CHEM789
Experimental Design and Statistics in Chemistry
Spring Term 2014

Instructor: Dr. Kevin Owens
Class Time: Mon 6:00-7:20 pm
Wed 7:30-8:50 pm
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Class Room: Curtis 452
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Required Textbook:
Note there is a student companion website for the textbook at http://bcs.wiley.com/he-bcs/Books?action=index&itemId=0470128666&bcsId=4460

Note: If you have access to the 7th edition (while it is no longer available directly from Wiley, it is still available from 3rd-party sellers such as Amazon) you may use it, but you will have to carefully check any problems assigned from the text.

Course Objectives:

- To develop basic statistical analysis skills, including the calculation of summary statistics, propagation of error and confidence intervals
- To develop an understanding of methods for comparing means (t-test) and variances (F-test)
- To gain an understanding of the calibration process, including selection of a model, calculation of experimental parameters from measured values, evaluation of the fitness of the model using an analysis of variance (ANOVA) approach, and application of the model to the analysis of unknowns, including the calculation of the appropriate confidence intervals of predicted values
- To gain an understanding of basic experimental design, specifically factorial and fractional factorial approaches
- To gain an understanding of experimental optimization methodology, particularly steepest ascent and simplex methods
- To gain a proficiency with Microsoft Excel and other freeware packages to solve basic statistical problems

Topic Outline:

Basic Statistics (Chapter 2)
- measures of central tendency
- measures of dispersion
- confidence intervals
- pooling of standard deviations
- treatment of outliers
- means testing
Experimental Design and Statistics in Chemistry Spring 2014

variance testing

Error Analysis
propagation of error

Regression Analysis Chapter 10
derivation of normal equations
regression analysis tables (analysis of variance of regression)
treatment of outliers
use of regression lines
  prediction
discrimination
confidence intervals
sensitivity
detection limits

Analysis of Variance Chapter 3
one-way designs
two-way designs

Experimental Design Methods Chapter 5
factorial designs Chapter 6-7
fractional factorial designs Chapter 8
central composite designs
Three-level and mixed-level designs Chapter 9

Optimization Methods Chapter 11
  steepest ascent methods
  simplex optimization
  genetic algorithms

Proposed Schedule:
May 5 EXAM I (possibly including take-home section)
May 26 No class, Memorial Day Holiday
Finals week EXAM II (possibly including take-home section)

Course Grading:
  Mid-term exam 35%
  Final exam 40%
  Problem sets (several of which will total) 25%

Additional Texts of Interest:


**Recorded Lectures**

The lectures for this class will be recorded; the screencasts will be made available on the Lecture Archive page available on the course homepage on Bb Learn. Every effort will be made to have the screencasts posted within 48 hours of the class. They will be available in both Shockwave (Flash) and zipped Ipad (*.m4v) format. In some cases additional material will be assigned as recorded lectures only. You are responsible for the material presented in those lectures as well.

**Microsoft Office Availability**

Unfortunately, the university decided approximately a year and a half ago to discontinue the student license for Microsoft Office products as a cost-saving measure. This affects you if you downloaded and installed your copy of MS Office from the Drexel software server; if you purchased your own copy of Office when you purchased your computer you are not affected by this situation. This creates a problem in that we have extensively used Excel for problem solving and data analysis in CHEM789; in particular we use many of the tools in Excel’s Data Analysis Toolpack Add-on that do not have good replacements in either Calc (as part of Open Office) or Spreadsheets (as part of Google Docs). After a good deal of hunting I have found an alternative freeware spreadsheet program named Gnumeric that in my opinion has better statistical analysis tools than those in Excel’s Data Analysis Toolpack. You should download the software (the current version is 1.12.9) from [http://projects.gnome.org/gnumeric/](http://projects.gnome.org/gnumeric/). The on-line User's Manual for the program can be found at [http://projects.gnome.org/gnumeric/doc/gnumeric.shtml](http://projects.gnome.org/gnumeric/doc/gnumeric.shtml). Another package that is highly recommended is R (see [http://www.r-project.org/](http://www.r-project.org/)), an amazingly complete (and free) statistical analysis environment. An overview can be found at [http://www.r-project.org/about.html](http://www.r-project.org/about.html) (the current version is 3.0.2). It is a "statistical analysis environment" much like Maple is a "mathematical computing environment" as opposed to a spreadsheet like Excel, Google Spreadsheet or Gnumeric. There are extensive on-line manuals at [http://cran.r-project.org/manuals.html](http://cran.r-project.org/manuals.html). I will provide further information about R in class.

