CHEM 454L – Chemometrics Spring 2007
Class Syllabus
Dr. Grady Hanrahan

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Office Hours: P.S. 807 M, W, F 11:00am -12:00pm, TH 1:00pm – 2pm or by appointment

Lecture: T/TH 9:50 am-11:30 am, SH-C168

Course Description & Objectives:

CHEM 454L - *Chemometrics* will offer a more practical training experience for students compared to traditional statistical method courses. An array of powerful chemometric techniques for experimental design and data analysis will be covered, ultimately providing students with modern analytical training.

The <u>purpose</u> of this course is to train students in chemometric methods for optimizing experimental design, data processing, calibration and quality control.

Upon completion of this course, students will be able to:
1. Apply basic statistical methods to their independent research efforts;
2. Perform advanced chemometric analysis on large data sets;
3. Apply the knowledge learned to all scientific data analyses during their studies and future career-related activities.

Prerequisites:

CHEM 201, MATH 206 and PHYS 103.

Required Textbook:

Statistics and Chemometrics for Analytical Chemistry, 5th Edition, James N. Miller & Jane C. Miller, Pearson/Prentice Hall Publisher.

Lecture Style: PowerPoint slides, overheads, scientific papers and take home exercises. Both independent research (computer-based) and group learning will be offered to compliment the classroom lectures.

Lecture Schedule: CHEM 454L - Spring 2007

<u>Dates</u>	<u>Subject</u>	<u>Chapter(s)</u>
Week 1	Class Introduction, Errors in Chemical Analysis, Descriptive Statistics, Intro to JMP Chemometric Software (computer lab exercise).	Chapters 1 & 2
Week 2	Significance Tests and computer lab exercise	Chapter 3
Week 3	Regression and Correlation – Calibration Methods, computer lab exercises.	Chapter 5
Week 4	Non-parametric and Robust Methods	Chapter 6
Week 5	Intro to Experimental Design, Exam 1	Chapter 7, Handout
	MIDTERM EXAM April 24	
Week 7	Experimental Design and Optimization, computer lab exercises.	Chapter 7
Week 8-9	Multivariate Methods of Analysis, Computer lab exercises.	Chapter 8
Week 10	Quality Assurance and Good Lab Practice	Chapter 4
Week 11	**FINAL PROJECT DUE – June 7th, 12:00 noon**	

*** Note: Dates subject to change (except for the Midterm and Final Project)

Point Distributions for Grades

Lecture: 1 x 100 point Midterm Exam
                  10 x 20 point quizzes (lowest dropped) = 180 points
                  5 x 10 point Computer Exercises
                  20 points - Class participation
                  Final Project - 200 points
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                  Total = 550 points

Grades will be assigned as traditional (A, B, C, D, & F) as follows:
A = 90-100%
B = 89-80%
C = 79-70%
D = 69-60%
F = 59%-below

However, class attendance, distribution of points and individual participation will be taken into consideration on final grades (+ and – considered). To pass this course, students <u>must complete all assigned work</u>. Students will receive an (F) if all work is not completed (unless a documented excuse, e.g., medical).

Final Project

You are to devise an experimental design research project on your current laboratory research (or data will be given to those students not performing independent research in a laboratory). You will use the various statistical, experimental design and optimization techniques learned in class to develop this project. You will need to use the JMP software to perform all experimental design and optimization techniques and include information on quality assurance. The more information and results presented, the better the grade for the research project. Project guidelines and expectations will be covered extensively during the 6-7th week by your instructor.

For the project, a formal, typed-written report must be handed in during finals week. This report must follow the format below. Reports must be a concise description of the experiment/data analysis with all appropriate data and graphs. The format includes (in order):

1. Cover page with title of experiment, name and date.
2. Abstract
3. Introduction
4. Experimental procedures
5. Results, including data and relevant graphs
6. Conclusion
7. References
8. Acknowledgments

Dropping the course/Incompletes

Hopefully, a student will not be dropping this course. However, in the event that this is necessary the student must meet all university rules and deadlines. In the case of an incomplete, the student must be making a (C) in the course and the reason for the incomplete an illness or an accident. An INCOMPLETE GRADE REPORT form must be completed and given to the instructor by the end of the examination week.

Formal Report Sections – Detailed Description

Abstract

A concise summary of the work performed and contains the key results. No introduction or background material should be placed here.

Introduction

Here one states the aim, the historical and theoretical context of the work. Include any relevant chemical equations or reactions. Should be concise, but have enough information for a complete introduction.

Experimental Procedures

This section is used for describing experimental procedures, conditions, apparatus and reagents used in the experiment.

Results

The data obtained in the experimental section is either tabulated and/or graphically displayed. Results from these data are calculated in this section. Show all data and calculations used.

Conclusion

This section contains a critical evaluation of the data gathered and the errors inherent in them. Be specific and thorough in your narrative.

References

Throughout the body of the manuscript, statements used which derive from external sources require defense based on previous work. These statements must be denoted numerically either with a superscript or in parenthesis in the text, and then the source listed in the Reference section by that number. ACS format is expected.

Acknowledgments

All assistance, funds and gifts should be acknowledged as a matter of courtesy. For example, financial support and scholarships, laboratory assistance, etc…should be stated.