**Universitat Autònoma de Barcelona**

# Numerical Calculus

**2022/2023**

Code: 104390
ECTS Credits: 6

| Degree | Type | Year | Semester |
|---|---|---|---|
| 2503740 Computational Mathematics and Data Analytics | FB | 1 | 2 |

## 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

A first course on calculus in one variable, and a first course on linear algebra.

## Objectives and Contextualisation

Modeling turns problems in science and engineering into mathematical problems. The complexity of the real world often gives rise to mathematical problems that cannot be addressed from an analytic approach. Or perhaps they can, but the analytic approach may be too complex in the context in which the solution of the problem is required. For instance, solving the problem could be part of a contract, for which limited time is available.

Numerical methods are techniques from which algorithms can be deduced in order to obtain approximate solutions of mathematical problems. Many times, especially when high precision is required, these algorithms demand a large amount of computations. The use of a computer is then mandatory. Computers are most efficient when using finite precision arithmetic (this is, working with a finite number of digits). This means that each operation introduces error, known as round-off. This is not usually a problem, in particular because we are looking for approximate solutions. Nevertheless, it is necessary to know how to avoid situations in which the propagation of round-off error could completely invalidate our computations.

This course is devoted to the analysis of basic numerical methods, related to the solution of the kind of mathematical problems studied in first-year courses. This analysis has as a goal being able to predict both the quality of the approximations produced by the different methods and the computational effort they involve. This course is also an introduction to scientific computing, this is, the set of techniques and skills needed for the implementation in a computer of the numerical solution of a problem.

The numerical methods studied in this course are building stones of numerical methods for the solution of more sophisticated problems, studied from the second year on, like ordinary and partial differential equations.

## Competences

- Apply a critical spirit and rigour for the validation or rejection of your own arguments and those of others.
- Calculate and reproduce certain mathematical routines and processes with ease.

- Demonstrate a high capacity for abstraction and translation of phenomena and behaviors to mathematical formulations.
- Formulate hypotheses and think up strategies to confirm or refute them.
- Make effective use of bibliographical resources and electronic resources to obtain information.
- Relate new mathematical objects with other known objects and deduce their properties.
- Students must be capable of collecting and interpreting relevant data (usually within their area of study) in order to make statements that reflect social, scientific or ethical relevant issues.
- Students must be capable of communicating information, ideas, problems and solutions to both specialised and non-specialised audiences.
- Students must have and understand knowledge of an area of study built on the basis of general secondary education, and while it relies on some advanced textbooks it also includes some aspects coming from the forefront of its field of study.
- Use computer applications for statistical analysis, numerical and symbolic computation, graphic visualisation, optimisation and other to experiment and solve problems.
- Using criteria of quality, critically evaluate the work carried out.
- Work cooperatively in a multidisciplinary context assuming and respecting the role of the different members of the team.

## Learning Outcomes

1. "Explain ideas and mathematical concepts pertinent to the course; additionally, communicate personal reasonings to third parties."
2. Apply a critical spirit and rigour for the validation or rejection of your own arguments and those of others.
3. Calculate and study function endpoints.
4. Calculate function integrals for a variable.
5. Classify matrices and linear applications according to different criteria (rank, diagonal and Jordan forms).
6. Contrast, if possible, the use of calculation with the use of abstraction in solving a problem.
7. Describe the concepts and mathematical objects pertaining to the subject.
8. Develop autonomous strategies for solving problems such as identifying the ambit of problems within the course, discriminate routine from non-routine problems, design an a priori strategy to solve a problem, evaluate this strategy.
9. Evaluate the advantages and disadvantages of using calculation and abstraction.
10. Identify the essential ideas in the demonstration of ceratin basic theorems and know how to adapt these to obtain other results.
11. In an orderly and accurately manner, draft brief mathematical texts (exercises, resolution of theoretical questions, etc.).
12. Make effective use of bibliographical resources and electronic resources to obtain information.
13. Read and understand a mathematical text at the current level of the course.
14. Solve problems by approaching them with integrals (lengths, areas, volumes, etc.).
15. Students must be capable of collecting and interpreting relevant data (usually within their area of study) in order to make statements that reflect social, scientific or ethical relevant issues.
16. Students must be capable of communicating information, ideas, problems and solutions to both specialised and non-specialised audiences.
17. Students must have and understand knowledge of an area of study built on the basis of general secondary education, and while it relies on some advanced textbooks it also includes some aspects coming from the forefront of its field of study.
18. Understand and work intuitively, geometrically and formally with the notions of limit, derivative and integral.
19. Using criteria of quality, critically evaluate the work carried out.
20. Work cooperatively in a multidisciplinary context, taking on and respecting the role of the distinct members in the team.

