Chemical Process Data Science
ECH 6845
Class Periods: -
Location: -
Academic Term: Fall xxxx

Instructor

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392-0862
CHE 223

Office Hours M,W 3 pm-4 pm, in person CHE 223 or Join Zoom Meeting
https://ufl.zoom.us/j/95675535395

Teaching Assistant/Peer Mentor/Supervised Teaching Student

Please contact through the Canvas website

- NA

Course Description

(3 credits) Applications of fundamental data science visualization methods and algorithms, with a strong emphasis on examples from science and technology.

Course Pre-Requisites / Co-Requisites

Basic working knowledge of Python programming or other languages such as MATLAB, C++, etc.

Course Objectives

In the modern chemical processing factory, data is recorded continually via sophisticated machines with numerous sensors. As process engineers, we must learn how to handle and analyze this data to our benefit. This becomes especially crucial to mitigate process variations, safety and quality events in highly integrated manufacturing processes for pharmaceutical drugs or semiconductor microchips. By the end of this course, students will be able to:

- Manipulate and visualize large datasets using Python packages, including numpy arrays, pandas, dictionaries, and data visualization aids, such as matplotlib and seaborn;
- Analyze large process datasets with supervised learning techniques for regression, including both regression and classification algorithms for data analysis;
- Analyze process data with unsupervised machine learning techniques, handle unlabeled datasets and learn how to harness the power of modern computers to identify patterns and commonalities in datasets using basic unsupervised machine learning algorithms.
- Learn how to use RDkit molecular package to featurize molecules for applications to molecular informatics.

Materials and Supply Fees

N/A

Required Textbooks and Software

None

Recommended Materials

N/A

Course Schedule

Week 1: Review of Python Basics / Pandas
Week 2: Review of Pandas / Data visualization
Week 3: Introduction to cheminformatics toolkit - RDkit
Week 4: RDkit Substructure searching, chemical reactions, coordinate generation (2D or 3D), fingerprinting
Week 5: Linear Regression
Week 6: Boot strapping and resampling for checking model accuracy
Week 7: Logistic Regression
Week 8: Midterm-1 / K Nearest neighbors – Algorithm and examples from chemical informatics/process
Week9: K means clustering – Algorithm and examples from chemical informatics
Week 10: Support Vector Machines – Algorithm and examples from chemical informatics
Week 11: Principal component analysis – dimensionality reduction in highly integrated processes
Week 12: Naïve Bayes Regression
Week 13: Gaussian Process Regression
Week 14: Midterm-2 / Deep Learning – Introduction for Process & Quality Control
Week 15: Review / practice problems / Final Exam

Attendance Policy, Class Expectations, and Make-Up Policy

Excused absences must be in compliance with university policies in the Graduate Catalog (http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#attendance) and require appropriate documentation. Additional information can be found here: https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/

Evaluation of Grades

Grades will be based on weekly assignments, two midterm tests and a final exam. Weekly assignments must be submitted online before class time on the date they are due.

Assignment	Percentage of Final Grade
Homework Assignments (10-12)	30%
Exams	70%

Grading Policy

Percent	Grade	Grade points
90.0 - 100	A	4.00
87.0 – 89.9	A-	3.67
84.0 - 86.9	B+	3.33
81.0 - 83.9	B	3.00
78.0 - 80.9	B-	2.67
75.0 - 77.9	C+	2.33
72.0 - 74.9	C	2.00
69.0 - 71.9	C-	1.67
66.0 - 68.9	D+	1.33
63.0 - 65.9	D	1.00
60.0 - 62.9	D-	0.67
0 - 59.9	E	0.00

More information on UF grading policy may be found at:
http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#grades

Students Requiring Accommodations

Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the Disability Resource Center (352-392-8565,

https://www.dso.ufl.edu/drc). It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

Course Evaluation

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/.

Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/.

In-Class Recording

Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A "class lecture" is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation, assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To "publish" means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third party note/tutoring services. A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student Honor Code and Student Conduct Code.

Commitment to a Safe and Inclusive Learning Environment

The Herbert Wertheim College of Engineering values broad diversity within our community and is committed to individual and group empowerment, inclusion, and the elimination of discrimination. It is expected that every person in this class will treat one another with dignity and respect regardless of gender, sexuality, disability, age, socioeconomic status, ethnicity, race, and culture.

If you feel like your performance in class is being impacted by discrimination or harassment of any kind, please contact your instructor or any of the following:

- Your academic advisor or Graduate Program Coordinator
- Jennifer Nappo, Director of Human Resources, 352-392-0904, jpennacc@ufl.edu
- Curtis Taylor, Associate Dean of Student Affairs, 352-392-2177, taylor@eng.ufl.edu
- Toshikazu Nishida, Associate Dean of Academic Affairs, 352-392-0943, nishida@eng.ufl.edu

University Honesty Policy

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 (https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) 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.

Software Use

All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Student Privacy

There are federal laws protecting your privacy with regards to grades earned in courses and on individual assignments. For more information, please see:
http://registrar.ufl.edu/catalog0910/policies/regulationferpa.html

Campus Resources:

Health and Wellness

U Matter, We Care:
If you or a friend is in distress, please contact umatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.

Counseling and Wellness Center: http://www.counseling.ufl.edu/cwc, and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

Sexual Assault Recovery Services (SARS)
Student Health Care Center, 392-1161.

University Police Department at 392-1111 (or 9-1-1 for emergencies), or http://www.police.ufl.edu/.

Academic Resources

E-learning technical support, 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu. https://lss.at.ufl.edu/help.shtml

Career Resource Center, Reitz Union, 392-1601. Career assistance and counseling. https://www.crc.ufl.edu/.

Library Support, http://cms.uflib.ufl.edu/ask. Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring. https://teachingcenter.ufl.edu/.

Writing Studio, 302 Tigert Hall, 846-1138. Help brainstorming, formatting, and writing papers. https://writing.ufl.edu/writing-studio/.

Student Complaints Campus*:* https://www.dso.ufl.edu/documents/UF_Complaints_policy.pdf

On-Line Students Complaints*:* http://www.distance.ufl.edu/student-complaint-process.