

CHM 6165
INTRODUCTION TO CHEMOMETRICS
Spring Semester 2023, 3 Credits
LEIGH 242

- Instructor:** John Bowden, Basic Science Building (BSB) 324
Phone: 352-294-4063, Email: john.bowden@ufl.edu
- Lectures:** Tuesday, 11:45AM-12:35PM (Period 5)
Thursday, 11:45AM-1:40PM (Periods 5 and 6)
- Office hours:** After class periods or by appointment.
- Course objectives:** To provide students with an introductory foundation in statistical and data management methods/tools often used by analytical chemists, using the programming language R as the teaching platform. Students will learn how to select the appropriate method, handle data, and effectively disseminate results.
- Textbooks:** Txt1 – "R in Action," **2nd Edition**, Robert I. Kabacoff; \$59.99 (list), \$50.50 (Amazon, new), \$34.05 (Amazon, used) AND Txt2 – "Practical Statistics for the Analytical Scientist", 2nd Edition, Stephen Ellison, Vicki Barwick, Trevor Farrant, \$69.00, \$45.99 (Amazon new) or \$35.85 (Amazon used). Both books are not required, but strongly suggested and may serve as useful references. Amazon has the option to rent these books as well, I believe.
- Grading:** Grades will be based out of 500 points:
150 points for midterm exam (take home)
200 points for final exam (in class)
70 points for in class quizzes
50 points for in class presentation (5 min)
30 points for attendance for guest zoom lectures.
- Grade scale: Course grades will be assigned based on the following grading scheme: A (100 – 94), A- (93.99-90), B+ (89.99 – 87), B (86.99 – 84), B- (83.99 – 80), C+ (79.99 – 77), C (76.99 – 74), C- (73.99 – 70), D+ (69.99 – 76), D (66.99 – 64), D- (63.99 – 61), E (60.99 – 0).
- Class Presentations: In an effort to provide an interactive element, there will be one class presentation mid-semester. Selected topics for the presentations should be made in consultation with Dr. Bowden.

Presentation – Students will select a case study on data ethics and will give a 5 min presentation to the class. The exercise will be graded based on the ability to communicate and present the material, with special attention to framing key concepts in data ethics.

Quizzes: There will be 7 rapid quizzes (no notes allowed) throughout the semester that will cover basic concepts covered prior to the quiz date.

Zoom Attendance: There were be several guest lectures on zoom, points will be given for attendance and participation. Full attendance points are only awarded with zoom cameras on during the lecture.

Mid-term: The mid-term exam will be take-home and will be handed out **March 2 and will be due March 9 at the beginning of class.**

Final exam: The cumulative final exam will be take-home and will be handed out **May 4th, 10am to 12 pm, LEIGH 242.**

Information on current UF grading policies is online: (<https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>).

Course policies:

Attendance will not be recorded (except for guest zoom lectures), but participation in lectures and demonstration periods is important for assimilating the course material. Any request for make-up exams or quizzes should be made to Dr. Bowden as far in advance as possible.

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

UF students are bound by The Honor Pledge which states: "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest

standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (<http://www.dso.ufl.edu/sccr/process/student-conduct-honorcode/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class."

Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at <https://evaluations.ufl.edu>. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at <https://evaluations.ufl.edu/results/>.

For counseling the following resources are available to students: **U Matter, We Care:** If you or a friend is in distress, please contact umatter@ufl.edu or 352-392- 1575. **Counseling and Wellness Center:** <http://www.counseling.ufl.edu/cwc/Default.aspx>, 352-392-1575; the University Police Department: 352-392-1111 or 911 for emergencies. **Sexual Assault Recovery Services (SARS):** Student Health Care Center, 352-392-1161.

In order to ensure student privacy, communication concerning grades will only be conducted through Canvas or in a personal meeting (zoom or face to face).

Course Schedule

Tuesday, January 10: Introduction and Preparation of R

Thursday, January 12: R Basics and Tidyverse

Tuesday, January 17: Graphing in R

Thursday, January 19: Graphing in R (**Quiz 1**)

Tuesday, January 24: Normal Distribution

Thursday, January 26: Significance Tests and ANOVA

Tuesday, January 31: ANOVA

Thursday, February 2: ANOVA (**Quiz 2**)

Tuesday, February 7: Bivariate Relationships

Thursday, February 9: Regression

Tuesday, February 14: Nonparametric Tests (**Quiz 3**)

Thursday, February 16: Student Presentations

Tuesday, February 21: Outliers, Missing Data, Non-Detects

Thursday, February 23: Principal Component Analysis

Tuesday, February 28: Other Multivariate Methods

Thursday, March 2: MetaboAnalyst and Clustering Methods (**Quiz 4**)

Midterm Exam (take home)

Tuesday, March 7: Classification Methods/QSAR

Thursday, March 9: AI Basics and Catch up/Niche Topics/MixOmics

Spring Break

Tuesday, March 21: Calibration

Thursday, March 23: Method Performance (**Quiz 5**)

Tuesday, March 28: Experimental Design/Sampling Strategies/Power

Thursday, March 30: QA/QC in the Analytical Laboratory and Metrology (**Quiz 6**)

Tuesday, April 4: Carlie Lalone (EPA), "Bioinformatics in Ecotoxicology" and
Jeremy Koelmel, Innovative Omics, "What do you do with omics
data?"

Thursday, April 6: **GUEST IN PERSON/TBD** and Angelos Barmpoutis, UF,
"Interdisciplinary Applications of Artificial Intelligence from
Medicine to the Arts"

Tuesday, April 11: **GUEST ZOOM/TBD**

Thursday, April 13: **GUEST ZOOM/TBD** and Kelly Elkins, Towson University,
"TBD"

Tuesday, April 18: Categorical Distribution and Models

Thursday, April 20: Advance Graphing with ggplot2 and Data Management

Tuesday, April 25: Resampling Statistics and Time Series (**Quiz 7**)

Final Exam, May 5: 10:00 AM - 12:00 PM, Leigh 242