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BOARD # 38: ”Enhancing Undergraduate Research in Machine Learning with MATLAB: The Role of AI Assistance”

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Enhancing Undergraduate Research in Machine Learning with MATLAB: The Role of AI Assistance

(Work in progress - Poster)

Abstract

With the growing incorporation of machine learning (ML) in chemical engineering, students must develop proficiency in a range of tools and techniques. ML is widely applied in areas such as process optimization, predictive modeling of chemical reactions, material property prediction, and fault detection in industrial processes. Gaining expertise in these methods equips students to tackle complex challenges and drive innovation within the field. In 2018, I formed a research group focused on tackling a range of machine learning problems, despite the absence of formal programming instruction in the curriculum. To streamline our workflow and improve efficiency, we selected MATLAB for its machine learning toolbox, which minimized the amount of manual coding required for implementing and testing algorithms.

This poster examines how ChatGPT, an AI language model, has functioned as an educational tool to assist chemical engineering students in bridging the gap between their core discipline and machine learning, with a focus on MATLAB. It highlights examples of ChatGPT's capabilities, such as offering step-by-step guidance for implementing ML algorithms in MATLAB, helping with code debugging, simplifying complex ML concepts, and providing personalized learning support. The aim is to inspire and accelerate efforts by other faculty looking to integrate machine learning into their courses or research projects.

Introduction/Challenges

To better equip students to engage with these advancements and understand their potential impact, an undergraduate research class was developed. This course provides students with firsthand opportunities to explore ML techniques and their applications, fostering critical thinking and innovation in addressing complex challenges within the field. However, many students face inherent challenges due to the lack of formal programming prerequisites in the undergraduate curriculum. Without prior exposure to coding concepts, students often struggle to navigate the technical aspects of ML, such as data preprocessing, algorithm implementation, and model interpretation. This gap in programming proficiency can hinder their ability to fully engage with ML tools and techniques, making it critical to design instructional approaches that address these foundational barriers.

This poster examines how ChatGPT, an AI language model, has served as an educational tool to assist chemical engineering students in bridging the gap between their core discipline and machine learning, with a focus on MATLAB. It highlights examples of ChatGPT's capabilities, such as providing step-by-step guidance for implementing ML algorithms in MATLAB, aiding in code debugging, simplifying complex ML concepts, and offering personalized learning support. The aim is to inspire and accelerate efforts by other faculty to integrate ML into their courses or research projects.

Course Design

This course is a semester-long class designed to provide students with a foundational knowledge and hands-on experience in ML. Students typically enroll for one credit hour, which requires a commitment of at least 3 hours per week towards their research. The course begins with lectures introducing essential ML concepts, including supervised learning, unsupervised learning, and reinforcement learning. These foundational topics provide students with a basic level of theoretical knowledge needed to effectively apply ML tools and techniques in practical scenarios.

An example of one of the foundational topics is where students download wine quality data from the University of California Irvine's Machine Learning Repository (Cortez, 2009). Using MATLAB's Regression Learner Toolbox, they employ supervised learning techniques, such as regression, to predict wine quality. A key feature of MATLAB is its ability to simultaneously compare multiple models, enabling users to select the most effective one (see **Figure 1**).

