FACULTY OF ENGINEERING AND APPLIED SCIENCE

CHEE 418 – STRATEGIES FOR PROCESS INVESTIGATIONS

Course Syllabus – Fall 2020

This is your course syllabus. Please download the file and keep it for future reference.

TEACHING TEAM

COURSE INSTRUCTOR

Jim McLellan, PhD
Professor
Department of Chemical Engineering
Queen's University

E-mail: james.mclellan@queensu.ca

TEACHING ASSISTANTS

Judith Ogwuru
judith.ogwuru@queensu.ca

Bexi Bustillo
18bmb3@queensu.ca

Shamimeh Azimi
sa204@queensu.ca

COURSE INFORMATION

COURSE DESCRIPTION[1]

This is a course about identifying systematic relationships between variables, and selecting and estimating appropriate models for making predictions about process behaviour and developing insights into the process structure. Different data types and data collection approaches are considered, including quantitative and qualitative data. Graphical and quantitative techniques are presented for exploratory data analysis, identifying possible model structures and parameterizations, and assessing the quality of estimated models and predictions. Both linearly parameterized and nonlinear regression models are discussed, and machine learning techniques are introduced. The distinctions between supervised and unsupervised learning in machine learning are made, and are compared to regression estimation. The roles of designed experiments and data analysis procedures in process investigations are discussed. Applications of two-level factorial and fractional factorial designs in screening studies and higher-order experimental designs are examined. The design component of this course is the planning and execution of an experimental investigation, the analysis of the resulting data, and the formulation of recommendations on the basis of those results. (12/0/0/18/12)

Prerequisites: CHEE 209 – Analysis of Process Data (or equivalent) or permission of the department. Exclusion: STAT 361.

PRE-REQUISITE KNOWLEDGE

This course is a requirement for all fourth year Chemical Engineering students at Queen's University. Learners must complete the following prerequisite course prior to registering for CHEE 418: CHEE 209 – Analysis of Process Data (or equivalent).

CHEE 418 develops further concepts in probability and statistics to achieve a comprehensive understanding of how models are estimated from data, and how experimental programs can be designed to make the resulting data as informative as possible. It also places recently developed approaches in machine learning and use of passively collected data (e.g., historical operating data) in the context of statistically-based analysis and designed experiments.

[1] The CHEE 418 Course Author is James McLellan.

COURSE LEARNING OUTCOMES (CLO)

By the end of this course, students should be able to:

	Course-level Learning Outcomes (CLOs)	Program Indicators
CLO 1:	Assess the existence of systematic relationships between variables using appropriate graphical and quantitative techniques	KB-Mathematics KB-ES-ApplMath (b) IN-Synthesis TOO (a), (c)
CLO 2:	Estimate empirical models between variables using statistical model building and machine learning techniques including multiple linear and non-linear regression	KB-Mathematics KB-ES-ApplMath (b)
CLO 3:	Assess the quality of estimated models using graphical and quantitative techniques	IN-Synthesis ET-Create ET-Limitations
CLO 4:	Evaluate and interpret estimated models taking into account sources of uncertainty and variability	IN-Synthesis ET-Create ET-Limitations
CLO 5:	Propose programs of experimental investigation taking into account the goals and context of the investigation, screen and prioritize process variables using 2-level factorial designs, and higher-order experimental designs	KB-ES-ApplMath (b) IN-Conduct IN-Synthesis

GRADUATE INDICATORS

This course develops the following attributes at the 4th year level:

Knowledge Base (KB): Mathematics Demonstrate competence in university-level mathematics.

Knowledge Base, Engineering Science (**KB-ES**): **Applied Math (b)** Apply numerical and statistical methods to analyze, interpret and model data.

Investigation (IN): Conduct Conduct investigations to test hypotheses related to complex problems. **Synthesis** Synthesize information from investigations, considering sources of unbcertainty and limitations to reach substantiated conclusions.

Engineering Tools (ET): Create Develop, adapt and/or extend appropriate software, equipment, models and simulations for a range of engineering activities. **Limitations** Evaluate

limitations and errors of instrumentation/measurement techniques/models/simulations to assess appropriateness of the results.

COURSE EVALUATION

ASSESSMENT WEIGHTING

Assessment instructions are available in full detail on the course website.

