Course unit (module) title	Code
Mathematical Modelling	

Lecturer(s)	Department(s) where the course unit (module) is delivered
Coordinator: prof. Julius Žilinskas, prof. Olga Štikonienė **Other(s):**	Institute of Data Science and Digital Technologies Institute of Applied Mathematics Faculty of Mathematics and Informatics

Study cycle	Type of the course unit (module)
Second cycle	Compulsory

Mode of delivery	Period when the course unit (module) is delivered	Language(s) of instruction
Face-to-face, self-study Lectures, seminars and practice	2nd semester	English

Requirements for students	
Prerequisites: Basic concepts of Calculus and Linear Algebra	**Additional requirements (if any):**

Course (module) volume in credits	Total student's workload	Contact hours	Self-study hours
10	272	136	136

Purpose of the course unit (module): programme competences to be developed
The purpose of this course unit is to develop key mathematical skills related to theory of differential equations and its applications in mathematical modeling of dynamics of various biological components as well as to graph theory and optimization and their applications to model and solve problems in systems biology. The students will be introduced to differential equations including initial and boundary value problems, graph theory and search algorithms on graphs, optimization theory and algorithms. In addition, students should gain a good understanding of the underlying principles and concepts in order to be able to choose proper models and algorithms to solve their problems.

Learning outcomes of the course unit (module)	Teaching and learning methods	Assessment methods
2.1. Be able select an appropriate mathematical model for a given biological domain and problem	Lectures, debates, group discussion and practical assignments	Completion of practical assignments (two tests); Research project (written report and presentation); Written examination.
3.2. Perceive differential methods, graph theory, optimization algorithms used in evolutionary processes of biological systems		
3.5. Be able to apply differential methods, graph theory, optimization algorithms to describe evolutionary processes of biological systems		
4.1. Perform duties within the deadlines and goals of a project		
5.1 Be able to work autonomously and as a part of a multidisciplinary team; act honestly and according to ethical obligations		
5.2. Be able to critically analyse their own research quantitative results and know possible ways for improvement		

Content: breakdown of the topics	Contact hours							Self-study work: time and assignments	
	Lectures	Tutorials	Seminars	Exercises	Laboratory work	Internship/work placement	**Contact hours**	**Self-study hours**	**Assignments**
Part A. Differential equations	**28**			**28**			**56**	**56**	
1 Ordinary differential equations. Basic concepts and techniques.	8			8			**16**	**16**	Self-study of ordinary differential equations (P.Blanchard, R.LDevaney, G.R.Hall. Differential equations, 1.2, 1.8, 1.9, Chapter 3. Paul's Online Math Notes, Differential equations).
2. Modelling with differential equations. Numerical solution of differential equations.	4			4			**8**	**8**	Self-study of modelling with differential equations and numerical solution of differential equations. (P.Blanchard, R.L.Devaney, .R.Hall. Differential equations, Chapters 1-5, 7, Taubes Modeling Differential Equations in Biology, Burstein. MATLAB in Bioscience and Biotechnology, Nagle, . Saff, Snider. Fundamentals off Differential Equations, Projects)
3. Qualitative theory of differential equations.	8			8			**16**	**16**	Self-study of qualitative theory of differential equations. (P.Blanchard, R.L.Devaney, .R.Hall. Differential equations, 1.3-1.7, 2.2, 3.3-3.7, 5.2, D.K. Arrowsmith, C.M. Place)
4 Laplace transform. Solving linear integral and differential equations using Laplace transform.	2			2			**4**	**4**	Self-study of Laplace transform. (P.Blanchard, R.L.Devaney, .R.Hall. Differential equations, Chapter 6)
5 Partial differential equations.	6			6			**12**	**12**	Self-study of partial differential equations.

									(Y. Pinchover, J. Rubinstein. An Introduction to Partial Differential Equations.)
Part B. Graph theory	**18**			**18**			**36**	**20**	
6. Basic graph theory	2			2			**4**	**4**	Self-study of Basic graph theory (W. Kocay, D. L. Kreher, Graphs, Algorithms, and Optimization, Chapter 1)
7. Paths and walks	4			4			**8**	**4**	Self-study of Paths and walks (W. Kocay, D. L. Kreher, Graphs, Algorithms, and Optimization, Chapter 2)
8. Special classes of graphs	4			4			**8**	**4**	Self-study of Special classes of graphs (W. Kocay, D. L. Kreher, Graphs, Algorithms, and Optimization, Chapter 3)
9. Hamilton cycles	4			4			**8**	**4**	Self-study of Hamilton cycles (W. Kocay, D. L. Kreher, Graphs, Algorithms, and Optimization, Chapter 9)
10. Colorings and cliques	4			4			**8**	**4**	Self-study of Colorings and cliques (W. Kocay, D. L. Kreher, Graphs, Algorithms, and Optimization, Chapter 11)
Part C. Optimization	**18**			**18**			**36**	**20**	
11. Basics of optimization, one-dimensional optimization	2			2			**4**	**4**	Self-study of Basics of optimization (E. K. P. Chong, S. H. Zak, An Introduction to Optimization, Chapter 6-7)
12. Unconstrained optimization	4			4			**8**	**4**	Self-study of Unconstrained optimization (E. K. P. Chong, S. H. Zak, An Introduction to Optimization, Chapter 8-11)
13. Nonlinear programming	4			4			**8**	**4**	Self-study of Nonlinear programming (E. K. P. Chong, S. H. Zak, An

