University of Gdańsk

Subject card

Subject name and code	Statistics and chemometrics in chemical analytics, PG_00082093		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
Education level	Bachelor's studies	Subject group	Obligatory subject group in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish polish
Semester of study	2	ECTS credits	3.0
Learning profile	academic	Assessment form	credit
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Karolina Jagiełło	
	Teachers	dr inż. Karolina Jagiełło dr hab. Łukasz Haliński	

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	0.0	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	5.0	40.0	75

Subject objectives	To develop the ability to perform basic calculations and statistical tests with particular emphasis on the ability to select appropriate statistical methods for the specific problem under investigation. - To introduce students to the range of applicability of chemometric methods in chemistry. - To provide students with the skills to use the most important chemometric methods - To familiarise students with available software implementing chemometric methods.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEML3_W09] Describes the practical applications of IT tools (computer programmes) for chemical calculations and data analysis.	On completion of the course each student: 1. understands that making a measurement involves comparing the measurand with a standard; 2. understands the need to reliably document results, identify potential problems that may arise from inadequate maintenance of the test documentation 3. knows for what purpose individual descriptive statistics are calculated (mean, state-dependent deviation and others); 4; 4. understands the idea of statistical inference about characteristics of the general population on the basis of a based on a representative statistical sample; 5. understands the concept of the significance level of a test; 6. knows the basic statistical distributions (normal distribution, Student's t distribution, F distribution and chi square) and their parameters; 7. knows the assumptions and limitations of basic statistical tests; 8. knows the basic division of chemometric methods, the applications of of these methods in chemistry (chemical analytics, forensic science, cosmetology forensic science, cosmetology and others); 9; 9. knows which computer software implements which methods; 10. knows the theoretical basis (algorithm of operation) of the most important methods of chemometric methods, e.g: HCA, PCA and LR/MLR. 11. is aware that measurements are subject to uncertainty; will indicate potential sources of measurement error and uncertainty in the research process; understands the phenomenon of uncertainty propagation in indirect measurement.	[SW4] test/exam - oral or written

Course outcome	Subject outcome	Method of verification
[CHEML3_U05] Uses basic statistical methods and IT techniques to describe chemical processes and analyse experimental data.	Upon completion of the course, each student: 1. is able to calculate basic descriptive statistics; 2. uses the resolution series and histogram to correctly infer the nature of the distribution of a series of results; 3. uses statistical tables; 4. is able to select and apply a statistical test appropriate to the problem under consideration problem; 5. uses KNIME or R software for chemometric calculations; 6; 6. is able to prepare data appropriately for chemometric analyses; 7. will carry out analyses of the internal structure of a set of data using HCA and PCA methods and will correctly interpret the results obtained; 8. will build a regression model (using the LR/MLR method), correctly perform the process of validation, and will make a prediction of the dependent variable based on the independent variable independent variable(s); 9. is able to estimate the uncertainty of direct and indirect measurement (based on the based on the law of propagation of uncertainty).	[SU8] observation of student's independent or team work
[CHEML3_U06] Uses basic application software packages to solve problems from the field of science.	Upon completion of the course, each student: 1. is able to calculate basic descriptive statistics; 2. uses the resolution series and histogram to correctly infer the nature of the distribution of a series of results; 3. uses statistical tables; 4. is able to select and apply a statistical test appropriate to the problem under consideration problem; 5. uses KNIME or R software for chemometric calculations; 6; 6. is able to prepare data appropriately for chemometric analyses; 7. will carry out analyses of the internal structure of a set of data using HCA and PCA methods and will correctly interpret the results obtained; 8. will build a regression model (using the LR/MLR method), correctly perform the process of validation, and will make a prediction of the dependent variable based on the independent variable independent variable(s); 9. is able to estimate the uncertainty of direct and indirect measurement (based on the based on the law of propagation of uncertainty).	[SU8] observation of student's independent or team work

