Department of Chemical Engineering
Indian Institute of Technology Kanpur

Proposal for a new course

Title: Artificial Intelligence in Systems Biology

Course No.:   ChE6XX

Structure: 3 lectures per week. (3-0-0-9) (Total 40 lectures)

Duration of Course: Full semester

Prerequisite: None

Open to: PG students and third-year and fourth-year UG students.

Proposer: Sana Khanum (FB-466, skhanum@iitk.ac.in), Department of Chemical
                   Engineering

Other faculties interested in teaching the course: Indranil Saha Dalal, Salman Ahmad Khan

Course objectives: This course aims to build on the fundamentals (theory and programming) of artificial intelligence (AI), machine learning (ML), and deep learning (DL), and expose students to the applications of AI/ML/DL in chemical engineering. The course will also introduce the students to the recent advances in the field.

Course contents:

S. No	Title	Topics	No. of Lectures
1.	Introduction to Artificial Intelligence (AI)	Introduction to AI and its applications in various fields of ChE. Introduction to Jupyter Notebook, Python Libraries, PyTorch, and TensorFlow	3
2.	Applied Mathematics and Machine Learning (ML) basics	Linear Algebra, Probability, Density Estimation, Information Theory, ML Basics Principal Component Analysis, and relevant Python libraries	3

3.	Applications of ML	Applications of ML in Chemical Engineering, including biochemical process design, optimization, and control, biomaterial and product property prediction	2
4.	Deep Learning Basics	Single-layer NN, Multi-layer Perceptron, ANN, CNN (Theory and Computing)	3
5.	Optimization algorithms for Deep Learning	Convexity, Gradient Descent, Stochastic Gradient Descent, Minibatch Stochastic Gradient Descent, Momentum, Adagrad, RMSProp, Adadelta, Adam, Learning Rate Scheduling	3
6.	Deep Learning (DL)	Vanishing gradients, skip connections, batch normalization, transfer learning, and data augmentation	3
7.	Deep Learning Techniques	RNN, GRU Networks, LSTM, Transformers, Autoencoders, Diffusion Models (Theory and Computing)	5
8.	Applications of Deep Learning	Applications of Deep Learning in Chemical Engineering, including Physics-informed neural networks, deriving causality for gene regulatory networks	2
9.	Computer Vision	Introduction to Image Augmentation, Fine-tuning, Object detection and bounding boxes, Anchor boxes, Multiscale object detection (Theory and Computing)	3
10.	Applications of Computer Vision	Applications of Computer Vision in Chemical Engineering, including computer vision in cell biology, and computer vision for material discovery	2
11.	Natural Language Processing	Introduction, Various NLP techniques: Word Embedding (word2vec), Word Embedding with Global Vectors (GloVe), Bidirectional Encoder Representations from	5

		Transformers (BERT) (Theory and Computing)	
12.	Applications of Natural Language Processing (NLP)	Applications of Natural Language Processing in Chemical Engineering, including studying protein-ligand interactions, analysing single-cell data	2
13.	Large Language Models (LLMs)	Introduction to LLMs, Fine-tuning, distillation, and prompt engineering, overview of the LLM architecture, and some use cases of LLMs	4
		Total:	40

Expected enrolment: ~50-60

Other departments to which the proposed course will be of interest: AE, ME, CE

References:

1. [PY] Python Data Science Handbook by Jake VanderPlas, 2016. https://jakevdp.github.io/PythonDataScienceHandbook/
2. [PPA] Patterns, predictions, and actions: A story about machine learning by Moritz Hardt and Benjamin Recht, 2022, https://mlstory.org/pdf/patterns.pdf
3. [DL] Deep Learning by Ian Goodfellow, Yoshua Bengio, and Aaron Courville, 2016. http://www.deeplearningbook.org
4. [DD] Dive into Deep Learning by Aston Zhang, Zachary C. Lipton, Mu Li, and Alexander J. Smola, 2023. https://d2l.ai/
5. [LLM] Build a Large Language Model from Scratch by Manning Publications

Dated: 26/09/2025   Proposer: Sana Khanum

Dated: DPGC Convener:

The course is approved / not approved

Chairman,   **SUGC**

Dated: