Advanced Artificial Intelligence: Diffusion Models

CSCI 546

Instructor Info

Dr. Michael Wojnowicz (Mike)

Office Hrs: Tues 12:15-1:15, Thurs 12-2

Barnard 352

https://mikewojnowicz.github.io/

michael.wojnowicz@montana.edu

Course Info

Prerequisites: Ability to code in some language (ideally Python). Integral and Differential Calculus. Previous experience with or strong interest in probability.

Class meetings: Tues, Thurs 10:50-12:05p

Wilson 1123

Course description

This course provides an in-depth study of diffusion-based generative models in machine learning, including score-based models, denoising diffusion probabilistic models (DDPMs), and conditional and spatiotemporal variants. Students will explore the theoretical foundations, including Markov chains, stochastic differential equations, and score matching. Students will also learn how transformers can be used within diffusion modeling. Practical aspects of diffusion modeling will be explored in a final project.

Readings

- *First half of the course*: Here we will focus on mathematics behind diffusion modeling. We will use the textbook:

  Grimmett, G., & Stirzaker, D. (2020). *Probability and random processes.* (4th Edition). Oxford university press.
- *Second half of the course:* Here we will focus on the machine learning of diffusion modeling, and will use the various resources given in the Class Schedule.

Learning Outcomes

- To develop fluency in the mathematics underlying diffusion modeling (probability, Markov chains, and diffusion processes).
- To understand the fundamentals of diffusion modeling in machine learning;
- To apply diffusion modeling to a real or simulated dataset.

Learning Philosophy

This course will use an "inquiry-based learning" approach. This means that classes will not be lecture-oriented. Instead, to quote Dr. Dana Ernst,

> *You will be expected to work actively to construct your own understanding of the topics at hand with the readily available help of me and your classmates. Many of the concepts you learn and problems you work on will be new to you and ask you to stretch your thinking. You will experience frustration and failure before you experience understanding. This is part of the normal learning process. If you are doing things well, you should be confused at different points in the semester.*

Active learning has been shown to increase student performance in STEM courses (e.g. see [1, 2]).

Class activity

A typical class meeting will be structured (approximately) as follows:

Mathematics Module
- Review prev. exercises: 30 mins
- Mini-lecture: 15 mins
- New group exercises: 30 mins

ML Module
- Reaction card: 5 mins
- Peer lightning Pres: 10 mins
- Paper discussion: 60 mins

Daily readings

Before each class meeting, you will be assigned a reading (or task). These tasks are listed on the class schedule at the end of the syllabus. The reading serves as preparation for actively participating in the class that day.

Group exercises

For each class meeting within the mathematics module, students will be split randomly into groups of three to work on problems using the whiteboards. Mathematics is not a spectator sport!

Grading

- Midterm: 30%
- Participation: 10%
- Reading reactions: 20%
- Presentations: 15%
- Project: 25%

Grades will be assigned as follows:
A: 93-100, A-: 90-93, B+: 87-90, B: 83-87, B-: 80-83, C+: 77-80, C: 73-77, C-: 70-73, D+: 67-70, D: 63-67, D-: 60-63, F: 0-60.

Makeup policy. It is highly recommended to keep up with the class, as the material is cumulative. However, I drop 2 participation days with no consequence. Missed material beyond that (with a valid explanation and documentation) can be replaced with by increasing the weight of the midterm and final project grades.

Diversity and Inclusivity Statement. I consider this classroom to be a place where you will be treated with respect, and I welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability - and other visible and non-visible differences. All members of this class are expected to contribute to a respectful, welcoming and inclusive environment for every other member of the class. Your suggestions about how to improve the value of diversity in this course are encouraged and appreciated. Please let me know ways to improve the effectiveness of the course for you personally or for other students or student groups.

Accommodations for Students with Disabilities. If you are a student with a disability and wish to use your approved accommodations for this course, contact me during my office hours to discuss. Please have your Accommodation Notification available for verification of accommodations. Accommodations are approved through the Office of Disability Services located in 137 Romney Hall. www.montana.edu/disabilityservices.

Student Conduct. You are expected to abide by MSU's Code of Student Conduct.

Scholarly Responsibilities. The class has no homework. However, to be successful in the course, you need to do the following:

- Before class: *Read the assigned section.* Be sure to read actively , with a pencil and paper in hand. For the mathematics module, work out some of the examples within the section on your own, using the textbook to check your work.
- During class: *Attend class.* This allows you to participate in the group activities and discussions.
- After class: *Finish working through the group exercises.* Solutions to group exercises are posted in Canvas. During class time, you will probably just get the gist of some problems. After class, you should make sure you know how to do all of the group exercises.

