Math 557: Topics in Num. Ana. Machine Learning in Computational Science **Fall 2023**

TIME Tues. and Thurs. 9:30 - 10:45 am PLACE CENT 1030

Credit Hours: 3
Instructor: Professor Jehanzeb Chaudhry
Office: SMLC 310
Office Hours: Monday 1 - 2:30 pm and Wednesday 8:30 - 10 am
Or by appointment or walk-in.
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Description: The course will cover machine learning techniques, with a focus on DNNs, to solve two important problems in computational science: i. Partial Differential Equations (PDEs) ii. Approximating probability distributions for statistical inference

We will cover the basics of DNNs and learn PyTorch to implement neural network architectures. PyTorch is a widely used machine learning library in the Python programming language and is easy to learn and apply. After covering the basics, we will dive into methods for solving PDEs using Neural Networks. In particular, we will study:

- Physics-Informed Neural Networks (PINNs) - Basics of PINNS - PINNS to solve nonlinear elliptic, parabolic, hyperbolic PDEs - PINNS for interface problems - PINNS for fluid-flow problems - Galerkin Neural Networks

The final part of the course will cover approximating probability densities. The main tool for this will be Normalizing Flows. Normalizing flows use DNNs to learn an invertible transformation between an arbitrary probability distribution, and a much simpler base distribution (e.g. a Normal distribution). This area has seen explosive growth in the recent years. In this course, we will cover not only the theory behind Normalizing Flows, but also focus on implementing them in PyTorch. Finally, time permitting, we will contrast Normalizing Flows with traditional techniques like Optimal Flow.

Texts: There is no assigned text for this course. The course will be conducted by lecture notes and research articles.

Grading: 20% class participation/class presentation, 50% homework, 30% project. Letter grades will be assigned according to the following scheme: A, 90 or above, B, 80 or above, C, 70 or above, F below 70. However, the instructor reserves the right to "curve" grades to offset unforeseen circumstances.

Target Audience and Pre-reqs This course is targeted towards any mathematics, statistics, engineering or physical sciences graduate student interested in solving PDEs and/or approximating probability densities. Some familiarity with basic numerical analysis and PDEs is preferred. The course will not assume any prior knowledge

of DNNs or PyTorch, and we will spend time learning these tools during the semester.

Class participation/ class presentation

There are two main components for class participation/ class presentation:

- Every student will lead class discussion for one topic. You should plan on leading this discussion for at least one lecture, and perhaps two if required. I will upload literature sources for the discussion on Canvas. The presentation can be lead via a powerpoint (or similar) presentation, or simply by the use of the blackboard.

- I will assign reading assignments prior to every lecture. You are expected to read these literature sources (posted on canvas), and contribute positively in the discussion of the material during the lecture. These contributions may consist of asking questions, answering questions, highlighting interesting aspects of the paper, commenting on results, your opinions on the strong and weak parts of the paper etc.

Homeworks: Each homework will consist of a number of computer and theoretical problems. You need submit a report on the due date in class. All plots/figures in the report must be generated in a programming language and not hand drawn, unless otherwise specified in the question.

Computer Implementation: Some basic familiarity in a programming language is needed for the computer implementation aspects of the class. For the purposes of this course, we will be using the Python programming language.

Project: A final project will be assigned which will comprise 30% of the course grade. Each student will have a distinct final project and will involve literature survey and replication of results from the various literature sources surveyed for the project. The instructor will work with each student to identify suitable articles, books and other resources needed for the final project. Students will present their findings in a class presentation and also turn in a report documenting their work. The class presentation will be carried out during the last week of classes.

Attendence Policy: Regular and punctual attendance is required. UNM Pathfinder policies apply, which in part means instructor drops based on non-attendance are possible. This policy applies regardless of the grading option you have chosen.

Accomodations and Title IX

I can make appropriate accommodations that will support you in this class by collaborating with you and the Accessibility Resource Center (https://arc.unm.edu/). It is important that you take the initiative to inform me of your accommodations needs, as I am not legally permitted to inquire. In accordance with University Policy 2310 and the Americans with Disabilities Act (ADA), academic accommodations may be made for any student who notifies the instructor of the need for an accommodation. Students who may require assistance in emergency evacuations should contact the instructor as to the most appropriate procedures to follow.

In an effort to meet obligations under Title IX, UNM faculty, Teaching Assistants, and Graduate Assistants are considered "responsible employees." This designation requires that any report of gender discrimination which includes sexual harassment, sexual misconduct and sexual violence made to a faculty member, TA, or GA must be reported to the Title IX Coordinator at the Office of Equal Opportunity (oeo.unm.edu). For more information on the campus policy regarding sexual misconduct, see: https://policy.unm.edu/university-policies/2000/2740.html

Credit-hour statement

This is a three credit-hour course. Class meets for two 75-minute sessions of direct instruction for fifteen weeks during the Fall 2023 semester. Please plan for a minimum of six hours of out-of-class work (or homework, study, assignment completion, and class preparation) each week.

Academic Integrity: The University of New Mexico believes that academic honesty is a foundation principle for personal and academic development. All University policies regarding academic honesty apply to this course. Academic dishonesty includes, but is not limited to, cheating or copying, plagiarism (claiming credit for the words or works of another from any type of source such as print, Internet or electronic database, or failing to cite the source), fabricating information or citations, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the academic work of other students. The University's full statement on academic honesty and the consequences for failure to comply is available in the college catalog and in the Pathfinder.

Cell Phones and Technology: As a matter of courtesy, please turn off cell phones, pagers, and other communication and entertainment devices prior to the beginning of class. Notify me in advance if you are monitoring an emergency, for which cell phone ringers should be switched to vibrate.