Syllabus
Course Program
Course Program

Programming of Modern Numerical Methods

Specialty
113 – Applied Mathematics

Institute
Institute of Computer Modeling, Applied Physics and Mathematics

Educational program
Computer and Mathematical Modeling

Department
Mathematical Modelling and Intelligent Computing in Engineering (161)

Level of education
Master's level (1 year 4 months)

Course type
Special (professional), Elective

Semester
1

Language of instruction
English

Lecturers and course developers

Oleksiy Larin (responsible lecturer)

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Doctor of Technical Sciences, Professor, work experience - 15 years
Specialist in the field of computational mechanics, probabilistic modeling and reliability prediction. The main focus of scientific works is devoted to the development of models, methods, approaches and algorithms of computer modeling and statistical analysis of engineering systems, in particular with random parameters. Author of more than 150 scientific and methodical works

More information about the teacher on the website of the department

General information

Summary
This course covers selected areas of nonlinear problems that arise in data analysis and pattern discovery through approximation. The course covers a number of topics, including spline approximation and nonlinear regression. The main focus of the material is on the accompanying problem of solving nonlinear algebraic problems that arise in these frameworks. A peculiarities of different methods, problems of convergence, accuracy and relevant comparative analysis are the methodological and pedagogical goals of the course. Students will gain practical experience in programming for individual methods, which is supposed to be done from scratch to understand the algorithmic features and tuning parameters of the respective methods.

Course objectives and goals
The course aims to provide students with a deep understanding of the mathematical and algorithmic foundations of computational solution of nonlinear algebraic problems arising in applied problems of nonlinear approximation and regression and is the basis for their effective use in data analysis and solving complex modelling problems

The course objectives:

1) Mastering the theoretical foundations of nonlinear approximation and regression for effective data analysis and pattern identification. Understand the features of various numerical methods for solving nonlinear algebraic problems.

2) Gain practical experience in programming to implement and analyse approximation and regression methods, in particular in the Python programming language.

3) Study of convergence and accuracy problems and comparative analysis of various numerical methods for the purpose of making a reasonable choice and applying the most effective tools in practice.

Format of classes

Lectures, practical classes. Final control in the form of a credit.

Competencies

GC1. Ability to generate new ideas (creativity) and non- standard approaches to their implementation.
GC7. Ability to think abstractly, analyse and synthesise..
PC1. Ability to solve tasks and problems that can be formalised, require updating and integrating knowledge, in particular in conditions of incomplete information.
PC2. Ability to conduct scientific research aimed to develop new and adapt existing mathematical and computer models to study various processes, phenomena and systems, conduct appropriate experiments and analyse the results.
PC3. Ability to develop methods and algorithms for the
construction, research and software implementation of mathematical models in engineering, physics, biology, medicine and other fields and to analyse them.
PC7. Ability to design and develop software to solve formalised problems, including systems with large amounts of data.

Learning outcomes

LO4. Build mathematical models of complex systems and choose methods of their research, implement the built models in software and check their adequacy using computer technologies.
LO5. Justify and, if necessary, develop new algorithms and software tools for solving scientific and applied problems, apply, modify and investigate analytical and computational methods for solving them.
LO8. Develop and implement algorithms for solving applied problems, system and application software of information systems and technologies.

Student workload

The total volume of the course is 90 hours (3 ECTS credits): lectures - 16 hours, laboratory classes - 16 hours, self-study - 58 hours.

Course prerequisites

For a general understanding of lectures, it is assumed that students have a background in the following disciplines: Mathematical Analysis (Differential, Integral calculus and Series); Linear Algebra (matrix, vector algebra); Numerical methods and fundamentals of optimisation theory.
Skills in basic Python coding is welcomed but not mandatory.

Features of the course, teaching and learning methods, and technologies

The course teaching and learning methods include traditional lectures for theoretical foundations and practice. The practice is structured in such a way that students are given a task for self-study in advance of the practical assignment. It can be a task or a series of mathematical tasks to solve or a task for independent programming. The practical lesson itself is devoted to consultations on problems that have arisen during the independent solution of the tasks and the defense of the results obtained. It is important to answer theoretical questions about the topic from the given practice, as well as to interpret the results and make conclusions.

