

**MEMORANDUM FOR STUDENTS ENROLLED IN CHEN 4341**  
**SUBJECT: CHEN 4341 – Special Topics - Administrative Instructions**

**Lecture times:** MW, 9:00 am - 10:20 am

**Location:** RBN 2011

**Instructor:** Dr. Ning Wang, office RBN 3014

**E-mail:** [nwang@uttyler.edu](mailto:nwang@uttyler.edu)

**Phone:** 903-566-7306

**Office hours:** M 12:30-2:00 pm & W 1:00-2:30 pm (and by appointment)

**TA:** Damola Agboola, [dagboola@patriots.uttyler.edu](mailto:dagboola@patriots.uttyler.edu)

**TA office hours:** T & F 4:00-5:30 pm, RBN 1034

Welcome to CHEN 4341 - Special Topics: Machine Learning in Chemical Engineering, a course designed to introduce students to the foundational concepts of machine learning (ML) and their application in chemical engineering. Students will become familiar with topics such as regression, supervised learning, unsupervised learning, and feature extraction. An overview of ML methods will be included. The course will emphasize practical programming skills using Python implementations and will use case studies in chemical engineering.

**Course Objectives:**

Upon successful completion of this course, students will be able to:

- Compare, analyze, and assess different ML algorithms and their applications in different scenarios
- Implement their own ML routine from scratch that does linear regression and logistic regression
- Implement their own ML routine for neural networks
- Obtain improved problem-solving, written, and oral communication skills
- Describe and communicate importance of ML for technological and societal challenges

The course has one prerequisite which must be completed successfully prior to taking this course:

- ✓ CHEN 3360 (Chemical Reaction Engineering)

The goal of our faculty is to be commonly available to you for assistance, so you are encouraged and expected to seek **additional instruction**. Take advantage of it, it is FREE and really will help! There are several ways you can seek help:

- ✓ You are welcome to stop by the instructor's office at any time. However, for your own satisfaction, you can ensure the instructor is available at the office by using the following options:
  - Come to office hours. This is the time the instructor has set aside to answer your questions.
  - E-mail the instructor to set up a mutually agreeable time to meet with the instructor.

- E-mail your questions to the instructor (this is the least preferred option because of the limited effectiveness of e-mail communication), but it is acceptable if other options are not possible.

### **Use of Artificial Intelligence (AI):**

UT Tyler is committed to exploring and using artificial intelligence (AI) tools as appropriate for the discipline and task undertaken. We encourage discussing AI tools' ethical, societal, philosophical, and disciplinary implications. All uses of AI should be acknowledged as this aligns with our commitment to honor and integrity, as noted in UT Tyler's Honor Code. Faculty and students must not use protected information, data, or copyrighted materials when using any AI tool. Additionally, users should be aware that AI tools rely on predictive models to generate content that may appear correct but is sometimes shown to be incomplete, inaccurate, taken without attribution from other sources, and/or biased. Consequently, an AI tool should not be considered a substitute for traditional approaches to research. You are ultimately responsible for the quality and content of the information you submit. Misusing AI tools that violate the guidelines specified for this course (see below) is considered a breach of academic integrity. The student will be subject to disciplinary actions as outlined in UT Tyler's Academic Integrity Policy.

For this course, you can use AI programs (ChatGPT, Copilot, etc.) in this course. These programs can be powerful tools for learning and other productive pursuits, including completing assignments in less time, helping you generate new ideas, or serving as a personalized learning tool. However, your ethical responsibilities as a student remain the same. You must follow UT Tyler's Honor Code and uphold the highest standards of academic honesty. This applies to all uncited or improperly cited content, whether created by a human or in collaboration with an AI tool. If you use an AI tool to develop content for an assignment, you must cite the tool's contribution to your work.

*Mode of delivery:* This is a face-to-face course.

