University of Gdańsk

Subject card

Subject name and code	Machine learning in chemistry, PG_00051252		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2025/2026
Education level	postgraduate studies	Subject group	Obligatory subject group in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	2	Language of instruction	English
Semester of study	3	ECTS credits	3.0
Learning profile	academic	Assessment form	
Conducting unit	Pracownia Chemoinformatyki Środowiska -> Katedra Chemii i Radiochemii Środowiska -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr Alicja Mikołajczyk	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	45.0	0.0	0.0	45

E-learning hours included: 0.0

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	45	8.0	22.0	75

Subject objectives

Familiarizing the students with machine learning theory and its applications in chemistry presenting the advantages and disadvantages of various types of machine learning algorithms in chemistry.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Ability to choose and apply the appropriate machine learning algorithm to solve a particular problem under consideration in the chemistry science domain.	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report
[CHEMMU2_W09] Classifies specialist IT tools used in statistical evaluation of experiment results.	The ability to select the proper computer chemistry tools for given data.	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report
[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.	Ability to work with a scientific text.	[SU2] presentation/project/paper/ report [SU4] test/exam - oral or written
[CHEMMU2_K02] Works in a team taking on various roles in it.	Ability to cooperate in a group.	[SK2] presentation/project/paper/ report [SK4] test/exam - oral or written
[CHEMMU2_K03] Understands the need for systematic work on various projects of a long-term nature and knows how to set priorities for the implementation of undertaken tasks.	Knowledge of the principles of REACH in Europe and the resulting legal obligations	[SK2] presentation/project/paper/ report [SK4] test/exam - oral or written
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	Knowledge of basic types of chemical structure descriptors and methods of their calculation	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report
[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	Ability to perform chemoinformatic analyses that allow to reduce costs and time of research.	[SK2] presentation/project/paper/ report [SK4] test/exam - oral or written
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	Ability to assess the effectiveness of the developed model and critically interpret the results obtained using specific machine learning methods	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report

Subject contents

This course is designed to provide students with foundational knowledge of practical aspects of machine learning in chemistry, including: introduction to machine learning theory and its applications,overview of various types of machine learning algorithms (supervised and semi-supervised machine learning methods; classification and regression methods; reinforcement learning algorithms; generative versus discriminative models),challenges in application of machine learning in chemistry (methods for handling uncertain, limited, imbalanced and noisy data; feature selection; model selection and assessment),open source chemoinformatics software.

Prerequisites and co-requisites

Repetitory in mathematics· Repetitory in general and inorganic chemistry· Introduction to Python programming· Introduction to R programmingExploratory analysis of multidimensional chemical space

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
exam	51.0%	100.0%

Recommended reading

Basic literature	S. D. Brown, R. Tauler, B. Walczak (ed): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009 R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005
Supplementary literature	J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopulos, H. Reis, M. Shukla (ed): Handbook of Computational Chemistry (2nd Edition). Springer 2016. Volume 5: Chemoinformatics, Puzyn T (ed.).
eResources addresses	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed

Work placement	Not applicable

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