GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Chemometrics and artificial intelligence in spectroscopic data analysis, PG_00069261						
Field of study	Chemistry						
Date of commencement of studies	February 2025		Academic year of realisation of subject	2025/2026			
Education level	second-cycle studies		Subject group				
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	3.0			
Learning profile	general academic profile		Assessment form	assessment			
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Wydziały Politechniki Gdańskiej						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Piotr Bruździak				
	Teachers						
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	8.0	16.0	0.0	21.0	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	The objective of the course is to familiarize students with the characteristics of spectroscopic data and modern methods for their analysis using chemometrics and artificial intelligence. Students will learn to process, interpret, and model spectral data using the Python language and AI models that support the programming process. The course develops practical skills in data analysis, critical thinking, and teamwork through the completion of programming projects.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U101] is able to formulate complex research problems and adopts appropriate methods, obtaining innovative solutions, cooperating with other people, both as a leader and a team member	Working in a team, students are able to identify a research problem and select the optimal method of spectroscopic data analysis to address it.	[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
[K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	Students are able to prepare a presentation and a report summarizing their work, with a particular focus on its objectives, the proposed solutions, and any technical challenges encountered.	[SU1] Assessment of task fulfilment [SU5] Assessment of ability to present the results of task
[K7_U01] integrates and interprets information from literature, databases and other sources	Students are able to find the best solutions for pre-processing, spectroscopic data analysis, and software implementation from available knowledge sources. They can also leverage the capabilities of AI solutions when designing approaches to the problems being studied.	[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
[K7_W101] is able to make an in-depth identification of key objects and phenomena related to the field of study, as well as theories that describe them and applicable analytical and design methods	Students are able to evaluate the quality of spectroscopic data and select appropriate methods for its preparation and processing.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects
[K7_K101] acknowledges the importance of knowledge related to the field of study in solving cognitive and practical problems, critically assessing the information obtained	Students are able to extrapolate their acquired knowledge and skills to other types of chemical and technical problems, including, in particular, the analysis of signals and data seemingly unrelated to spectroscopy.	[SK5] Assessment of ability to solve problems that arise in practice

Subject contents

1. Introductory Part (8 weeks: 1h lecture & 2h laboratory session per week):
a) Types and characteristics of spectroscopic data: spectra types, signal shapes, sources of noise and artifacts, data formats.
b) Fundamentals of Python programming for chemists: development environment, NumPy, Pandas, Matplotlib, and SciPy libraries.
c) Introduction to interactive web applications with Streamlit.
d) Using AI language models (e.g., Google AI Studio) to assist in code development and debugging.
e) Chemometrics and Exploratory Data Analysis (EDA): statistical characterization of spectral data, input data requirements.
g) Spectroscopic data pre-processing methods: baseline correction, denoising (Savitzky-Golay filter, wavelet analysis), derivative calculation, normalization.
h) Dimensionality reduction: PCA, t-SNE, UMAP.
i) Data decomposition methods: EFA, MCR-ALS.
j) Regression and classification: PLS, LDA, SVM; model validation methods.
2. Project Part (7 weeks: 3 hours per week):
a) Team-based design and implementation of two tools:
- A generator for synthetic spectral data with user-defined parameters.
- A spectroscopic data analyzer (pre-processing, decomposition, analysis).
b) Peer testing and validation of the developed applications.
c) Option to develop a custom thematic project, subject to instructor approval.
d) Presentation of results, discussion of the project's objectives and implementation, identification of challenges and their solutions.

Prerequisites and co-requisites

Prerequisites: Knowledge of general chemistry and the fundamentals of spectroscopy.

Recommended (optional): Basic knowledge of Python programming.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Presentation of project results	60.0%	50.0%
Completion of the project assignment	60.0%	50.0%

Recommended reading

Basic literature	1. Chu X., Huang Y., Yun Y.-H., Bian X., Chemometric Methods in Analytical Spectroscopy Technology, Springer, 2022. 2. Mark H., Workman Jr J., Chemometrics in Spectroscopy, Wiley, 2018.
Supplementary literature	Other relevant academic publications and textbooks on the subject.
eResources addresses	

Example issues/ example questions/ tasks being completed	Implementation of a Streamlit application with the following capabilities: - Loading and saving spectroscopic data. - Applying preprocessing methods (normalization, smoothing, derivatives, denoising). - Performing PCA and MCR-ALS analysis with visualization of the resolved profiles. - Generating synthetic spectra with user-defined parameters (peak types, noise, concentrations).
Work placement	Not applicable

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