CHM 6165 – Chemometrics

Spring 2024

Instructor: Tim Garrett, MSB M641, 273-5050, tgarrett@ufl.edu

Lectures: T – 11:45-1:40 and R 12:50-1:40, LEI 242

Office hours: F 9:00-10:00

Textbook: "Chemometrics: Statistics and Computer Application in Analytical Chemistry", Matthias Otto, 3rd edition, 2017

Exams: Exams will cover material from lecture and any related reading material from assigned references or handouts.

Exam 1 will be an in class 2-hour exam, scheduled for approximately Tuesday, February 13th. This exam will cover material from lectures up to this point.

Exam 2 will be an in 2-hour exam

The final exam will be a take home exam that will cover all material.

Project: Every student will be provided data (or can use data from their research) and they will be required to prepare a report or present an oral report that describes the results of various chemometrics methods in analyzing and interpreting that data. The report would be written in a way to describe the results to another person such as a collaborator or client. A select number of oral presentations (~10) will be available depending on the enrollment.

Grading: Course grades will be assigned on the basis of the exams and the project, each counting for 25%.

Lecture Schedule (tentative)

Date	Topic
9-Jan	Introduction: chemometrics
11-Jan	Introduction: chemometrics
16-Jan	Basic statistics
18-Jan	Basic statistics
23-Jan	Experimental Design
25-Jan	Experimental Design
30-Jan	Analytical figures of merit (sensitivity, specificity, LOD)
1-Feb	Analytical figures of merit (sensitivity, specificity, LOD)
6-Feb	Quantitation and Calibration
8-Feb	Quantitation and Calibration
13-Feb	Exam 1
15-Feb	Introduction to the 'Omics sciences
20-Feb	Metabolomics
22-Feb	Lipidomics
27-Feb	Proteomics
Feb-29	Data reduction and filtering
5-Mar	Data reduction and filtering
8-Mar	Normalization and scaling
12-Mar	No Class, Spring break
14-Mar	No Class, Spring break
19-Mar	Normalization and scaling
21-Mar	Multivariate Methods
26-Mar	Exam 2
28-Mar	Multivariate Methods
2-Apr	Machine learning/Artificial intelligence
4-Apr	Machine learning/Artificial intelligence
9-Apr	Practical data analysis strategies
11-Apr	Practical data analysis strategies
16-Apr	Student presentations
18-Apr	Student presentations
23-Apr	Student presentations
30-Apr	Final exams Due