### **Classroom Procedures:**

- a. Bring study notes, **textbooks**, note-taking material, calculator, and laptop to every class. You may not borrow or exchange calculators during graded events. If your calculator fails during a graded exercise, I am not responsible to furnish a substitute. Class preparation is your individual responsibility.
- b. Textbook:

#### **Required:**

1. Python Programming and Numerical Methods: A Guide for Engineers and Scientists, freely available [here](#). We will call this book "PPNM"
2. Deisenroth, M. P., Faisal, A. A., & Ong, C. S. (2020). [Mathematics for machine learning](#). Cambridge University Press.
3. An Introduction to Statistical Learning, freely available [here](#). We will call this book "ISL".

Additional **free** resources:

- Bishop, C. M., & Bishop, H. (2023). [Deep learning: Foundations and concepts](#). Springer Nature.

- [https://scikit-learn.org/stable/user\\_guide.html](https://scikit-learn.org/stable/user_guide.html) - This is the online user-guide for the main machine learning library we will be using known as Scikit-learn. It is an outstanding resource.
  - <https://machinelearningmastery.com/> - This is one of the best blogs out there for beginners and I strongly suggest consulting it regularly. Everything is done in Python and Keras, like this course.
  - Deep Learning for Molecules & Materials by White. <https://dmol.pub/>
- c. Students will need a **laptop** during class to participate in hands-on programming activities.

## Evaluations:

- a. *ACADEMIC DISHONESTY:* Representation of others' work as your own will not be tolerated. Cheating on examinations, quizzes, and homework and the false representation of work will be interpreted as academic dishonesty. Academic dishonesty will be subject to disciplinary action as outlined by the UT Tyler Student Guide on Conduct and Discipline.
- b. *Participation grade:* Students are expected to be engaged in class and outside of the class. The instructor will assign a participation grade to each student based on the following observations:
- ✓ Attendance in class and punctuality.
  - ✓ Level of participation in class, asking questions about the material and answering questions from the instructor.
  - ✓ Engagement in recitation sessions, demonstrating initiative to work on problems, and actively participating in the discussions.
  - ✓ Asking questions outside class: after class, during office hours, and by e-mail.
- Attendance in class is the component with more weight on participation. A student that attends every class but otherwise is not active will receive a 2.0/4.0 as participation grade. **A student who is absent for the majority of classes without a valid excuse will not pass the course, regardless of other grades.**
- c. *Homework:* A total of six homework assignments will be distributed during the semester, corresponding to the progression of course topics. All homework is mandatory and becomes part of your grade. As an engineer, your goal is to make a clear, logical, and professional presentation of your work, which is both accurate and correct. As such, both the presentation and the accuracy of your work are important, and both will be graded. It is critical that you show all of your work and leave "footprints" so that it can be easily followed. No guess work should be required to see what you did. For each homework problem, the corresponding topic and numerical answers will be provided. You are encouraged to work in groups, but the work that you turn in should be your own. Homework must be submitted online via Canvas before the **due** date.
- d. *Journal Club:*

As part of this course, students will participate in three *Journal Clubs* designed to develop critical reading, presentation, and discussion skills. Each student will present three peer-reviewed research articles during the semester, as outlined below:

- Journal Club 1:

This session will take place during the first half of the semester. At this stage, you may not have learned many machine learning techniques yet, and that's perfectly fine. For this presentation, choose any research paper that interests you but applies machine learning **outside** of chemical engineering (for example, computer vision, natural language processing, drug discovery, healthcare, or related fields). You are encouraged to focus on what excites you most about the paper, summarize it in your own words, and explain the key ideas based on your current understanding. The goal is to help you become familiar with how machine learning is used across different disciplines and to build confidence in interpreting research articles early in the course.

- Journal Club 2:

This session will take place in the middle of the semester, once you have learned some foundational machine learning concepts and techniques. For this presentation, focus on **best practices for applying machine learning in chemical engineering**. Choose a paper that demonstrates how ML methods are effectively integrated into chemical engineering problems, such as process modeling, materials discovery, reaction prediction, or molecular simulation. Emphasize how the authors applied ML responsibly and thoughtfully, including aspects like data quality, model validation, uncertainty quantification, and interpretation of results.

