CSE741 course webpage Documentation

Release 2019

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Contents:

Computer Science and Engineering, University at Buffalo

Fall Semester 2019

CHAPTER 1

Instructors

- Varun Chandola (lead instructor; chandola[at]buffalo.edu)

CHAPTER 2

Meeting times and locations

- Wednesdays 10.00 AM - 12.20 PM, 212 Capen Hall (CARA Suite Conference Room)
- Chandola Office Hours: Tuesdays, 1.00 PM - 3.00 PM, 213 Capen Hall.

CHAPTER 3

Prerequisites

CSE 574 - Introduction to Machine Learning or equivalent (*This will be strictly enforced*)

CHAPTER 4

Piazza Page

https://piazza.com/class/k02huzljak83nh

- We will use Piazza as the primary medium for communication.

CHAPTER 5

Description

Machine learning (ML) has become an invaluable tool for almost every sector in the world, including business, finance, environment, technology, government, and scientific research. New powerful ML based tools for scientists, allow them to extract essential information from large amounts of data, either from experiments or simulations. Significant steps forward in every branch of the physical sciences could be made by embracing, developing and applying the methods of machine learning to interrogate high-dimensional complex data in a way that has not been possible before.

So far, most applications of machine learning to scientific research has been limited, mostly focusing on fitting pre-existing physical models to data and on discovering strong signals. However, recent research has shown that advancements in ML, including deep learning research, can allow learn much more complex physical principles and structures from the data, which can accelerate scientific discovery to unprecedented levels. However, scientists do not just want to learn data-driven models. They want models that can be interpreted within the paradigms of their disciplines. This is has led to a unique body of work that integrates the capabilities of current ML models with the physical laws governing all physical processes (`ml4physics`). At the same time, the field of machine learning continues to benefit from methods from physics (`physics4ml`). Many modern machine learning tools, such as variational inference and maximum entropy, are refinements of techniques invented by physicists. Physics, information theory and statistics are intimately related in their goal to extract valid information from noisy data, and there has been exciting recent work in advancing the cross-pollination further in the specific context of discovering physical principles from data.

So, what is the seminar about?

In this seminar, we will discuss some of the latest work in the area of ML and Physics (both `ml4physics` and `physics4ml`). Each lecture, we will discuss 1-2 papers from leading ML conferences and journals on these topics. To better understand these papers, we will also build/refresh our knowledge of the necessary concepts in ML and physics. The course will also include a semester long project where you will put these ideas into practice.

What will I learn?

For computer science students, this will be an opportunity to delve into a new topic within ML, especially deep learning, and see how concepts from Physics can help us build better interpretable ML models. For students from engineering and science areas, this will be a chance to see what ML can offer in your own disciplines.

CHAPTER 6

Grading

This course is only for a Satisfactory/Non-satisfactory credit. You can sign up for 1,2, or 3 credits. To pass the course, you need to:

- Present 1-2 research papers (see below for a tentative list of papers)
- Submit a critique on every presented paper (details below)
- A term project that builds upon concepts discussed in class (*optional for students signing up for 1 credit*)

CHAPTER 7

Reading list

Number	Paper	Type	Date	Presenter
1	Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data	physics4ml	Sept 4	`chandola`
2	Machine learning and the physical sciences	physics4ml	Sept 4	`chandola`
3	Gaussian Processes	tutorial	Sept 11	`aelazar`
4	Machine learning of linear differential equations using Gaussian processes	ml4physics	Sept 11	`chandola`
5	Physics-guided Neural Networks (PGNN): An Application in Lake Temperature Modeling	physics4ml	Sept 18	`aelazar`
6	Solving Ordinary Differential Equations	tutorial	Sept 18	`chandola`
7	Neural Ordinary Differential Equations	ml4physics	Sept 25	`hwang79`
8	Solving partial differential equations	tutorial	Sept 25	`binganfe`
9	Physics Informed Deep Learning (Part I): Data-driven Solutions of Nonlinear Partial Differential Equations	physics4ml	Oct 2	`rs268`
10	Physics Informed Deep Learning (Part II): Data-driven Discovery of Nonlinear Partial Differential Equations	physics4ml	Oct 2	`rs268`
11	Learning Neural PDE Solvers with Convergence Guarantees	ml4physics	Oct 9	`vbhavsar`
12	AI Feynman: a Physics-Inspired Method for Symbolic Regression	physics4ml	Oct 9	`jtmalina`
13	Toward an AI Physicist for Unsupervised Learning	ml4physics	Oct 16	`Jtmalina`
14	Hidden Physics Models: Machine Learning of Nonlinear Partial Differential Equations	ml4physics	Oct 16	`vbhavsar`
15	Visual Causal Feature Learning	physics4ml	Oct 23	`wzhang52`
16	Accelerating Eulerian Fluid Simulation With Convolutional Networks	ml4physics	Oct 30	`wzhang52`
17	Machine learning strategies for systems with invariance properties	physics4ml	Oct 30	`binganfe`
18	A Comprehensive Physics-Informed	physics4ml	Nov 6	`chandola`

CHAPTER 8

Submitting paper feedback

Every student will submit a short report on the papers discussed every lecture. This will be due by Tuesday night of the week those papers are discussed in class. The report should include key strengths and weaknesses that you perceived in the paper. Additional comments are welcome but not required. We will use UB Box to manage the feedback submission. More details will be provided soon.

See also:

The UB Box folder is here - https://buffalo.app.box.com/folder/52956982460

CHAPTER 9

Project

More details will be provided soon.

CHAPTER 10

Resources and Links

- UB Box Folder for feedback submission You will receive an invitation from the instructor when the semester starts
- AWS resources for UB Students
- Center for Computational Research (CCR) resources for UB Students

CHAPTER 11

Accessibility Services and Special Needs

If you have any disability which requires reasonable accommodations to enable you to participate in this course, please contact the Office of Accessibility Resources in 60 Capen Hall, 716-645-2608 and also the instructor of this course during the first week of class. The office will provide you with information and review appropriate arrangements for reasonable accommodations, which can be found on the web at: http://www.buffalo.edu/studentlife/who-we-are/departments/accessibility.html.

CHAPTER 12

Academic Integrity

Academic integrity is a fundamental university value. Through the honest completion of academic work, students sustain the integrity of the university and of themselves while facilitating the university's imperative for the transmission of knowledge and culture based upon the generation of new and innovative ideas. For more information, please refer to the Graduate Academic Integrity policy.

This course will operate with a zero-tolerance policy regarding cheating and other forms of academic dishonesty. Any act of academic dishonesty will subject the student to penalty, including the high probability of failure of the course (i.e., assignment of a grade of "F"). It is expected that you will behave in an honorable and respectful way as you learn and share ideas. Therefore, recycled papers, work submitted to other courses, and major assistance in preparation of assignments without identifying and acknowledging such assistance are not acceptable. All work for this course must be original for this course. Additionally, you are not allowed to post course homeworks, exams, solutions, etc., on a public forum. Please be familiar with the University and the School policies regarding plagiarism.