

Faculty of Science Course Syllabus
Department of Chemistry
Chemistry 4205B/5205B
Chemometrics
Winter 2021

Professor: Dr. Michael Freund
Chemistry e-mail: michael.freund@dal.ca

Teaching Assistant: Jamie Stark e-mail: jm353545@dal.ca

Lectures: Asynchronous on Brightspace

Discussions: Synchronous, weekly 30 min discussions (TBD, required)

Office Hours: Brightspace by appointment

Course Description (from Calendar)

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

Required Course Materials

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

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

Software: The class will make extensive use of the MATLAB programming environment, particularly in the latter half. This software is available on most Dalhousie computers and is available for download through a Dalhousie license. To download the software, go to www.dal.ca/dept/its/its-services/software-download.html.

Web Site

A web-site has been 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.

Lectures

Asynchronous **online lectures** based on the Lecture Notes, are posted on Brightspace. Synchronous 30 minute meetings of small groups will be scheduled for interactive discussion of course material and progress (attendance required).

Assignments

Assignments will be distributed weekly. While not to be handed in or marked, they serve as the basis for quizzes and tests and are essential tools for study of the material and should be completed each week. A **Brightspace discussion forum for assignments** will be established and should be the first stop for questions and discussion related to each assignment. Students are encouraged to share information and work together to complete assignments.

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.

Although MatLab will be used more in the latter part of the course, students are expected to develop a familiarity with the language and the environment early. For this purpose, a series of MatLab Tutorials, specifically targeted for this course, have been posted on Brightspace and assignments will include MatLab components. A **Brightspace discussion forum** for MatLab will field questions and provide course information related to use of the software and will be monitored by Jamie Stark (TA). Alternatively, 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 Assessment

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

<u>Component</u>	<u>Chem 4205</u>	<u>Chem 5205</u>	<u>Dates (subject to change)</u>
Quizzes	20%	15%	Weekly (see schedule)
Participation	10%	10%	Weekly and discussion forum
Term Test #1	20%	20%	Wednesday, Feb. 22
Term Test #2	20%	20%	Tuesday, Apr. 5
Project	NA	15%	Due last week of classes
Final Exam	30%	20%	To be scheduled

Quizzes: Quizzes will be administered on approximately a weekly basis. Only the six best quizzes will be counted.

Participation: Students are required to attend and participate in synchronous small group discussions (approximately weekly) as well as to participate in the Brightspace assignment discussion board.

Tests: Tests will be administered online on the dates specified unless changed by consensus of the class. The first test (closed-book) is not computer-based. The second test (open-book) will be computer-based (involving MatLab).

Final Exam: The final examination (three hours) is scheduled by the Registrar and will be primarily computer-based (involving MatLab). The exam is open book.

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 and an in-class presentation at the end of term. Students are encouraged to start thinking about their project early and discuss it with the Instructor.

Grade Scale

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

	A+	A	A-	B+	B	B-	C+	C	C-	D	F
Chem 4205	90+	85+	80+	77+	73+	70+	65+	60+	55+	50+	<50
Chem 5205	90+	85+	80+	77+	73+	70+	-	-	-	-	<70

Course Policies

Absences. If students are unable to complete a test or participate in synchronous discussions 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 under “Assessments/Assignments”. This form applies for illnesses lasting no longer than three days and may only be used twice during the term. See Section B for more information

Absence from **quizzes** requires no notification or documentation. No make-up quizzes will be given, since the best six quiz marks are used.

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, assignments and common issues should be directed through the discussion boards (assignment and MatLab). 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 assignment question, MSF will review the discussion board and arrange a tutorial.

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 in the context of submitted material will be considered an academic offense.

Course Content

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

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

Course Objectives/Learning Outcomes

- 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.

Faculty of Science Course Syllabus (Section B) Winter 2021

Chemistry 4205B/5205B: Chemometrics

University Policies and Statements

(rev. June 2020)

This course is governed by the academic rules and regulations set forth in the University Calendar and by Senate

Missed or Late Academic Requirements due to Student Absence

As per Senate decision instructors may not require medical notes of students who must miss an academic requirement, **including the final exam**, for courses offered during fall or winter 2020-21 (until April 30, 2021). Information on regular policy, including the use of the Student Declaration of Absence can be found here: https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.html.

Academic Integrity

At Dalhousie University, we are guided in all of our work by the values of academic integrity: honesty, trust, fairness, responsibility and respect (The Center for Academic Integrity, Duke University, 1999). As a student, you are required to demonstrate these values in all of 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.

Information: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Advising and Access Services Centre is Dalhousie's centre of expertise for student accessibility and accommodation. The advising team works with students who request accommodation as a result of a disability, religious obligation, or any barrier related to any other characteristic protected under Human Rights legislation (Canada and Nova Scotia).

Information: https://www.dal.ca/campus_life/academic-support/accessibility.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.

Code: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

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

Statement: <http://www.dal.ca/cultureofrespect.html>

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 (1321 Edward St) (elders@dal.ca).

Information: https://www.dal.ca/campus_life/communities/indigenous.html

Important Dates in the Academic Year (including add/drop dates)

https://www.dal.ca/academics/important_dates.html

University Grading Practices

https://www.dal.ca/dept/university_secretariat/policies/academic/grading-practices-policy.html

Student Resources and Support

Advising

General Advising https://www.dal.ca/campus_life/academic-support/advising.html

Science Program Advisors: <https://www.dal.ca/faculty/science/current-students/academic-advising.html>

Indigenous Student Centre: https://www.dal.ca/campus_life/communities/indigenous.html

Black Students Advising Centre: https://www.dal.ca/campus_life/communities/black-student-advising.html

International Centre: https://www.dal.ca/campus_life/international-centre/current-students.html

Academic supports

Library: <https://libraries.dal.ca/>

Writing Centre: https://www.dal.ca/campus_life/academic-support/writing-and-study-skills.html

Studying for Success: https://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html

Copyright Office: <https://libraries.dal.ca/services/copyright-office.html>

Fair Dealing Guidelines <https://libraries.dal.ca/services/copyright-office/fair-dealing.html>

Other supports and services

Student Health & Wellness Centre: https://www.dal.ca/campus_life/health-and-wellness/services-support/student-health-and-wellness.html

Student Advocacy: <https://dsu.ca/dsas>

Ombudsperson: https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html

Safety

Biosafety: <https://www.dal.ca/dept/safety/programs-services/biosafety.html>

Chemical Safety: <https://www.dal.ca/dept/safety/programs-services/chemical-safety.html>

Radiation Safety: <https://www.dal.ca/dept/safety/programs-services/radiation-safety.html>

Scent-Free Program: <https://www.dal.ca/dept/safety/programs-services/occupational-safety/scent-free.html>