pattern recognition, exploratory data analysis and mixture analysis. Students are introduced to programming in MatLab.

Course Prerequisites

CHEM 2201 or equivalent with a grade of C- or better.

The class will begin at a fundamental level and will assume a basic familiarity with chemical measurements, calculus, and computers (Windows/Mac, spreadsheets, etc.). A background in statistics, linear algebra, and/or programming will be helpful, but these are not required.

Course Structure

Lectures

The **classroom lectures (MW) 8:35-9:25** in room 1108 Mona Campbell Building. Fridays will involve completing and submitting exercises through Brightspace on your own computer.

Exercises

Exercises will be distributed approximately weekly. They must be submitted through Brightspace but are not marked. However, they serve as the basis tests and on-time, online submissions will be part of the participation grade.

MatLab and MatLab Tutorials

A main objective of this course is to develop computer programming skills. The programming language MatLab, widely used in science and engineering, will be used to introduce computer programming in the context of data analysis techniques central to scientific measurements.

Students are expected to develop a familiarity with the language and the environment. For this purpose, MatLab self-paced online courses will be completed (matlabacademy.mathworks.com). A range of resource material is available on the MathWorks website (e.g. www.mathworks.com/videos.html), on YouTube, and within the MatLab environment.

Information on installing MatLab using the Dalhousie site license is available on Brightspace under "General Information".

Course Materials

Required Course Materials

Text: Material is drawn from several sources and there is no formal text for the class. There are several useful reference texts in the library.

Lecture Notes: Copies of the Lecture Notes will be available in Brightspace and consist of reproductions of the lecture slides.

Software: The class will make extensive use of the MATLAB programming environment. This software is available on most Dalhousie computers and is available for download through a Dalhousie license. To download the software, go to https://software.library.dal.ca and follow instructions to create a MathWorks account with your Dal email address.

Web Site

A website will be set up through Brightspace to provide information and act as a repository for files. Online lectures, tutorials, lecture notes and other materials will be available through this resource.

Assessment

The following grading schemes will be used for Chemistry 4205 and 5205

Component	Chem 4205	Chem 5205	Dates (subject to change)
Participation	25%	20%	Attendance and exercises
Term Test #1	25%	20%	Friday, Jan. 30
Term Test #2	25%	20%	Friday, Mar. 6
Term Test #3	25%	20%	Wednesday, Apr. 8
Project	NA	20%	Thursday Ap. 9

***Participation*:** Students are required to attend lectures, complete tasks and submit exercises. The overall percentage will include 5% lecture attendance and the remainder determined by tasks and exercise completion.

***Tests*:** Tests will be administered on the dates specified unless changed by consensus of the class. The first test (closed-book, in class) is not computer-based. The second and third test will have a closed-book, in-class portion as well as an open book take-home computer-based portion involving MatLab.

***Projects*:** For **graduate students** (Chem 5205) there will be a project component to the class. Projects can take on various forms, but typically involve the application of some of the methods discussed in class to real data from a research problem. Completion of the project involves the preparation of a report at the end of term. A one-page project proposal is due before the winter break and by the end of class on February 13th. Students are encouraged to start thinking about their project early and discuss it with the instructor prior to the proposal deadline.

Conversion of numerical grades to final letter grades follows the Dalhousie Grade Scale

A+ (90-100)	B+ (77-79)	C+ (65-69)	D (50-54)
A (85-89)	B (73-76)	C (60-64)	F (0-49)
A- (80-84)	B- (70-72)	C- (55-59)	

Course Policies on Missed or Late Academic Requirements

Absences. If students are unable to complete a test at the scheduled time due to illness or other valid reasons, they are responsible for notifying the instructor as follows.

- E-mail the instructor (michael.freund@dal.ca) within 24 hours, preferably in advance.
- Submit a **Student Declaration of Absence** (available on Brightspace under "General Information) on Brightspace. This form applies for illnesses lasting no longer than three days and may only be used twice during the term.