- Journal Club 3:

This session will take place in the second half of the semester, when most course topics have been covered and you have developed a strong foundation in machine learning, making you the course "expert." For this presentation, focus on machine learning in chemical engineering, especially those involving advanced or emerging techniques **not** covered in this course. Possible topics include Recurrent Neural Networks (RNNs), Convolutional Neural Networks (CNNs), Graph Neural Networks (GNNs), Reinforcement Learning, Large Language Models (LLMs), and Generative AI. Your goal is to explore how these methods are being applied to cutting-edge problems in chemical engineering and to demonstrate your ability to critically analyze, interpret, and communicate complex ML-driven research.

Presentation Guidelines:

- ✓ ~10 minutes per presentation.
- ✓ Each presentation will be followed by a brief Q&A and discussion.

Presentations should include:

- ✓ A brief overview of the problem addressed in the paper.
- ✓ A clear explanation of the machine learning methodology used.
- ✓ Key findings and their implications.
- ✓ Critical evaluation of the paper's strengths, limitations, and potential future directions.

Participation:

Students are expected to actively participate in discussions. Thoughtful questions, comments, and connections to course material will be part of the participation grade.

Presentation Schedule:

The sequence of presentations will be posted later via Canvas.

e. *Mid-Term Exam:*

There will be one midterm exam and no final exam. The midterm exam will be conducted during the regular class period and will last the full class time. The date for midterm is included in the course schedule. Official reasons for missing an exam are outlined in the “Student Handbook”. You are required to take a make-up Exam, regardless of your reason for missing the scheduled Exam. Report any conflict to me as soon as possible prior to the Exam.

f. *Final project (with peer-evaluation):* A multi-part project will be assigned at the beginning of the semester and due as outlined on the schedule below – in the form of a written report and oral presentation.

As practicing engineers (or professionals in other fields), you will need to solve open-ended problems and write a final report on advanced topics in ML. For example, students can present their implementation of an ML algorithm not shown in class or an application of an ML algorithm to research data in chemistry, chemical and bioengineering, materials science, etc. They will also make a conference-style presentation (~15-20 minutes) to the class about their results. Your paper must be turned in via Canvas as pdf, formatted in a journal style. Students will also **submit their topic of choice and an outline of their paper for approval** and evaluation. Your written work may be electronically tested for plagiarized content. Plagiarism is a serious offense and will result in severe consequences. Python codes must be in **.ipynb or .py format**. Handwritten work for final project will not be accepted.

The frontier of machine learning changes at breakneck speed, so the lecture content of this course serves as a survey of the “greatest hits” of machine learning and builds the foundation to understand the methods emerging every day. To provide students a chance to dig deep into exciting new topics, the final course project is encouraged to be conducted on an advanced topic not covered (or only minimally covered) in the course. I provide a (non-definitive) list of potential topics below, but if you’d like to work on something else, just come ask!

Possible advanced topics: Recurrent Neural Networks, Convolutional Neural Networks, Graph Neural Networks, Reinforcement Learning, large language models, generative AI

Important Dates:

1. Individual topics due: 01/28/2026
2. Class presentations: 04/20/2026 and 04/22/2026
3. Written reports with code submissions due: 04/22/2026

g. *Late Submissions.* It is a basic principle of professionalism that “**Professionals are not Late.**” A “COORDINATED LATE” submission occurs when you will miss the due date

for a graded assignment, and you contact me in advance. Notification immediately before the submission will not suffice. Point cuts up to the amounts below **may** be assessed for a “COORDINATED LATE” submission:

1. 0-24 hours late                      a deduction of 25% of the earned grade
2. 24-48 hours late                    a deduction of 50% of the earned grade
3. More than 48 hours late No credit.

Obviously, there are circumstances that will occur and make a timely submission impossible, and I will work with you when and if they occur.

