ChBE 4803/8803 AI for Experimental Chemical Engineers (and Beyond!)
Spring 2025

Location: MoSE G021
Time: 8-9:15 am
Credits: 03

Prerequisites:

Background in chemical engineering and Python programming

Pre- and/or Co-Requisites:

- 8803: Graduate students are encouraged to take ChBE 6745 and ChBE 6746 prior to taking this course. Students should be familiar with basic concepts in math, linear algebra, numerical methods, optimization, python programming, and data analytics to be successful in this course.
- 4803: Prerequisites are: CHBE 3215 OR BMED 3310 OR MSE 3210

For both undergraduate and graduate students taking this course, you do not need to have taken any Python course before, but be aware that we will use Python codes in this course. If you already know how to program in Python, great; if not, you will need to invest time to become literate in Python (all your knowledge from MATLAB can be easily transferred to Python). **Module 0** of this course will offer resources that you can use to improve your Python programming.

Instructor:
Professor Vida Jamali (she/her/hers).
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Office hours: TBD

Teaching Assistants:
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Course Description: This course has two primary objectives: (a) to introduce students to advanced deep learning and AI methods and (b) to teach students how to use such models on experimental data relevant to chemical engineering and other disciplines, including biomedical engineering, materials science and engineering, and chemistry. Chemical (as well as bio and materials) engineers work with experimental data of various modalities that span microscopy images, time series data, spectrophotometry data, and texts, to name a few. This course will first introduce students to the foundations of popular AI models developed in the last 10 years and their application in analyzing experimental data. In addition to covering various model architectures (e.g., CNN, VAE, LLM, etc.), we will cover foundational topics related to AI,

including framing loss function, initialization, error backpropagation, gradient computation, and model fitting. The course will maintain a balance between neural network basics and application to experimental data at hand, such that the students obtain key knowledge on how to efficiently select the most suitable AI model and apply it to the data, know the mathematical principles of the model operation, test the model performance, and relevant statistical analysis. Overall, by the end of the course, the students will have a good understanding of how to apply AI models to experimental data relevant to chemical engineers and extract useful information.

Specific Outcome: At the end of this course, the student will:

- have a good understanding of how AI models operate: Students will be able to explain the principles and operation of popular AI models (e.g., Convolutional Neural Networks (CNN), Variational Autoencoders (VAE), and Large Language Models (LLM)) and understand their relevance to analyzing experimental data,
- be able to apply AI models to experimental data: Gain hands-on experience in applying AI models to various types of experimental data common in chemical engineering, including microscopy spectroscopy, synthesis, biomolecular engineering, and electrochemistry,
- be able to select a model and implement it: Students will be able to assess which type of AI model is suitable for their data,
- have a mathematical understanding of the AI models: This includes loss functions, optimization, and regularization, and implement the appropriate algorithms accordingly,
- be able to evaluate the performance of the model: Students will learn the relevant tests and statistical methods to evaluate the performance of the AI model and how to report the results,
- be able to communicate their results and present them to their peers.

Recommended textbook and other resources:
Simon Prince, Understanding Deep Learning (available for free or purchase)

Useful resource:

Terence Parr and Jeremy Howard, The Matrix Calculus You Need for Deep Learning, arXiv
Justin Johnson, Python NumPy tutorial
Basic Linear algebra review
Zico Kolter, Linear algebra review and reference

Class website: TBD

Web: Course material, homework assignments, screencasts, announcements and grades will be posted on Canvas (https://canvas.gatech.edu/). Materials needed for each week will be organized in the Files section. All announcements for this course will be posted on Canvas.

Attendance: Attendance is encouraged. Material presented in class will appear on homework. You are responsible for obtaining class materials if absent for non-health or institute-approved reasons. In the case of an absence when an exam is given, make-up will only be given when the absence is caused by an official Georgia Tech event or illness; such absences must be documented with a letter from the

appropriate Georgia Tech official, a physician or the Dean of Students. **Everyone should feel comfortable asking questions in our class, and should respect the questions of their classmates.**