For tests and exams, the option of a make-up test or prorating of marks is at the discretion of the professor.

E-mail. In order to manage email traffic and to receive responses in a timely manner, use e-mail for administrative or personal matters. Questions related to content, exercises and common issues should be addressed during scheduled office hours. MSF will not be able to reply to e-mails asking how to solve problems or asking to repeat information from the lecture. In cases where students working together are unable to tackle an exercise question, a meeting can be scheduled during office hours.

Course Policies related to Academic Integrity

This course maintains the usual expectations for academic integrity (see Section B for more information). In particular, program code written is expected to represent the original work of the student. While program elements may be extracted from course notes and examples, ***exchange of code with other students or generation of code by generative AI and large language models in the context of submitted material will be considered an academic offense.***

Learning Objectives

- Calculate basic statistical parameters (mean, standard deviation, confidence intervals, etc.).
- Apply the operations and principles of basic linear algebra to vectors and matrices.
- Devise and implement algorithms relevant to the concepts below in the MatLab programming environment, including data input and output, manipulation, subfunctions, and graphics.
- Calculate simple and complex probabilities using basic rules.
- Describe the origins, properties and relevance of common probability distributions (binomial, Poisson, normal, etc.) and distinguish between discrete and continuous distributions.
- Apply the binomial distribution to problems of sampling uncertainty.
- Characterize the nature and origins of instrumental noise.
- Calculate probabilities and confidence intervals from statistical tables.
- Describe the origins of measurement errors and apply methods for their evaluation.
- Evaluate uncertainty in a calculated result using the general method for error propagation.
- Apply and interpret statistical tests for common comparisons (means, variances, distributions, etc).
- Apply analysis of variance (ANOVA) for multiple comparisons.
- Describe the principles of good experimental design and recognize/construct basic designs.
- Evaluate regression parameters for linear, curvilinear and multilinear regression (weighted and unweighted cases).
- Assess the regression model and calculate properties of regression parameters (variance, confidence intervals, etc.) and of linear calibration (e.g. limit of detection).
- Develop first-order calibration models using classical least squares (CLS), inverse least squares (ILS) and principal components regression (PCR).
- Calculate and assess figures of merit associated with first-order calibration (sensitivity, etc.).
- Decompose a matrix by principal components analysis (PCA) and interpret the results in terms of scores, loadings, eigenvalues, variance, etc.
- Describe the differences between errors of calibration, validation, prediction and cross-

validation and their roles in model selection.
- Apply PCA to exploratory data analysis and interpret the results.
- Describe and apply common methods for clustering and classification.
- Apply PCA for the determination of the number of components in a mixture.
- Apply target-testing to evaluate the presence of a component in a complex mixture.

Course Content

The following is a list of topics covered in this course. A detailed list of learning outcomes follows

1. Introduction
2. Probability and Probability Distributions
3. Binomial Distribution and the Sampling of Solids
4. Poisson Distribution and Instrumental Noise
5. Gaussian Distribution and Confidence Intervals
6. Chi-Squared Distribution and Uncertainty in Variance
7. Student-t Distribution and Confidence intervals
8. Propagation of Errors
9. Hypothesis Testing
10. Analysis of Variance (ANOVA)
11. Experimental Design
12. Univariate Regression and Calibration: Conventional Formulation
13. Linear, Curvilinear and Multilinear Regression: Matrix Formulation
14. Multivariate Calibration: Part 1
15. Principal Components Analysis
16. Multivariate Calibration: Part 2
17. Pattern Recognition and Exploratory Data Analysis
18. Mixture Analysis

Faculty of Science Course Syllabus (Section B)

Winter 2025

Chemistry 4205B/5205B: Chemometrics

University Policies and Statements

Recognition of Mi'kmaq Territory

Dalhousie University would like to acknowledge that the University is on Traditional Mi'kmaq Territory. The Elders in Residence program provides students with access to First Nations elders for guidance, counsel, and support. Visit or e-mail the Indigenous Student Centre at 1321 Edward St or elders@dal.ca. Additional information regarding the Indigenous Student Centre can be found at: https://www.dal.ca/campus_life/communities/indigenous.html

