USC Viterbi

AME 508 Machine Learning and Computational Physics

Units: 4

Fall 2022—Monday/Wednesday—9:00-11:50 AM

Location: MHP B7B

Instructor: Assad Oberai

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Office Hours: 4:30-6 PM Thursday

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TA: Orazio Pinti

Office Hours: 2-3:30 PM Tuesday and Friday

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Guest Lecturer: Dr. Deep Ray

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Course Description
Algorithms in computational physics rely on encoding physical principles to perform predictive tasks on a computer. On the other hand, machine learning algorithms and models do not rely on an explicit set of instructions to perform a predictive task. Despite this obvious difference between these two classes of algorithms there is a remarkable overlap between them. In this course we will develop an understanding of this overlap and use it to design better predictive algorithms.

Learning Objectives
The learning objectives associated with this course are:

1. Ability to differentiate different classes of problems in machine learning: supervised, semi-supervised and unsupervised learning, and to select the appropriate algorithm for each class.
2. Ability to describe in detail the inner workings of select techniques in machine learning, with an emphasis on methods from deep learning.
3. Ability to make connections between certain continuous differential operators and algorithms from machine learning. These include, PDEs and convolutional neural networks (CNNs), nonlinear ODEs and deep residual neural networks, and spectral clustering methods and weighted Laplacians.
4. Ability to develop hybrid predictive models that utilize physics-based methods and machine learning algorithms for optimal performance.
5. Ability to apply tools for quantifying uncertainty in physics-based models and machine learning algorithms.

Prerequisite(s): AME 525 or equivalent.
Co-Requisite(s): none.
Concurrent Enrollment: none.
Recommended Preparation: Basic familiarity with Python/Matlab.

Course Notes
Course will include lectures presented in the classroom. These lectures will be saved on pdf files, and all students will have access to the pdf files.
Students will also have access to latexed version of the course notes which will be developed during the course.

Required Readings and Supplementary Materials

Required text:
There is no required text for the course. Most of the material is very recent and is covered in several papers that will be assigned for reading.

Supplementary reading material:

Papers and tutorials covered in this course:

He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 770-778).

Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. K. (2018). Neural ordinary differential equations. In Advances in neural information processing systems (pp. 6571-6583).

Patel, D., Tibrewala, R., Vega, A., Dong, L., Hugenberg, N., & Oberai, A. A. (2019). Circumventing the solution of inverse problems in mechanics through deep learning: Application to elasticity imaging. Computer Methods in Applied Mechanics and Engineering, 353, 448-466.

Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics, 378, 686-707.

Von Luxburg, U. (2007). A tutorial on spectral clustering. Statistics and computing, 17(4), 395-416.

Dunlop, M. M., Slepčev, D., Stuart, A. M., & Thorpe, M. (2020). Large data and zero noise limits of graph-based semi-supervised learning algorithms. Applied and Computational Harmonic Analysis, 49(2), 655-697.

Kipf, Thomas N., and Max Welling. "Semi-supervised classification with graph convolutional networks." arXiv preprint arXiv:1609.02907 (2016).

Karpathy, Andrej, Justin Johnson, and Li Fei-Fei. "Visualizing and understanding recurrent networks." arXiv preprint arXiv:1506.02078 (2015).

Lu, Lu, et al. "Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators." Nature Machine Intelligence 3.3 (2021): 218-229.

Description and Assessment of Assignments

Learning outcomes will be assessed by testing students on their performance in:

1. Homework that will be assigned every week or every other week. These will include programming assignments in Python. Students will write and run their code in Google colab and submit the HW as well as a Jupyter Notebook with the accompanying Python code. Students will make heavy use of Pytorch in most assignments, and will be provided with Introductory material about Python, Pytorch, and the Google Colab Environment on the first day of class.
2. Final Project that will test the summative understanding of multiple concepts learned in this course.

Tentative Grading Breakdown

Assignment	Points	% of Grade
7 Homeworks	210	60
Final Project	100	40
TOTAL	310	100
TOTAL		

Grading Scale

Course final grades will be determined using the performance on the total grade for the course.

Course Project

Every student will be required to propose a final summative project that demonstrates their understanding in one of the following major areas:

1. Overlap in the analysis and design of ML and Computational Physics algorithms.
2. Blended ML/Computational Physics algorithms.
3. Deep Operator Networks.
4. U-Nets for solving physics-based problems.
5. ML algorithms that highlight the role of Uncertainty Quantification.

