University of Gdańsk

Subject card

Subject name and code	Chemometrics, PG_00080780						
Field of study	Chemical Business						
Date of commencement of studies	October 2024		Academic year of realisation of subject	2026/2027			
Education level	Bachelor's 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	3		Language of instruction	English			
Semester of study	5		ECTS credits	1.0			
Learning profile	academic		Assessment form	exam			
Conducting unit	Laboratory of Environmental Chemoinformatics -> Department of Environmental Chemistry and Radiochemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor	dr Artur Mirocki					
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	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	15		2.0	8.0	25	
Subject objectives	Course objectives are: • Introducing students to the wide range of applications for chemometric and statistical methods in analyzing chemical data. • Students will become proficient in using essential statistical and chemometric methods to analyze and interpret results. • Students will be introduced to available software that implements statistical and chemometric methods, as well as data visualization software to aid in preparing figures and plots for a master's thesis.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[BCHINŻ_W04] Describes the role of experiment and computer simulation in the design process of engineering issues.	At the end of the course every student understands the principles of presenting and communicating information obtained from data.	[SW4] test/exam - oral or written
[BCHINŻ_U04] In the course of carrying out engineering tasks, s/he uses basic statistical methods, IT techniques and uses application software packages to describe chemical processes and experimental data.	At the end of the course every student: (1) be able to calculate basic descriptive statistics; (2) utilizes the R/KNIME environment for chemometric calculations; (3) correctly prepares data for further chemometric analyses; (4) performs HCA and PCA analyses and correctly interpret the results; (5) develops regression model using the LR/MLR algorithms, validate the models correctly and apply the models for predictions.	[SU4] test/exam - oral or written
[BCHINŻ_W03] Describes the techniques of higher mathematics and IT tools necessary to describe and model chemical phenomena and technological processes.	At the end of the course every student knows the theoretical basis and operating algorithms of key chemometric methods such as HCA, PCA, LR/MLR.	[SW4] test/exam - oral or written
[BCHINŻ_U08] Uses the chemical nomenclature and engineering terminology properly.	At the end of the course every student: (1) knows how to perform measurements; (2) understands the importance of reliable documentation of results and identifies potential problems that may arise from improper record-keeping; (3) understands the purpose of calculating descriptive statistics (e.g., mean, standard deviation) and their applications; (4) identifies potential sources of measurement errors and uncertainty in the research process.	[SU4] test/exam - oral or written

Subject contents

Course contents:

- Introduction to chemometrics: specificity of multivariate data; differences between statistics and chemometrics; areas of interest in chemometrics; classification of chemometric methods; overview of computer software implementing chemometric methods (including MATLAB, Statistica, Origin, SPSS, QSARINS, KNIME).
- Methods of analyzing the internal structure of multidimensional chemical data: similarity of objects in a multidimensional feature space; hierarchical cluster analysis (HCA) as an example of a similarity analysis method; principal components analysis (PCA) as an example of a projection search method; examples of the use of these methods in various areas of chemistry;
- Modeling of phenomena and processes using regression and classification methods: linear regression with one and multiple variables (LR and MLR); principal components regression (PCR), partial least squares regression (PLS); linear discriminant analysis (LDA), non-linear k-nearest neighbors (kNN) classifier; methods for selecting the optimal set of variables in the model (stepwise selection, genetic algorithm selection); validation of regression and classification models; examples of the use of these methods in various areas of chemistry.

Prerequisites and co-requisites

Knowledge of the basics of mathematics and statistics

Assessment methods and criteria

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

Recommended reading

Basic literature	J.Mazerski: Podstawy chemometrii. Gdańsk: Wydawnictwo Politechniki Gdańskie, 2000
Supplementary literature	S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009 R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005 D. Zuba, A Parczewski (red.): Chemometria w analityce: wybrane zagadnienia. Kraków: Wydawnictwo Instytutu Ekspertyz Sądowych, 2008
eResources addresses	

Example issues/ example questions/ tasks being completed	
Work placement	Not applicable

Document generated electronically. Does not require a seal or signature.