

Centre for Machine Learning and Intelligence
Multidisciplinary Course
Machine Learning for Chemistry
(Applicable for the PG Students admitted from 2022 – 2023 onwards)

Semester: III
Subject Code : 23MAIM02

Hours of Instructions / Week: 2
No. of Credits: 2

Objectives:

1. To understand the fundamentals of Machine Learning
2. To familiarize working with Google Colab environment
3. To learn how to design and develop chemistry related applications in Google Colab.

Unit I : Fundamental Concepts of Machine Learning **-6Hrs**
Machine Learning (ML) - Supervised Vs Unsupervised Learning - Reinforcement Learning - Regression - Classification – (Clustering)*

Unit II: Basics of Google Colaboratory **-6Hrs**
Introduction to Google Colab - Advantages of Google Colab - Features of Google Colab - GPU and TPU Facility in Google Colab - Colabpro - Installation of Google Colab - Starting up with New ColabNotebook - Setting the Notebook Name - Adding Cells and Entering Code in Google Colab - Executing Code in Google Colab - Modifying Cell Order and Deleting Cell in Google Colab - Saving and Sharing Notebook in Google Drive – (Arithmetic Operations)*

Unit III: Working with Google Colaboratory **-6Hrs**
Loading File System: Uploading Files from your Local File System - Downloading Files to your Local File System - Mounting Google Drive - Loading Image in Google Colab: Accessing Images from Google Drive - Accessing Images from Computer - Loading Imageset in Google Colab - Displaying a Single and Multiple Images in Google Colab - Loading Data in Google Colab: Accessing Data from Google Drive - Accessing Data from Computer – (Loading Data from Google Colab - Displaying Data using Colab.)*

Unit IV: Data Importing, Exporting and Visualization **-6Hrs**
Importing and Displaying Data from Kaggle - Importing and Displaying Data from Github- Importing and Extracting Zip Files in Google Colab - Saving and Sharing Notebook in Github - Exporting Code and Dataset to Github and Kaggle - Cloning Git Repository in Google Colab - Charting: Line Plotting - Bar Plotting - Scatter Plotting - Histogram - Pie Chart – (Fill_ between and alpha - Sub Plotting)* - 3D Graph - Saving Charts and Plots.

Unit V: Prediction of Chemical Formula and 3D Molecular Structure

-6Hrs

Package Installation: RDKit- Numpy - Pandas - Matplotlib. Data Accessing: Reading csv file using read_csv() - Importing and Visualization of chemical molecules - Unsupervised Learning: Regression. Performance Evaluation: Mean Square Error (MSE) – (Mean Absolute Error (MAE).)*

* Indicates Self - Study Component

Total Hours: 30

References:

1. Chris Albon. (2019). "*Machine learning with python cookbook*". 2nd edn. USA: O'Reilly Media, Inc.
2. John Paul Mueller and Luca Massaron. (2019). "*Python for data science for dummies*", 2nd edn. New Jersey: John Wiley & Sons, Inc.
3. Google Colab (2020) "*Google Colaboratory*" Available at: <https://colab.research.google.com/notebooks> (Accessed 10 November 2020)
4. Kaggle (2018) "*Kaggle Repository*". Available at: <https://www.kaggle.com/vladislavkisin/tutorial-ml-in-chemistry-research-rdkit-mol2vec> (Accessed 8 September 2021)

Course Outcomes

- CO1: Enhance the knowledge about machine learning
- CO2: Able to apply Machine Learning concepts for Chemistry related application
- CO3: Write programmes in Google Colab
- CO4: Experiment Chemistry applications using Google Colab
- CO5: Explain how datasets can be imported and used in Google Colab