Project Timeline:
- Week 3: Project announced in class; students asked to think about topics.
- Weeks 3-9: Discussion with students about appropriate projects.
- Week 10: Project finalized.
- Week 14/15: Project presentation (open to all students). To be done off-line if the enrolment is large.
- Finals week: Final report due along with code.

Sample project:
- Develop a Physics-Informed Deep Neural Network to solve a nonlinear PDE in two or three dimensions. Explore (a) the use of different activation functions and their effect on the accuracy of the solution; (b) the convergence of the numerical solution to a benchmark solution with increasing numbers of training points and network weights; (c) compare and contrast the performance of this network with more traditional computational methods for solving PDEs.

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Project Presentation: A 10-minute presentation of the main aspects of the project. A total of 8 slides permitted – to be made using Latex or Powerpoint. Slides to be uploaded to the course website prior to the presentation. The number of slides and the time of presentation will be reduced if the enrolment is large.

Final Report: A 8-page report that describes all aspects of the project will be required from all students. This report will be accompanied by a Jupyter notebook that contains the code for the project.

Grading breakdown: All aspects of the project combined are 30% of the semester grade, with a breakdown:
- Project formulation (novelty of the topic, relevance to course objectives and clarity of definition): 5%
- Final presentation: 7%
- Final report: 10%
- Evaluation of the accompanying code: 8%

Assignment Submission Policy
Homework assignments are to be submitted in class on the due date.

Additional Policies
No late assignments will be accepted barring documented illness or emergency.

Course Schedule: A Weekly Breakdown

	Topics/Daily Activities	Readings and Homework	Deliverable/ Due Dates
Week 1	Review of methods of computational physics		
Week 2	Introduction to select techniques Machine Learning	HW 1 assigned	HW due in one week
Week 3	Introduction to Deep Learning	HW2 assigned	HW due in two weeks
Week 4	Deep neural networks and ODEs.		
Week 5	Deep neural networks and ODEs.	HW 3 assigned	HW due in two weeks
Week 6	Convolutional neural networks and PDEs.		
Week 7	Convolutional neural networks and PDEs.	HW 4 assigned	HW due in two weeks
Week 8	U-Nets and their applications.		
Week 9	Physics-Informed Neural Networks.	HW 5 assigned	HW due in one week
Week 10	Deep Operator Networks.	HW 6 assigned Final Project Confirmed	HW due in two weeks
Week 11	Deep Operator Networks. Reinforcement Learning.		
Week 12	Reinforcement learning and Control theory.	HW 7 assigned	HW due in one week
Week 13	Graph Neural Networks. Project Presentations.		
Week 14	Graph Neural Networks. Project Presentations.		
Week 15	Review		
FINAL		**Final Project Due**	Date: For the date and time of the final for this class, consult the USC *Schedule of Classes* at www.usc.edu/soc.

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else's ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, "Behavior Violating University Standards" policy.usc.edu/scampus-part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, policy.usc.edu/scientific-misconduct.

Support Systems:

Counseling and Mental Health - (213) 740-9355 – 24/7 on call
studenthealth.usc.edu/counseling
Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

National Suicide Prevention Lifeline - 1 (800) 273-8255 – 24/7 on call
suicidepreventionlifeline.org
Free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week.

Relationship and Sexual Violence Prevention Services (RSVP) - (213) 740-9355(WELL), press "0" after hours – 24/7 on call
studenthealth.usc.edu/sexual-assault
Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

Office of Equity and Diversity (OED) - (213) 740-5086 | Title IX – (213) 821-8298
equity.usc.edu, titleix.usc.edu
Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

Reporting Incidents of Bias or Harassment - (213) 740-5086 or (213) 821-8298
usc-advocate.symplicity.com/care_report
Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity |Title IX for appropriate investigation, supportive measures, and response.

The Office of Disability Services and Programs - (213) 740-0776
dsp.usc.edu
Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.

USC Campus Support and Intervention - (213) 821-4710
campussupport.usc.edu
Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity at USC - (213) 740-2101
diversity.usc.edu
Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call
dps.usc.edu, emergency.usc.edu
Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-120 – 24/7 on call
dps.usc.edu
Non-emergency assistance or information.