Advanced Numerical Methods for Computational and Data Sciences Winter 2024

AMATH 840

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Class Schedule

Section	Location	Time	Instructor(s)
AMATH 840 001 *[LEC]*	MC 6460	Tuesdays & Thursdays 4 p.m. - 5:20 p.m.	Giang Tran giang.tran@uwaterloo.ca

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Instructor & TA (Teaching Assistant) Information

Office Hour: TBD at MC 6526

Course Description

> *Calendar Description for AMATH 840*
>
> Theory and practice of a selection of advanced numerical methods for computational and data sciences. Algorithms for eigenvalues and singular value decomposition. Multigrid methods for linear and nonlinear systems. Sparse optimization and compressed sensing. Low-rank tensor and matrix decomposition. Nonlinear convergence acceleration. Randomized numerical linear algebra. Adjoint methods and automatic differentiation for neural networks and optimal control. Stochastic gradient descent and variants. Efficient computer implementation of the algorithms and applications with real-world data. Students should have completed an introductory course on numerical methods.

The course will present some computational and mathematical perspectives of machine learning and data science. We will discuss some theoretical results as well as have some programming experiences.

Tentative Topics for Winter 2024:

1. Introduction to Data-Driven Methods (2 lectures)
2. Sparse Optimization and Compressive Sensing (~8 lectures)
    1. Sparse Optimization Methods: Orthogonal Matching Pursuit, Thresholding-Based Methods, Fast Proximal Gradient Methods, Alternating Direction Method of Multipliers, Primal-Dual Proximal Methods
    2. Compressive Sensing: Reconstruction Guarantees (Null Space Property, Coherence, Restricted Isometry Property), Analysis of some Sparse Optimization Algorithms
    3. Applications of Compressive Sensing and Sparse Optimization in Signal and Image Processing, Model Selection, and System Identification
3. Deep Neural Networks (~8 lectures)
    1. Mathematical Formulation, Derivation, and Properties of Popular Architectures including Feed Forward Neural Networks, Convolution Neural Networks, ResNet, Transformer, and Diffusion Model; Universal Approximation Theorem
    2. Backpropagation, Adjoint Methods and Automatic Differentiation, Implicit and Explicit Regularizations, Stochastic Gradient Method and its Acceleration
    3. Relation to Differential Equations and Stochastic Differential Equations
    4. Applications to Image Classification, System Identification, and Solving Differential Equation
4. Randomized Linear Algebra (~4 lectures)
    1. Johnson-Lindenstrauss Lemma
    2. Matrix Approximation by Sampling
    3. Randomized Matrix Multiplication
    4. Randomized SVD
    5. Applications to Model Reduction and Large-Scale Problems
5. Final Project Presentations (~2 lectures)

Learning Outcomes

By the end of this course students should be able to:

Know the fundamental concepts and results mentioned in the course description.

Tentative Course Schedule

See the Course Description.

Texts / Materials

Title / Name	Notes / Comments	Required
A Mathematical Introduction to Compressive Sensing	Book by Holger Rauhut and Simon Foucart	No
Randomized Numerical Linear Algebra: Foundations and Algorithms	Survey by Per-Gunnar Martinsson and Joel Tropp	No
Lectures on Randomized Numerical Linear Algebra	Article by Petros Drineas, Michael W. Mahoney	No
Deep Learning	Book by Ian Goodfellow, Yoshua Bengio, and Aaron Courville	No
Deep Residual Learning for Image Recognition	Article by Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun	No
Approximation by superpositions of a sigmoidal function	Article by G. Cybenko	No
Universal Approximation Bounds for Superpositions of a Sigmoidal Function	Article by Andrew Barron	No
Weighted Sums of Random Kitchen Sinks: Replacing minimization with randomization in learning	Article by Ali Rahimi and Benjamin Recht	No
Multilayer feedforward networks are universal approximators	Article by Kurt Hornik, Maxwell Stinchcombe, and Halbert White	No
Neural ordinary differential equations	Article by Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud	No
Kernel methods in machine learning	Article by Thomas Hofmann, Bernhard Schölkopf, and Alexander J. Smola	No
Attention is all you need	Article by Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin	No
Diffusion Models: A Comprehensive Survey of Methods and Applications	Article by Ling Yang, Zhilong Zhang, Yang Song, Shenda Hong, Runsheng Xu, Yue Zhao, Yingxia Shao, Wentao Zhang, Bin Cui, Ming-Hsuan Yang	No
Denoising Diffusion Probabilistic Models	Article by Jonathan Ho, Ajay Jain, Pieter Abbeel	No