All forms of evaluation in this course must be properly documented. As you are having your work reviewed, it is likely that you might receive help from your classmates, just simply document it. Information from the course textbooks (equations and outlines of procedures), class notes, or me is considered immediately available to all students and need not be acknowledged or documented with one exception. **YOU ARE REQUIRED TO ACKNOWLEDGE AND DOCUMENT ALL OTHER ASSISTANCE AND REFERENCES USED.** Documentation will be accomplished in accordance with any manual for writing, footnote or endnote, for papers, but for written homework, just place the documentation right at the point you received help using “Who and what” assistance.

### **Course Feedback and Collection of Student Work:**

Throughout the semester you will be asked to fill out anonymous non-graded feedback to help me guide course development. Even though these do not count for your grade, you are required to complete them to pass the course. I will also collect student work (best, average, and worst) for the ABET course and outcomes notebooks, for course improvement purposes. This will require me to make a copy of your work, keep your original and return a copy of the graded work to you. I will not draw attention as to what level of work you accomplished.

### **Grading:**

Grades will be based entirely on the student’s demonstrated ability to develop detailed, neat, organized, and correct solutions to the problems presented. Correct answers accompanied by incorrect, incomplete, or untidy solutions may receive no credit.

### **Course Points**

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Homework (6 at 3.0 points each)	18 (18 %)
Journal Club (3 at 10.0 points each)	30 (30 %)
Participation (1 at 7.0 points)	7 (7 %)
Midterm Exam (1 at 15 points each)	15 (15%)
Final Project (1 at 30 points)	30 (30%)
<b>Total</b>	<b>100 (100%)</b>

### **Grade Scale**

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85.0 points or higher

A

Between 70.0 and 84.0	B
<b><i>Between 60.0 points and 69.9</i></b>	<b>C</b>
Between 30.0 and 59.9 points	D
Less than 30.0 points	F

You need at least 60 points total to pass the course with a C grade. You need to be at the class average to receive a B grade.

### Other Resources:

1. **UT Tyler Honor Code** - Every member of the UT Tyler community joins together to embrace: Honor and integrity that will not allow me to lie, cheat, or steal, nor to accept the actions of those who do.
2. **Students Rights and Responsibilities:** to know and understand the policies that affect your rights and responsibilities as a student at UT Tyler, please follow this link: <http://www.uttyler.edu/wellness/rightsresponsibilities.php>.
3. **Campus Carry** - We respect the right and privacy of students 21 and over who are duly licensed to carry concealed weapons in this class. License holders are expected to behave responsibly and keep a handgun secure and concealed. More information is available at <http://www.uttyler.edu/about/campus-carry/index.php>.
4. **UT Tyler a Tobacco-Free University** - All forms of tobacco will not be permitted on the UT Tyler main campus, branch campuses, and any property owned by UT Tyler. This applies to all members of the University community, including students, faculty, staff, University affiliates, contractors, and visitors. Forms of tobacco not permitted include cigarettes, cigars, pipes, water pipes (hookah), bidis, kreteks, electronic cigarettes, smokeless tobacco, snuff, chewing tobacco, and all other tobacco products. There are several cessation programs available to students looking to quit smoking, including counseling, quitlines, and group support. For more information on cessation programs please visit [www.uttyler.edu/tobacco-free](http://www.uttyler.edu/tobacco-free).
5. **Grade Replacement/Forgiveness and Census Date Policies** - Students repeating a course for grade forgiveness (grade replacement) must file a Grade Replacement Contract with the Enrollment Services Center (ADM 230) on or before the Census Date of the semester in which the course will be repeated. Grade Replacement Contracts are available in the Enrollment Services Center or at <http://www.uttyler.edu/registrar>. Each semester's Census Date can be found on the Contract itself, on the Academic Calendar, or in the information pamphlets published each semester by the Office of the Registrar. Failure to file a Grade Replacement Contract will result in both the original and repeated grade being used to calculate your overall grade point average. Undergraduates are eligible to exercise grade replacement for only three course repeats during their career at UT Tyler; graduates are eligible for two grade replacements. Full policy details are printed on each Grade Replacement Contract. The Census Date is the deadline for many forms and enrollment actions of which students need to be aware. These include:

- Submitting Grade Replacement Contracts, Transient Forms, requests to withhold directory information, approvals for taking courses as Audit, Pass/Fail or Credit/No Credit.
  - Receiving 100% refunds for partial withdrawals. (There is no refund for these after the Census Date)
  - Schedule adjustments (section changes, adding a new class, dropping without a “W” grade)
  - Being reinstated or re-enrolled in classes after being dropped for non-payment
  - Completing the process for tuition exemptions or waivers through Financial Aid
- 6. State-Mandated Course Drop Policy** - Texas law prohibits a student who began college for the first time in Fall 2007 or thereafter from dropping more than six courses during their entire undergraduate career. This includes courses dropped at another 2-year or 4-year Texas public college or university. For purposes of this rule, a dropped course is any course that is dropped after the census date (See Academic Calendar for the specific date). Exceptions to the 6-drop rule may be found in the catalog. Petitions for exemptions must be submitted to the Enrollment Services Center and must be accompanied by documentation of the extenuating circumstance. Please contact the Enrollment Services Center if you have any questions.
- 7. Disability/Accessibility Services** - In accordance with Section 504 of the Rehabilitation Act, Americans with Disabilities Act (ADA) and the ADA Amendments Act (ADAAA) the University of Texas at Tyler offers accommodations to students with learning, physical and/or psychological disabilities. If you have a disability, including a non-visible diagnosis such as a learning disorder, chronic illness, TBI, PTSD, ADHD, or you have a history of modifications or accommodations in a previous educational environment, you are encouraged to visit <https://hood.accessiblelearning.com/UTTyler> and fill out the New Student application. The Student Accessibility and Resources (SAR) office will contact you when your application has been submitted and an appointment with Cynthia Lowery, Assistant Director of Student Services/ADA Coordinator. For more information, including filling out an application for services, please visit the SAR webpage at <http://www.uttyler.edu/disabilityservices>, the SAR office located in the University Center, # 3150 or call 903.566.7079.
- 8. Student Absence due to Religious Observance** - Students who anticipate being absent from class due to a religious observance are requested to inform the instructor of such absences by the second class meeting of the semester.
- 9. Student Absence for University-Sponsored Events and Activities** - Revised 05/19 If you intend to be absent for a university-sponsored event or activity, you (or the event sponsor) must notify the instructor at least two weeks prior to the date of the planned absence. At that time the instructor will set a date and time when make-up assignments will be completed.
- 10. Social Security and FERPA Statement** - It is the policy of The University of Texas at Tyler to protect the confidential nature of social security numbers. The University has changed its computer programming so that all students have an identification number. The electronic transmission of grades (e.g., via e-mail) risks violation of the Family Educational Rights and Privacy Act; grades will not be transmitted electronically.



**11. Emergency Exits and Evacuation** - Everyone is required to exit the building when a fire alarm goes off. Follow your instructor's directions regarding the appropriate exit. If you require assistance during an evacuation, inform your instructor in the first week of class. Do not re-enter the building unless given permission by University Police, Fire department, or Fire Prevention Services.

**12. Student Standards of Academic Conduct** - Disciplinary proceedings may be initiated against any student who engages in scholastic dishonesty, including, but not limited to, cheating, plagiarism, collusion, the submission for credit of any work or materials that are attributable in whole or in part to another person, taking an examination for another person, any act designed to give unfair advantage to a student or the attempt to commit such acts.

i. "Cheating" includes, but is not limited to:

