

Chemistry 526
Chemometrics
Spring 2008

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3 credit hours
MWF 10:00-10:50 AM
Shelby 251
Office Hours: 11-12 Tues & Wed

Text: Robert L. Anderson, "Practical Statistics for Analytical Chemists"

The book is out of print and can not be purchased. Chapters will be handed out in class as needed. Plus, supplemental material from other books will be used.

Course Goals: To gain knowledge on the use of mathematical manipulations to enhance data interpretation, data description, and experimental design in chemistry. We are concerned with the use of mathematical and statistical techniques, not with their derivation.

General Topics: Statistical Data and Error Analysis
Calibration
Experimental Design
Signal Processing and Transform Techniques
Data Description and Enhancement

Notice of Requirements: Graduate standing in Chemistry or permission of the instructor.

Assigned Problems: This is a very problem intensive course!

- Significant figures are always important in reporting the final answer.
- You will receive homework assignments approximately each week. Most problems will be graded and are due at the start of class either 4 or 7 days after you receive the assignment.
- Each student must hand in their own individual assignments. You may discuss the problems among yourselves or with Dr. Cassady. You may use your textbook or any other printed resources.
- Provide enough detail so that it is clear how you worked each graded problem.
- There will be 12 graded homework assignments worth 20 points each.

Exams: More Problems!

- There will be a midterm exam and a "final homework set," each worth 200 points. Both are take-home and open-book. However, you may NOT discuss exam questions among yourselves. If you do so it will be considered as academic misconduct and reported to the appropriate university officials. You may only discuss the exam material with Dr. Cassady if you wish to have the meaning of a question clarified.

	<u>Received</u>	<u>Due</u>
Midterm	2/22, 10:50 AM	3/3, 10:00 AM
Final	4/25, 10:50 AM	5/7, 11:30 AM

Computers and Calculators:

- Bring your calculator to each class.
- You may use spreadsheets such as Lotus, Quattro Pro, or Excel—but only their basic math functions (e.g., +, -, /, x, square root, 10^x , sin, cos, tan, log, ln, inverse of these functions, etc.). For other procedures that use these functions (e.g., standard deviation calculation, curve fits), you must write your own spreadsheet equations using the basic math functions.

Grading: 531-640 pts (83-100 %) = A
 416-530 pts (65-83 %) = B
 281-415 pts (44-65 %) = C
 <281 pts (<44 %) = don't let things get this bad

Important Notes:

- Class begins at 10:00 AM. Be on time!
- We will have a few class periods when there will be no lecture. These can be considered as time to compensate for the take-home exams.

Course Website:

- <http://bama.ua.edu/~ccassady/ch526/ch526.html>
- Keys for homework assignments will be posted on the website.

Academic Misconduct: All acts of dishonesty in any work constitute academic misconduct. The Academic Misconduct Disciplinary Policy will be followed in the event of academic misconduct.

Disability Accommodations: To request disability accommodations, please contact Disability Services (348-4285). After initial arrangements are made with that office, contact your professor.

Tentative Study Calendar

<u>Date</u>	<u>Topic</u>	<u>Anderson Chapter</u>
1/9	Types of Errors	1
1/11	Describing Data with Statistics	1, 2, 3
1/14	Data Distributions	2
1/16	Testing Distributions for Normalcy	2, 4
1/18	No Class	
1/21	No Class - Martin Luther King Holiday	
1/23	Confidence Limits	4
1/25	No Class	
1/28	“Advanced” Precision Procedures	4
1/30	Precision (cont.), “Advanced” Accuracy Procedures	4
2/1	Advanced Accuracy Procedures (conti.)	5

2/4	Bivariate Data and Least Square Linear Regressions	6
2/6	Evaluation of Linear Regressions	6
2/8	Evaluation of Linear Regressions (conti.)	6
2/11	One-Way ANOVA	7
2/13	Two-Way ANOVA	8
2/15	Multivariate, and Nested ANOVAs, Collaborative Testing	8, 9, 10, 11
2/18	Collaborative Testing, Experimental Design and Systems Analysis	
2/20	Experimental Optimization, Simplex Techniques	
2/22	Simplex (conti.), Multivariate Data Analysis	
2/25	No Class	
2/27	Principal Component Analysis, Clustering Techniques	
2/29	Clustering, Pattern Recognition	
3/3	Pattern Recognition (conti.), Fuzzy Clustering	
3/5	Neural Networks	
3/7	Monte Carlo Techniques	
3/10	Calculation of Calibration Curves with Matrix Algebra	12
3/12	Evaluation of the Calibration Equation, Non-Straight Line Fits	13
3/14	Non-Straight Line Curve Fitting (cont.)	
3/17-21	No Class - Spring Break	
3/24	Multiple Linear Regression, Principal Component Regression	
3/26	Partial Least Squares, More on Calibration	
3/28	More on Calibration	
3/31	Even More on Calibration, Fourier Transform Calculations	
4/2	Fourier Transform Calculations (conti.)	
4/4	Fourier Transform Convolution	
4/7	Fourier Transform Sampling and Noise	
4/9	Fourier Transform in Optical Spectroscopy	
4/11	Hadamard Transform	
4/14	Analytical Figures of Merit	
4/16	Signals and Noise	
4/18	No Class - Honors Day	
4/21	Signal Processing and Data Enhancement	
4/23	Real Life Examples Using Chemometrics	
4/25	No Class	
4/28	More Real Life Examples Using Chemometrics	
4/30	Chemometrics Today	
5/2	No Class - Continue With Take Home Assignment	
5/7, 11:30 AM	(final exam slot) - Turn in Take Home Final Homework Set	