Assessment Tool	Due Date	Weight	Alignment with CLOs
Online Quiz 1: Statistical Foundations	Week 5	**10%**	1, 2, 3
Online Quiz 2: Statistical Model Building and Estimation	Week 8	**10%**	1, 2, 3, 4
Online Quiz 3: Linear and Non-linear Regression and Machine Learning	Week 11	**10%**	2, 3, 4
Discussion Forum	Weeks 2, 3, 7, 9	**10%**	All CLO's
Individual Modeling Project (25% project, 10% pitch/Q&A)	Week 10	**35%**	All CLO's
Individual Experimental Design Project (20% project, 5% pitch/Q&A)	Week 12	**25%**	5
		100%	

WEEKLY LEARNING OUTCOMES

Week	Learning Outcomes
	MODULE 1: Getting Started – Data and Foundations
1	By the end of this module, students will be able to: • Recognize different types of data, the way data are collected and the implications for analysis and inference [CLO1] • Describe what is machine learning, identifying overarching concepts [CLO2] • Describe the difference between supervised and unsupervised learning [CLO2]
	MODULE 2: Systems Thinking and Design Thinking for Process Investigations
2	By the end of this module, students will be able to: • Idenfity systems, their components and interconnections [CLO1,CLO5], • Design and incorporate human-centred approaches for investigating socio-physical processes [CLO5] • Use a Systems Thinking approach to understand the interconnection of a system with its surrounding [CLO1, CLO5] • Propose and assess appropriate measurement points for gaining meanful data for process investigation [CLO5]
	MODULE 3: Data, Learning and Systematic Relationships
3	By the end of this module, students will be able to: • Describe the similarities and differences between statistical learning and machine learning in general [CLO2] • Recognize the different types of data (quantitative/qualitative) and natural language processing [CLO1, CLO2] • Describe the importance of how data are collected and the implications for analysis and making decisions [CLO1] • Assess the existence of the systematic relationships between variables using graphical and quantitative techniques [CLO1]
	MODULE 4: Estimating Regression Models, Assessing Quality of Fit, Inference, and Model Predictions
4-6	By the end of this module, students will be able to: • Estimate linear regression models from data [CLO2] • Assess the quality of the estimated models using appropriate qualitative and quantitative techniques [CLO3] • Make predictions using estimated models, taking into account uncertainty and variability [CLO4]

Week	Learning Outcomes
	• Assess the importance of and interpret model terms using appropriate statistically based techniques [CLO3, CLO4]
	MODULE 5: Non-linear Regression Models
7	By the end of this topic, learners will be able to: • Recognize when parameters appear non-linearly in a regression model [CLO2] • Describe the Gauss-Newton solution procedure, and linearization for inference Make decisions about parameters and predictions using statistical inference [CLO2, CLO3]
	MODULE 6: Machine Learning
8,9	By the end of this module, students will be able to: • Recommend the appropriate machine learning approach (e.g., Supervised or unsupervised learning, type of machine learning model, and training approach) [CLO2] • Select and implement appropriate training and validation data approaches [CLO2]
	MODULE 7 – Design and Implementation of Experiments
10-12	By the end of this module, students will be able to: • Propose experimental programs based on 2-level factorial and higher-order designs [CLO5] • Screen variables for importance using experimental designs [CLO5] • Identify limitations in experimental programs and data arising from design and collection decisions [CLO5]

COURSE MATERIALS

Recommended Textbook

- Montgomery, D.C., Runger, G.C. and N.F. Hubele, Engineering Statistics, Wiley, New York (2010), 5th Edition (Note: Editions 3, 4, and 5 are acceptable).

Other Materials

Software

The following software will be used:

- JMP (available from the FEAS software distribution "AppsAnywhere" at no charge (university license)). Please see OnQ course pages for details and instructions.

Additional software that can be used includes:

- JASP (available for free from the University of Amsterdam). Please see OnQ course pages for details and instructions.
- R (available for free download from CRAN). Please see OnQ course pages for details and instructions.

- Matlab (available from the FEAS software distribution "AppsAnywhere" at no charge (university license)). Please see OnQ course pages for details and instructions.

Datasets

Datasets will be made available for practicing analysis and model building. Datasets will be posted on the CHEE418 OnQ pages.

Slides and Readings

Slides, readings and supplemental materials will be posted on the CHEE418 OnQ pages.

