

GDAŃSK UNIVERSITY

Subject card

Subject name and code	, PG_00052326							
Field of study	Chemical Technology							
Date of commencement of studies	October 2020		Academic year of realisation of subject			2023/2024		
Education level	first-cycle studies		Subject group			Optional subject group		
Mode of study	Full-time studies		Mode of delivery			at the university		
Year of study	4		Language of instruction			Polish		
Semester of study	7		ECTS credits		2.0			
Learning profile	general academic profile		Assessment form		assessment			
Conducting unit	Department of Analytical Chemistry -> Faculty of Chemistry							
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Piotr Konieczka						
	Teachers		prof. dr hab. inż. Piotr Konieczka					
		dr inż. Tomasz Majchrzak						
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Projec	:t	Seminar	SUM
	Number of study hours	30.0	15.0	0.0	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		2.0		13.0		60
Subject objectives	The aim of the course is to learn useful mathematical statistics and chemometric methods used at the stage of developing measurement results.							
Learning outcomes	Course outcome		Subject outcome		Method of verification			
	K6_U11		is able to plan and implement the learning process			[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools		
	K6_W01		knows the basics of mathematics, statistics, data analysis			[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects		

Subject contents	LECTURE
	Introduction to probability
	Basic statistical tools: mean, standard deviation, regression, verification of statistical hypotheses
	Measures of position, measures of dispersion, measures of asymmetry, measures of focus
	Distributions of random variables
	Estimation theory
	Description of basic statistical tests and algorithm for their application
	a. Nonparametric tests (Kolmogorov-Smirnova)
	b.Parametric tests (Q-Dixon, Grubbs, F-Snedecor, ² , F max-Hartley, t-Student)
	Verifying statistical hypotheses
	Correlation and regression analysis, study of the significance of regression coefficients
	Correlation matrix, heat map
	ANOVA Analysis of Variance
	Graphical presentation of research results charts, histograms.
	Use Excel to calculate, analyze, and present research results.
	Data normalization methods; standardization
	Introduction to experiment planning; a factorial experiment plan; RSM (response surface method); optimization
	Distance in n-dimensional data space; Euclidean distance; Hierarchical beam analysis (HCA); HCA with heat map
	Main Component Analysis (PCA)
	Introduction to machine learning; Classifiers; artificial neural networks (ANN)
	SEMINAR
	Calculations using Excel:

	 Series of analytical measurement results (simple analytical techniques titration, mass measurement, pH measurement). Calculation of the values of basic statistical parameters along with their interpretation. Application of the regression method to determine the calibration curve along with the interpretation of the obtained values of regression coefficients. Comparison of precision and correctness of the results of two series of measurements (independent series) using statistical tests. Application of CRM recovery study analysis of the obtained results and comparison with the reference value. Reporting and inference. Preparation of reports from classes 1-4 along with a graphical presentation of the results. Introduction to Chemometrics Big Data Analysis Introduction to free data analysis tools: Excel, Orange Data Mining, R Studio Use data analysis tools to interpret results Group project Scientific poster main assumptions and tools Presentation of the result of the work in the form of a scientific poster. 				
Prerequisites and co-requisites	Basics of mathematics and useful statistics.				
Assessment methods	Subject passing criteria	Passing threshold	Percentage of the final grade		
and criteria	passing classes in the form of a presentation	60.0%	100.0%		
Recommended reading	 Example d reading Basic literature F.M. Dekking, C. Kraaikamp, H.P. Lopu Modern Introduction to Probability and S Why and How, Springer, 2005. W. Dyczka, W. Krysicki, J. Bartos, Rach i statystyka matematyczna w zadaniach A. Maksimowicz-Ajchel, Wstęp do staty: statystycznego, WUW Warszawa 2007 Sobczyk M: Statystyka, PWN, Warszaw P. Konieczka, J. Namieśnik, B. Zygmun Zawadka, A. Naganowska-Nowak, E. K kontrola jakości wyników pomiarów ana Konieczka, J. Namieśnik, Warszawa, W P. Konieczka, J. Namieśnik, Quality Ass in the Analytical Chemistry Laboratory. Second Edition, CRC Press/Francis and 2018. J. Mazerski, CHEMOMETRIA PRA wyniki swoich pomiarów, wyd. II, W 		P. Lopuha a, L.E. Meester, A lity and Statistics. Understanding os, Rachunek prawdopodobieństwa adaniach, cz. II, PWN, 2016. do statystyki. Metody opisu va 2007 Warszawa 2007 Zygmunt, E. Bulska, A. Świtaj- vak, E. Kremer, M. Rompa: Ocena i arów analitycznych, red. P. zawa, WNT, 2007 Jality Assurance and Quality Control oratory. A Practical Approach, ancis and Taylor, Boca Raton, FL, RIA PRAKTYCZNA - Interpretuj vyd. II, Wydawnictwo Malamut, 2016		
	Supplementary literature	available literature on the subject			
	eResources addresses	Adresy na platformie eNauczanie: Statystyka i chemometria w chemii analitycznej - Technologia Chemiczna, Analityka Techniczna i Przemysłowa, 1 st. sem. 7 - 2023/2024 - Moodle ID: 33454 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=33454			

Example issues/ example questions/ tasks being completed	 List and characterize the basic statistical parameters. Provide the algorithm used to verify the statistical hypothesis. Characterize the selected statistical test by its range of applicability, prerequisites, procedure and inference. Provide a range of applications of the regression method in analytics. Specify the statistical steps used in compiling the measurement results. A range of applications of the ANOVA method univariate and multifactorial. Provide basic ways of graphical presentation of results and the scope of their applicability. How you can compare two series of results in terms of precision and correctness provide the algorithm of conduct. The role and importance of standard deviation in the development of measurement results. Arithmetic mean vs. median similarities and differences. Normal distribution characteristics and significance in chemical measurements. For what purpose is data normalization carried out. Give examples of standardization methods Characterize the Box-Behnken plan What are the connection methods in beam analysis? What is the main component? Methods for validating classifiers
Work placement	Not applicable