Piazza: (accessible from Canvas plug-in) https://piazza.com/gatech/spring2025/chbe4803vjchbe8803vj
Piazza is the main communication channel in this course. Emails are strongly discouraged. You will be getting an email from Piazza (to your official GT email) inviting you to join the class Piazza site. We will be conducting all class-related discussions here this semester. The quicker you begin asking questions on Piazza, the quicker you'll benefit from the collective knowledge of your classmates and instructors. We encourage you to ask questions when you're struggling to understand a concept or a homework problem or just have a general question about class procedures—you can even do so anonymously. Here are the ground rules:

1. TAs and instructor will only respond to questions 24 hours after they are posted. This is to encourage you to help and answer each other -- part of what Piazza is all about!
2. We will "endorse" answers from students as soon as possible so you know that the answers your classmates posted are "correct".
3. We will not answer any questions via email, except those of a personal nature. Please use Piazza so everyone can benefit.

Grading Scheme:

Homework	30% (for undergrads 40%)
Midterm Exam	20%
Student Paper Presentation	10%
Project	40% (for undergrads 30%)

Homework:
Homework (electronic copy uploaded on Canvas unless problem statement specifies otherwise) is due at the beginning of class (8:00 am). Assignments will be considered late if uploaded after 8:05 am. Unfortunately, we won't be able to accept late HWs to be fair and so solutions can be posted promptly. Everyone is entitled to a one-time, 1-day (business day) extension (i.e., homework due Thursday would be due by 8:00 am Friday). No need to email me to indicate the reason. a) This is separate from any other accommodation from the Office of Disability Services, and b) This is only valid for HWs, not the project.

Solutions will be posted on Canvas ~at the end of class (or next business day if late submitters). Students are responsible for determining their mistakes from the solutions or office hours. Working with others is allowed and encouraged to help each other learn, but each student must write up and turn in their own work (see Honor Code). Homework copied from classmates, former students, solutions from previous semesters, or solution manuals is considered cheating and will be reported.

Homework Grading:
All problems are worth 3 points.
0 = didn't try it at all
1 = tried some of the problem, or tried most of it but did it mostly wrong
2 = tried most or all of the problem but had some errors
2.5 = tried the whole problem and it was nearly correct with very minor error

3 = tried the whole problem and it was entirely correct

Project: Semester-long project for developing an AI model for experimental data sets coming from a lab at GT. The project will be completed in teams. You must form a team at the beginning of the semester for the group project and submit the project proposal by Jan 30th. Collaboration and teamwork are essential components of these projects, and professional behavior and respect for your teammates are critical. You and your teammates will pick a project topic and discuss it with the instructor during office hours in January to ensure that it is suitable for this course. The final project will be graded based on the following breakdown. More details/guidelines will be provided for each assignment and are subject to change. Detailed rubrics and deadlines are posted on Canvas. Assignments in **bold will be instructor-graded, and non-bold assignments will be peer-graded**.

- 10% - **Project proposal** (grads only): ~1-page proposal on the description of dataset and project goals
- 10% - Data preparation: Dataset ready for analysis (no missing values, etc.)
- 10% - **Baseline model:** Simple model evaluated with an appropriate assessment metric.
- 15% - Improved model: More accurate or efficient model with assessments.
- 10% - **Report draft:** Draft of ~5 page project report detailing approach and results.
- 25% - **Final Report:** Finalized version of the project report.
- 5% - Work ethics and team work (graded by teammates):
- 15% - Final Poster Presentation: Last day of class.

Note: Some parts of the project will be due before a topic is covered in the course (e.g., data preparation). You may revise your strategies after we cover a topic in the course but should be able to establish a simple strategy before a topic is covered by attending office hours and looking at course notes ahead of time.

Faculty-led student paper presentations:
There will be **six** student paper presentations and faculty-led discussions with days indicated on the syllabus (two papers each time, twelve papers total). Students will form groups of two. Each paper will be assigned a defense and offense team. The defense team will defend the paper for 15 min (as if this is their own research paper), and then the offense team will attach the paper for 15 min, followed by 5 min Q&A. We will have a five-minute break before starting the discussion on the second paper of that day. The papers preselected (by the instructor) cover various topics of chemical engineering research in which using AI (AI models covered in lectures) resulted in significant advancement in that research area. The papers will also introduce new directions that could be useful for the final project. **All students in the class must sign up by January 14th to present one of the papers. Please use this link to sign up:**
PaperDisussion-Team-SignUp.xlsx

Lecture Notes:
The lecture notes for the course are presented in PowerPoint slides and will be shared with students on the course Canvas page. Lecture notes will be continuously updated throughout the course so please check back regularly.

