Universitat Autònoma de Barcelona

Numerical calculus

2022/2023

Code: 100120
ECTS Credits: 6

Degree

2500149 Mathematics

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities

Contact

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Use of languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

Teachers

Carles Barril Basil

Prerequisites

It is advisable to have successfully completed all mandatory courses, and also to know a programming language.

Objectives and Contextualisation

Systems of linear and non-linear equations, and ordinary differential equations (ODEs) are present in many mathematical models of physical processes.

In this course we will study numerical techniques for the approximate solution of systems of linear and non-linear equations, and both initial and boundary value problems for ordinary differential equations. We will also study algorithms for the computation of eigenvalues of matrices.

The course's main goal is for the students to learn these methods using their mathematical foundation while learning their convergent properties and becoming proficient programmers. An essential component of the assignment is computer practice, which aims to help the students better understand the characteristics of the various numerical methods.

Skills and learning outcomes

Skills:

- To be able to define new mathematical objects, be able to relate them to known objects, and determine their properties.
- To quickly and accurately reproduce predetermined mathematical routines and processes. And to be able to create innovative and competitive research and professional activity proposals.
- To apply realistic situations with a moderate level of complexity, gather and analyze pertinent data and information, propose and validate models using appropriate mathematical tools, and ultimately arrive at conclusions.
- Students must have and understand knowledge of an area of study built on the basis of general secondary education. This knowledge is typically found at a level that, while supported by advanced text books, also includes some elements that suggest knowledge that is at the cutting edge of the student's field of study.
- That students can convey knowledge, concepts, issues, and solutions to both specialized and non-specialized audiences.

Learning outcomes:
1. To control the computation errors that the machines make.
2. Understanding how computers work internally and being critical of the results they produce.
3. Developing innovative and competitive research and professional activity proposals.
4. Acquire and comprehend the knowledge acquired in the study area.
5. To acquire the ability to disseminate the new acquired knowledge to both specialized and non-specialized audiences.
6. Being able to program mathematical computation algorithms

Content

1. Initial value problems for ordinary differential equations
    - 1.1. One-step methods: Euler and Taylor.
    - 1.2. Numerical method's errors.
    - 1.3. Analysis and convergence of one-step methods.
    - 1.4. Runge-Kutta method.
    - 1.5. Fehlberg step-size control.
    - 1.6. Comments on multi-step methods.
    - 1.7. Introduction to stiff problems.
2. Numerical solution of systems of non-linear equations
    - 2.1. Matrix norms.
    - 2.2. Fixed point method: convergence and error estimation.
    - 2.3. Newton and *Quasi*-Newton methods in several variables.
3. Boundary value problems for ordinary differential equations
    - 3.1. Single shooting method.
    - 3.2. Multiple shooting method.
    - 3.3. Finite difference methods.
4. Numerical linear algebra
    - 4.1. Perturbation analysis of linear systems.
    - 4.2. QR method for square and over-determined systems
    - 4.3. Iterative methods for linear systems: convergence and error estimation.
    - 4.4. Methods for the computation of eigenvalues and eigenvectors.
5. Introduction to approximation of functions
    - 5.1. Gaussian quadrature.
    - 5.2. Brief introduction to the Discrete Cosine and fast Fourier transform.

Methodology

The theoretical and problem sessions will be carried out in a classroom. These sessions will be devoted to the presentation of theoretical aspects of numerical methods, their basic properties and the solution of problems, some of them of theoretical nature and some of them requiring the use of a calculator. Problem lists will be supplied along the course.

The seminar sessions with will be carried out in a computer room. In these sessions, students will solve an applied problem through the implementation in the C or MATLAB programming languages of methods studied in the course. These practical sessions will be evaluated from the delivery towards the end of the course (a date will be announced) of the code and a report.