Course outcome	Subject outcome	Method of verification
[CHEML3_W06] Chooses higher mathematics techniques to the extent necessary to understand and describe the physical processes important for understanding chemistry.	On completion of the course each student: 1. understands that making a measurement involves comparing the measurand with a standard; 2. understands the need to reliably document results, identify potential problems that may arise from inadequate maintenance of the test documentation 3. knows for what purpose individual descriptive statistics are calculated (mean, state-dependent deviation and others); 4; 4. understands the idea of statistical inference about characteristics of the general population on the basis of a based on a representative statistical sample; 5. understands the concept of the significance level of a test; 6. knows the basic statistical distributions (normal distribution, Student's t distribution, F distribution and chi square) and their parameters; 7. knows the assumptions and limitations of basic statistical tests; 8. knows the basic division of chemometric methods, the applications of of these methods in chemistry (chemical analytics, forensic science, cosmetology forensic science, cosmetology and others); 9; 9. knows which computer software implements which methods; 10. knows the theoretical basis (algorithm of operation) of the most important methods of chemometric methods, e.g: HCA, PCA and LR/MLR. 11. is aware that measurements are subject to uncertainty; will indicate potential sources of measurement error and uncertainty in the research process; understands the phenomenon of uncertainty propagation in indirect measurement.	[SW4] test/exam - oral or written

Course outcome	Subject outcome	Method of verification
[CHEML3_W07] Understands and describes physicochemical patterns, phenomena and processes using the language of mathematics.	On completion of the course each student: 1. understands that making a measurement involves comparing the measurand with a standard; 2. understands the need to reliably document results, identify potential problems that may arise from inadequate maintenance of the test documentation 3. knows for what purpose individual descriptive statistics are calculated (mean, state-dependent deviation and others); 4; 4. understands the idea of statistical inference about characteristics of the general population on the basis of a based on a representative statistical sample; 5. understands the concept of the significance level of a test; 6. knows the basic statistical distributions (normal distribution, Student's t distribution, F distribution and chi square) and their parameters; 7. knows the assumptions and limitations of basic statistical tests; 8. knows the basic division of chemometric methods, the applications of of these methods in chemistry (chemical analytics, forensic science, cosmetology forensic science, cosmetology and others); 9; 9. knows which computer software implements which methods; 10. knows the theoretical basis (algorithm of operation) of the most important methods of chemometric methods, e.g: HCA, PCA and LR/MLR. 11. is aware that measurements are subject to uncertainty; will indicate potential sources of measurement error and uncertainty in the research process; understands the phenomenon of uncertainty propagation in indirect measurement.	[SW4] test/exam - oral or written
[CHEML3_K01] Identifies the level of her/his own knowledge and skills and the need for continuous learning and personal development.	On completion of the course each student: 1. based on his/her knowledge and skills, critically evaluate the results of research using statistical methods (scientific research, reports, surveys, etc.); 2. is convinced of the benefits of using a computer and introducing the methods of chemometric methods into their everyday research practice; 3. understands the need for further training in chemometric methods; 4. is aware that every numerical result is subject to measurement uncertainty.	[SK8] observation of student's independent or team work

<table>
<tr><td>Subject contents</td><td>1. basics of chemical metrology and documentation of results: history and essence of measurements, standards, scales, significant figures, rules for rounding numbers,principles for documenting measurement results.Basics of statistical description: general population versus statistical samples; characteristics of a single series of results: measures of central tendency anddispersion of results, statistical distributions, descriptive statistics and their interpretation, the distribution series and the histogram, identification of outliers; hypothesis testing.outliers; statistical hypothesis testing based on selected parametric and non-parametric tests; correlation analysis.3 Introduction to chemometric methods: specificities of multivariate data; differences between chemical statistics and chemometrics;area of interest of chemometrics; division of chemometric methods; overview of computer software implementing chemometric methods (e.g.chemometric methods (e.g. R environment, MATLAB, Statistica, Ori-gin, SPSS, KNIME).4 Methods for analysing the internal structure of multidimensional chemical data: similarity of objects in a multidimensional feature space;hierarchical cluster analysis (HCA) as an example of a similarity analysis method; principal component analysis (PCA) as an example of a method ofsearching for projections. Examples of the use of this group of me-tods in different areas of chemistry.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>chemistry and mathecatics</td></tr>
<tr><td>Assessment methods and criteria</td><td>
<table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>egzam</td><td>51.0%</td><td>100.0%</td></tr>
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</td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td>A. Łomnicki: Wprowadzenie do statystyki dla przyrodników. Wydawnictwo Naukowe PWN, Warszawa 2003. J. Mazerski: Podstawy chemometrii. Gdańsk: Wydawnictwo Politechniki Gdańskiej, 2000 P. Konieczka, J. Namieśnik i in.: Ocena i kontrola jakości wyników analitycznych. Centrum Doskonałości Analityki i Monitoringu Środowiskowego, Gdańsk 2004.</td></tr>
<tr><td>Supplementary literature</td><td>scientific publications</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td></td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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