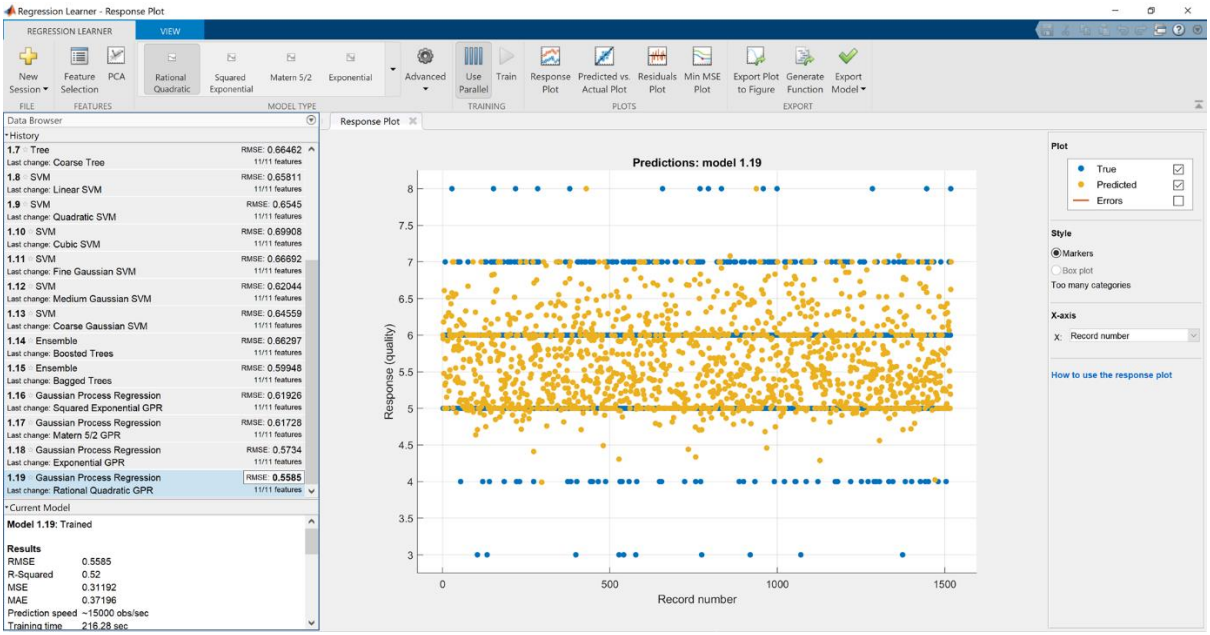

Figure 1: Screenshot of Matlab Regression Learner Toolbox (The MathWorks Inc., 2023).

Following this introduction, the majority of the course focuses on research-driven projects that allow students to explore ML applications in real-world scenarios. Some projects are pre-defined, such as using ML to predict diffusion coefficients of chromatographic solvents or predicting the efficiency of concrete corrosion inhibitors through ML and computer-aided molecular design. Alternatively, students can propose their own projects, exploring unique applications like using a classification learner for analyzing Spotify data or employing ensemble bagged machine learning to predict baseball win classifications by team.

For students who enroll in the course for three semesters, the program qualifies as a chemical engineering elective, encouraging deeper engagement. The objective of the course is not to produce peer-reviewed papers but to provide students with the experience of tackling open-ended, research-oriented questions, mirroring the challenges encountered in graduate-level studies.

Examples of ChatGPT Enhancements

Initially, the curriculum did not include formal programming or MATLAB instruction, which posed significant challenges for students. Many struggled with fundamental tasks such as preparing datasets for analysis in MATLAB's Regression Learner Toolbox. Data preprocessing tasks, including variable elimination and row or column manipulations, proved difficult and time-consuming for both students and instructors. These bottlenecks consumed countless hours, diverting focus away from meaningful research and exploration of machine learning concepts.

The integration of ChatGPT transformed this dynamic, enabling students to overcome technical hurdles quickly and efficiently. With AI assistance, students could directly ask how to perform specific MATLAB tasks, streamlining their workflows and allowing them to concentrate on higher-order problem-solving and project development. This approach not only accelerated progress but also empowered students to tackle more advanced challenges with confidence.

For instance, in preparation for analyzing real data that was not yet available, students generated random dentist data in Excel to use in MATLAB with the Regression Learner Toolbox. While students were familiar with Excel, they sought to perform all tasks in MATLAB to streamline their workflow and deepen their understanding of the software. To achieve this, students attempted to write MATLAB code independently and used ChatGPT to debug and refine their work. ChatGPT provided corrected code, as shown in **Figure 2**, with detailed comments explaining each line's purpose and incorporating a verification step to ensure accuracy. This guidance helped bridge the gap between their familiarity with Excel and their desire to fully utilize MATLAB.

