

Faculty of Science Course Syllabus
Department of Chemistry

Chemistry 4205B/5205B
Chemometrics
Winter 2018

Professor: Dr. Peter D. Wentzell
Room 511, Chemistry Ph. 902-494-3708 e-mail: peter.wentzell@dal.ca

Lectures: MWF 9:35-10:25, Chemistry 223
Some lectures will also be held in Room 2019 of the McCain Arts and Social Sciences Building (computer lab)

Tutorials: Scheduled as needed.

Office Hours: Assistance in the Advanced Resource Centre: **W 11:30-12:30, Th 4:00-5:00.**
Also available 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 a requirement.

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 the Dalhousie Bookstore (~\$30). These contain 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

Formal **online lectures** based on the Lecture Notes, are available on Brightspace. The **classroom lectures** will be used to review material, illustrate concepts, and solve problems. These are intended to be interactive, but may not be as comprehensive as online lectures. Students are encouraged to consult the online lectures for a more complete discussion of the material.

Assignments

Assignments will be distributed approximately weekly. These do not need to be handed in and are not be marked, but serve as the basis for quizzes and tests. Some assignments are computer-based. Students are encouraged to complete the assignments as a primary tool for study.

Office Hours

Assistance in the Chemistry Resource Centre: **M 4:00-5:00, T 11:30-12:30, F 3:30-4:30.**

Also available by appointment.

MatLab and MatLab Tutorials

A main objectives 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 mainly in the latter part of the course, students are encouraged 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. 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.

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)
Term Test #1	20%	20%	Wednesday, Feb. 13 (in class)
Term Test #2	20%	20%	Tuesday, Mar. 26 (evening)
Project	NA	15%	Due last week of classes
Final Exam	40%	30%	To be scheduled

Quizzes: Quizzes will be administered in class on approximately a weekly basis. Some of these will make use of the computer. Only the five best quizzes will be counted.

Tests: Tests will be administered on the dates specified unless changed by consensus of the class. The first test (closed-book) will be conducted in class and is not computer-based. The second test (open-book) will be held in the evening and will be computer-based.

Final Exam: The final examination (three hours) is scheduled by the Registrar and will be primarily computer-based. 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 at the scheduled time due to illness or other valid reasons, they are responsible for notifying the instructor as follows.

- E-mail the instructor (peter.wentzell@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 five 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. Use e-mail for issues related to administrative matters or short queries related to content. PDW will not reply to e-mails asking how to solve problems or asking to repeat information from the lecture.

Electronics. Cell phones should be turned off while in lecture; laptop computers may be used and their use is encouraged to follow examples done in class.

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

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

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 elements of data input and output, data manipulation, flow control, 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 appropriate statistical tests for common comparisons (means, variances, distributions, outliers).
 - 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.
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Faculty of Science Course Syllabus (Section B)

Chemistry 4205B/5205B: Chemometrics

University Policies and Statements

(rev. June 2018)

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

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

Missed or Late Academic Requirements due to Student Absence (policy)

https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.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>