GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Chemometrics, PG_00036535		
Field of study	Chemistry		
Date of commencement of studies	October 2021	Academic year of realisation of subject	2024/2025
Education level	first-cycle 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	4	Language of instruction	Polish
Semester of study	7	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Tomasz Laskowski	
	Teachers		

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	30.0	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	5.0	25.0	75

Subject objectives

Student:

- designs, collects, and controls multidimensional data,
- creates graphical presentations of multidimensional data,
- selects the variables necessary to describe the basic properties of the analyzed set of objects (samples),
- uses principal component analysis to analyze data,
- creates multivariate regression models and determi their significance and adequacy,
- classifies the examined objects according to the value of many explanatory variables.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U03] can make detailed documentation of the results of self-conducted experiments and prepare a report describing these results	The student is able to correctly prepare a summary documentation of the results of the experiments and prepare a study containing a discussion of these results	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
[K6_U04] can use professional vocabulary, can prepare and communicate technical information in the form of text documents, spreadsheets, charts and technological schema	The student is able to use professional vocabulary and prepare and transfer technical informations.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU5] Assessment of ability to present the results of task
K6_W02	A student possesses knowledge on basic and advanced chemometric techniques, particularly regarding the mathematics fueling the methods used.	[SW1] Assessment of factual knowledge

Subject contents	The lectures will include following issues: • experimental design with particular regard to factor and minimum design, • data collection, archiving and pre-processing, • methods of graphic presentation of multidimensional data, • application of the principal components analysis to multidimensional data sets, • mathematical modeling of relationships with particular emphasis on the rules of models creation and assessment of their adequacy, • classification, i.e. determining the rules of belonging of objects to predefined classes, • similarity analysis, i.e. searching for natural clusters of objects. As part of the laboratory, students will independently carry out chemometric analysis of their multidimensional data sets using various chemometric techniques.
Prerequisites and co-requisites	Prerequisite subjects: mathematics, computer science. Prerequisites: knowledge of basic concepts of statistics, skills in using a spreadsheet computer program (e.g. Excel)

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
practical exercises	60.0%	40.0%
compilation of results	60.0%	10.0%
lecture test	60.0%	50.0%

Recommended reading

Basic literature	J.Mazerski: "Chemometria Praktyczna", Wydawnictwo Malamut,Warszawa 2009J.Koronacki, J.Mielniczuk: Statystyka dla studentów kierunkówtechnicznych i przyrodniczych. WN-T, W-wa 2001
Supplementary literature	E.Steiner: "Matematyka dla chemików", Wydawnictwo Naukowe PWN,Warszawa 2001S.Brandt: Analiza danych, Wydawnictwo Naukowe PWN, Warszawa1998
eResources addresses	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed

1. Design a series of measurements whose results will allow you to create a model of relationship between yield the chemical synthesis and its conditions: temperature, time and catalyst content.
2. Based on the attached results of the regression analysis, determine an adequate model of a relationship
3. Evaluate the prognostic capacity of the obtained model.

Work placement	Not applicable