									Introduction to Optimization, Chapters 20-23)
14. Linear programming	4			4			**8**	**4**	Self-study of Linear programming (E. K. P. Chong, S. H. Zak, An Introduction to Optimization, Chapters 15-16)
15. Global optimization	4			4			**8**	**4**	Self-study of Global optimization (E. K. P. Chong, S. H. Zak, An Introduction to Optimization, Chapter 14)
Part D. Research project			**8**				**8**	**40**	Self-study of literature on individual topic, preparation for implementation and investigation, preparation of presentation at a seminar.
Total	**64**		**8**	**64**			**136**	**136**	

Assessment strategy	Weight,%	Deadline	Assessment criteria
Practicals with computer	10	During Part A	In the laboratory work problems are being solved (with the programs like Matlab, Octave). During the laboratory work in the computer class students have to demonstrate and explain their solution. Maximum number of points is given for full and correct solution; some points are given for partial solutions.
Midterm written exam	30	After Part A	Midterm exam consists of various complexity exercises. The scoring of each exercise is presented. The maximal grade of the midterm exam is 10 points. The evaluation criteria for the exercises are presented one week before the midterm exam.
Two tests in computer lab. Test 1 Test 2	 10 10	 After Part B After Part C	Tests consisting of various complexity exercises. The scoring of each task is presented. The maximal grade of the test is 10 points. The evaluation criteria for the exercises are presented one week before the test.
Course project	10	During Part D	Students perform a research project on optimization of an individually assigned problem. A written project report supposed to be presented and discussed with colleagues. The maximum grades for the written work and presentation are 10 points each. Written report assessment criteria (2 points each): 1. Consistency of presentation; 2. Arguments; 3. Generalization; 4. Correct solution; 5. Correct citation and references.

			Presentation assessment criteria (2 points each): • Quality of speech (clearity, distinction); • Eye contact with audience; • Quality of visually presented material; • Management of questions (quality of answers to the presented questions); • Management of time (is the time given for presentations used properly).
Written exam	30	After all parts	Written exam on topics of Parts B and C. The scoring for each exam question is given. The maximum grade is 10 points. The evaluation criteria of exam questions are presented during the last lecture.
Final grade			Weighted average according to the weights specified above

Author	**Year of publication**	**Title**	**Issue of a periodical or volume of a publication**	**Publishing place and house or web link**
Compulsary reading				
Paul Blanchard, Robert L. Devaney, Glen R. Hall	2012	Differential Equations, Fourth Edition		Cengage Learning
Leonid-Burstein.	2011	MATLAB in Bioscience and Biotechnology.		Biohealthcare Publishing (Oxford) Limited
R. Kent Nagle, Edward B. Saff, Arthur David Snider,	2018	Fundamentals off Differential Equations. Ninth Ed.		Pearson
William Kocay, Donald L. Kreher	2016	Graphs, Algorithms, and Optimization, Second Edition		Chapman and Hall/CRC
Edwin K. P. Chong, Stanislaw H. Zak	2013	An Introduction to Optimization		Wiley
Y. Pinchover and J. Rubinstein	2005	An Introduction to Partial Differential Equations.		Cambridge University Press,
Optional reading				
D.K. Arrowsmith, C.M. Place	1992	Dynamical Systems: Differential Equations, Maps, and Chaotic Behaviour		Chapman Hall/CRC Mathematics Series
D G. Zill, M.R. Cullen,	2008	Differential Equations with Boundary-Value Problems		Cengage Learning
Clifford Henry Taubes	2009	Modeling Differential Equations in Biology		Cambridge Univesity Press
D.S. Jones, M.J. Plank, B.D. Sleeman	2009	Differential Equations and Mathematical Biology	Second Edition	CRC Press

J. Stewart, T. Day	2015	Biocalculus: Calculus for the Life Sciences		Cengage Learning
P. Dawkins		Paul's Online Math Notes		http://tutorial.math.lamar.edu/
Dieter Jungnickel	2013	Graphs, Networks and Algorithms		Springer
B. Guenin, J. Könemann, L. Tunçel	2014	A Gentle Introduction to Optimization		Cambridge University Press

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