Honor Code:
Students are expected to follow the Georgia Tech Honor Code at all times.
http://www.honor.gatech.edu
Copying from other students (current or former), instructor/TA solutions from previous semesters, solution manuals, websites, AI-generated solutions, pay for work services, or any other form of word is considered an honor code violation and will be reported along with receiving a zero on the assignment.

Diversity and Disability Statement: Georgia Tech values diversity and inclusion, so do I. I am committed to a climate of mutual respect and full participation. **All of you belong here**. My goal is to create a learning environment that is usable, equitable, inclusive, and welcoming. Please be kind, respectful and professional both in and out of our classroom. If there are aspects of the instruction or design of this course that result in barriers to your inclusion, accurate assessment, or achievement, please notify me as soon as possible. Students with disabilities should contact the Office of Disability Services to discuss options for removing barriers in this course, including accommodations. ODS can be reached at 404-894-2563, dsinfo@gatech.edu, or disabilityservices.gatech.edu. If you need accommodations for exams, please contact the ODS office as soon as possible and make reservations for the days based on the schedule below for all quiz and exam dates.

Institute-Approved Absences: As per Georgia Tech policy, you are permitted to be absent from class to participate in athletic events, official field trips, and religious observances. For planning purposes, please provide me with written notice of your upcoming absence at least two weeks before the event, and ideally within the first two weeks of class. When I receive this notice, you and I will discuss opportunities to make up work you will miss in your absence. Please see http://catalog.gatech.edu/rules/4/ for more information about receiving official notice from the Registrar about the nature and timing of your upcoming Institute-approved absence.

Campus Resources for Students: If physical or mental health, hunger, or homelessness are affecting your studies, please reach out to one of these resources or to me.

- Counseling Center
  - Crisis Line: 404.894.2575 (M-F 8 a.m.- 5 p.m.)
  - After-hours counselors: 404.894.2204
- Dean of Students and Student Life (404.894.2565)
  - Student Temporary Assistance and Resources (STAR) (for services like the food pantry, emergency funds, and temporary housing)
- Georgia Tech Police Department (404.894.2500)
- LGBTQIA Resource Center
- Office of Institute Diversity
- Veterans Resource Center
- Women's Resource Center

Health and Well-being: Wellness is about maintaining an overall quality of life and the pursuit of optimal emotional, mental, physical, and interpersonal health. Wellness is not the absence of disease, illness, or stress but the presence of purpose in life, active involvement in satisfying work and play, joyful relationships, a healthy body and living environment, and happiness.

Ten Tips for Better Mental Health

1. **Build Confidence**- identify your abilities and weaknesses together, accept them, build on them and do the best you can with what you have.
2. **Accept Compliments**- many of us have difficulty accepting kindness from others but we all need to remember the positive in our lives when times get tough.
3. **Make Time for Family and Friends**- these relationships need to be nurtured; if taken for granted, they will dwindle and not be there to share life's joys and sorrows.
4. **Give and Accept Support**- friends and family relationships thrive when they are "put to the test." Just as you seek help when you are having a tough time, a friend or family member might come to you in their time of need.
5. **Create a Meaningful Budget**- financial problems are big causes of stress, especially in today's economy. Over-spending on our "wants" instead of our "needs" can compound money worries. Writing down where your money is going helps you keep a closer eye on your finances.
6. **Volunteer**- being involved in community gives a sense of purpose and satisfaction that paid work cannot. Find a local organization where your life skills can be put to good use.
7. **Manage Stress**- we all have stressors in our lives but learning how to deal with them when they threaten to overwhelm us will help to maintain our mental health.
8. **Find Strength in Numbers**- sharing a problem with others who have had similar experiences may help you find a solution and will make you feel less isolated. Even talking about the situation with people who have not experienced what you are going through is a good way to gain outside perspective.
9. **Identify and Deal with Moods**- we all need to find safe and constructive ways to express our feelings of anger, sadness, joy and fear. Channeling your emotions creatively is a wonderful way to work off excess feelings. Writing (keeping a journal), painting, dancing, making crafts, etc. are all good ways to help deal with emotions.
10. **Learn to Be at Peace with Yourself**- get to know who you are, what makes you really happy and learn to balance what you can and cannot change about yourself.