- copying from another student's test paper;
- using, during a test, materials not authorized by the person giving the test;
- failure to comply with instructions given by the person administering the test;
- possession during a test of materials which are not authorized by the person giving the test, such as class notes or specifically designed "crib notes". The presence of textbooks constitutes a violation if they have been specifically prohibited by the person administering the test;
- using, buying, stealing, transporting, or soliciting in whole or part the contents of an unadministered test, test key, homework solution, or computer program;
- collaborating with or seeking aid from another student during a test or other assignment without authority;
- discussing the contents of an examination with another student who will take the examination;
- divulging the contents of an examination, for the purpose of preserving questions for use by another, when the instructor has designated that the examination is not to be removed from the examination room or not to be returned or to be kept by the student;
- substituting for another person, or permitting another person to substitute for oneself to take a course, a test, or any course-related assignment;
- paying or offering money or other valuable thing to, or coercing another person to obtain an unadministered test, test key, homework solution, or computer program or information about an unadministered test, test key, home solution or computer program;
- falsifying research data, laboratory reports, and/or other academic work offered for credit;
- taking, keeping, misplacing, or damaging the property of The University of Texas at Tyler, or of another, if the student knows or reasonably should know that an unfair academic advantage would be gained by such conduct; and
- misrepresenting facts, including providing false grades or resumes, for the purpose of obtaining an academic or financial benefit or injuring another student academically or financially.

ii. "Plagiarism" includes, but is not limited to, the appropriation, buying, receiving as a gift, or obtaining by any means another's work and the submission of it as one's own academic work offered for credit.

iii. “Collusion” includes, but is not limited to, the unauthorized collaboration with another person in preparing academic assignments offered for credit or collaboration with another person to commit a violation of any section of the rules on scholastic dishonesty.

iv. All written work that is submitted will be subject to review by plagiarism software.

### 13. UT Tyler Resources for Students

- UT Tyler Writing Center (903.565.5995), writingcenter@uttyler.edu
- UT Tyler Tutoring Center (903.565.5964), tutoring@uttyler.edu
- The Mathematics Learning Center, RBN 4021, this is the open access computer lab for math students, with tutors on duty to assist students who are enrolled in early-career courses.
- UT Tyler Counseling Center (903.566.7254)

### Tentative schedule:

Week		January	Material	Assigned Reading	Evaluation due
1	M	12	Syllabus, Intro to ML	PPNM	-
	W	14	Intro to Python	PPNM	-
2	M	19	no classes	-	-
	W	21	Intro to Python	PPNM	HW 1
3	M	26	Intro to Python	PPNM	-
	W	28	Intro to Python	PPNM	HW 2
		<b>February</b>	<b>Material</b>	<b>Assigned Reading</b>	<b>Evaluation due</b>
4	M	2	Journal Club 1	-	Journal Club 1 Presentation
	W	4	Intro to Python	PPNM	HW 3
5	M	9	Math review	Mathematics for Machine Learning	-
	W	11	Math review	Mathematics for Machine Learning	HW 4
6	M	16	Math review	Mathematics for Machine Learning	-
	W	18	Midterm	-	HW 5, Midterm
7	M	23	Linear Regression	ISL Ch. 3.1-3.3, 7.1	-
	W	25	MLR	ISL Ch. 3.1-3.3, 7.1	-
		<b>March</b>	<b>Material</b>	<b>Assigned Reading</b>	<b>Evaluation due</b>
8	M	2	Model Selection	ISL Ch. 2.2, 5.1-5.3	-
	W	4	Journal Club 2	-	Journal Club 2 Presentation
9	M	9	No class - Spring break	-	-
	W	11			
10	M	16	Classification: SVM	ISL Ch. 9.1-9.5	-
	W	18	Classification: Trees, Ensemble Learning	ISL Ch. 8.1-8.2	-
11	M	23	Neural Networks	ISL Ch. 10	-
	W	25	Molecular Representation	-	-
12	M	30	Best Practices	-	HW 6
		<b>April</b>	<b>Material</b>	<b>Assigned Reading</b>	<b>Evaluation due</b>
12	W	1	Journal Club 3	-	Journal Club 3 Presentation
13	M	6	Clustering	ISL Ch. 12.4	-
	W	8	PCA	ISL Ch. 12.2, 12.3	-
14	M	13	Attention and Transformers	Bishop Ch. 12	-
	W	15	Research talk + guest speakers	-	-
15	M	20	Final Presentations	-	-
	W	22	Final Presentations	-	Final reports