

Numerical Calculus

Code: 104390
ECTS Credits: 6

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

Contact

Name: Jose Maria Mondelo Gonzalez
Email: JoseMaria.Mondelo@uab.cat

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 converts problems from science and engineering in 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 a set of techniques from which algorithms can be deduced for the approximate solution of mathematical problems. Many times, especially when high precision is required for the approximate solution, these algorithms need a large amount of computations. The use of a computer then mandatory. Computers are most efficient when using finite precision arithmetic (this is, when they work with a finite number of digits). This means that each operation is done not exactly but with error, known as round-off error. This is not usually a problem, because we are looking for approximate solutions in the first place. Nevertheless, it is necessary to know how to avoid situations in which the propagation of round-off error could completely invalidate our (presumed) approximations.

This course is devoted to the analysis of basic numerical methods, related to the solution of the kind of mathematical problems studied in the remaining first-year courses. Analysis stands for 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, like ordinary and partial differential equations, which are part of courses of the second year and above.

Skills

- 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 certain 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

Interpolation, differentiation, integration

Numerical solution of non-linear equations

Methodology

The theoretical sessions will be devoted to the explanation by the lecturer of the different methods and their analysis. The explanation of the different methods will be accompanied by examples of their behavior, done with computer, that will have as a goal both a better understanding of the methods by the students and an introduction to their analysis.

The problem sessions will be devoted to the solution of problems of both a theoretical and a computational nature. Some of the computational problems 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 the part of the course devoted to introduce 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 implementing basic numerical methods.

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 | | | |
| 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 |

Evaluation

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 succeed, it is mandatory that $\max(0.35*EP+0.65*EF, EF, ER) \geq 4$ and $PR \geq 4$.

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.

Evaluation 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.