Modern computational methods in physics

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Exam - Modern computational methods in physics

One **project** with

- a numerical program (e.g. in Mathematica);
- supporting theory (physics/ mathematics and numerical methods used).

Processing of Physical Data and Numerical Methods - Overview

I. Solution of Linear Algebraic Equations

II. Non-linear Equations and Roots of Polynomials

III. Least Squares Methods for Curve Fitting

IV. Interpolation and Extrapolation

V. Numerical Evaluation of Derivatives

VI. Numerical Evaluation of Integrals

VII. Numerical Solution of Ordinary Differential Equations

VIII. Numerical Solution of Partial Differential Equations

IX. Numerical Solution of Integral Equations

I. Solution of Linear Algebraic Equations

1. Direct Methods
    1. Upper (Superior) Triangular Matrix
    2. Gaussian Elimination
    3. Gauss-Jordan Elimination
2. Iterative Methods
    1. Jacobi Method
    2. Gauss-Seidel Method
    3. Successive Over Relaxation
3. Solution by Matrix Decomposition
    1. Doolittle Factorization
    2. Crout Factorization
    3. Cholesky Factorization
4. Tridiagonal and Band Diagonal Systems of Equation
    1. Gaussian Elimination
    2. Doolittle Factorization
5. Singular Value Decomposition
    1. Singular Value Decomposition of a Square Matrix
    2. Singular Value Decomposition for Fewer Equations than Unknowns
    3. Singular Value Decomposition for More Equations than Unknowns

II. Non-linear Equations and Roots of Polynomials

- II.1 Bisection Method
- II.2 Newton-Raphson Method
- II.3 False Position and Secant Method
- II.4 Müller's Method
- II.5 Graeffe's Method
- II.6 (Lin-)Bairstow Method
- II.7 Laguerre's Method
- II.8 Methods for Non-linear Systems of Equations
  - II.8.1 Fixed Point Iteration Method
  - II.8.2 Newton-Raphson Method

III. Least Squares Methods for Curve Fitting – Linear Least Squares

- III.1 Least Squares Line
- III.2 Least Squares Polynomials

IV. Interpolation and Extrapolation

- IV.1 Polynomial Interpolation
  - IV.1.1 Lagrange Interpolation
  - IV.1.2 Newton Interpolation
- IV.2 Rational Function Interpolation
- IV.3 (Cubic) Spline Interpolation
- IV.4 Interpolation with Orthogonal Polynomials

V. Numerical Evaluation of Derivatives

- V.1 Classical Difference Formulas
- V.2 Richardson Extrapolation

VI. Numerical Evaluation of Integrals

- VI.1 Classical Formulas for Equally Spaced Abscissas
  - VI.1.1 Closed Formulas
  - VI.1.2 Open Formulas
  - VI.1.3 Semi-open Formulas
- VI.2 Gaussian Quadratures and Orthogonal Polynomials
- VI.3 Monte-Carlo Integration (for one and two variables)

VII. Numerical Solution of Ordinary Differential Equations

Direct Methods for Initial Value Problems

- VII.1 Euler's Method
- VII.2 Runge-Kutta Methods
- VII.3 Second-Order Conservative Equations

VIII. Numerical Solution of Partial Differential Equations

- VIII.1 Elliptic PDE
- VIII.2 Hyperbolic PDE
- VIII.3 Parabolic PDE

IX. Numerical Solution of Integral Equations

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I. Review of Solution of Linear Algebraic Equations
II. Review of Non-linear Equations and Roots of Polynomials
III. Review of Numerical Evaluation of Derivatives and Integrals
IV. Numerical Solution of Ordinary Differential Equations
V. Numerical Solution of Partial Differential Equations
- VIII.1 Elliptic PDE
- VIII.2 Hyperbolic PDE
- VIII.3 Parabolic PDE

VI. Numerical Solution of Integral Equations

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Laborator 1 – tasks:

Compute in Mathematica:

- **Determine the eigenvalues and eigenvectors of a 3 x 3 matrix (using both, Mathematica's predefined commands and a direct algorithm)**