CHEM 528 Syllabus

April 3, 2018

Data Analysis for Chemistry

3 Credits
Spring 2018

Course:	CHEM 528 Data Analysis for Chemistry
Instructors:	Brian Clowers, Ph.D. and Aurora Clark, Ph. D.
Contact Info:	Phone: 509-335-4300 e-mail: brian.clowers@wsu.edu & auclark@wsu.edu
Office Hours:	Mondays and Tuesdays 9:00—10:00 am
Course Time:	Tuesdays and Thursdays Time: 10:35-11:50 am
Location:	Fulmer 438

Text: 1. Introduction to Python for Science, Release 0.9.23, David Pine (Distributed via CoCalc)

1. Hand-outs, review articles, and other information will be provided via CoCalc.

Computing Requirements

- Access to a computer with a functional, modern web-browser (e.g. Chrome, Firefox, etc.).
- Registration at http://cocalc.com

Goals and Learning Objectives: To address modern challenges across the chemical sciences and add clarity to complex, multidimensional data sets a solid foundation related to data analysis and interpretation is necessary. Additionally, to effectively place this knowledge into practice a range of computational skills are required. Consequently, this class aims to develop a student's understanding of data collection, processing, and statistical analysis while providing them with an introductory skill set in computer scripting languages.

Using Python as a learning and processing platform, students will be exposed to a range of case studies aimed at demonstrating the effective use of data analysis, reduction, and interpretation

techniques. Underpinning these examples will be a tractable application of statistics specifically geared to towards the chemical and physical sciences.

Upon successful completion of this course students will:

Student Learning Outcome	Evaluation of Outcome
Become familiar with core Python scripting language and understand its basic usage as a scientific computing tool.	Homework Assignments, Scripting Proficiency Exam
Code organization, Data structures, File I/O, introduction to numerical techniques, and basic GUI programing	Homework Assignments, Scripting Proficiency Exam, Class Presentation
Develop the core skills to graphically present scientific data from a variety of input formats	In class presentations and graded course work.
Understand the underlying assumptions of the most common data reduction and clustering approaches used in modern chemometric applications	Homework assignments and participation in class discussions
Apply course exercises to a student driven data analysis challenge.	Course project and class presentation

GRADED ACTIVITIES:

Homework	**40%**	**100 points**
Scripting Proficiency Exam	**20%**	**50 points**
Class Presentations	**10%**	**25 points**
Final Project	**30%**	**75 points**

GRADING SCALE:

A: >=90%	**A-: 85–89.9%**	**B+: 80–84.9%**	**B: 75–79.9%**	**B-: 70–74.9%**
C+: 65–69.9%	**C: 60–64.9%**	**C-: 55–59.9%**	**D: 50–54.9%**	**F: <50%**

Homework—10 points each

- **10 of 13 assignments will be counted towards the final grade**

Throughout the semester and following in-class demonstrations homework will be assigned to demonstrate competency for a given topic or skill. Sample datasets will be posted on the course website (www.cocalc.com) along with the example code presented in lecture. Homework is to be turned in electronically via CoCalc. Comments and corrections to students' submissions will also be provided electronically using CoCalc as well. Innovative solutions provided by students will anonymously be highlighted in subsequent class periods.

Scripting Proficiency Exam—50 points

A single take-home exam will be assigned during the 6th week of the class. Focusing on the basic use of scripting languages in the physical sciences, this exam is to be completed independently. Electronic and textual resources may be utilized to complete the exam provided sources leading to solutions are adequately cited.

Class Presentation—25 points each

- **One 25 minute presentation**

Beginning the 5th week of class, students will actively present the solution to an assigned challenge problem building upon the concepts previously covered in class. The dates of these presentations will be selected during the second week of class to provide adequate time for preparation. Student solutions are to be posted electronically prior to the presentation class period to allow others to follow. For each challenge question the topic data set will be assigned or chosen by the student with instructor approval. Students are encouraged to select a topic dataset relevant to the research interests. Students will be expected to provide a 10-minute introduction to the topic, followed by 10 minutes outlining a detailed rationale for the approach selected, with the final portion of the presentation focusing on the interpretation of the result.

Final Projects—75 points

- **10 points for the initial proposal**
- **25 points for a written report**
- **40 points for the class presentation**

During the 8th week of class students will be tasked with providing a 2-page project proposal focusing the application of computational approaches to solving a problem related to the physical sciences. Topics focusing on the student's research interests are encouraged and assistance in

project selection will be provided if necessary. Example projects may include, molecular dynamics, signal processing, experimental design optimization, and database mining. A written report (5 pages excluding code solution) and an annotated solution will be provided to the instructor. This written report will be due at the beginning of the class period in which the student is to present the solution to the project proposal.

