Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2023-2024
Course Handout Part II

Date: 09-01-2024

In addition to part-I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No.	:	*ChE F315*
Course Title	:	Machine Learning in Chemical Engineering
Instructor-in-Charge	:	Lakshminarayanan Samavedham

Scope and Objective of the Course:

Scope:

Chemical engineering, as a discipline, has largely been influenced by the advances in Machine learning (ML), and artificial intelligence (AI). Increasing availability of data, cheaper and powerful hardware and significant algorithmic advances have made possible several breakthroughs in processing of various kinds of process data – numbers, text, images, videos etc. Process industries are rapidly adopting ML to enable higher efficiencies in process operations and discovering new functional products. While the applications of ML can span many areas even within chemical engineering, this course intends to provide a solid foundational base in the use of several machine learning techniques with applications to process modeling, process monitoring, fault diagnosis and optimization. The course will focus on analyzing numerical data covering steady state, dynamic, linear and nonlinear data. In addition to the theory and principles, there will be a significant emphasis on industry case studies and research articles. MATLAB will be used for demonstrating the ideas as well as for student learning and assessments.

Course Learning Outcomes:

Upon completing this course, the student must be able to:
1. Describe the concepts and principles behind the ML algorithms
2. Choose the most appropriate machine learning technique for analyzing the given data
3. Demonstrate the capability to construct and validate regression, classification and clustering models from data using **MATLAB**
4. Articulate operational insights and process/product improvement opportunities based on the constructed models

Mode of Delivery:

The class will emphasize both theory and industry/research applications of the concepts learnt. It will introduce fundamentals and classical methods and go on to describe some established modern techniques that you will be able to use in the industry. The class lectures will be augmented with invited lectures from academics and industrial practitioners.

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For this 3 credit (unit) course, my expectation will be that you spend 7.5 hours each week. That means, after 3 hours of class attendance, you must spend 4.5 hours of work each week on self-study, assignments and project work. I am committed to support your learning process. If you have any doubts, drop by my office during the announced chamber consultation hours or via CMS/email and get the doubts sorted out. Do not postpone learning!

Textbooks:
1. Sridhar, S. and Vijayalakshmi, M., 2021, Machine Learning. 1st ed., Oxford University Press, ISBN-13 (print edition): 978- 0-19-012727-5 **(SV)**
2. Russell, E.L., Chiang, L. H. and Braatz, R.D., 2000, Data-driven Methods for Fault Detection and Diagnosis in Chemical Processes, 1st ed., Springer London, ISBN 978-1-4471-1133-7 **(RCB)**
3. Gramacy, R.B., 2020, Surrogates: Gaussian Process Modeling, Design, and Optimization for the Applied Sciences, 1st ed., Chapman and Hall/CRC. https://doi-org.libproxy1.nus.edu.sg/10.1201/9780367815493 **(GRB)**

Reference books:
1. Gopal, M., 2019, Applied Machine Learning. 1st ed., New York: McGraw-Hill Education. https://www.accessengineeringlibrary.com/content/book/9781260456844

Course Plan:

Lecture No.	Theme	Topic	Text Book Chapter/Section
1		Course Overview and Logistics	None
2		Technical Introduction to Problem Types	None
3	Dimensionality Reduction	Principal Components Analysis (PCA)	SV 2.10.3
4		Application of PCA for Fault Detection	RCB 4.4 and 4.5
5		Canonical Correlations Analysis (CCA)	RCB 7.2
6 & 7	Regression Methods	Ordinary Least Squares (OLS)	SV 5.5
8		Stepwise Regression	SV 2.10.1 and 2.10.2
9		Principal Components Regression (PCR)	SV 5.2
10		Partial Least Squares (PLS)	RCB 6.1 to 6.7
11		Regularization - LASSO, ElasticNet	SV 5.8
12		Genetic Programming (GP) / Symbolic Regression (SR)	SV 15.6.2
13 & 14		Introduction to Artificial Neural Networks (ANNs)	SV 10
15		Gaussian Process Regression (GPR)	GRB 5
16	Analysis of Time Series Data	Introduction to Time Series Data	RCB 7.1
17		Linear and Nonlinear Time Series Models	RCB 7.1
18		State Space Models - Continuous and Discrete Time	SV 7.4
19 & 20		Canonical Variate Analysis (CVA)	SV 7.3
21		Long Short Term Memory Networks (LSTM)	SV 16.8
22	Classification and Clustering	Classification and Regression Trees (CART)	SV 6
23 & 24		Support Vector Machines (SVM and SVR)	SV 11
25		k-means Clustering	SV 13.1 and 13.2
26 & 27		Introduction to Reinforcement Learning	SV 14.1 to 14.4 and 14.9
28		Dr. Rohit Patwardhan, Saudi Aramco, Saudi Arabia	
29		Prof. Ravindra Gudi, IIT Bombay	
30		Dr. Raghuraj Rao, AKXATECH India	
31		Dr. Kanchi Lakshmi Kiran, DBS Bank Singapore	
32		Dr. Aditya Tulsyan, AMGEN USA	
33		Dr. Ravishankar Sethuraman, ExxonMobil USA	
34		Dr. Yelneedi Sreenivas, SABIC, Saudi Arabia	

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35	**Industry and Academic Guest Seminars**	Mr. Aswin Venugopal, Shell India	
36		Dr. Sabareesh, BITS Pilani Hyderabad Campus	
37		Dr. Sushant Garud, Aleph Technologies & NUS, Singapore	
38	**Physics informed Machine Learning**	Physics Informed Canonical Variate Analysis	Research Articles will be distributed
39		Uniform Manifold Approximation and Projection (UMAP)	
40		Physics Informed Symbolic Regression	

Evaluation Scheme:

Component	Duration	Weightage (%)	Date & Time	Nature of Component
3 Assignments to be done in groups of 2 members	-	18%	One assignment every four weeks	Continuous Assessment
Attendance at Industry Talks and completion of a 250 word reflective summary after each talk	60 minutes each session	10% + 10% = 20%	About 12 sessions mostly in March and April will be announced	Continuous Assessment
Midterm	90 minutes	27%	12/03 - 9.30 - 11.00AM	Open Book, Notes and using MATLAB
Comprehensive	3 Hours	35%	08/05 FN	Open Book, Notes and using MATLAB

Chamber Consultation Hours: 3-4 PM (Mondays, Wednesdays) at Block D, Room 319B. Students can contact me through CMS and I will try to respond as quickly as I can.

Notices: All notices and correspondences will be via the course management system (CMS). It is your responsibility to check the CMS and your BITS email for all information disseminated by me.

Make-up Policy: Make-up will be offered only for the mid-semester examination and will normally be held within one week of the mid-semester test. You need not give any proof to ask for the make-up. Only know that the make-up exam will be more difficult compared to the main test and the test format may also be different. If you are not able to take the make-up test on the day it is held, you will be awarded zero credit for the mid-semester test.

Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Lakshminarayanan Samavedham
INSTRUCTOR-IN-CHARGE