Internationalization

At Dalhousie, 'thinking and acting globally' enhances the quality and impact of education, supporting learning that is "interdisciplinary, cross-cultural, global in reach, and orientated toward solving problems that extend across national borders." Additional internationalization information can be found at: https://www.dal.ca/about-dal/internationalization.html

Academic Integrity

At Dalhousie University, we are guided in all our work by the values of academic integrity: honesty, trust, fairness, responsibility, and respect. As a student, you are required to demonstrate these values in all the work you do. The University provides policies and procedures that every member of the university community is required to follow to ensure academic integrity. Additional academic integrity information can be found at: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Student Accessibility Centre is Dalhousie's centre of expertise for matters related to student accessibility and accommodation. If there are aspects of the design, instruction, and/or experiences within this course (online or in-person) that result in barriers to your inclusion, please contact the Student Accessibility Centre (https://www.dal.ca/campus_life/academic-support/accessibility.html) for all courses offered by Dalhousie with the exception of Truro. For courses offered by the Faculty of Agriculture, please contact the Student Success Centre in Truro (https://www.dal.ca/about-dal/agricultural-campus/student-success-centre.html)

Conduct in the Classroom – Culture of Respect

Substantial and constructive dialogue on challenging issues is an important part of academic inquiry and exchange. It requires willingness to listen and tolerance of opposing points of view. Consideration of individual differences and alternative viewpoints is required of all class members, towards each other, towards instructors, and towards guest speakers. While expressions of differing perspectives are welcome and encouraged, the words and language used should remain within acceptable bounds of civility and respect.

Diversity and Inclusion – Culture of Respect

Every person at Dalhousie has a right to be respected and safe. We believe inclusiveness is fundamental to education. We stand for equality. Dalhousie is strengthened in our diversity. We are a respectful and inclusive community. We are committed to being a place where everyone feels welcome and supported, which is why our Strategic Direction prioritizes fostering a culture of diversity and inclusiveness (Strategic Priority 5.2). Additional diversity and inclusion information can be found at: http://www.dal.ca/cultureofrespect.html

Student Code of Conduct

Everyone at Dalhousie is expected to treat others with dignity and respect. The Code of Student Conduct allows Dalhousie to take disciplinary action if students don't follow this community expectation. When appropriate, violations of the code can be resolved in a reasonable and informal manner - perhaps through a restorative justice process. If an informal resolution can't be reached, or would be inappropriate, procedures exist for formal dispute resolution. The full Code of Student Conduct can be found at: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

Fair Dealing Policy

The Dalhousie University Fair Dealing Policy provides guidance for the limited use of copyright protected material without the risk of infringement and without having to seek the permission of copyright owners. It is intended to provide a balance between the rights of creators and the rights of users at Dalhousie. Additional information regarding the Fair Dealing Policy can be found at: https://www.dal.ca/dept/university_secretariat/policies/academic/fair-dealing-policy-.html

Originality Checking Software

The course instructor may use Dalhousie's approved originality checking software and Google to check the originality of any work submitted for credit, in accordance with the Student Submission of Assignments and Use of Originality Checking Software Policy. Students are free, without penalty of grade, to choose an alternative method of attesting to the authenticity of

their work and must inform the instructor no later than the last day to add/drop classes of their intent to choose an alternate method. Additional information regarding Originality Checking Software can be found at:
https://www.dal.ca/dept/university_secretariat/policies/academic/student-submission-of-assignments-and-use-of-originality-checking-software-policy-.html

Student Use of Course Materials

Course materials are designed for use as part of this course at Dalhousie University and are the property of the instructor unless otherwise stated. Third party copyrighted materials (such as books, journal articles, music, videos, etc.) have either been licensed for use in this course or fall under an exception or limitation in Canadian Copyright law. Copying this course material for distribution (e.g. uploading to a commercial third-party website) may lead to a violation of Copyright law.