University of Gdańsk

Subject card

Subject name and code	Exploratory analysis of multidimensional chemical space, PG_00054860		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
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	1	Language of instruction	English
Semester of study	1	ECTS credits	4.0
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 hab. Agnieszka Gajewicz-Skrętna	
	Teachers	mgr Klaudia Chmielewska Sattibabu Merugu mgr inż. Michał Kałapus	

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	47.0	100

Subject objectives

Course objectives are:

- Achieving advanced skills in exploratory analysis of multidimensional chemical space (performing analyses and interpreting the results)
- Familiarizing the students with the available software allowing to perform the multidimensional analysis
- Familiarizing the students with Pythons scripts used to data analysis

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	At the end of the course every student knows classification of advanced methods of data analysis and provides examples of their applications in multidimensional chemical problems	[SW4] test/exam - oral or written
[CHEMMU2_W04] Applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis.	At the end of the course every student explains theoretical background (algorithm) of the advanced methods, including HCA, PCA	[SW4] test/exam - oral or written
[CHEMMU2_W09] Classifies specialist IT tools used in statistical evaluation of experiment results.	At the end of the course every student knows basic software packages to be used for multidimensional data analyses	[SW4] test/exam - oral or written
[CHEMMU2_U06] Presents the results of scientific discoveries in chemistry and related disciplines in an understandable way.	At the end of the course every student performs various multidimensional data analyses and correctly interprets the results	[SU4] test/exam - oral or written
[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	At the end of the course every student is convinced that the use of a computer and exploratory analysis strengthens the potential of data analysis and can critically evaluate experimental results and understand the necessity of their control	[SU4] test/exam - oral or written
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Pod koniec kursu każdy student rozumie potrzebę głębszego poznania metod wielowymiarowej analizy danych	[SK4] test/exam - oral or written
[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	At the end of the course every student uses Python environment for multidimensional analyses of chemical space	[SW4] test/exam - oral or written

Subject contents

Course contents:

- Introduction to multivariate data, review of the basic software allowing to perform the multidimensional analysis
- Advanced methods of analyzing the internal structure of the data: similarity in the multivariable feature space, methods of similarity analysis, dimensionality reduction, hierarchical cluster analysis (HCA), principal component analysis (PCA), k-Means clustering, fuzzy c-Means clustering, Self-organizing maps, Gaussian Mixture models, and other deep learning algorithms Density-based spatial clustering of applications with noise.
- Examples of applying these methods in chemical data analysis.

Prerequisites and co-requisites

Assessment methods and criteria

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

Recommended reading

Basic literature	R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005
Supplementary literature	S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009 scientific publication in the field
eResources addresses	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed

Work placement

Not applicable