Indian Institute of Technology, Kanpur

Department of Chemistry

Course Title	AI/ML in Chemistry
Course No.:	CHM669
Credits:	3-0-0-0 (9)

Course Contents

S. No.	Broad Title	Topics	No. of lectures
1.	Introduction	• Uses and impact of AI in Chemistry: An overview. • Fundamental tasks of machine learning: Regression, classification, clustering. • Mathematical preliminaries: Crash courses in multivariable calculus, linear algebra, and graph theory. • Basics of Python programming. • Regression and classification tasks. • Some elementary machine learning models: Gaussian processes, feed-forward neural networks, tree models and random forests.	12

2.	Machine learning and the electronic structure problem:	• Machine learning interatomic potentials (MLIPs)
		  ○ Behler-Parrinello networks.
		  ○ Deep graph neural networks.
		  ○ Atomic cluster expansion (ACE) and MACE architecture.
		• Learning the electron density.
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3.	Machine learning for chemical compound design:	• Defining chemical space.
		• The problem of representing molecules for machines.
		• Machine learning architectures and strategies.
		  ○ Recurrent neural networks.
		  ○ Generative adversarial networks.
		  ○ Autoencoders and variational autoencoders.
		• Sequential graph generation.
		• 3D Shape generation.
		• Point clouds.
		• Molecular property prediction.
			8

	Machine learning for materials characterization and design:	• Atomic versus molecular materials
		• The problem of representing bulk crystals for machines.
		• Machine learning architectures and strategies extended to periodic structures.
		  ○ Deep graph neural networks.
		  ○ Generative adversarial networks.
		  ○ Autoencoders and variational autoencoders.
		• Predicting crystal structures and materials properties.
		• Models and strategies for materials discovery.
		  ○ Latent spaces and 3D structure searching and generation.
		  ○ Use of points clouds.
			8

	Brief overview of other models and their uses in other areas of chemistry (Instructors can adjust the topics based on the state-of-the-art areas which he/she wishes to cover at the time of teaching)	• Large language models and transformer networks. • Flow networks, generative flow networks, and diffusion models. • ML and its uses in molecular simulation. • ML and its uses in molecular spectroscopy or protein structure prediction	7

Recommended Books:

- Bishop, Christopher M. Pattern Recognition and Machine Learning. New York :Springer, 2006.
- Y. Wang et al., "On the design space between molecular mechanics and machine learning force fields", *Applied Physics Reviews* **12**, 021304 (2024). DOI 10.1063/5.0237876.
- Jon Paul Janet and Heather J. Kulik, *Machine Learning in Chemistry*; American Chemical Society, 2020. DOI: 10.1021/acs.infocus.7e4001
- Hugh M Cartwright (Ed.), Machine Learning in Chemistry: The Impact of Artificial Intelligence, The Royal Society of Chemistry, 2020.
- Python Machine Learning, Sebastian Raschka & Vahid Mirjalili , Packt Publishing; 3rd ed. Edition, 2019