GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	CHEMOMETRICS, PG_00064394		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2025/2026
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	2	Language of instruction	Polish
Semester of study	4	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Tomasz Laskowski	
	Teachers	dr inż. Julia Borzyszkowska-Bukowska dr hab. inż. Tomasz Laskowski	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	15.0	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	2.0	18.0	50

Subject objectives

The aim of the course is to familiarize the student with methods for working with multidimensional datasets, with particular emphasis on extracting so-called useful (actionable) information. An additional objective is to develop practical skills in using the R and Python programming languages for data analysis.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_W01] applies his/her knowledge of selected branches of mathematics and physics to analyse, interpret and solve problems and to describe physical, chemical phenomena and technological processes	The student has the knowledge necessary to use specialized vocabulary. They are ready to prepare and communicate technical information, as well as use advanced numerical and statistical techniques to solve chemometric problems.	[SW3] Assessment of knowledge contained in written work and projects
[K6_K03] is aware of the importance of caring for the quality and diligence of the tasks performed, being responsible for their consequences	The student is aware of the importance of the reliable application of basic and advanced chemometric techniques, with particular emphasis on the mathematical foundations of the methods, and is responsible for the correct interpretation of the results of the optimization process and their consequences in research and professional work.	[SK2] Assessment of progress of work [SK5] Assessment of ability to solve problems that arise in practice
[K6_U04] creates detailed documentation of the results obtained from the experiments carried out individually or as part of a team, analysing and interpreting the results in the form of text documents, spreadsheets, graphs, technological diagrams, multimedia presentations using correct chemical nomenclature	Student is able to correctly compile a consolidated record of experimental results and prepare a written report that includes a discussion and interpretation of these results.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools

Subject contents

Course content – lecture

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.

Course content – laboratory

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%
lecture test	60.0%	50.0%
compilation of results	60.0%	10.0%

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	

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.

Practical activites within the subject

Not applicable

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