*Note to Macintosh Users:* For some reason, Microsoft has decided not to include the Data Analysis Toolpack Add-on in the latest versions of Microsoft Office for the Macintosh. There is
a free alternative for the missing Add-on: StatPlus:mac LE offered by a company named AnalystSoft, Inc (see http://www.analystsoft.com/en/products/statplusmacle/ for details). The free LE version includes ANOVA and linear regression. The free edition can be upgraded to the regular version (student price of $90 for a single license and $199 for a 4-pack) which includes polynomial regression, amongst other tools. IF anyone finds other possible solutions for this Mac issue, please let me know.

Bb Learn

We will be using Bb Learn 9, Drexel’s on-line Course Management System, extensively to enhance communication in CHEM789. The instructions below tell you how to log on and begin using Bb Learn:

1) Login through DrexelOne at http://one.drexel.edu.
2) Enter your Drexel domain ID and password, click on Login.
3) Click on the Students Tab.
4) Click on the My Courses link.

or

1) Enter the Drexel Bb Learn website directly at https://learn.dcollege.net/.
2) Enter your Drexel domain ID and password, click on OK.

If you enter these correctly you will now be on your Bb Learn dashboard. Select CHEM789 Statistics & Experimental Design from the list of courses in the center pane of the screen under the heading My Courses. You will now be on the course homepage. Please note that ALL of your homework assignments will be posted as assignments on the homepage. The Announcements page will be used for assignment and exam reminders, etc.

Communication

It is assumed that all students have a Drexel computer account for email and easy access to the Internet and to the Drexel University network.

Academic Integrity

As you are working towards becoming a chemical professional, you are expected to maintain the highest degree of integrity in your work, as reflected by the Ethical & Professional Guidelines as published by the American Chemical Society (available at the ACS website under Careers, Professional Development, Ethics and Professional Guidelines). Your efforts as a student here at Drexel are covered by the academic dishonesty policy found at http://www.drexel.edu/provost/policies/academic_dishonesty.asp.

Course Drop/Withdrawal

Courses may only be dropped during the “drop period” lasting from the beginning of the enrollment period through the end of the second week of the quarter. Dropping a course results in the course being removed from the student’s academic record without a “W” appearing on the transcript; i.e., neither the course nor the grade of “W” appears on the student’s transcript. Students may withdraw from a course during the “withdrawal period” lasting from the beginning of the third week through the end of the seventh week of the quarter. Withdrawing from a course
causes both the name of the course and the grade of “W” to appear on the student’s transcript. Before withdrawing from a course, students should consult with the instructor. You should consult the information found on the Provost’s office website http://www.drexel.edu/provost/policies/academic_transactions.asp for complete details.

Disability Services

Students with disabilities who wish to request accommodations and services at Drexel University need to present a current accommodation verification letter (“AVL”) to the instructor before accommodations can be made. AVL's are issued by the Office of Disability Resources, which is based in the Office of Equality & Diversity (see http://www.drexel.edu/oed/disabilityResources/).

Syllabus Modification

I reserve the right to modify the syllabus, including the course schedule and list of topics, at anytime during the course. I will announce any changes both in lecture and by posting on Bb Learn.

Rev 3/29/14 kgo