The gender perspective goes beyond the contents of courses, since it implies also a revision of teaching methodologies and interactions between students and lecturers, both inside and outside the classroom. In this sense, participative teaching methodologies that give rise to an equality environment, less hierarchical in the classroom, avoiding examples stereotyped in gender and sexist vocabulary, are usually more favorable to the full integration and participation of all students in the classroom.

Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning outcomes
Type: Directed			
Problem classes	14	0,56	1,3,4,5
Computer sessions	12	0,44	1,2,3,4,5,6

Theoretical classes	24	0,96	1,3,4,5
Type: Autonomous			
Personal study	50	2	3,4,5
Problem solving and computer work	44	1,76	1,2,3,4,5,6

Assessment

La evaluación del curso se llevará a cabo a partir de tres actividades:

- Partial exam (PE): the resolution of problems that deal with the first part of the course will be evaluated (details will be announced during the course in class and at the Campus Virtual)
- Final exam (FE): an exam of all the course, with theoretical questions and problems.
- Practical work (PR): delivery of the algorithms (software) and a report

Además, se seguirán los siguientes criterios

- The students will have the option of taking an additional recovery exam (RE) with the same format as FE.
- Nor the partial exam nor the practical work will be recoverable
- In order to succeed this course, it is mandatory that max(EF, ER)>=3.5 y que PR>=3.5. If one student does not reach the minimum required in any of the evaluation activities, and the calculation of the final grade is equal to or greater than 5, a grade of 4 will be placed in the file
- A student is considered "Non-Evaluable" (NE) only if he / she has not done any assessment activity. Remember that the NE grade means that one examination sitting is lost.
- The final grade will be calculate following: max(0.1 EP+0.5EF+0.4PR, 0.6 EF+0.4PR).
- Honor grades will be granted at the first complete evaluation. Once given, they will not be withdrawn even if another student obtains a larger grade after consideration of the RE exam.

Assessment activities

Title	Weighting	Hours	ECTS	Learning outcomes
Recovery exam	0,5	3	0,12	1,3,4,5
Final exam	0,5	3	0,12	1,3,4,5
Partial exam	0,1	2	0,08	1,3,4,5
Delivery of practical work	0,4	0	0	1,2,3,4,5,6

Bibliography

General:

- J. Stoer and R. Burlisch, Introduction to numerical analysis, 3a ed, Springer, 2002.
- A. Ralston and P. Rabinowitz, A first curse in numerical analysis, McGraw-Hill, 1988.
- G. Dahlquist and A. Björck, Numerical methods, Englewood Cliffs (N.J.) : Prentice-Hall, 1974.
- A. Aubanell, A. Benseny y A. Delshams, Eines bàsiques del càlcul numèric, Manuals de la U.A.B., 1991.
- A. Quarteroni, R. Sacco and F. Saleri, Numerical Mathematics, TAM, Springer, 2000.
- C. Vuik, F. J. Vermolen, M. B. Gijzen, and M. J. Vuik, Numerical Methods for Ordinary Differential Equations, TU Delft OPEN, 2023 (1st edition VSSD, 2007).

Specialized:

- R. L. Burden and J. D. Faires, Análisis Numérico, Grupo Editorial Iberoamérica, México D. F., 1985.
- G. W. Gear, Numerical initial value problems in ordinary differential equations, Prentice-Hall, 1971.
- E. Hairer, S.P. Nørsett, G. Wanner, Solving ordinary differential equations. Vol. 1, Springer-Verlag, 1987.
- E. Hairer, S.P. Nørsett, G. Wanner, Solving ordinary differential equations. Vol. 2, Springer-Verlag, 1991.
- L. Elden, L. Wittmeyer-Koch, & H. B. Nielsen, Introduction to Numerical Computation, Studentlitteratur AB, 2004.

Software

It will either be MATLAB (matrix laboratory) or C for the practical lessons for this assignment. According to MATLAB, the UAB has a license that "permits use of the full functionality of the products of software from this platform by the entire university community and without restriction."
Link: https://www.uab.cat/web/serveis-dtic/matlab-1345826750494.html?detid=1345838118031