SUGGESTED TIME COMMITMENT

This course represents a study period of one semester spanning 12 consecutive weeks. Learners can expect to invest on average 2 hours per week online in this course, 2 hours per week in class discussions that supplement the online material, one hour per week in tutorials working on practice problems, plus 3 hours of independent study. Learners who adhere to a pre-determined study schedule are more likely to successfully complete the course on time.

Assessment Descriptions

Online Quizzes

There will be three one-hour duration online quizzes (week 6, week 8, week 11) throughout the term that contain a variety of questions pertaining the foundations of statistical analysis, model development, estimation and inference, and machine learning techniques. These quizzes will help you to check for understanding and interpretation of key concepts, terms and techniques.

In addition, there will be practice quizzes which you will be able to use to test your knowledge. These practice quizzes do not contribute to the grade.

Discussion Forum

There will be five discussion forum exercises in which you will have the opportunity to discuss concepts and applications in the course.

Individual Modeling Project

There will be an individual modeling project in which you will analyze data, propose and estimate models, and provide a justification and critical assessment of your model, using regression and/or machine learning techniques. This project will include a short pitch/Q&A of your results, in which you will provide an overview of your results, and be asked questions about your results.

Individual Experimental Design Project

There will be an individual experimental design project in which you will propose an experimental design and program to investigate a problem that is posed. This project will include a short pitch/Q&A of your results, in which you will provide an overview of your results, and be asked questions about your proposed experimental design and program implementation.

There is no final exam in CHEE418.

Late Policy

Please refer to the Department of Chemical Engineering policies regarding late submission of assignments, and quizzes, midterms and examinations. Note that unacceptable reasons include malfunctioning computer, travel plans to go home for holidays, and being generally behind on schoolwork.

GRADING

All assessments in this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to the established Grade Point Index.

Feedback on Assessments

The teaching team will provide feedback on graded activities. You can expect feedback on your assessments within ten days of the due date.

Accessing Your Final Grade

Your final grades will show on SOLUS. Official transcripts showing final grades will be available on the Official Grade Release Date. Please note that in official transcripts, a mark of IN (incomplete) is considered a grade, and your transcript is released with this grade.

COURSE COMMUNICATION

QUESTIONS ABOUT COURSE MATERIAL

Questions or comments regarding the course material that can be of benefit to other students should be posted in the Q&A forum on the class website. The instructor, TAs, and students are encouraged to answer these questions directly in the discussion forum for the benefit of everyone in the course.

COURSE ANNOUNCEMENTS

The instructor will routinely post course news in the Announcements section on the main course homepage on OnQ. Please sign up to be automatically notified by email when the instructor posts new information in the Announcements section. Instructions on how to modify your notifications are found in the **Begin Here** section of the class website.

OFFICE HOURS

In addition to interaction in the Q&A discussion forums, you will have the opportunity to interact in a synchronous fashion with either a TA or the instructor through office hours. The instructor will provide a schedule of availability at the beginning of the term.

CONFIDENTIAL MATTERS

If you have a confidential matter you would like to discuss with your instructor, their contact details are on the first page of this document. Expect email replies within 48 hours and in some cases within 24 hours.

COURSE POLICIES

Please review the following policies below concerning copyright, academic integrity, absences and academic accommodations. Please note that CHEE418 is governed by policies of the Department of Chemical Engineering, in additioned to those of the Faculty of Engineering and Applied Science.

COPYRIGHT

Unless otherwise stated, the material on the course website is copyrighted and is for the sole use of students registered in BWRC 802. The material on the website may be downloaded for a registered student's personal use but shall not be distributed or disseminated to anyone other than students registered in this course.

ACADEMIC INTEGRITY

Information on policies concerning academic integrity is available in the Queen's University Code of Conduct, in the Senate Academic Integrity Policy Statement, on the Faculty of Engineering and Applied Science website, and from your instructor.

ABSENCES (ACADEMIC CONSIDERATION) AND ACADEMIC ACCOMMODATIONS

For absences and academic accommodations please review the information on the FEAS website.

TECHNICAL SUPPORT

No specialized computer-related technical skills are required for this course. If you require technical assistance, please contact Technical Support.

PERSONAL SUPPORTIVE COUNSELLING

If at any time you find yourself feeling overwhelmed, anxious, sad, lonely, or distressed, consider confidential supportive counselling offered by the Faculty of Engineering and Applied Science.