ARTIFICIAL INTELLIGENCE IN CHEMICAL ENGINEERING
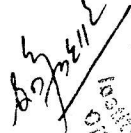## ENCH 204

Lecture : 3

Tutorial : 1

Practical : 0

Year : II

Part : I

Course Objectives:

The objective of this course is to provide students with a thorough understanding of data visualization, data quality, and key machine learning techniques, including classification, regression, and clustering. By the end of the course, students will have gained hands-on experience with machine learning packages and learned to fine-tune hyperparameters to optimize model performance. This knowledge will be solidified through a group project that encourages practical application of these skills in a collaborative setting.

1   Fundamentals of AI and Applications   (2 hours)

    1.1   Definition, historical overview, applications
    1.2   AI, ML, deep learning: Differences and overlap
    1.3   Ethical considerations (Bias, transparency, interpretability)
    1.4   Applications in chemical engineering

2   Python Basics and Data Handling   (6 hours)

    2.1   Intro to python and Jupyter notebooks
    2.2   Data handling with python: Data manipulation with pandas
    2.3   Python for basic statistics

3   Data Visualization and Scientific Computing   (8 hours)

    3.1   Basic libraries: Numpy, Scipy, Matplotlib, Seaborn
    3.2   Solving linear, nonlinear, interpolation, curve-fitting and ordinary differential
            equation problems
    3.3   Data visualization with Matplotlib
    3.4   Solving chemical engineering problems

4   Data Engineering   (9 hours)

    4.1   Data gathering, types of data, data quality
    4.2   Data cleaning, handling missing values, outlier detection
    4.3   Feature engineering (Selecting and transforming features)
    4.4   Data scaling and normalization, dealing with imbalanced data

5 **Introduction to Machine Learning**   (10 hours)

   5.1   Overview of supervised learning and applications

   5.2   Regression models: Linear regression, K-nearest neighbors (KNN), simple neural network regressor

   5.3   Classification Models: Decision trees, random forests, KNN classifier

   5.4   Evaluation metrics for regression and classification (MAE, MSE, accuracy, confusion matrix)

6 **Introduction to Neural Networks**   (10 hours)

   6.1   Neurons, layers activation functions

   6.2   Neural network architectures

   6.3   Simple neural network example using Keras

   6.4   Applications in chemical engineering: Process optimization, predictive maintenance (Time-series data)

   6.5   Clustering techniques (K-means) for anomaly detection in chemical processes

Tutorial   (15 hours)

1. AI, ML overview, differences, chemical related applications
2. Data handling with Pandas data frame.
3. Interpolation, ODEs and data visualization
4. Data handling, cleaning, scaling, feature engineering
5. Regression, classification problems with evaluation metrics
6. Neural network application in chemical engineering

Final Exam

The questions will cover all the chapters in the syllabus. The evaluation scheme will be as indicated in the table below.

Chapters	Hours	Marks distribution*
1 and 2	8	12
3	8	12
4	9	12
5	10	12
6	10	12
Total	45	60

* There may be minor deviation in marks distribution.

References

1. McClarren, R.G. (2021). Machine learning for engineers. Springer.
2. Quantrille, T.E., Liu, Y.A. (2012). Artificial intelligence in chemical engineering. Elsevier.
3. Muller, A.C., Guido, S. (2016). Introduction to Machine Learning with Python: A Guide for Data Scientists. O'Reilly Media.
4. Gopal, M. (2019). Applied Machine Learning. McGraw Hill.