KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI
FUNDUSZ SPOŁECZNY

Course title	ECTS code
Exploratory analysis of multidimensional chemical space	13.3.1292

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	Digital Chemistry
		specialization	wszystkie

Teaching staff

dr Agnieszka Gajewicz-Skrętna; dr inż. Karolina Jagiełło; Michał Kałapus; prof. dr hab. Tomasz Puzyn; Sattibabu Merugu; dr Alicja Mikołajczyk; mgr Annemarie Danielsson

Forms of classes, the realization and number of hours

Forms of classes

Laboratory classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Laboratory classes: 45 hours

ECTS credits

7
Lecture – 30 h
Classes - 45 h
student's own work – 30 h
tutorial classes – 70 h
TOTAL: 175 h – 7 ECTS

The academic cycle

2023/2024 winter semester

Type of course

obligatory

Language of instruction

English

Teaching methods

- multimedia-based lecture
- •In the computational laboratory students will conduct hands on exercises, based on the instructions prepared by the teacher

Form and method of assessment and basic criteria for eveluation or examination requirements

Final evaluation

- Graded credit
- Examination

Assessment methods

Lectures – final exam with multiple-choice questions
Laboratories – the final grade is based on partial grades received during the semester for written reports and/or presentation of assignments.

The basic criteria for evaluation

Assessment criteria in accordance with the University of Gdańsk Study Regulations
Lab classes: the arithmetic mean of partial grades received during the semester for written reports on laboratory exercises and presentation of the final assignment; the main criteria for evaluation of reports are the correct answers to the questions in the exercise instructions.
Lectures: passing the final exam in the form of a multiple-choice question test (a score of 50% or more required to pass the exam).

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
lack

B. Prerequisites
lack

Aims of education

Achieving advanced skills in exploratory analysis of multidimensional chemical space (performing analyses and interpreting the results)
Familiarizing the students with the available software allowing to perform the multidimensional analysis
Familiarizing the students with Python's scripts used to data analysis

Course contents

Introduction to multivariate data, review of the basic software allowing to perform the multidimensional analysis
Advanced methods of analyzing the internal structure of the data: similarity in the multivariable feature space, methods of similarity analysis, dimensionality reduction, hierarchical cluster analysis (HCA), principal component analysis (PCA), k-Means clustering, fuzzy c-Means clustering, Self-organizing maps, Gaussian Mixture models, and other deep learning algorithms Density-based spatial clustering of applications with noise.
Examples of applying these methods in chemical data analysis.

Bibliography of literature

Literature required to pass the course
• R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005
B. Extracurricular readings
• S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009
• scientific publication in the field

The learning outcomes (for the field of study and specialization)

K_W04: applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis

K_W07: selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of extended complexity chemical processes

K_W09: classifies specialist IT tools used in statistical evaluation of experiment results

K_W11: demonstrates in-depth knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field

K_U04: applies acquired knowledge of chemistry and related scientific disciplines

K_U06: presents the results of scientific discoveries in chemistry and related disciplines in an understandable way

K_K01: knows the limitations of her/his own knowledge; understands the need for further education

Knowledge

At the end of the course every student:
knows classification of advanced methods of data analysis and provides examples of their applications in multidimensional chemical problems
knows basic software packages to be used for multidimensional data analyses
explains theoretical background (algorithm) of the advanced methods, including HCA, PCA

Skills

At the end of the course every student:
uses Python environment for multidimensional analyses of chemical space
correctly prepares data for further analysis
performs various multidimensional data analyses and correctly interprets the results

Social competence

At the end of the course every student:
is convinced that the use of a computer and exploratory analysis strengthens the potential of data analysis
can critically evaluate experimental results and understand the necessity of their control
understands the need of deeper learning of multidimensional data analysis methods

Contact

agnieszka.gajewicz@ug.edu.pl