

Graduate course

MACHINE LEARNING

March 11th – March 12th

Applied Mechanics and Data Analysis MS3 Department Faculty of Engineering Technology University of Twente

UNIVERSITEIT TWENTE.







General

This course is a collaborative effort spearheaded by the Dutch graduate school Engineering Mechanics, with active participation from research groups at various universities, including University of Twente, TU Eindhoven, University of Groningen and TU Delft. In addition to covering the theoretical and computational facets of machine/deep learning, special emphasis will be placed on connecting the field of Machine Learning with the established theory of mechanics of materials. Importantly, this course is an integral component of the 4TU Engineering Mechanics training program designed for PhD students.

Objective

In the field of mechanics and dynamics analysis of materials/structures, the integration of machine and deep learning techniques has revolutionized innovation, enabling researchers to analyse intricate material behaviours, predict structural responses, and optimize designs, manufacturing processes and systems. Utilizing machine learning algorithms, valuable insights are extracted from extensive datasets. enhancing our understanding of material properties and related mechanical performance. This synergy between artificial intelligence and classical mechanical and dynamics theories has become beneficial in for example multiscale analysis of materials. However, amidst these advancements, few challenges have emerged. Notably the training of deep learning models demands large training datasets that usually are not existing in the everyday industrial practice. Next to this, the reliance on historical data may hinder adaptability to novel scenarios, and the deployment of complex models requires significant computational resources and specialized expertise. On the other hand, the models designed are known to have interpretability and explainability issues.

Despite these challenges, ongoing research seeks to address these limitations, fostering more robust and interpretable machine and deep learning applications in the mechanics of materials. The goal of this graduate course in Engineering Mechanics is to offer a thoughtful introduction to this broad and rapidly evolving interdisciplinary field. The course aims to explore various facets within this domain, with a specific emphasis on classical machine learning theory, physicsinformed neural networks, operator networks and their integration with traditional theories. The course covers both theoretical foundations and computational frameworks, employing realworld examples from research to illustrate the advantages of machine learning in the multiscale analysis of materials.

Local organization

The course is organized by the Applied Mechanics and Data Analysis group of University of Twente. The local organizing committee is composed of

- Bojana Rosic (chairwoman)
- Abhishek Chatterjee
- Vasos Arnaoutis
- Debbie Vrieze-Zimmerman (group secretary)
- Rachel van Outvorst (EM secretary)

Lecturers

Iuri Rocha Delft University of Technology Bojana Rosic University of Twente Michael Abdelmalik Eindhoven University of Technology Francesco Maresca University of Groningen Ondrej Rokos Eindhoven University of Technology

Lecture notes

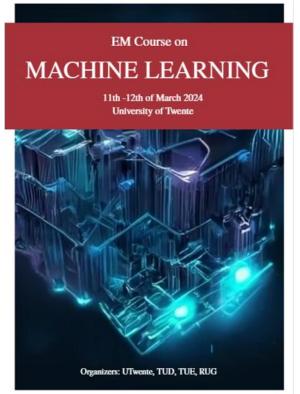
Lecture notes will be distributed during the course.

Poster session

An informal poster session will be organized on the first day of the course. This session aims to share all challenges in machine learning applications in engineering mechanics from the perspective of the participants, providing a clear view of the background of all related research projects and individuals. All participants are invited to prepare a poster and present it on the first day.

Prerequisites

Basic undergraduate courses in linear algebra, probability theory, partial differential equations and mechanics/dynamics.



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Contents

I INTRODUCTION TO ML

- Decision theory for regression
- From linear regression to neural networks
- Towards deep learning: curse of dimensionality and inductive biases
- Bayesian machine learning with Gaussian Processes
- II PHYSICS RELATED AND PHYSICS INFORMED MACHINE LEARNING
 - Physics-based deep learning. Basic mathematical foundation of neural networks and universal approximation theorem
 - Connection between neural networks approach with finite elements and classical mesh-free methods
 - Physics-informed and variational physics-informed neural networks
 - Deep Galerkin and deep Ritz method for elliptic problems, convergence analysis and error estimates
 - Bayesian physics-informed neural networks
- III NEURAL OPERATOR NETWORKS
 - From partial differential equations to neural operators
 - Architectures for neural operators
 - Learning neural operators

IV ML FOR COMPUTATIONAL HOMOGENISATION

- Basics of computational homogenization, data generation.
- Learning constitutive models using Gaussian process regression.
- Equivariant graph neural networks in computational homogenization.

VI ML FOR ATOMISTIC-SCALE MECHANICS

- Database generation.
- Descriptors of local atomic environments, and regression methods.
- Performance: Gaussian Processes, Neural Networks, Moment Tensor Potentials, Atomic Cluster Expansion, Message passing frameworks.
- Prediction of mechanical properties and defects (dislocations, cracks).
- Model uncertainty quantification and active learning.

Location/date

The course will take place at University of Twente (MS3 Department) over two days, i.e. March 11th - 12th 2024, respectively. The course language is English. A list of hotel accommodations in the vicinity of the course-location is available upon request. Participants are required to contact the hotels directly.

Further information

- On the <u>contents</u> of the course: Prof. Dr. Ing. Bojana Rosic, UT, Tel.: +31- (0)53-489 87 57 E-mail: <u>b.rosic@utwente.nl</u>
- On the <u>organization</u> of the course: Mrs. Rachel van Outvorst, TU/e, Tel.: +31-(0)40-247 8306
 E-mail: <u>Engineering.Mechanics@tue.nl</u>

Fee/Registration

The course is free for registered members of the graduate schools Engineering Mechanics and GrasMech and for the research members of the contributing research groups. The course fee for non-EM members is € 100 for PhD students and € 400 for other participants. The fee includes lunch and coffee breaks, but does not include lodging and other meals. Participants will receive an invoice after accepted registration. Participants need to register via our website https://engineeringmechanics.nl/courses/

before 26th of February.

Members of the Graduate School Engineering Mechanics receive priority in case of over-subscription.

Upcoming courses

In addition to the present course, the Graduate School Engineering Mechanics organizes a series of graduate courses on several subjects. For further information on these courses and on other activities of the Graduate School Engineering Mechanics please visit the WWW-pages at:

http://www.engineeringmechanics.nl https://engineeringmechanics.nl/courses/

or contact:

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