University of Gdańsk

Subject card

Subject name and code	Statistics and Chemometrics in Chemical Analytics, PG_00188282		
Field of study	Statystyka i chemometria w analityce chemicznej (Wykład)		
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	2.0
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	30.0	0.0	0.0	0.0	0.0	30

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	30	5.0	15.0	50

Subject objectives

Teaching students how to perform basic and advanced statistical calculations and tests, with particular emphasis on selecting the appropriate statistical methods for the specific problems encountered in forensic analysis.
Presenting students with the possibilities of using chemometric methods in chemistry and in the analysis of forensic traces and evidence.
Acquisition by students of practical skills in the application of 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_W06] The graduate knows and understands the principles of statistical processing of measurement data and the basics of chemometrics and validation of analytical methods.	Student: knows and understands the principles of statistical analysis of measurement data, including the rules for selecting appropriate descriptive statistics, distributions, and statistical tests, as well as their significance for assessing the quality of research results. has a solid knowledge of the basics of chemometrics, including the main methods of multidimensional analysis and their application in the interpretation of data obtained from techniques used in forensic analysis. understands the basics of analytical method validation, including the assessment of uncertainty, repeatability, selectivity, and sensitivity, and the importance of these parameters for the reliability and evidential value of analytical results.	[SW4] test/egzamin - ustny lub pisemny
	[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. is aware of measurement uncertainties, is able to identify potential sources of error, and knows how their presence affects data interpretation. understands the importance of reliable research documentation and is able to identify the consequences of incorrect documentation. knows basic descriptive statistics, the basics of statistical inference, the most important statistical distributions and tests, and their application in laboratory and forensic practice. 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, as well as knowledge of 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

Subject contents	Fundamentals of chemical metrology and documentation of results in forensic investigations: history and essence of measurements in the context of trace analysis; the role of standards and calibration in forensic laboratories; measurement scales, significant digits, and rules for rounding numbers; requirements for reliable documentation of measurement results for evidentiary proceedings; potential consequences of errors in documentation for the evaluation of evidence. Basics of statistical description in the analysis of evidence: general population vs. forensic samples; characteristics of series of results from chemical and physicochemical trace analysis; measures of central tendency and data dispersion; basic statistical distributions used in the interpretation of results; descriptive statistics and their importance for the assessment of the reliability of results; distribution series, histograms, and identification of outliers in forensic data; testing statistical hypotheses using parametric and non-parametric tests; correlation analysis in comparative studies. 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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