Chemical Engineering 4G3, Winter 2015
Optimization in Chemical Engineering

Instructor

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Class time and location

Class: JHE 326H, on Monday and Wednesday, 11:30 to 12:20

Tutorials: Computer labs in BSB, room 249. Monday (group M) at 15:30 to 17:20, and Friday (group F) from 10:30 to 12:20.

Disclaimer

This outline **may be modified**, as circumstances change, by the instructor or university.

1 About the course

Official description

The application of optimization methods to important engineering problems in thermodynamics, statistics, design, control, economics and scheduling. The course will emphasize problem definition, model formulation and solution analysis, with sufficient details on existing algorithms and software to solve problems.

Prerequisites

CHEM ENG `3E4` (all those programming tools are important in 4G), and all your basic chemical engineering courses will be used in the case studies and problems: `2O4` (fluid mechanics), `3G4` (process simulation and modelling), `3M4` (mass transfer and basic separations), `3P4` (process control).

What you must be able to demonstrate by the end of the course

This course will provide the student with the ability to formulate, solve and interpret meaningful optimization problems in engineering, science and business. Emphasis will be placed on the formulation of mathematical models for use with commonly available solution techniques. Software packages will be used for solving realistic engineering problems. Correct interpretation of the software output is critical.

Here are some further objectives:

- Understand that we seek the best solution with reasonable computation.
- Recognize that all mathematical models have errors, and we must evaluate and understand the effects of these errors on the solution; thus, we will perform sensitivity analyses.
- An engineer must be able to apply a problem solving strategy to translate an opportunity into a mathematical model and optimization solution.
- The engineer must test, debug, verify and apply mathematical models for optimization. This requires programming and software tools, and thoughtful interpretation using your brain.
- Then, the engineer must explain the solution in terms that a non-specialist in optimization can understand.
- We must recognize opportunities for optimization and whether the optimum is likely to be located at an extreme point or the interior of the feasible region.

- We must select the appropriate model complexity to achieve the goals defined in the engineering problem.
- We must match the solution approach to the model structure, problem definition, and required accuracy.
- Comprehensively interpret mathematical optimization results to yield decisions to be implemented.
- Be aware of "weird events" that can misdirect you. We will apply appropriate methods of results analysis to prevent implementation of incorrect decisions.
- There is an art to optimization: it is not just straightforward application of mathematics.

Course materials

The course website will be permanently available at: http://learnche.mcmaster.ca/4G3. Course materials, assignments and solutions, project postings, *etc* will be available from the website.

Course announcements will only be posted to the main page of the website - students are expected to check the website at least 3 times per week. Please note that this is not an Avenue course website. If you want to automatically receive all course notifications, please subscribe to the course Twitter feed at @opt4eng.

Required textbook

There is no official course textbook. We will be using the departmental material based on notes from previous instructors: Dr. Benoit Chachuat (a previous professor here), Dr. Thomas Marlin (now retired), Dr. San Yip (a graduate student from McMaster, and an industrial practitioner of optimization), and myself.

The following text is highly recommended, though extremely expensive: Rardin, R., "Optimization in Operations Research", Prentice-Hall, Upper Saddle River, NJ, 1998.

Additional reference texts are listed on the course website and are generally available in Thode Library or online.

Course structure

The class time (Monday and Wednesday) will consist of classroom instruction, which will include lectures and interactive activities. There will be occasional guest lecture(s). Topics covered in class time include:

1. Introduction to Optimization concepts
2. Creating mathematical models
3. Linear programming (LPs): formulation and interpretation of the solution
4. Mixed Integer Linear Programming (MILPs)
5. Nonlinear Programming (NLPs) with a single variable (unconstrained)
6. Nonlinear Programming (NLPs) with multi variables (unconstrained)
7. Nonlinear Programming (NLPs) adding constraints
8. Optimization in Industrial Practice

There are tutorials (Monday and Friday), which will involve solving problems posed by the instructor. Group work will occur during the tutorial. Computer exercises will be performed throughout the course.

A major course project will be performed in small groups.

Several assignments will be posted on the course website. These may be completed in groups (see below).

2 Grading

To assess your understanding of the course materials, the grading for the course will be:

Component	Fraction	Notes
Assignments	12%	Expect around 6 or 7 assignments; can be completed individually, or in groups of 2 (no exceptions).
Midterm	20%	A written midterm exam.
Project	20%	A short project report done in groups of 2 (no exceptions)
Final exam	48%	A written exam, lasting 3 hours.

