CHEM ENG 752 – OPTIMIZATION OF CHEMICAL PROCESSES
Term I, 2025-26 (September–December 2025)

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Overview and Objectives:

Optimization is a central theme that impacts most areas of process systems engineering including process design, process control, process operations and scheduling, and parameter estimation. The primary goals of this course are to provide an overview of state-of-the-art optimization algorithms, the theoretical principles that underpin them, and their use for solving several types of practically relevant optimization problems arising in process systems engineering. The course will also cover aspects of numerical computation (such as the solution of systems of nonlinear algebraic equations, solution of initial-value ODE/DAE problems, and orthogonal collocation on finite elements) that would be useful in many areas of process engineering. Course assignments will include analysis, hand calculations, problem formulation, and solution of optimization problems of various types using computing environments such as GAMS and Matlab, and state-of-the-art commercial grade optimization solvers.

Assessment: Assignments: 65%
Project : 35%

Reference Texts:
I - Optimization

Biegler, L.T., *Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes*, SIAM, 2010.

Chvatal, V., *Linear Programming*, Freeman, New York, 1983.

Edgar, T.F. and D.M. Himmelblau and L.S. Lasdon, *Optimization of Chemical Processes*, 2nd Edn., McGraw-Hill, 2001.

Floudas, C.A., *Nonlinear and Mixed-Integer Optimization*, Oxford University Press, 1995.

Griva, I., Nash, S.G., Sofer, A., *Linear and Nonlinear Optimization*, 2nd Edn., SIAM, 2009.

Grossmann, I.E., *Advanced Optimization for Process Systems Engineering*, Cambridge University Press, 2021.

Nocedal, J. and S. J. Wright, *Numerical Optimization*, Springer, 1999.

Peressini, A.L., F.E. Sullivan and J.J. Uhl, *The Mathematics of Nonlinear Programming*, Springer-Verlag, 1988.

Ravindran, A., Ragsdell, K.M., Reklaitis, G.V., *Engineering Optimization*, 2nd Edn., Wiley, 2006.

Wright, S.J., *Primal-Dual Interior-Point Methods*, SIAM, 1997.

II – Numerical Methods

Burden, R.L., Faires, J.D., Reynolds, A.C., *Numerical Analysis*, 2nd Edn., PWS Publishers, 1981.

Conte, S.D., and de Boor, C., *Elementary Numerical Analysis*, 3rd Edn., McGraw-Hill, 1980.

PROVISIONAL COURSE OUTLINE

1. Fundamentals/Mathematical Preliminaries
   - Overview and optimization applications in process systems engineering
   - Linear equation systems and matrix factorization
   - Vector and matrix norms; condition number

2. Linear Programming
   - Fundamental theorem of Linear Programming
   - Simplex method
   - Sensitivity analysis
   - Implementation/computational issues

3. Optimization Software Environments
   - Spreadsheets
   - Low-level programming
   - Modeling languages

4. Solution of Nonlinear Algebraic Equation Systems
   - Newton's method
   - Rates of convergence

5. Optimization Fundamentals
   - Concepts and definitions
   - Convexity

6. Unconstrained Optimization
   - Optimality criteria
   - Direct search methods
   - Descent directions and line search strategies
   - Steepest descent, Newton and quasi-Newton methods

7. Constrained, Nonlinear Optimization
   - Optimality criteria
   - Sequential quadratic programming (SQP)
   - Generalized reduced gradient (GRG) method
   - Barrier/interior-point (IP) methods

8. Dynamic Optimization
   - Numerical solution of ODE and DAE initial-value problems
   - Sequential solution, sensitivity equations
   - Simultaneous approach, orthogonal collocation on finite elements

9. Mixed-Integer Programming
   - Branch-and-bound paradigm
   - Mixed-integer linear programming (MILP)
   - Mixed-integer nonlinear programming (MINLP)
   - MIP formulation issues
   - Process systems engineering applications

10. Optimization Under Uncertainty
    - Robust optimization
    - Chance constraints
    - Stochastic programming

11. Global Optimization
    - Deterministic strategies (branch-and-bound based)
    - Metaheuristic methods (Genetic algorithms, Simulated annealing)

12. Selection from
    - Mixed-integer dynamic optimization (MIDO)
    - Parametric programming
    - Mathematical programs with complementarity constraints (MPCCs)

13. Project presentations

APPROVED ADVISORY STATEMENTS

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. **It is your responsibility to understand what constitutes academic dishonesty.**

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. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at https://secretariat.mcmaster.ca/university-policies-proceduresguidelines/

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.
- copying or using unauthorized aids in tests and examinations.

Generative AI

Students are not permitted to use generative AI in this course. In alignment with McMaster academic integrity policy, it "shall be an offence knowingly to … submit academic work for assessment that was purchased or acquired from another source". This includes work created by generative AI tools. Also stated in the policy is the following, "Contract Cheating is the act of "outsourcing of student work to third parties" (Lancaster & Clarke, 2016, p. 639) with or without payment." Using Generative AI tools is a form of contract cheating. Charges of academic dishonesty will be brought forward to the Office of Academic Integrity.

Authenticity / Plagiarism

Some courses may use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. Avenue to Learn, etc.) using plagiarism detection (a service supported by Turnitin.com) so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster's use of Turnitin.com please go to www.mcmaster.ca/academicintegrity.

Courses with an On-line Element

Some courses may use on-line elements (e.g. e-mail, Avenue to Learn, LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, private information such as first and last names, user names for the McMaster e-mail accounts, and program affiliation may become apparent to all other students in the same course. The available information is dependent on the technology used. Continuation in a course that uses on-line elements will be deemed consent to

this disclosure. If you have any questions or concerns about such disclosure please discuss this with the course instructor.

Online Proctoring

Some courses may use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.

Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all of our living, learning and working communities. These expectations are described in the Code of Student Rights & Responsibilities (the "Code"). All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online**.

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students' access to these platforms.

Academic Accommodation of Students with Disabilities

Students with disabilities who require academic accommodation must contact Student Accessibility Services (SAS) at 905-525-9140 ext. 28652 or sas@mcmaster.ca to make arrangements with a Program Coordinator. For further information, consult McMaster University's Academic Accommodation of Students with Disabilities policy.

Requests for Relief for Missed Academic Term Work

In the event of an absence for medical or other reasons, students should review and follow the Policy on Requests for Relief for Missed Academic Term Work.

Academic Accommodation for Religious, Indigenous, or Spiritual Observances (RISO)

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the RISO policy. Students should submit their request to their Faculty Office **normally within 10 working days** of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

Copyright and Recording

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, **including lectures** by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by

a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

Extreme Circumstances

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, Avenue to Learn and/or McMaster email.