Student Assessment

Component	Value
Assignments	50%
Final Project	50%

Assignments: There will be several assignments that consist of both theoretical and computational problems. All assignments will be posted on LEARN and you will submit your solutions via Crowdmark. You are encouraged to discuss assignment problems with your classmates and consult sources such as textbooks and the internet. However, you must **write your solutions in your own words** without copying other students or sources, and you must credit all of your collaborators on your assignments. **Late submissions will not be accepted.**

Final Projects: Each student or a group of two students will present a topic to the whole class. You can choose your own topic or can discuss potential topics with the instructor. Each presentation is around 25 minutes during the Final Exam Week -- time TBA. Students need to submit the slides and a short report (10 to 25 pages) about their topics.

Assignment Screening

No assignment screening will be used in this course.

Administrative Policy

IMPORTANT WEBSITES

- **LEARN:** To check course outline, course notes, recorded videos, assignments, supplementary materials, and important announcements.
- **Crowdmark:** To submit and see marked assignments. For each assignment, you will receive an invitation from Crowdmark to submit your assignment.
- **Discussion Forum:** To pose questions about lectures, assignments, textbooks, ..., please sign up for the course discussion board at Piazza, via the following link: https://piazza.com/uwaterloo.ca/winter2024/amath840 (https://piazza.com/uwaterloo.ca/winter2024/amath840) . The instructor will monitor the discussion board daily and will respond to unanswered questions. You are welcome to discuss and answer questions yourselves on Piazza. **The instructor will not answer course content-related questions sent via emails. Please use Piazza for those questions.**

University Policy

Academic integrity: In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect and responsibility. [Check the Office of Academic Integrity (https://uwaterloo.ca/academic-integrity/) for more information.]

Grievance: A student who believes that a decision affecting some aspect of their university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy 70, Student Petitions and Grievances, Section 4 (https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-70). When in doubt, please be certain to contact the department's administrative assistant who will provide further assistance.

Discipline: A student is expected to know what constitutes academic integrity to avoid committing an academic offence, and to take responsibility for their actions. [Check the Office of Academic Integrity (https://uwaterloo.ca/academic-integrity/) for more information.] A student who is unsure whether an action constitutes an offence, or who needs help in learning how to avoid offences (e.g., plagiarism, cheating) or about "rules" for group work/collaboration should seek guidance from the course instructor, academic advisor, or the undergraduate associate dean. For information on categories of offences and types of penalties, students should refer to Policy 71, Student Discipline (https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-71). For typical penalties, check Guidelines for the Assessment of Penalties (https://uwaterloo.ca/secretariat/guidelines/guidelines-assessment-penalties).

Appeals: A decision made or penalty imposed under Policy 70, Student Petitions and Grievances (https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-70) (other than a petition) or Policy 71, Student Discipline (https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-71) may be appealed if there is a ground. A student who believes they have a ground for an appeal should refer to Policy 72, Student Appeals (https://uwaterloo.ca/secretariat/policies-procedures-guidelines/policy-72).

Note for students with disabilities: AccessAbility Services (https://uwaterloo.ca/accessability-services/), located in Needles Hall, Room 1401, collaborates with all academic departments to arrange appropriate accommodations for students with disabilities without compromising the academic integrity of the curriculum. If you require academic accommodations to lessen the impact of your disability, please register with AccessAbility Services at the beginning of each academic term.

Turnitin.com: Text matching software (Turnitin®) may be used to screen assignments in this course. Turnitin® is used to verify that all materials and sources in assignments are documented. Students' submissions are stored on a U.S. server, therefore students must be given an alternative (e.g., scaffolded assignment or annotated bibliography), if they are concerned about their privacy and/or security. Students will be given due notice, in the first week of the term and/or at the time assignment details are provided, about arrangements and alternatives for the use of Turnitin in this course.

It is the responsibility of the student to notify the instructor if they, in the first week of term or at the time assignment details are provided, wish to submit alternate assignment.