Policies regarding grading

- We encourage you to complete the assignments in groups of no more than 2 members. You, and your group, will receive the greatest benefit if you each do **all** the questions yourselves. Arrange to meet and review your solutions, discussing various approaches. Assemble a **single submission** for the group – the TAs will not grade loose sheets handed in after the first submission. Submissions must show the names of all group members.
- You are defeating the purpose of the group-based assignment if you simply divide the assignment into sections, one for each group member. This is definitely not recommended, because you are losing out on the learning opportunity of seeing your mistakes and the group member's mistakes, and learning from them.
- No sharing of any work may be done between groups for assignments and projects. This includes handwritten documents and electronic files of any type. Reusing solutions from previous years will be considered plagiarism. Please ensure that you have read the University's academic integrity policy (part of which is reproduced below).
- This is a large class of about 80 students, so late hand-ins interfere with the TAs to efficiently grade your assignments. Late assignments will be penalized by deducting 30% per day for every late day. A grade of zero will be given for submissions handed in after the solutions are posted (usually within 2 days of assignment hand-in). Note: a "day" in this outline refers to any day of the week, not only working days.
- Emergencies and such arise, so each person has 2 "late day" credits for assignments. So you can hand in one assignment 2 days late, or 2 assignments each one day late, without penalty. Late day credits cannot be used for midterms or projects, only for assignments.
- Grading of all work will include contributions for clarity and organization of presentation.
- No make-ups will be given for assignments, tutorials or the midterm. Using an MSAF for the course might require handing in the assignment or performing a work submission, at the discretion of the instructor. It is not automatic that the MSAF material's weight is moved to the final exam.
- The midterm might be followed by a collaborative review session. You will work on the midterm again in groups and submit a single submission per group. That group submission will count 15% of the midterm grade, and the individual portion will be 85% of the midterm grade. Your overall midterm grade will be that weighted sum, or 100% of your individual portion, whichever is highest.
- The midterm and the final exam will be closed-notes. A page of formulas will be provided to you. The class will jointly decide what appears on this page 5 to 10 days prior to the test or exam, and this page will be available on the course website for you, so you are aware of what is provided.
- Only the standard McMaster calculator may be used during tests and exams.
- All assignments will be graded, and the mean of **all** assignments used to calculate the assignment grade. You should expect $N \approx 6$ or 7, and the assignments will be more frequent at the start of the course.
- The final exam will be cumulative, based on the entire semester's material.
- The course project **must** be submitted electronically. Grading will be done electronically in the document to minimize the use of paper reports. Please see the website for more details and a video demonstration.
- The final percentage grades will be converted to letter grades using the Registrar's recommended procedure. Adjustment to the final grades may be done at the discretion of the instructor.

3 Important notes

Class participation:

Please bring a calculator to every class. A cell phone, laptop, tablet computer, or some sort of device to connect to the internet in the class rooms, while not mandatory, will help you for tutorials and answering questions during class.

Course software

Several software packages will be used, demonstrated and encouraged during the course. There isn't one software package for optimization, and furthermore, when you use these tools in industry your company may already have a specific software license for a package. The most important part of the course is to set up your optimization problem and interpret the software output.

Software packages used might include: GAMS, Excel, Gurobi, OpenOpt, and MATLAB. Other software packages are under consideration. All details about the software packages will be posted on the course website.

Out-of-class access and email

Office hours and contact information are posted on the instructor's website, http://learnche.mcmaster.ca.

The TAs for this course can be contacted by email - please see their email address above. Try to send email from your McMaster account - email from personal accounts are sometimes discarded by spam filters. Your instructor filters his email, so emails from `@mcmaster.ca` addresses receive higher priority than personal addresses.

4 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.

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:

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

Consider this course outline to be a first warning; any lack of academic integrity will not be accepted.

5 Accessibility

The instructor aims to make this class accessible to all students. Please forward and optionally discuss any accommodation granted by Student Accessibility Services 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.

6 Important dates

A list of *tentative* dates:

Date	Description
5 January 2015	First class: course overview
16-22 February	Midterm break
25 February	Written midterm (tentative)
27 March	*Kipling*
08 April	Project due
10 to 30 April	Final exams