uc3m Universidad Carlos III de Madrid

Numerical methods in biomedicine

Academic Year: (2022 / 2023) Review date: 16-05-2022

Department assigned to the subject: Mathematics Department

Coordinating teacher: GUTIERREZ DIEZ, RICARDO

Type: Basic Core ECTS Credits: 6.0

Year: 2 Semester: 2

Branch of knowledge: Engineering and Architecture

REQUIREMENTS (SUBJECTS THAT ARE ASSUMED TO BE KNOWN)

Calculus I, Calculus II, Linear Algebra, Differential Equations, Computer Programming, Systems and Signals.

OBJECTIVES

Using NUMERICAL METHODS (NM) to calculate approximate solutions of models of physiological, cellular, and molecular systems.

Studying the stability and accuracy of NM.

Calculating numerical solutions of systems of nonlinear equations.

Approximating the minimum of a function of several variables.

Developing, analyzing, and implementing finite difference methods.

Solving ordinary differential equations and systems by means of numerical integration methods.

Using software environments to test the efficiency, pros and cons of different NM.

DESCRIPTION OF CONTENTS: PROGRAMME

PROGRAMME

1- PRINCIPLES OF NUMERICAL MATHEMATICS.

Well-Posedness and Condition Number of a Problem.

Stability of Numerical Methods.

The Floating-Point Number System.

2- ROOTFINDING OF NONLINEAR EQUATIONS.

Conditioning of a Nonlinear Equation.

The Newton-Raphson Method.

Newton's Methods for Systems of Nonlinear Equations.

3- UNCONSTRAINED OPTIMIZATION.

Necessary and Sufficient conditions for Optimality. Convexity.

Optimization Methods.

4- FINITE DIFFERENCE METHODS: INTERPOLATION, DIFFERENTIATION AND INTEGRATION.

Backward, Forward, and Central Differences.

Interpolation and Extrapolation methods.

5- NUMERICAL SOLUTIONS OF ORDINARY DIFFERENTIAL EQUATIONS (ODEs).

ODEs and Lipschitz Condition.

One Step Numerical Methods.

Zero-Stability, Convergence Analysis and Absolute Stability.

Consistency.

Numerical methods for ODEs.

Systems of ODEs.

Stiff Problems.

6- APROXIMATION THEORY. Least-Squares Solutions Fast Fourier Transform.

LEARNING ACTIVITIES AND METHODOLOGY

One of the purposes of this course is to provide the mathematical foundations of numerical methods, to analyze their basic theoretical properties (stability, accuracy, computational complexity), and demonstrate their performances on examples and counterexamples which highlight their pros and cons. The primary aim is to develop algorithmic thinking emphasizing essential computational concepts. Every chapter is supplied with examples, exercises and applications of the theory developed in class. The course relies throughout on well tested numerical procedures for which we include codes and test files.

Students should write their own codes by studying and eventually rewriting the codes given by the Teacher in Aula Global. The codes written by the students should be run, tested and uploaded to Aula Global in the Computer Room classes.

Throughout the course we emphasize graphic 2D and 3D representations of solutions. Through this visual approach, students will become familiar with results at a more intuitive level, and will be able to gain insight into the behavior of numerical solutions.

ASSESSMENT SYSTEM

The final grade will be calculated as follows: 50% final exam score + 50% continuous assessment score, which includes grades obtained in midterm exams and computational assignments.

% end-of-term-examination: 50 % of continuous assessment (assignments, laboratory, practicals...): 50

BASIC BIBLIOGRAPHY

- [A] K. Atkinson Elementary Numerical Analysis, John Wiley & Sons, 2004
- [BC] A. Belegundu and T. Chandrupatla Optimization Concepts and Applications in Engineering, Cambridge University Press, Second Edition. 2011., 2011
- [BC] A. Belegundu and T. Chandrupatla Optimization Concepts and Applications in Engineering, Cambridge University Press, Second Edition., 2011
- [BC] A. Belegundu and T. Chandrupatla Optimization Concepts and Applications in Engineering, Cambridge University Press, Second Edition., 2011
- [DCM] S. Dunn, A. Constantinides and P. Moghe Numerical Methods in Biomedical Engineering, Elsevier Academic Press, 2010
- [KC] D. Kincaid and E. W. Cheney Numerical Analysis: Mathematics of Scientific Computing, American Mathematical Society, 2002
- [MF] J. H. Mathews and K. D. Fink Numerical Methods Using Matlab, 4th ed., Pearson Prentice Hall, 2004
- [QSG] A. Quarteroni, F. Saleri and P. Gervasio Scientific computing with MATLAB and Octave, Springer, 2010
- [QSS] A. Quarteroni, R. Sacco and F. Saleri Numerical Mathematics, Springer, 2007

ADDITIONAL BIBLIOGRAPHY

- [HH] D. Higham and N. Higham Matlab Guide, Second Edition., 2005.
- [K] C. Kelley Iterative Methods for Optimization, SIAM, 1999.
- [NW] J. Nocedal and S. J. Wright Numerical Optimization, Springer, 2006