UNIWERSYTET GDAŃSKI

Course title
Metody numeryczne z algorytmami analizy danych / Numerical methods with algorithms for data analysis

ECTS code
13.3.0983

Name of unit administrating study
Faculty

Studies

Field of study	Type	Form	
Chemistry	Masters	Full-time studies	

Teaching staff
Prof. dr hab. Adam Liwo

Forms of classes, the realization and number of hours

A. Forms of classes, in accordance with the UG Rector's regulations
lecture, laboratory class

B. The realization of activities
in-class learning

C. Number of hours
60 h (30 h lecture, 30 h laboratory class)

ECTS credits 5

classes - 60 h
tutorial classes – 10 h
student's own work – 55 h

Total: 125 h - 5 ECTS

The academic cycle
2019/2020 summer semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods

Designing experiments
Lecture with multimedia presentation

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

A. Final evaluation, in accordance with the UG study regulations
course completion (with a grade)

B. Assessment methods
Exam, multiple-choice question test
Final assignment completion in the form of written report or presentation

C. The basic criteria for evaluation or exam requirements

Lab classes: Completion of the assigned project(s) (carried out individually or in teams of 2-3 students) and reporting the results to the teacher. 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).

Required courses and introductory requirements
Mathematics, Physics, Basic chemistry, Analytical Chemistry, Information Technology, Programming I,
Basics of calculus and linear algebra, Ability to use the UNIX operation system, Basic skills in C/Fortran programming.

Aims of education
• Familiarizing the students with the numerical agorithms applied in chemistry.
• Preparing the students to write own numerical applications, including using existing numerical libraries in the proces.

Course contents

Algorithm and its correctness. Errors in numerical calculations; Wilkinson's lemmas. Condition number of a problem. Overflow (INF), underflow, NaN. Interpolation: Lagrange and Newton schemes. Numerical differentiation. Numerical integration: the Newton-Coates and Gauss quadratures. Solution of linear equations systems: the Gauss, Gauss-Jordan, Cholesky, Householder, and QR algorithms. Solution of eigenproblem in quantum chemiatry. Solution of nonlinear equations: the Newton, regula falsi, secant, Pegasus, and bisection algorithms. Solution of systems of nonlinear equations; calculation of equilibrium concentrations in multicomponents systems as an example. Local minimization of functions in single and several variables in relation to conformational analysis with molecular mechanics. Introduction to global optimization algorithms and their relation to the problem of finding the most stable structures of molecules and crystals. Least-squares algorithms in fitting models to experimental data: linear and nonlinear regression (the Newtona-Gauss, Newtona, i Levenberg-Marquardt methods): application in the

determination of equilibrium constants. Statistical assessment of the goodness of fit and of the confidence levels of the determined parameters. Determination of parameters from noisy or insufficient data: the maximum entropy method. Algorithm for solving ordinary differential equations: application to chemical kinetics and molecular dynamics. Algorithms for solving partial differentia equations: applications to the electrochemical analysis (e.g., calculation of cyclic voltamperometry and polarography profiles) and to the calculation of electrostatic solvation energy of macromolecules. Fourier transformation and its application to the processing of IR and NMR spectra. Cluster analysis algorithms. Factor analysis algorithms and their application to the decomposition of UV spectra, QSAR, and conformational analysis.

Bibliography of literature

A. Literature required to pass the course

Z. Fortuna, B. Macukow, J. Wąsowski. Metody numeryczne, WNT, Warszawa
S. Brand, Analiza danych, PWN, Warszawa

B. Extracurricular readings

J. i M. Jankowscy, Przegląd metod i algorytmów numerycznych, WNT, Warszawa.
S. Brand, Analiza danych, PWN, Warszawa
J. Stoer. Wstęp do metod numerycznych. PWN, Warszawa.
J. B. Czermiński, A. Iwasiewicz i in.: Metody statystyczne w doświadczalnictwie chemicznych. Wydawnictwo Naukowe PWN, Warszawa 1992.
C.R. Rao, Modele liniowe statystyki matematycznej, PWN, Warszawa.
G.A.F., Seber, C.J. Wild, Nonlinear regression, Wiley.
R.G. Brereton, Chemometrics, Wiley.

Knowledge

The student describes floating point arithmetics problems and explains the causes and implications of floating point round-offs. Defines the concept of the algorithm. Describes the basic numerical algorithms applied in solving equations and systems of linear and nonlinear equations, target function minimization and solving the initial and boundary problems for ordinary and partial differential equations, respectively. The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry.

Skills

The student defines and solves the problems connected with the specific features of floating-point arithmetics, which arise when using the available quantum chemistry, molecular mechanics and dynamics, chemometry, etc., packages. Solves the computational problems that arise in chemistry and related subjects while using the software libraries available in the computer centers or from the web. Designs, for this purpose, simple numerical applications that use own or library procedures.

Social competence

The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the responsibility for his/her personal account on the workstation.Develops the ability of working in a team.