Chemical Engineering 4G03

Optimization Formulation and Solution

Course Outline - Winter 2024

Course Details

Instructor:		**Dr. Jake Nease**	**neasej@mcmaster.ca** **+1 (905) 599-3165**	**BSB/B105**
Teaching Assistants:		Lauren Weir	See A2L	See A2L
		Adekunle Omoniyi	See A2L	See A2L
		Reza Farzadnia	See A2L	See A2L
		Nilou Seyyedizadeh	See A2L	See A2L
Website:		Avenue2Learn	avenue.mcmaster.ca	
Lectures:		See A2L	See A2L	See A2L
Tutorials:		See A2L	See A2L	See A2L
		See A2L	See A2L	See A2L
		Tutorials begin January 15 *Tutorials are MANDATORY and will be used to introduce software, work on practice activities, give project consultation time, and cover lecture material*		
Office Hours:	**JAKE**:	Wed 15:00-16:30, or by appointment (always happy to chat)		
	TAs:	TBD, and by appointment		
Prerequisites:		ChE {2O04, 2E04, 3P04, 3G04, 3M04}		
Software:		MATLAB – Expected prerequisite but will be refreshed throughout the term EXCEL – Expected prerequisite but will be refreshed throughout the term GAMS – **G**eneral **A**lgebraic **M**odel **S**olver (will be introduced in this course)		
Course Materials:		Lecture modules, tutorials, assignments, readings, and solutions will be posted on A2L Grades will also be posted on A2L but are not official		
Recommended Textbook:		R. Rardin: *Optimization in Operations Research*. Pearson Education		
		First Edition (1997):	Pearson	Amazon
		Second Edition (2017):	Pearson	Amazon

Formal Course Description

The application of optimization methods to important engineering problems in thermodynamics, statistics, design, control, economics, and scheduling. Emphasis on problem definition, model formulation and solution analysis, with applications of existing algorithms and software tools to solve industry-related problems.

Informal Course Description

A course dedicated to determining the **best way** to do something given a **clear objective** and set of **constraints**.

Learning Objectives

After completing this course, the student should be able to:

LO.1. Demonstrate the ability to identify the **best outcome** possible for a given problem

LO.2. Recognize and exploit opportunities for optimization in **real-world scenarios**

LO.3. Compare the trade-offs between **accuracy** and **computational effort**

LO.4. Demonstrate that mathematical models have **inherent errors** that can be minimized through appropriate **solution methods**, sensitivity **analysis tools** and **interpretation** of results

LO.5. Apply problem-solving strategies that can **translate a real-world problem** or opportunity into a **mathematical model** to be solved via optimization

LO.6. Interpret and explore the mathematical concepts that define the basis for **optimization theory**

LO.7. Test, debug, and apply mathematical strategies for optimization using a variety of **software tools**

LO.8. **Explain** an optimal solution and other results to an **audience unfamiliar** with formal optimization

LO.9. Select appropriate **model complexity** to achieve the **desired accuracy** and solution approach

LO.10. Identify **misleading results** and apply appropriate analyses to **judge their accuracy** or applicability

Grading Policies

Please be aware of the following grading policies for ChE 4G03:

- Late submissions of any take-home portions of exams will not be accepted without an appropriate MSAF
- Valid MSAF submissions will result in either a make-up examination or rolling of that component's weight into the final exam, depending on the situation
- The midterm and the exam will be open-book (any book) and open-notes (any hard copies), **EXCEPT** any old midterms, exams, or associated solutions
- Any calculator may be used for examinations
- All grades are unofficial until final grades are posted on McMaster's student and faculty software: MOSAIC
- The instructor retains the right to modify course weights or components, typically only enforced for the student's benefit
- Final grades will be converted to the standard McMaster 12-point scale
- All submissions for assignments, projects, and take-home examinations must be done **electronically**
- Any copying of code, formulations, or interpretations from other students, prior versions of this course, or resources online will be considered a violation of McMaster's academic integrity policy

Grading Breakdown

Weight	Component	Comments
0%	Tutorial Activities	Are there to prepare you for exams, projects, and assignments
0-25%	Assignments	5 optional assignments (5% each); submitted in groups of ≤ 3
0-25%	Midterm Test	Classic in-person midterm. Deferred to exam in your favour
20%	Course Project	Proposal (2%), presentation (10%), formulation (8%)
25-75%	Final Exam	Classic final exam. Assignments displace weight if better
5%	Tutorial Participation	Attendance in tutorial sessions (0.5% each, 10 sessions)

Assignments

There will be 5 assignments for this course, each counting for 5% of the student's final grade **if they are better than the final exam**, up to a maximum of 25%. If more than 5 assignments are released, only the best 5 results will count at 5% each. Please note the following considerations:

- Assignments may be completed in groups of **up to three (3) students**. Groups may change between assignments and can be different from project groups.
- Assignments must be submitted **electronically** to the appropriate A2L dropbox prior to the due date.
- All relevant code, with appropriate comments and guidance for grading, must also be submitted with each assignment.
- Assignments will typically focus on each of the five main topics of this course (broken down below), but the instructor reserves the right to modify coverage.
- All assignments will have a *demerit system* for presentation and professionalism. Any submissions that are poorly formatted, have no discussion, or show any other lack of professionalism will be penalized.

