Universitat Autònoma de Barcelona

2018/2019

Numerical calculus

Code: 100120
ECTS Credits: 6

Degree	Type	Year	Semester
2500149 Mathematics	OT	4	0

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

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 are present in many mahtematical 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 main goal of the course is that students learn all these methods from their mathematical foundation by studying their convergence properties, ant also that they are able to program them. Computer sessions are a fundamentel part of the course, and they are intended for students to valuebetter understand the features of the different numerical methods.

Skills

- Assimilate the definition of new mathematical objects, relate them with other contents and deduce their properties.
- Calculate and reproduce certain mathematical routines and processes with agility.
- For the students to be able to transmit information, ideas, problems and solutions to both specialised and non-specialised audiences.
- For the students to have shown that they possess and understand knowledge in a study area on the basis of general secondary education and tend to have reached a level that, though supported by advanced textbooks, also includes some aspects that imply knowledge acquired from latest developments in their field of study.
- Generate innovative and competitive proposals for research and professional activities.
- When faced with real situations of a medium level of complexity, request and analyse relevant data and information, propose and validate models using the adequate mathematical tools in order to draw final conclusions

Learning outcomes

1. Control for errors produced by machines when computing.
2. For the students to be able to transmit information, ideas, problems and solutions to both specialised and non-specialised audiences.
3. For the students to have shown that they possess and understand knowledge in a study area on the basis of general secondary education and tend to have reached a level that, though supported by advanced textbooks, also includes some aspects that imply knowledge acquired from latest developments in their field of study.
4. Generate innovative and competitive proposals for research and professional activities.
5. Know how to program algorithms for mathematical calculation.
6. Understand the internal workings of computers and be critical of the results received.

Content

1. **Initial value problems for ordinary differential equations**
    1. One-step methods: Euler and Taylor.
    2. Local discretization error.
    3. Runge-Kutta methods.
    4. Convergence of one-step methods.
    5. Fehlberg step-size control.
    6. Comments on multistep methods.
    7. Stiff problems.
2. **Numerical solution of systems of non-linear equations**
    1. Matrix norms.
    2. Fixed point methods: convergence and error estimation.
    3. Newton's method in several variables.
3. **Boundary value problems for ordinary differential equations**
    1. Single shooting method.
    2. Multiple shooting method.
    3. Finite difference methods.
4. **Numerical linear algebra**
    1. Perturbation analysis of linear systems.
    2. QR method for square and over-determined systems.
    3. Iterative methods for linear systems. Convergence and error estimation.
    4. Power and inverse power methods for the computation of eigenvalues and eigenvectors.
    5. QR method for the computation of eigenvalues and eigenvectors.
5. **Approximation of functions**
    1. Gaussian quadrature.
    2. 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, studens will solve an applied problem through the implementation in the C programming language 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 C 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 female students in the classroom. Because of this, their effective implementation will be attempted in this course.

Activities

Title	Hours	ECTS	Learning outcomes
Type: Directed			
Computer sessions	12	0.48	1, 6, 4, 3, 2, 5
Problem classes	8	0.32	4, 3, 2
Theoretical classes	30	1.2	4, 3, 2
Type: Autonomous			
Personal study	50	2	4, 3, 2, 5
Problem solving and computer work	44	1.76	1, 6, 4, 3, 2, 5

Evaluation

The course will be graded from three evaluation activities:

- Final exam (FE): an exam of all the course, with theoretical questions and problems.
- Practical work (PR): delivery of C programs and a report.
- Optional delivery of Octave/Matlab problems: code and a report.

Besides that, the students will have the option of taking an additional recovery exam (RE) with the same format as FE. The practical work will not be recoverable.

In order to succeed in this course, it is mandatory that max(FE,RE)>=4 and PR>=4.

The final grade will be

max(0.5*FE,0.5*RE)+0.5*PR

Students will be given the option (and encouraged) to solve some problems of the problem list consisting in computer experiments on the properties of some of the numerical methods explained in the course. These problems will be designed to be solved with Octave/Matlab, and will be a good opportunity for students to be introduced in this language. These problems will be graded and will add up to one point (out of ten) to the grades of EF and ER.

Honor grades will be granted at the first complete evaluation. Once given, they will no be withdrawn even if another student obtains a larger grade after consideration of the RE exam.

Evaluation activities

Title	Weighting	Hours	ECTS	Learning outcomes
Delivery of Octave/Matlab problems	0.05	0	0	1, 6, 4, 3, 2, 5
Final exam	0.45	3	0.12	4, 3
Practical work	0.50	0	0	1, 6, 4, 3, 2, 5

Recovery exam	0.50	3	0.12	4, 3

Bibliography

General references:

- 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.

Specialized references:

- 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.