## Content

Error propagation

Numerical linear algebra

Numerical solution of non-linear equations

Interpolation, differentiation, integration

## Methodology

In the theoretical sessions, the lecturer will explain the different methods and their analysis. The explanation of the different methods will be accompanied by computer examples of their behavior, both for a better understanding of the methods and in order to introduce their analysis.

The problem sessions will be devoted to the solution of both theoretical and computational problems. Some of the computational ones will require the use of a calculator, whereas other problems will require the use of a computer. In this last case, the problems will not be computationally intensive, so the algorithms needed for their solution will be of a fast implementation in an interpreted Octave-type language. Problems will be solved by either the lecturer, a student for all the class, or all the students for themselves with the support of the lecturer.

The computer sessions are designed as an introduction to scientific computing. In these sessions, students will work in more computationally intensive problems, by implementing their solution in a compiled language. In doing this, students will progressively develop their personal library of routines for basic numerical methods.

Annotation: 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 sessions | 15 | 0.6 | 2, 19, 9, 3, 4, 18, 6, 7, 8, 10, 17, 16, 11, 14, 20, 12 |
| Theoretical sessions | 30 | 1.2 | 2, 19, 9, 3, 4, 18, 6, 7, 8, 1, 10, 13, 17, 16, 15, 14, 12 |
| Type: Supervised | | | |
| Computer sessions | 8 | 0.32 | 2, 19, 9, 3, 4, 18, 6, 7, 8, 1, 13, 17, 16, 15, 11, 14, 20, 12 |
| Type: Autonomous | | | |
| Computer work | 16 | 0.64 | 2, 9, 6, 7, 8, 1, 13, 17, 16, 15, 11, 12 |
| Personal study | 76 | 3.04 | 2, 19, 9, 3, 4, 5, 18, 6, 7, 8, 10, 13, 17, 16, 15, 14, 12 |

## Assessment

The course will be evaluated from three activities:

- Partial exam (PE): an exam of a part of the course, with theoretical questions and problems.
- Final exam (FE): an exam of the whole course, with theoretical questions and problems.
- Practical computer work (PR): delivery of code and a report.

Students will be given the option of taking an additional recovery exam (RE), of the same format of the FE exam. The practical work (PR) will not be recoverable.

In order to suceed, it is mandatory that max(0.35*PE*0.65*FE,FE,RE)>=3.5 and PR>=3.5.

The final grade of the course will be

0.6*max(0.35*PE+0.65*FE,FE,RE)+0.4*PR

Honor grades will be granted at the first complete evaluation. 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 |
| --- | --- | --- | --- | --- |
| Computer work | 0.4 | 0 | 0 | 2, 19, 9, 6, 7, 1, 13, 17, 16, 15, 11, 20, 12 |
| Final exam | 0.39 | 3 | 0.12 | 2, 19, 9, 3, 4, 5, 18, 6, 7, 8, 1, 10, 17, 16, 15, 11, 14 |
| Partial exam | 0.21 | 2 | 0.08 | 2, 19, 9, 4, 6, 7, 8, 1, 10, 17, 16, 15, 11, 14 |

## Bibliography


Basic references:

- A. Aubanell, A. Benseny, A. Delshams. Eines bàsiques de càlcul numèric. Manuals de la UAB 7, Publ. UAB, 1991.
- M. Grau, M. Noguera. Càlcul numèric. Edicions UPC, 1993.
- J.D. Faires, R. Burden. Métodos numéricos, 3a ed. Thomson, 2004.
- R. Burden, J.D. Faires. Numerical analysis, 6a ed. Brooks/Cole, 1997.
- G. Hämmerlin, K.-H. Hoffmann. Numerical mathematics. Springer, 1991.

Advanced references:

- E. Isaacson, H.B. Keller. Analysis of numerical methods. Wiley, 1966.
- J. Stoer, R. Bulirsch. Introduction to numerical analysis, 3a ed. Springer, 2002.
- G. Dahlquist, A. Björk. Numerical methods. Prentice Hall, 1964.
- A. Ralston and P. Rabinowitz. A first course in numerical analysis. McGraw-Hill, 1988.
- A. Quarteroni, R. Sacco and F. Saleri. Numerical Mathematics. Springer, 2000.


## Software

- Preferably a Linux environment
- code-oriented text editor (e.g. Kate)
- GNU C compiler
- gnuplot
- image manipulation tools (e.g. imagemagick)
- GNU Octave