PROFESSIONAL EDUCATION

MACHINE LEARNING FOR MATERIALS INFORMATICS

SEPTEMBER 26–29, 2022 | Instructor: Markus J. Buehler (email: mbuehler@mit.edu)

Note: All times are US Eastern Daylight Time. Schedule is subject to change.

DAY 1: MONDAY, SEPTEMBER 26 (9:00AM–7:00PM)	
9:00-10:30 AM	L1 Foundations in materials informatics I (data science and basic concepts of machine learning)
10:30-10:45 AM	**COFFEE BREAK**
10:45-12:30 PM	L2 Foundations in materials informatics II (multiscale modeling; datasets, experimental methods for data collection)
12:30-1:00 PM	**LUNCH**
1:00-2:30 PM	**CLINIC #1** • Convolutional neural network (classifier, regression, and peeking inside via interpretable methods)
2:30-2:45 PM	**COFFEE BREAK**
2:45-4:00 PM	L3 Digging deeper: Deep neural nets, loss functions, Stochastic optimization methods (e.g., stochastic gradient descent and variants), Regularization
4:00-5:00 PM	**CLINIC #2:** • Material failure analysis • Physics informed neural networks
5:00-7:00 PM	**VIRTUAL RECEPTION** (includes participant introductions)

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DAY 2: TUEDAY, SEPTEMBER 27 (9:00AM–7:00PM)	
9:00-10:30 AM	L4 Hands-on introduction to PyTorch (example application to fine-tuning a BERT NLP model applied to protein molecular design)
10:30-10:45 AM	**COFFEE BREAK**
10:45-12:30 PM	L5 Hands-on introduction to TensorFlow (example application to developing an adversarial neural network) Practical guide to tensor algebra and other important math concepts needed
12:30-1:00 PM	**LUNCH**
1:00-2:30 PM	L6 Ethics, bias and sustainability in materials informatics Data science, statistics and visualization (includes review of relevant Python toolkits)
2:30-2:45 PM	**COFFEE BREAK**
2:45-4:00 PM	**LAB 1** Data, data, everywhere…*De novo* dataset construction (imaging lab) and application to build a deep neural network (covers computer vision tools, live imaging using depth camera
4:00-5:00 PM	L8 Introduction to graph neural networks (applications to molecular systems, truss systems, alloys, proteins, and healthcare; graph transformers)
5:00-7:00 PM	**Optional:** Time for Group Work and Assignments (can be arranged within groups at other times), Instructor is available for personal meetings

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DAY 3: WEDNESDAY, SEPTEMBER 28 (9:00AM–7:00PM)	
9:00-10:30 AM	L9 Transforming AI and healthcare with attention (AlphaFold, RoseTTAFold and OpenFold; applications to protein design, synthesis)
10:30-10:45 AM	**COFFEE BREAK**
10:45-12:30 PM	L5 Deepening the understanding of language models applied to materials (pre-training and fine-tuning); BERT, GPT-3, PaLM and other large language models (applications to materials problems; category theory; time-dependent material phenomena; fracture)
12:30-1:00 PM	**LUNCH**
1:00-2:30 PM	**CLINIC #3** • Transformer models for inverse materials design (develop multiscale transformer model from scratch)
2:30-2:45 PM	**COFFEE BREAK**
2:45-4:00 PM	L11 Adversarial neural networks and applications to materials design (manufacturing, inverse problem, characterization)
4:00-5:00 PM	L12 Case study: Image segmentation in microscopy, medical imaging, and analysis
5:00-7:00 PM	**Optional:** Time for Group Work and Assignments (can be arranged within groups at other times), Instructor is available for personal meetings

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DAY 4: THURSDAY, SEPTEMBER 29 (9:00AM–7:00PM)	
9:00-10:30 AM	L13 Autoencoders (vision, graphs, NLP, proteins) and variants
10:30-10:45 AM	**COFFEE BREAK**
10:45-12:30 PM	**CLINIC #4:** • To fail or not to fail: Buckling modeling (time-dependent phenomena) • Interpretable machine learning (includes: dependent features, causal interpretation, and uncertainty estimation)
12:30-1:00 PM	L14 Concluding discussion Graduation ceremony and certificates