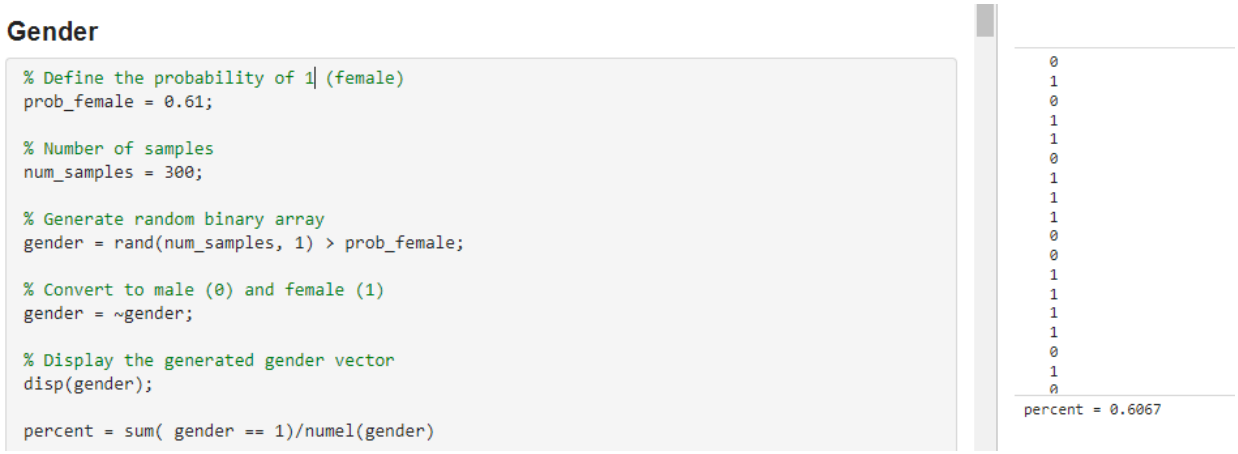

Figure 2: Code Generated with comments by ChatGPT.

ChatGPT also assisted in brainstorming solutions for inputting data into MATLAB. For instance, to generate random age data in MATLAB, ChatGPT provided guidance that led to the code shown in **Figure 3**, meeting the parameters of average and standard deviation.

