Numerical Methods for Differential Equations

Course objectives and preliminaries

Tony Stillfjord, Gustaf Söderlind

Numerical Analysis, Lund University

Contents

1. Course structure and objectives *Learning by doing*

Main objectives

- Learn basic *scientific computing* for solving differential equations
- Understand *mathematics–numerics interaction*, and how to match numerical method to mathematical properties
- Understand *correspondence* between principles in physics and mathematical equations
- Construct and use *elementary* MATLAB*/Python programs* for differential equations

A motto

The computer is to mathematics what the telescope is to astronomy, and the microscope is to biology

– Peter D Lax

The operators we will deal with

Initial value problems

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{t}}$$

The operators we will deal with

Boundary value problems

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} \qquad \frac{\mathrm{d}}{\mathrm{d}x}$$

Partial differential operators

Parabolic

$$\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}$$

Hyperbolic

$$\frac{\partial}{\partial t} - \frac{\partial}{\partial x}$$

Course topics

- **IVP** *Initial value problems* first-order equations; higher-order equations; systems of differential equations
- **BVP** *Boundary value problems* two-point boundary value problems; Sturm–Liouville eigenvalue problems
- **PDE** *Partial differential equations* diffusion equation; advection equation; convection–diffusion; wave equation
- **Applications** in all three areas

A first-order equation without elementary analytical solution

$$\frac{\mathrm{d}y}{\mathrm{d}t} = y - \mathrm{e}^{-t^2}, \qquad y(0) = y_0$$

A second-order equation Motion of a pendulum

$$\ddot{\theta} + \frac{g}{L}\sin\theta = 0, \qquad \theta(0) = \theta_0, \quad \dot{\theta}(0) = \dot{\theta}_0$$

A system of equations Predator–prey model

$$\begin{aligned} \dot{y}_1 &= k_1\, y_1 - k_2\, y_1\, y_2 \\ \dot{y}_2 &= k_3\, y_1\, y_2 - k_4\, y_2 \end{aligned}$$

where y_1 is the prey population and y_2 is the predator species

Second-order two-point BVP Electrostatic potential u between concentric metal spheres

$$\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}u}{\mathrm{d}r} = 0, \qquad u(R_1) = V_1, \quad u(R_2) = 0$$

at distance r from the center

A Sturm–Liouville eigenvalue problem Euler buckling of a slender column

$$y'' = \lambda y, \qquad y'(0) = 0, \quad y(1) = 0$$

Find eigenvalues λ and eigenfunctions y

Some application areas in ODEs

Initial value problems

- mechanics $M\ddot{q} = F(q)$
- electrical circuits $C\dot{v} = -I(v)$
- chemical reactions $\dot{c} = f(c)$

Boundary value problems

- materials $u'' = M/EI$
- microphysics $-\frac{\hbar}{2m}\psi'' = E\psi$
- eigenmodes $-u'' = \lambda u$

The Poisson Equation

$$u_{xx} + u_{yy} = f(x, y)$$

subject to

$$u(x, y) = g(x, y)$$

on the boundary $x = 0 \vee x = 1$, and $y = 0 \vee y = 1$ is an *elliptic PDE* modelling e.g. the displacement u of an elastic membrane under load f

The Diffusion Equation

$$u_t = u_{xx} + f(x)$$

subject to

$$\begin{aligned} &u(x,0) = g(x), \qquad x \in [0, L] \\ &u(0,t) = c_1, \quad u(L,t) = c_2, \qquad t \in [0, T] \end{aligned}$$

is a *parabolic PDE* modelling e.g. temperature u as a funtion of time, in a rod with temperature c_1 and c_2 at its ends, with initial temperature distribution $g(x)$ and source term $f(x)$

The Wave Equation

$$u_{tt} = u_{xx}$$

subject to

$$\begin{aligned} u(x,0) = g(x), \qquad & x \in [0, L] \\ u(0,t) = 0, \quad u(L,t) = 0, \qquad & t \in [0, T] \end{aligned}$$

is a *hyperbolic PDE* modelling e.g. the displacement u of a vibrating elastic string fixed at $x = 0$ and $x = a$

2. What is Numerical Analysis?

Categories of mathematical problems

Category	Algebra	Analysis
linear	*computable*	*not computable*
nonlinear	*not computable*	*not computable*

Algebra Only finite constructs

Analysis Limits, derivatives, integrals etc. (transfinite)

Computable *Exact solution obtained with finite computation*

What is Numerical Analysis?