Class Schedule

MODULE 0: Course Overview

Tues	Jan 13	Course Overview	

MODULE 1: Mathematics

MODULE 1A: Probability Fundamentals

Thurs	Jan 15	Events and their probabilities	GS Sec 1.1-1.7
Tues	Jan 20	Random variables and their distributions	GS Sec 2.1-2.3
Thurs	Jan 22	Random variables and their distributions	GS Sec 2.4-2.6
Tues	Jan 27	Discrete random variables	GS Sec 3.1-3.5
Thurs	Jan 29	Discrete random variables	GS Sec 3.6-3.10
Tues	Feb 3	Continuous random variables	GS Sec 4.1-4.5
Thurs	Feb 5	Continuous random variables	GS Sec 4.6-4.11

MODULE 1B: Markov Chains

Tues	Feb 10	Markov Chains	GS Sec 6.1, 6.2
Thurs	Feb 12	Markov Chains	GS Sec 6.3, 6.4
Tues	Feb 17	Markov Chains	GS Sec 6.5, 6.6, 6.9

MODULE 1C: Diffusion Processes

Thurs	Feb 19	Brownian motion	Chang Sec 5.1-5.6, GS Sec 8.1, 8.5
Tues	Feb 24	Diffusion Processes	Chang Sec 6.1-6.4, GS Sec 13.3
Thurs	Feb 26	Stochastic Calculus	Chang Sec 6.7-6.8, GS Sec 13.7
Tues	Mar 3	Itô integral	Chang Sec 6.9, 6.11, GS Sec 13.8-13.9

MIDTERM

Thurs	Mar 5	MIDTERM EXAM	

MODULE 2: Machine Learning

MODULE 2A: Introduction to Diffusion

Tues	Mar 10	Variational Inference	Blei, D. M., Kucukelbir, A., & McAuliffe, J. D. (2017). Variational inference: A review for statisticians. *Journal of the American statistical Association*, 112(518), 859-877.
Thurs	Mar 12	Variational Autoencoders	Kingma, D. P., & Welling, M. (2014). Auto-encoding variational Bayes. In *Proceedings of the International Conference on Learning Representations (ICLR)*.
		No Classes — Spring Break	
Tues	Mar 24	The Original Diffusion Model	Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., & Ganguli, S. (2015, June). Deep unsupervised learning using nonequilibrium thermodynamics. In *International conference on machine learning* (pp. 2256-2265).
Thurs	Mar 26	Overview of Diffusion Models	Christopher Bishop (2023), *Deep Learning* (Chapter 20: Diffusion Models).

MODULE 2B: Diffusion and Score Matching

Tues	Mar 31	Score Matching	Hyvärinen, A., & Dayan, P. (2005). Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6(4).
Thurs	Apr 2	Diffusion Modeling with Score Matching	Ho, J., Jain, A., & Abbeel, P. (2020). Denoising diffusion probabilistic models. *Advances in neural information processing systems*, 33, 6840-6851.
Tues	Apr 7	Diffusion and variational inference	Kingma, D., & Gao, R. (2023). Understanding diffusion objectives as the elbo with simple data augmentation. *Advances in Neural Information Processing Systems*, 36, 65484-65516
Thurs	Apr 9	Diffusion and SDEs	Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., & Poole, B. (2021). Score-based generative modeling through stochastic differential equations. In *Proceedings of the International Conference on Learning Representations (ICLR).*

MODULE 2C: Diffusion with Transformers

Thurs	Apr 9	Intro to Transformers	Christopher Bishop (2023), *Deep Learning* (Chapter 12: Transformers). Supplemental: Sasha Rush's *LLMs in 5 formulas*
Tues	Apr 14	Attention Exercises	https://classic.d2l.ai/chapter_attention-mechanisms/index.html
Tues	Apr 21	Diffusion with transformers	Peebles, W., & Xie, S. (2023). Scalable diffusion models with transformers. In *Proceedings of the IEEE/CVF international conference on computer vision* (pp. 4195-4205).

MODULE 2D: Spatiotemporal Diffusion

Thurs	Apr 23	Conditional score-based diffusion	Tashiro, Y., Song, J., Song, Y., & Ermon, S. (2021). Csdi: Conditional score-based diffusion models for probabilistic time series imputation. *Advances in neural information processing systems*, 34, 24804-24816.
Tues	Apr 28	Probabilistic weather forecasting	Price, I., Sanchez-Gonzalez, A., Alet, F., Andersson, T. R., El-Kadi, A., Masters, D.... & Willson, M. (2025). Probabilistic weather forecasting with machine learning. *Nature*, 637(8044), 84-90.

MODULE 2E: Projects

Thur	Apr 30	Final project workshop	
Thurs	May 7	Project Submission Deadline	

Note: The class schedule is tentative; it is subject to change as the course progresses.

* References

[1] Louis Deslauriers, Ellen Schelew, and Carl Wieman. Improved learning in a large-enrollment physics class. *science*, 332(6031):862–864, 2011.

[2] Scott Freeman, Sarah L Eddy, Miles McDonough, Michelle K Smith, Nnadozie Okoroafor, Hannah Jordt, and Mary Pat Wenderoth. Active learning increases student performance in science, engineering, and mathematics. *Proceedings of the national academy of sciences*, 111(23):8410–8415, 2014.