Mental Health Crisis: If you are experiencing a crisis that requires immediate attention you may speak with a counselor at any time 24 hours a day, 7 days a week. All students, **including graduate students**, currently registered in a degree-seeking program are eligible for services at the Counseling Center.

> ***During regular business hours*** (Monday-Friday 8-5) Students are initially assessed through GT CARE, a separate department working closely with the Counseling Center to meet student needs. A student who wishes to initiate serves should come by the CARE office on the first floor (Room 102B) of the Smithgall Student Services building (Flag Building) between 8:00 am and 4:00 pm, Monday through Friday. Students will need about 30 minutes to complete the initial information forms. The CARE clinician will provide a brief triage and assessment. Students will also be given a written CARE Plan which is a plan of action to address the student's described needs. Students who

are not actively in counseling may walk-into GT CARE or call CARE at 404-894-3498. Established Counseling Center clients may walk-in or call 404-894-2575.

After business hours, please call either 404-894-2575 or 404-894-3498 and select the option to speak to the after-hours counselor. You may also call the Georgia Tech police at 404-894-2500.

Life Threatening Emergency: Students who are experiencing an immediate life-threatening emergency on campus, call the **Georgia Tech Campus Police** at 404-894-2500. If off campus, please immediately call 911.

Tentative Class Schedule

Module 0

Resources for Python Programming:

https://cs231n.github.io/python-numpy-tutorial/

Matplotlib tutorial:

https://github.com/rougier/matplotlib-tutorial

Resources for reviewing linear algebra, vector calculus, and probability

https://stanford-cs221.github.io/spring2023/modules/index.html

Resources for reviewing linear algebra

Linear Algebra Review by Zico Kolter

Week	Lec #	Date	Lecture Title
1	1	1/7/25	Introduction- what is AI?
1	2	1/9/25	Supervised vs. unsupervised models
2	3	1/14/25	Generalized linear models and their application in thermodynamic property prediction
2	4	1/16/25	Deep Neural Networks (DNNs) and example application to Vapor-liquid equilibrium prediction
3	5	1/21/26	DNN: Loss Functions
3	6	1/23/25	DNN: Optimization, backpropagation
4	7	1/28/25	DNN: Initialization, Regularization, and Performance
4	8	1/30/25	Supervised, self-supervised, and unsupervised models in ChemE
5	9	2/4/25	DNNs to lower experimental cost: a battery research case study
5	10	2/6/25	Convolutional Neural Networks (CNNs)
6	11	2/11/25	Dilated CNNs
6	12	2/13/25	**Midterm Exam**
7	13	2/18/25	Faculty led paper discussion: Application of CNNs in 1) Raman spectroscopy data analysis 2) super resolution microscopy
7	14	2/20/25	Application of CNN in particle tracking and time series data analysis
8	15	2/25/25	Unsupervised models (AEs), UNet architecture
8	16	2/27/25	Faculty-led paper discussion: UNet for 1) fluorescence microscopy image restoration 2) cellular segmentation
9	17	3/4/02	Generative AI, Variational Auto Encoders (VAEs)
9	18	3/6/25	Faculty Led paper Discussion: VAE for 1) block co-polymer morphology characterization 2) scanning probe microscopy image segmentation
10	19	3/11/25	Shapley value
10	20	3/13/25	Faculty led paper discussion: Application of SHAP in 1) optimization of battery cathodes 2) high throughput quantum dot synthesis
		Spring break	

		spring break	
11	21	3/25/25	From Brownian motion to Diffusion models
11	22	3/27/25	Faculty led paper discussion: Diffusion models for 1) protein engineering 2) denoising microscopy images
12	23	4/1/25	Automating Chemical labs
12	24	4/3/25	Faculty led paper discussion: Automating chemical labs in practice: 1) autonomous self-driving fluidic technology for catalysis acceleration and testing; 2) Self-driving labs for small molecule discovery
13	25	4/8/25	Guest Lecture: TBD
13	26	4/10/25	Guest Lecture: TBD
14	27	4/15/25	Generative AI and process system engineering
14	28	4/17/25	Large Language Models
15	29	4/22/25	Poster Presentation