

Numeric Methods and Computer Applications

Code: 100966
ECTS Credits: 6

Degree	Type	Year	Semester
2500253 Biotechnology	FB	2	2

Contact

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Use of Languages

Principal working language: spanish (spa)
Some groups entirely in English: No
Some groups entirely in Catalan: No
Some groups entirely in Spanish: Yes

Prerequisites

It is strongly recommended that the student has passed the following subjects: Mathematics and the contents of Computer Science of the course Integrated Laboratory 1.
We understand that the students already know how to use calculators and computers.

Objectives and Contextualisation

In the Numerical Analysis course we will study computational algorithms to solve some of the basic problems that usually appear in the scientific calculation, such as the calculation of the solution of nonlinear equations, the resolution of systems of linear equations and the numerical resolution of differential equations.

The goal of the course is that the student learns about these methods from their mathematical foundation, studying the properties of convergence and stability and estimating errors and their applicability and possible limitations.

Computer laboratory sessions will have an important role in this course. The sessions are a complement to better understand the numerical methods. The computer lab sessions allow to show, in different examples, the properties of convergence and stability studied analytically in the seminars. The sessions will also help to compare different numerical methods to solve the same problem. Most examples will be considered at an easy level so they can be done by hand or with a calculator. Keep in mind that real problems are usually much more complicated and cannot be done without using a computer. It is in the later cases where the phenomena described in the theory seminars are produced.

The procedure we will follow consist of first, understand the methods studied in the seminars, then do a series of exercises by hand or with a calculator in order to master the algorithm and finally, codify the algorithm with which to solve more difficult problems. That is why the theory and problem seminars and the computer laboratory sessions have the same importance.

Capacities or skills to acquire.

- Understand the mathematical foundations of the methods.
- Ability to generate or build the different methods.
- Distinguish the different types of errors introduced by a method and understand how to estimate them.
- Understand convergence criteria for iterative methods.
- Learn how to compare different methods to solve the same problem.

- Ability to choose the most appropriate numerical method (s) to solve a given problem.
- Sufficient skills to implement these methods in the most efficient way.
- Give practical stopping iteration criteria in order to obtain a fixed accuracy.

Develop criteria to detect erroneous results and ability to find the source of errors (ill-conditioned problem, method not suitable for the problem considered, unstable numerical scheme, etc.) and correct them.

Competences

- Make decisions.
- Reason in a critical manner
- Use ICT for communication, information searching, data processing and calculations.
- Use the fundamental principles of mathematics, physics and chemistry to understand, develop and evaluate a biotechnological process.

Learning Outcomes

1. Analyse the different types of errors and their importance in problem solving. Apply certain numerical methods for equation-solving and integration.
2. Interpret the graphs of functions of one or more variables and relate them to their formulae.
3. Make decisions.
4. Reason in a critical manner
5. Use ICT for communication, information searching, data processing and calculations.

Content

REVIEW OF BASIC KNOWLEDGE FOR THE COURSE

- Derivation and integration in several variables. Function graphic representation
- Taylor's formulas in one and several variables.

1. ERRORS

- Sources of error.
- Absolute error and relative error.
- Propagation of errors in the data and the calculations.
- Ill-conditioned problems

2. RESOLUTION OF NON-LINEAR EQUATIONS

- Methods of Bisection and fixed point. Secant and Newton's methods.
- Order of convergence
- Systems of nonlinear equations.

3. INTERPOLATION AND INTEGRATION OF FUNCTIONS

- Lagrange Formula and divided differences.
- The error in polynomial interpolation.

- Trapezoidal rule
- Simpson's rule
- The error in numerical integration.
- Composite formulas.

4. DIFFERENTIAL EQUATIONS

- Introduction.
- Euler method.
- Taylor's method.
- Runge-Kutta Methods.
- Step adaptation techniques.
- Systems of differential equations.

5. REGRESSION AND APPROXIMATION

- Overdetermined systems
- Approximation by minimum squares
- Approximation of functions dependent on two parameters.

Methodology

This course consists of three hours per week that are divided into theoretical seminars and problem sessions. In addition, within the course "Integrated laboratory 4 " there are five computer laboratory sessions related to the course throughout the semester of three hours each.

In theory seminars, several numerical methods will be introduced and their basic properties will be studied. The problems sessions will be devoted to the resolution of problems of a theoretical nature and / or problems requiring the use of a calculator to be solved. Lists of problems will be provided throughout the semester and will be available on the website of the virtual campus. It is essential to bring a calculator to these sessions. Problems sessions will be intercalated within the usual schedule as the subjects are completed.

In the computer laboratory sessions the student will have to solve numerically certain problems with the help of the computer. These sessions will take place in the PC's laboratories of the faculty. The student will have a guide describing the steps to follow in each session which will consist of the implementation of some of the numerical methods studied and their use to solve the proposed problems.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Theory and problems seminars	45	1.8	1, 5, 2, 3, 4
Type: Supervised			
Continuous evaluation	5	0.2	1, 5, 2, 3, 4

Type: Autonomous

Personal study and problem resolution	95	3.8	1, 5, 2, 3, 4
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Assessment

The evaluation of the subject will be carried out through a continuous evaluation in which the student has to demonstrate his degree of achievement of the concepts of the subject through delivery of assignments and written tests of theory and problem solving.

Throughout the course there will be four evaluation blocks. Each of them will be formed by two different tests: one based on theory questions and the other on problem solving.

There will be four deliveries of assignments that will be properly announced and for which the student will have a week to complete each of them.

With the result of all the tests a qualification will be obtained that, if equal or bigger than 5, will give the final qualification of the course. It is not necessary to obtain any minimum grade for any of the partial tests to pass the subject.

The qualification of Honors will be assigned to the best grades obtained in the continuous evaluation.

There will be a retake examination at the end of the course in which the student can recover the blocks not passed if the total average obtained in the subject is at least 3.

In order to participate in the recovery exam, the student must have been previously evaluated in a set of activities, the weight of which equals a minimum of two thirds of the total grade of the subject. Therefore, the student will obtain the qualification of "Not Evaluable" when the evaluation activities carried out have a weight lower than 67% of the final grade.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Assignments delivery	4%	1	0.04	1, 5, 2, 3, 4
Partial theory test 1	5%	0.25	0.01	1, 5, 2, 3, 4
Partial theory test 2	5%	0.25	0.01	1, 5, 2, 3, 4
Partial theory test 3	5%	0.25	0.01	1, 5, 2, 3, 4
Partial theory test 4	5%	0.25	0.01	1, 5, 2, 3, 4
Test problem solving 1	19%	0.75	0.03	1, 5, 2, 3, 4
Test problem solving 2	19%	0.75	0.03	1, 5, 2, 3, 4
Test problem solving 3	19%	0.75	0.03	1, 5, 2, 3, 4
Test problem solving 4	19%	0.75	0.03	1, 5, 2, 3, 4

Bibliography

- A. Bjorck i G. Dahlquist, Numerical methods, Prentice Hall, Englewood Cliffs, New Jersey (1977)
- A. Aubanell, A. Benseny i A. Delshams, Eines bàsiques del Càlcul numèric, Manuals de la UAB, (1992)
- C. Bonet i altres, Introducció al Càlcul Numèric, Universitat Politècnica de Catalunya, (1989)
- R. L. Burden y J. D. Faires, Análisis Numérico, Grupo Editorial Iberoamérica, (1985)