Course Project

A significant portion of the student's grade will come in the form of a course project. The project will follow a guided self-directed learning (SDL) format in which the students will develop their own topic by applying course concepts to a problem that they consider to be interesting or noteworthy. Some additional comments about the course project:

- The project **MUST** be tackled in groups of **three (3)**. *Special circumstances* will permit groups other than three, at the discretion of the instructor
- A **proposal** (10% of project grade) will be due around reading week. A specific due date will be communicated by the instructor closer to the date
- After the proposal has been reviewed, each group will meet briefly with the instructor (10-minute meetings) to hammer out **specific project details and objectives**
- The remainder of your project grade comes from two deliverables:
    - A final presentation (20 minutes + questions) in which you will document the motivation, problem formulation, and results of your project and associated case studies. This presentation is mandatory and will be scheduled in an evening toward the last week of the term.
    - A formal written document outlining your **problem formulation**. Such a document will break down the assumptions, variables, sets, objective, and constraints in a clear manner such that the reader will understand the opportunity for optimization and how your project was formulated.

Midterm and Exams

The course midterm (0-25%) and exam (25-75%) will be written tests completed individually. Some comments:

- The final exam will be **cumulative** and may test all the components of the course. The final exam will be scheduled during the final exam break at the discretion of the registrar.
- For the date and time of the midterm exam, please see the posted schedule on A2L.
- The instructor reserves the right to adjust the weighting scheme and coverage of the test problem sets in a manner that benefits the students, if it is deemed appropriate.

Academic Integrity

You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity.

~ The use of generative AI is considered academic dishonesty in this course ~

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university. It is your responsibility to understand what constitutes academic dishonesty. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at http://www.mcmaster.ca/academicintegrity.

The following illustrates only **three forms** of academic dishonesty:

- Plagiarism, *e.g.* the submission of work that is not one's own or for which other credit has been obtained
- Improper collaboration in group work: this point is **particularly important** and will be strongly penalized in this course
- Copying or using unauthorized aids in tests and examinations (internet-enabled devices, for example)

Accessibility and Mental Health

The instructor aims to make this class accessible to all students. Please forward and optionally discuss any accommodation granted by Student Accessibility Services (SAS) with the instructor *before the third week of the course*. Please raise any other accessibility issues with the instructor as soon as possible, *e.g.* accessibility of the course website and course materials.

I am certified with the McMaster Professor Hippo on Campus Program for mental health awareness and aid to students in need. My office (or online video portal) is a **safe space** to discuss issues both academic and otherwise, and you are welcome to contact me at any time to chat. If I reach out to you at any time, be aware that it is not to embarrass or penalize you; it is because I care.

Course Feedback

Please do not hesitate to let me know your thoughts on the course or what you might want to change at any time. You can reach me at neasej@mcmaster.ca. If you would prefer to leave feedback **anonymously**, do not hesitate to use our anonymous feedback form posted to A2L.

Class Recordings

As has become standard in my courses, classes will be recorded each week and posted on YouTube. Please remember that these recordings should NOT be used as an excuse to skip class, and since they are one-take I cannot make any guarantees of their availability in the event of technical difficulties.

Classes will be recorded using Echo 360 and processed for closed captioning. Suggestions for improved video quality are welcome.

Anticipated Course Schedule and Topics

Lecture Date	Anticipated Topics	Anticipated Module Content (subject to change)
Week 01	Course Overview Intro to Optimization Formulation	• Review of course outline • Concept of optimization • Optimization in industry • Class example – "Make the most of final year" • Class workshop – "Play the game your way"
Week 02	Formulation Mathematical Concepts	• Types of constraints • Graphical interpretations • Local/Global optima • Gradients and optimality • Convexity and geometric interpretation • Feasible directions, types of constraints
Week 03	Linear Programming	• Introduction to linear programming • Properties of linear programs • Types of constraints • Slack variables
Week 04	Linear Programming	• Solution method **Simplex Search** • Simplex Tableau • Graphical interpretation
Week 05	Linear Programming	• Sensitivity analysis/Shadow Prices • Software tools
Week 06	Integer Programming	• Handling of integer variables • Formulating integer problems • Knapsack constraints • Integer relaxations
Week 07	Integer Programming	• Solution method: **Branch and Bound** • Types of BB searches with examples
Week 08	Integer Programming	• Branch and Bound continued
Week 09	Unconstrained Nonlinear Programming	• **Gradient Search** • **Line Search** • **Golden Search** (Bisection)
Week 10	Unconstrained Nonlinear Programming	• Linear relaxation • Derivative-free methods (**Nelder Mead**) • Quasi-Newton searches
Week 11	Constrained Nonlinear Programming	• Handling constraints • Penalty functions • Barrier functions
Week 12	Black-Box Optimization	• **Particle Swarm** Optimization • **Differential Evolutions** • Pros/cons of Black Box methods

The P.R.O.C.E.S.S.

As some of you may already be aware, the department of Chemical Engineering has a storied history of education. In addition to teaching and learning, the department is proud of our graduates not only for their academic success, but their more intrinsic traits that make them respected members of the engineering community.

Recently, several high-ranking graduates from the McMaster Chemical Engineering Program employed in various industries (oil/gas, financials, *etc*.) were interviewed to ask what traits they look for when hiring for engineering positions. Using this information, the department would like to present to you the **PROCESS**: a code of conduct that we hope will guide our students throughout this program and their careers to come.

- **P**rofessionalism
- **R**esponsibility
- **O**wnership
- **C**uriosity
- **E**mpathy
- **S**elflessness
- **S**ervice

It is up to YOU to interpret these traits and apply them to your time at McMaster and your career as you see fit. These traits will not be assessed for grades but will be strongly encouraged throughout your time at McMaster. We hope that you identify with these character traits and what they mean to you, and that you **trust the process**.