Numerical methods for ODEs: Introduction

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Introduction

- History of ODEs:
  - Leibniz, Newton: foundation of infinitesimal calculus.
  - Bernouilli dynasty:
    - Swiss family of scholars who made many contributions to ODEs.
    - Discovery of practically all known elementary methods for solving ODEs of the first-order.
  - Euler: reduction of a particular class of second-order ODEs to that of the first-order.
  - Lagrange, d'Alembert: problem of linear equations with constant coefficients.
  - Study of Bessel's functions, Laguerre, Legendre, and Hermite polynomials that are solutions to ODEs $\rightarrow$ modern numerical analysis.

Introduction

- Solve physical problems: mathematical models involving an equation in which a function and its derivatives play important roles.
- Theoretical developments of ODEs $\rightarrow$ independent discipline with the solution of such equations an end in itself:
  - Mathematical properties of solutions: existence, uniqueness, regularity, long-time behavior, ...
  - Numerical solutions: numerical schemes and their convergence, stability, and accuracy properties.

Introduction

- Interdisciplinary nature of ODEs: Applications physics, chemistry, biology, economy, social sciences, data sciences, ...
  - Modeling of tumor growth and treatment:
    - α and β: fraction of dividing and dying cells each time interval dt;
    - Difference in (number of cells)$/dt = \alpha$ (number of cells) - β (number of cells).
    - K: carrying capacity constraints;
    - Difference in (number of cells)$/dt = (\alpha - \beta)$ (number of cells) (1 - (number of cells)$/K$).
    - Treatment: Difference in (number of cells)$/dt = (\alpha - \beta)$ (number of cells) (1 - (number of cells)$/K$) $-\xi$ (number of cells).
    - ξ: strength of the tumor cell kill.

Introduction

- Modeling gene expression:
  - Variables: r: mRNA concentrations; p: protein concentrations;
  - Parameters: $f(p)$: transcription functions; L: translational constants; V: degradation rates of mRNAs; U: degradation rates of proteins.
  - Model:

$$\frac{dr}{dt} = f(p) - Vr, \quad \frac{dp}{dt} = Lr - Up.$$

Introduction

- Modeling crowd motion:
  - Variable: V_i: velocity of the ith pedestrian;
  - Parameters: v_i^0: desired velocity in direction e_i^0; τ_i: characteristic time; m_i: mass of the ith pedestrian; f_{ij}: interaction forces.
  - Model:

$$\frac{dV_i}{dt} = \frac{v_i^0 e_i^0 - V_i}{\tau_i} + \frac{1}{m_i} \sum_{j \neq i} f_{ij}.$$

Introduction

- Data sciences:
  - Functional inputs/ functional outputs.
  - System dynamics: modeling how the output changes in response to changes in input.
  - Noisy discrete data not necessary sampled at equally spaced times $\rightarrow$ system of differential equations that describes the data.
  - Learn the dynamics from data.

Introduction

- Hamiltonian systems:
  - Dynamical systems.
  - Evolution of physical systems.
- History of Hamiltonian systems:
  - Hamiltonian mechanics: born out of optics.
  - Theory for studying the propagation of the phase in optical systems guided by Fermat's principle for light rays (i.e. high frequency systems).
  - Similarity of Fermat's principle with the action principle $\rightarrow$ one could adapt the machinery to mechanics.
  - Hamilton, Poincaré, ...

Introduction

- Applications of Hamiltonian systems:
  - Hamiltonian methods: central topic in dynamics and mechanics.
  - Many interesting models appear as a limit of mechanical systems of many small particles (e.g. water waves, fluid mechanics, the equations of plasma physics);
  - Hamiltonian setting: essential for studying these types of models.
  - Practical scientists: appreciate the magic cancellations in the Hamiltonian setting $\rightarrow$ efficient calculations.
  - Interdisciplinary nature of Hamiltonian systems.
  - Applications in physics, space mechanics, and theoretical chemistry.

Introduction

- Pharmaceutical drug design:
  - Variables: q: $3D$ atomic positions; p: momenta;
  - Parameters: M: mass matrix; V: potential function;
  - Model:

$$\begin{cases} \dfrac{\mathrm{d}p}{\mathrm{d}t} = -\dfrac{\partial H}{\partial q}(p, q), \\ \dfrac{\mathrm{d}q}{\mathrm{d}t} = \dfrac{\partial H}{\partial p}(p, q). \end{cases}$$

  - Hamiltonian function:

$$H(p, q) = \frac{1}{2} p^T M^{-1} p + V(q).$$

subscript T: transpose.

Introduction

- Hamiltonian systems:
  - Geometrical aspects play an important role.
  - Construction of numerical methods that respect the geometry of the problem.
  - Benefits from using structure-preserving algorithms.

Introduction

- Plan:
  - Part I: Some basics;
  - Part II: Mathematical properties of solutions: existence, uniqueness, regularity.
  - Part III: Linear systems of ODEs.
  - Part IV: Numerical solutions of ODEs.
  - Part V: Geometrical integration of Hamiltonian systems.
  - Part VI: Finite difference methods.

Introduction

- Some information:
  - Webpage:
    http://www.sam.math.ethz.ch/~grsam/FS18/NAII/index.html
  - Lecture notes.
  - Assignment sheets.
  - Mid-term exams: one hour; bonus; March 26 and May 28th.
  - Last year exams.