Program of the course

Topics of the lectures

Topic 1. Special sections on approximation problems.
Short information on the general formulation of the approximation problem. Bezier curves. Spline approximations. Cubic splines.
Topic 2. Nonlinear regression problem.
Formulation of regression problems. The quality function and its impact on convergence.
Topic 3. Systems of nonlinear algebraic equations.
The difference between the statement and the solution of systems of linear equations. Multivaluedness. Impossibility of analytical solutions. The concept of linearisation.
Topic 4. Systems of nonlinear algebraic equations (continued).
Harmonic linearisation. Seidel's method. Newton's simplified method.
Topic 5. Systems of nonlinear algebraic equations (continued).
The concept of regularisation. The method of continuation by parameter.
Topic 6. Problems of finding extreme values of functions of many variables.
Formulation of the problem of finding extrema of functions. Connection with problems of solving systems of nonlinear algebraic equations.
Topic 7. Problems of finding extreme values of functions of many variables (continued).
Methods of the fastest descent and Newton-Hauss. Analytical calculation of Jacobi and Hesse matrices.
Topic 8. Problems of finding extreme values of functions of many variables (continued).
The Levenberg-Marquardt method.

Topics of the workshops

Not appliable

Topics of the laboratory classes

Practical class 1.
Software implementation of spline approximation.
Practical class 2.
Software implementation of approximation by Bezier curves and surfaces.
Practical class 3.
Nonlinear regression analysis using standard Python libraries. Investigation of convergence depending on different settings of the quality functional.
Practical class 4.
Software implementation (own code) for Newton's method of solving nonlinear algebraic equations.
Practical class 5.
Software implementation (own code) for the Newton-Raphson method for solving a system of nonlinear algebraic equations. Comparison of accuracy and convergence with the harmonic linearisation and the Seidel's method.
Practical class 6.
Software implementation (own code) for the method of continuation by the parameter of solving a system of nonlinear algebraic equations.
Practical class 7.
Software implementation of steepest descent and Newton-Gauss methods for the problem of finding extreme values of functions of many variables (continued). Comparative analysis of methods.
Practical class 8.
Software implementation of the Levenberg-Marquardt method.

Self-study

Processing of lecture material.
Completion of programming (coding) tasks, which are given after each lecture and are expected to be completed in advance of the practical class. It should be noted here that the practice time is mainly allocated for consultations on problems that arose during the previous performance of tasks and for

individual defense of reports on them, but not for their performance as such, which is expected within the framework of self-study.

Course materials and recommended reading

1. Samborska O.M. Numerical Methods. Study guide for students of higher technical educational institutions / O.M. Camborska, B.G. Shelestovskyi – Ternopil: Ivan Pulyuy TNTU, 2010. – 164 p. (in UA)
2. Goncharov O. A. Numerical methods for solving numerical problems: teaching. manual / O. A. Goncharov, L. V. Vasylieva, A. M. Yunda. – Sumy: Sumy State University, 2020. – 142 p. (in UA)
3. Dychka I. A. Numerical methods. Solving problems of mathematical analysis: laboratory workshop / I. A. Dychka, M. V. Onai, R. A. Hadynyak - Kyiv. - KPI named after Igor Sikorskyi, 2018. – 169 p. (in UA)

Assessment and grading

Criteria for assessment of student performance, and the final score structure

Theoretical part: **20 points**
in the form of an oral exam (2 questions in the exam paper for 10 points)

Practical part of the course: **80 points**
The work is formed from 8 individually completed tasks that are presented and defended in practical classes. Each practical class is worth 10 points.
Completion of all practical assignments is a prerequisite for the theoretical colloquium at the exam.

Grading scale

Total points	National	ECTS
90–100	Excellent	A
82–89	Good	B
75–81	Good	C
64–74	Satisfactory	D
60–63	Satisfactory	E
35–59	Unsatisfactory (requires additional learning)	FX
1–34	Unsatisfactory (requires repetition of the course)	F

Norms of academic integrity and course policy

The student must adhere to the Code of Ethics of Academic Relations and Integrity of NTU "KhPI": to demonstrate discipline, good manners, kindness, honesty, and responsibility. Conflict situations should be openly discussed in academic groups with a lecturer, and if it is impossible to resolve the conflict, they should be brought to the attention of the Institute's management.
Regulatory and legal documents related to the implementation of the principles of academic integrity at NTU "KhPI" are available on the website: http://blogs.kpi.kharkov.ua/v2/nv/akademichna-dobrochesnist/.

Approval

Approved by	Date August 30, 2023	Head of the department Oleksii VODKA
	Date August 30, 2023	Guarantor of the educational and professional program (1 year 4 months) Oleksiy LARIN