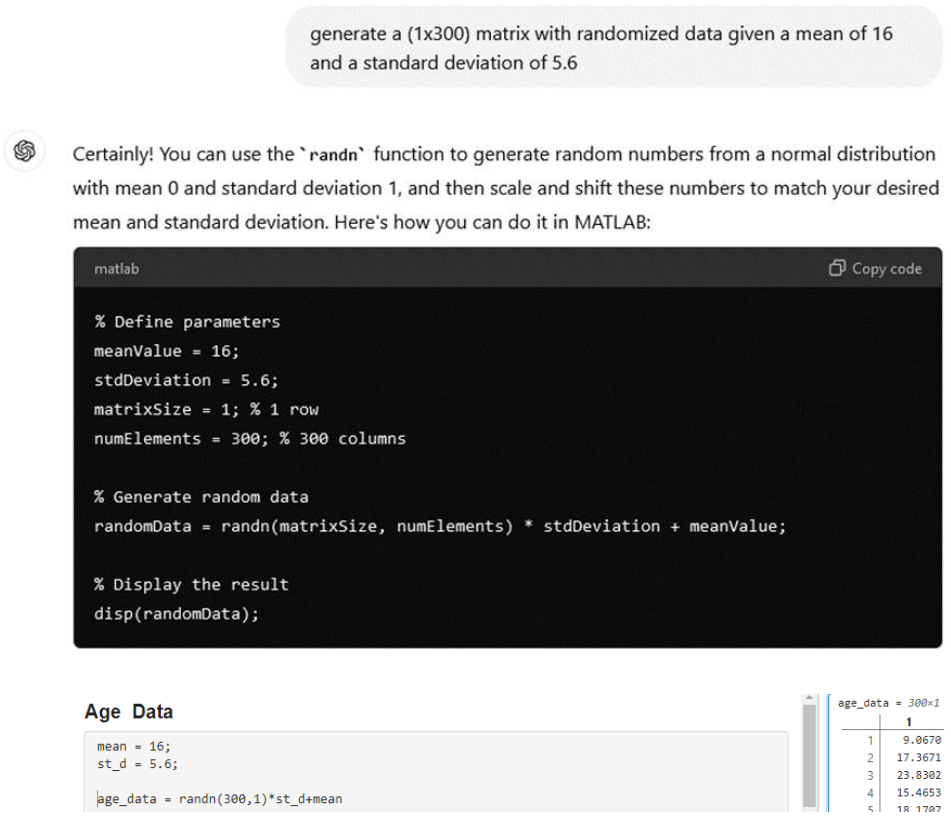

Figure 3: Integration of ChatGPT and MATLAB—ChatGPT's response guiding students in generating random age data, including subsequent MATLAB commands, and resulting outputs.

While the above examples are simplified for brevity, students have utilized ChatGPT in a variety of resourceful ways to enhance their projects. They have used it to research topics of interest that are well-suited for machine learning applications, as well as to deepen their understanding of the programming and mathematical foundations of their models. For example, students opted for ensemble bagged machine models to predict baseball game outcomes and K-Nearest Neighbors algorithms to analyze music preferences based on their accuracy. After selecting these models, ChatGPT offered comprehensive explanations of models, helping students to grasp and utilize them more effectively. This combination of AI-driven guidance and independent research has empowered students to tackle innovative projects with limited time.

Conclusion

The integration of ChatGPT into an undergraduate research course on machine learning has significantly streamlined the research process, enabling students to achieve meaningful results in less time. By addressing technical challenges such as data preprocessing, code debugging, and

algorithm implementation, ChatGPT has empowered students to focus on creative problem-solving and deeper exploration of machine learning applications in chemical engineering. Even students with limited programming experience have been able to approach complex, open-ended research projects.

For me, the use of AI tools like ChatGPT has been a transformative way to incorporate machine learning into undergraduate education. By streamlining tasks such as teaching programming fundamentals and troubleshooting code, ChatGPT has allowed me to dedicate more time to guiding students through the conceptual and applied aspects of machine learning. This experience has shown me how AI can bridge gaps in expertise and accelerate progress in both teaching and research. I hope that sharing this work-in-progress encourages other educators to consider how AI assistance might similarly enhance their efforts, making advanced topics like machine learning more accessible and impactful for both their students and themselves.

Future Work

With the introduction of a required introductory Python programming course for all chemical engineering students starting in 2023, the future direction of this machine learning course will shift to align with this new curriculum. Python, widely regarded for its versatility and extensive libraries for machine learning, will replace MATLAB as the primary platform for running machine learning algorithms. This transition will enable students to leverage tools such as scikit-learn, TensorFlow, and PyTorch,

However, ChatGPT will continue to play a critical role in this transition by supporting students as they navigate Python-based machine learning workflows. It will still assist in debugging Python code, providing guidance on implementing algorithms, and offering tailored explanations for complex ML concepts. I believe by integrating ChatGPT into Python-focused coursework, students will gain confidence and efficiency in their programming skills, ensuring a smooth transition while maintaining the innovative, research-oriented nature of the course. That said, ChatGPT is just one of many AI tools available, and future iterations of this course could benefit from exploring other platforms to enhance the learning experience further.

References

Cortez, P. (2009). *Wine Quality*. Retrieved from UC Irvine Machine Learning Repository: https://archive.ics.uci.edu/dataset/186/wine+quality

The MathWorks Inc. (2023). *Regression Learner App*. Retrieved from Mathworks: https://www.mathworks.com/help/stats/regression-learner-app.html