Workload Statement

For every equivalent lecture credit students are expected to spend at least 3 hours per week on work outside the classroom. This work may be in the form of homework, project preparation, take-home exams or any other work associated with the duties of the course.

Outline of Class Schedule:

Week Date	Dates	Topic	Assignment
1	1/9/2018	Introduction to Python	Scripting Exercise 1
	1/11/2018	Introduction to Python	HW1
2	1/16/2018	No Class -- Holiday	Scripting Exercise 2
	1/18/2018	Flow Control	HW2
3	1/23/2018	Plotting Basics	Array Indexing and Slicing
	1/25/2018	Data Structures and Storage	HW3
4	1/30/2018	Python in Chemistry	File Manipulation
	2/1/2018	Advanced Plotting	HW4
5	2/6/2018	Introduction to Numerical Techniques	Exam Assigned
	2/8/2018	Numpy in Depth	
6	2/13/2018	Introduction to OOP	Plot Class and Trends
	2/15/2018	Lessons Learned, Pitfalls, and Race Conditions	HW5
7	2/20/2018	No Class -- Holiday	Data Clustering
	2/22/2018	Classification Algorithms	HW6
8	2/27/2018	Clustering Algorithms	Data Reduction
	3/1/2018	Principle Component Analysis	HW7
9	3/6/2018	Partial Least Squares Discriminant Analysis	Similarities vs Differences
	3/8/2018	Putting it Together: Data, Processing, Clustering	HW8
10	3/13/2018	Spring Break	
	3/15/2018		
11	3/20/2018	Process and Experimental Design	Result Deconvolution
	3/22/2018		HW9
12	3/27/2018	Pattern Recognition/Introduction to Graph Theory	Node Exercise
	3/29/2018		HW10
13	4/3/2018	Case Study: Molecular Dynamics and Graph Theory	
	4/5/2018		HW11
14	4/10/2018	Case Study: Peak Picking and Deconvolution	
	4/12/2018	Student Presentations	HW12
15	4/17/2018	Student Presentations	
	4/19/2018		HW13
16	4/24/2018	Student Presentations	
	4/26/2018		

Attendance Policy: Though attendance will not be taken, class participation remains an integral to meeting the stated course objectives. It is incumbent upon each student to notify the instructor in advance and obtain approval for an absence when a student presentation is scheduled (i.e. challenge problems and final presentations). An unexcused absence for days on which a

student is to present information to the class will result in no credit for that particular assignment.

ACADEMIC INTEGRITY: Academic integrity is the cornerstone of higher education. As such, all members of the university community share responsibility for maintaining and promoting the principles of integrity in all activities, including academic integrity and honest scholarship. Academic integrity will be strongly enforced in this course. Students who violate WSU's Academic Integrity Policy (identified in Washington Administrative Code (WAC) 504-26-010(3) and -404) will be reported to the Office of Student Conduct. A confirmed violation of WSU's Academic Integrity Policy will result in a course failure.

Cheating includes, but is not limited to, plagiarism and unauthorized collaboration as defined in the Standards of Conduct for Students, WAC 504-26-010(3). It is expected that you are to read and understand all of the definitions of cheating: http://app.leg.wa.gov/WAC/default.aspx?cite=504-26-010. If you have any questions about what is and is not allowed in this course, you should ask the course instructor before proceeding. If you wish to appeal a faculty member's decision relating to academic integrity, please use the form available at conduct.wsu.edu.

When completing take-home exams and homework, students are not to collaborate, discuss, or share solutions to question with other students unless approved by the instructor. Additionally, consultation and solicitation via on-line forums is discouraged.

ACCOMMODATIONS: Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; 509-335-3417) to schedule an appointment with an Access Advisor. All accommodations MUST be approved through the Access Center. For more information contact a Disability Specialist at 509-335-3417, http://accesscenter.wsu.edu, or Access.Center@wsu.edu. Accommodations are also available for students whose course activities fall on days that are objectionable because of religious beliefs. Request for accommodations should be made at least a week before the accommodation is required.

SAFETY: WSU urges students to follow the "Alert, Assess, Act," protocol for all types of emergencies and the "Run, Hide, fight" response for an active shooter incident. Remain ALERT (through direct observation or emergency notification), ASSESS your specific situation, and ACT in the most appropriate way to assure your own safety (and the safety of others if you are able). Please sign up for emergency alerts on your account at MyWSU. For more information on this subject, campus safety, and related topics, please view the FBI's Run, Hide, fight video (https://www.fbi.gov/about/partnerships/office-of-partner-engagement/active-shooter-incidents) and visit the WSU safety portal (https://oem.wsu.edu/about-us/).