Categories of mathematical problems

Category	**Algebra**	**Analysis**
linear	*computable*	*not computable*
nonlinear	*not computable*	*not computable*

Problems from all four categories can be solved numerically:

Numerical analysis aims to construct and analyze quantitative methods for the automatic computation of approximate solutions to mathematical problems

Goal Construction of mathematical software

3. The four principles of numerical analysis

There are four basic principles in numerical analysis. Every computational method is constructed from these principles

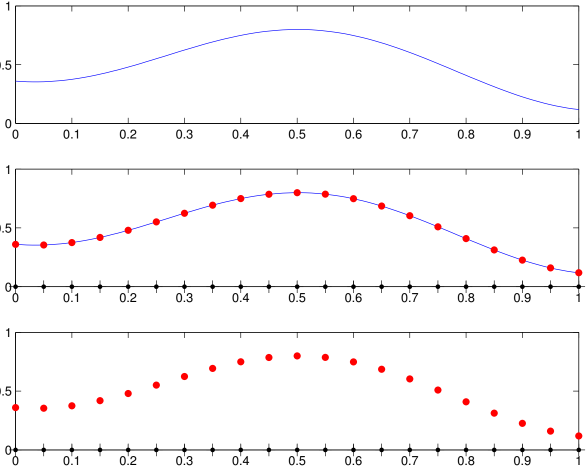
- **Discretization**
  To replace a continuous problem by a discrete one

- **Linear algebra** tools, including polynomials
  All techniques that are computable

- **Linearization**
  To approximate a nonlinear problem by a linear one

- **Iteration**
  To apply a computation repeatedly (until convergence)

Discretization



A continuous function is sampled at discrete points

Discretization ...

Reduces the amount of information to a finite set

Select a subset $\Omega_N = \{x_0, x_1, \ldots, x_N\}$ of distinct points from the interval $\Omega = [0, 1]$

Continuous function $f(x)$ is replaced by vector $F = \{f(x_k)\}_0^N$

The subset Ω_N is called *the grid*

The vector F is called a *grid function* or discrete function

Discretization yields a *computable problem*. Approximations are computed only at a finite set of grid points

Definition of derivative

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

Take $\Delta x = x_{k+1} - x_k$ finite and *approximate*

$$f'(x_k) \approx \frac{f(x_k + \Delta x) - f(x_k)}{\Delta x} = \frac{F_{k+1} - F_k}{x_{k+1} - x_k}$$

How accurate is this approximation?

Error and accuracy

Expand in Taylor series

$$\frac{f(x_k + \Delta x) - f(x_k)}{\Delta x} \approx \frac{f(x_k) + \Delta x\, f'(x_k) + \mathcal{O}(\Delta x^2) - f(x_k)}{\Delta x}$$

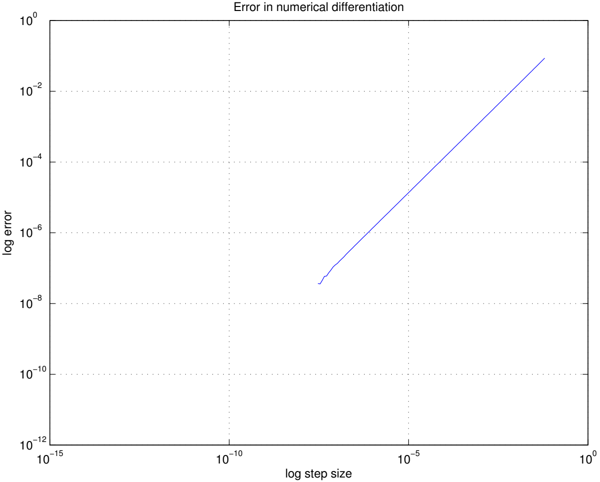
$$= f'(x_k) + \mathcal{O}(\Delta x)$$

The error is proportional to Δx

Try this formula for $f(x) = \mathrm{e}^x$ at $x_k = 1$ for various Δx

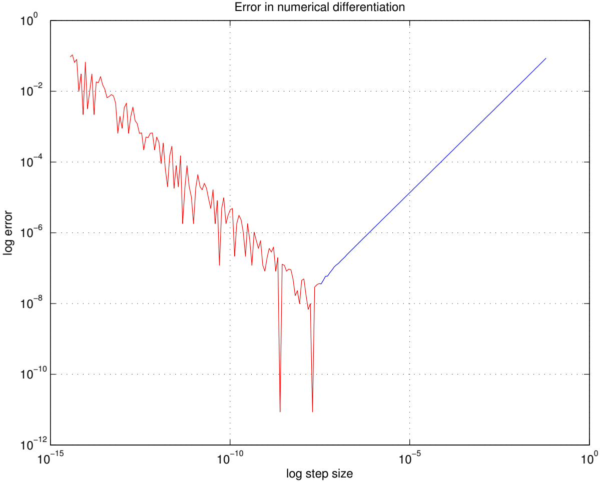
Numerical differentiation

Error in numerically calculated derivative of e^x at $x = 1$



Loglog plot of error vs. step size Δx

Error in numerically calculated derivative of e^x at $x = 1$



Loglog plot of error vs. step size Δx

$$\frac{f(x_k+\Delta x)-f(x_k-\Delta x)}{2\Delta x} = \frac{F_{k+1}-F_{k-1}}{x_{k+1}-x_{k-1}} = f'(x_k) + \mathcal{O}(\Delta x^2)$$

