University of Gdańsk

Subject card

Subject name and code	Statistics and Chemometrics in Chemical Analytics, PG_00188284		
Field of study	Statystyka i chemometria w analityce chemicznej (Ćw.laboratoryjne)		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2026/2027
Education level	Bachelor's studies	Subject group	Obligatory subject group in the field of study Subject group related to scientific research in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	2	ECTS credits	1.0
Learning profile	academic	Assessment form	credit
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Karolina Jagiełło	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	15.0	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

Acquisition by students of practical skills in applying the most important chemometric methods in the interpretation of data obtained from analytical techniques used in forensics
Familiarization of students with available software implementing statistical and chemometric methods and preparation of students for the independent use of these tools in analytical work and forensic research.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[AKRL3_W01] The graduate knows and understands, at an advanced level, the laws and theories in the field of chemistry, as well as the basics of biology, mathematics and law constituting general knowledge in the scientific disciplines forming the theoretical foundations relevant to the study program.	Student: has advanced knowledge and understanding of the chemical principles used in chemometric analysis, including the nature of data obtained from instrumental methods used in forensics. knows the basic mathematical laws and concepts that form the foundation of chemometric methods, such as multidimensional analysis, correlation, regression, and dimensional reduction, and is able to apply them in computer practice. understands the biological principles relevant to the interpretation of data in forensic investigations (e.g., biological variability, characteristics of biological samples), enabling the proper analysis and modeling of biological data. knows the basic legal conditions for data analysis and reporting in the context of forensic expertise, including the principles of responsibility, reliability, and documentation of research.	[SW2] prezentacja/projekt/referat/ raport
	[AKRL3_K01] The graduate is ready to critically evaluate their own knowledge, understand its importance for solving cognitive and practical problems, and to seek expert opinions when necessary.	Student: is ready to critically evaluate their knowledge of statistics and chemometrics, understands its importance in the analysis of measurement data and in solving research problems, particularly in the context of forensic analytics. is able to consciously select appropriate statistical and chemometric methods, assessing their assumptions, limitations, and impact on the reliability of the results obtained. understands the importance of reliable research documentation and is able to identify the consequences of incorrect documentation. has knowledge of the main chemometric methods (including PCA, HCA, LR/MLR), their operating algorithms, and their potential use in the analysis of traces and evidence is familiar with the software available for implementing these methods and is able to critically assess its usefulness in specific analytical tasks.	[SK4] test/egzamin - ustny lub pisemny

Course outcome	Subject outcome	Method of verification
[AKRL3_U01] The graduate is able to identify, analyse and solve complex research problems in chemistry and forensic science by selecting appropriate methods and information sources.	Student: is able to recognize and formulate research problems related to the analysis of chemical and forensic data, identifying the type of data, variables, and potential relationships. selects appropriate chemometric methods and IT tools (e.g., PCA, HCA, PLS, classification methods) according to the nature of the research problem being analyzed. analyzes and interprets complex data sets obtained from instrumental methods used in forensics, using multidimensional statistical models and computer visualizations. searches for and uses appropriate sources of information - scientific literature, methodological documentation, legal standards, and reference data - to justify the selection of methods and interpretation of results. is able to propose and evaluate various strategies for solving analytical problems, taking into account data limitations, uncertainty of results, and forensic expertise requirements.	[SU2] prezentacja/projekt/referat/ raport
[AKRL3_U04] The graduate is able to select appropriate equipment for experiments and prepare reports and expert opinions based on analytical results in compliance with legal and ethical standards.	Student: is able to select appropriate IT tools and software (e.g., KNIME) for chemometric analysis of data obtained in forensic experiments. is able to prepare a chemometric analysis report containing correct calculations, data visualizations, interpretation of results, and a description of the methods used. is able to formulate expert opinions based on the results of computer analyses, taking into account their limitations, reliability, and compliance with applicable legal and ethical standards in forensics. applies the principles of proper documentation of analytical processes, ensuring transparency and repeatability of analyses and preparing results in a form acceptable in evidentiary proceedings.	[SU2] prezentacja/projekt/referat/ raport

Course outcome	Subject outcome	Method of verification
[AKRL3_K06] The graduate is ready to follow occupational health and safety regulations in the laboratory and care for the safety of themselves and others.	Student: is prepared to comply with health and safety rules in the computer lab, including rules for proper workstation organization, ergonomics, and safe use of hardware and software. understands the importance of data security in forensic analysis and applies the principles of information protection, confidentiality, and data integrity when working with statistical and chemometric software. ensures their own safety and that of others by responding to potential hazards associated with working on a computer, storing measurement data, using storage media, and operating specialized IT tools used in forensic expertise.	[SK2] prezentacja/projekt/referat/ raport

Subject contents

Introduction to chemometric methods in forensics: specifics of multidimensional data obtained from analytical techniques used in trace evidence examination; differences between chemical statistics and chemometrics; scope of chemometric applications in forensic analysis (sample classification, evidence comparison, profiling); classification of chemometric methods; overview of software used in forensics (R, MATLAB, Statistica, Origin, SPSS, KNIME) and their typical applications.

Methods of analyzing the internal structure of multidimensional chemical data in forensics: the concept of similarity of objects in multidimensional feature space (e.g., comparing chemical profiles of drugs, fibers, paints); hierarchical cluster analysis (HCA) as a method for determining similarity and grouping samples; principal component analysis (PCA) as a tool for dimension reduction and visualization of similarities; examples of the use of HCA and PCA methods in various areas of forensics (e.g., identification of material sources, substance profiling, analysis of variance in trace populations).

Modeling phenomena and processes using regression and classification methods in the context of forensic investigations: linear regression (LR, MLR) and principal component regression (PCR) in quantitative analysis of evidence; methods for selecting optimal variables (stepwise selection, genetic algorithms) in modeling forensic data; validation of regression and classification models in terms of their reliability as tools supporting expert opinions.

Prerequisites and co-requisites

General chemistry, mathematics

Assessment methods and criteria

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

Recommended reading

Basic literature	*A. Łomnicki: Wprowadzenie do statystyki dla przyrodników. Wydawnictwo Naukowe PWN, Warszawa 2003. J. Mazerski: Podstawy chemometrii. Gdańsk: Wydawnictwo Politechniki Gdańskiej, 2000 P. Konieczka, J. Namieśnik i in.: Ocena i kontrola jakości wyników analitycznych. Centrum Doskonałości Analityki i Monitoringu Środowiskowego, Gdańsk 2004.*
Supplementary literature	Scientific publikaction
eResources addresses	

Example issues/ example questions/ tasks being completed

Work placement

Not applicable

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