

Machine learning/chemometrics – data analysis for scientists

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In short, chemometrics(machine learning) uses mathematical and statistical methods to extract information from experimental data. The course will introduce aspects necessary for successful data analysis starting from methods of collecting good data, pre-processing, and extracting information using both supervised and unsupervised methods.

Apart from lectures, course will also include a workshop (or workshops) that will allow all participants to make their own analyses in Python. Programming knowledge is not needed, ready Anaconda scripts and short intro how to run them will be provided. Participants are encouraged to bring their own data to be analyzed during the workshop, in other case chemical (spectroscopy, electrochemistry) and biological datasets will be used.

Starting date: 3rd of March 2023, the course will be given once a week for 10 weeks on Fridays 12:00

Deadline for registration: 21st of February 2022. Please register early by sending an email to ewitkowskanery@ichf.edu.pl

Syllabus:

Introduction to chemometrics/machine learning;

Data pre-treatment;

Unsupervised methods: Clustering

Unsupervised methods: Dimensionality reduction

Supervised methods: Regression

Supervised methods: Classification

Neural Networks

Workshop

Multivariate data visualization methods;