The approximation is *2nd order accurate* because error is Δx^2

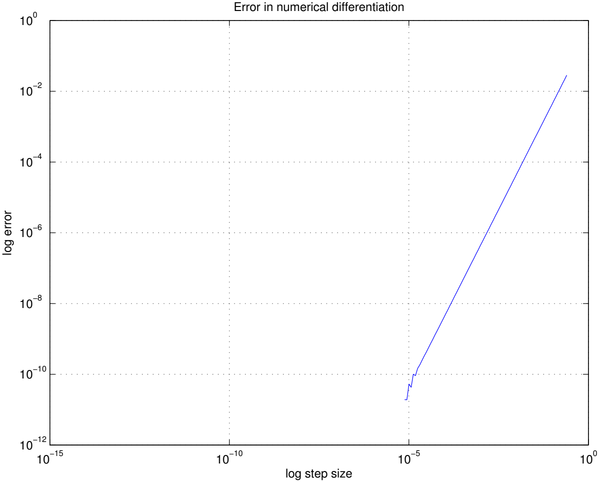
Whenever you have a power law, plot in log-log diagram

$$\text{err} \approx C \cdot \Delta x^p \quad \Rightarrow \quad \log \text{err} \approx \log C + p \log \Delta x$$

This is a *straight line of slope p*, easy to identify

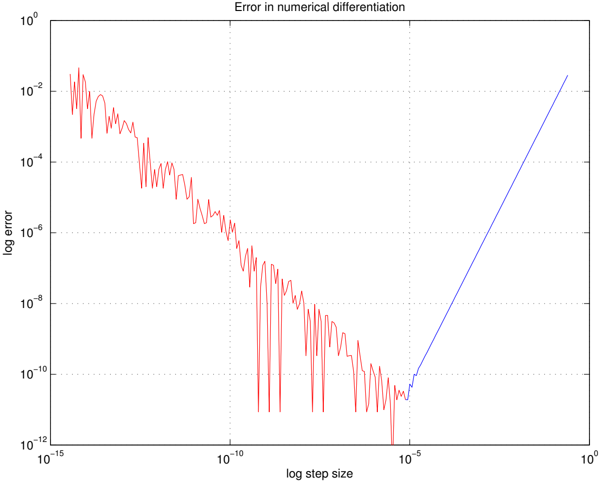
Numerical 2nd order differentiation

Error in numerically calculated derivative of e^x at $x = 1$



Loglog plot of error vs. step size Δx

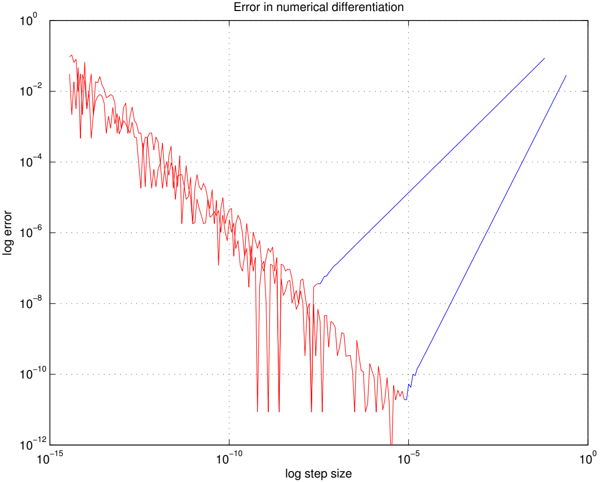
Error in numerically calculated derivative of e^x at $x = 1$



Loglog plot of error vs. step size Δx

1st and 2nd order comparison

Error in numerically calculated derivative of e^{x} at $x = 1$



2nd order approximation has much higher accuracy!

Discretization of a differential equation

Problem Solve $\dot{y} = qy$ numerically on $[0, T]$, with $y(0) = y_0$

The *analytical solution is a function* $y(t) = y_0 \mathrm{e}^{qt}$

The *numerical solution is a vector* $y = \{y_k\}_{k=0}^{N}$ with $y_k \approx y(t_k)$, where $t_k = kT/N$

Method Approximate derivative by difference quotient, using step size

$$\Delta t = t_{k+1} - t_k = T/N$$

Discretization of a differential equation ...

Discretization method Approximate derivative by finite difference quotient

$$\frac{y_{k+1} - y_k}{t_{k+1} - t_k} \approx \dot{y}(t_k)$$

to get the linear algebraic equation system ($k = 0, 1, \ldots, N$)

$$\frac{y_{k+1} - y_k}{t_{k+1} - t_k} = q y_k$$

or

$$y_{k+1} = \left(1 + \frac{qT}{N}\right) y_k \quad \Rightarrow \quad y_N = \left(1 + \frac{qT}{N}\right)^N y_0$$

Discretization of a differential equation . . .

Note The numerical approximation at time T is

$$y_N = \left(1 + \frac{qT}{N}\right)^N y_0$$

But

$$\lim_{N\to\infty} \left(1 + \frac{qT}{N}\right)^N = \mathrm{e}^{qT}$$

The numerical approximation *converges* to the exact solution as $N \to \infty$

Main course objective

The course centers on *discretization methods* for differential equations of all types

We will also encounter the other three principles of numerical analysis as we go

- linear algebra methods and polynomial techniques
- linearization
- and iterative methods