Scientific Computing I

Module 4: Numerical Methods for ODE

Michael Bader

Lehrstuhl Informatik V

Winter 2005/2006

Part I

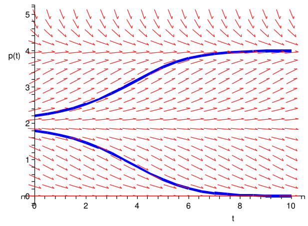
Basic Numerical Methods

Motivation: Direction Fields

- given: initial value problem:

$$\dot{y}(t) = f(t, y(t)), \qquad y(t_0) = y_0$$

- easily computable: direction field



- idea: "follow the arrows"

"Following the Arrows"

- direction field illustrates slope for given time t_n and value y_n:

$$\dot{y}_n = f(t_n, y_n)$$

- "follow arrows" = make a small step in the given direction:

$$y_{n+1} := y_n + \tau \dot{y}_n = y_n + \tau f(t_n, y_n)$$

- motivates numerical scheme:

$$\begin{aligned} y_0 &:= y_0 \\ y_{n+1} &:= y_n + \tau f(t_n, y_n) \qquad \text{for } n = 0, 1, 2, \ldots \end{aligned}$$

Euler's Method

- numerical scheme is called **Euler's method**:

$$y_{n+1} := y_n + \tau f(t_n, y_n)$$

- results from **finite difference** approximation:

$$\frac{y_{n+1} - y_n}{\tau} \approx \dot{y}_n = f(t_n, y_n)$$

(difference quotient instead of derivative)

- or from truncation of Taylor expansion:

$$y(t_{n+1}) = y(t_n) + \tau \dot{y}(t_n) + \mathcal{O}(\tau^2)$$

Euler's Method – 1D examples

- model of Maltus, $\dot{p}(t) = \alpha p(t)$:

$$p_{n+1} := p_n + \tau \alpha p_n$$

- Logistic Growth, $\dot{p}(t) = \alpha (1 - p(t)/\beta) p(t)$:

$$p_{n+1} := p_n + \tau \alpha \left(1 - \frac{p_n}{\beta}\right) p_n$$

- Logistic growth with threshold:

$$p_{n+1} := p_n + \tau \alpha \left(1 - \frac{p_n}{\beta}\right) \left(1 - \frac{p_n}{\delta}\right) p_n$$

Euler's Method in 2D

- Euler's method is easily extend to systems of ODE:

$$\mathbf{y}_{n+1} := \mathbf{y}_n + \tau f(t_n, \mathbf{y}_n)$$

- example: nonlinear extinction model

$$\begin{aligned} \dot{p}(t) &= \left(\tfrac{71}{8} - \tfrac{23}{12}p(t) - \tfrac{25}{12}q(t)\right)p(t) \\ \dot{q}(t) &= \left(\tfrac{73}{8} - \tfrac{25}{12}p(t) - \tfrac{23}{12}q(t)\right)q(t) \end{aligned}$$

- Euler's method:

$$\begin{aligned} \dot{p}(t) &= p_n + \tau\left(\tfrac{71}{8} - \tfrac{23}{12}p_n - \tfrac{25}{12}q_n\right)p_n \\ \dot{q}(t) &= q_n + \tau\left(\tfrac{73}{8} - \tfrac{25}{12}p_n - \tfrac{23}{12}q_n\right)q_n \end{aligned}$$

Discretized Model vs. Discrete Model

- simplest example: model of Maltus

$$p_{n+1} := p_n - \tau\alpha p_n, \qquad \alpha > 0$$

- compare to discrete model:

$$p_{n+1} := p_n - \delta p_n, \qquad \delta > 0$$

  with decay rate δ ("percentage")
- obvious restriction in the discrete model: $\delta < 1$
- obvious restriction for τ in the discretized model?

$$\tau\alpha < 1 \Rightarrow \tau < \alpha^{-1}$$

- not that simple in non-linear models or systems of ODE!

Implicit Euler

- Euler's method ("explicit Euler"):

$$y_{n+1} := y_n + \tau f(t_n, y_n)$$

- implicit Euler:

$$y_{n+1} := y_n + \tau f(t_{n+1}, y_{n+1})$$

- explicit formula for y_{n+1} not immediately available
- to do: solve equation for y_{n+1}

Implicit Euler – Examples

- example: Model of Maltus

$$p_{n+1} := p_n + \tau\alpha p_{n+1} \Rightarrow p_{n+1} = \frac{1}{1-\tau\alpha}p_n$$

- correct (discrete) model?

$$\begin{aligned} &\alpha < 0: \quad \text{then} \quad 0 < (1-\tau\alpha)^{-1} < 1 \text{ for any } \tau \\ &\alpha > 0: \quad \text{then} \quad \tau < \alpha^{-1} \text{ required!} \end{aligned}$$

- in physics $\alpha < 0$ is more frequent! (damped systems, friction, ...)
- implicit schemes preferred when explicit schemes require very small τ

Implicit Euler – 2D Example

- example: arms race

$$\begin{aligned} p_{n+1} &= b_1 + a_{11}p_{n+1} + a_{12}q_{n+1} \\ q_{n+1} &= b_2 + a_{21}p_{n+1} + a_{22}q_{n+1}) \end{aligned}$$

- solve linear system of equations:

$$\begin{aligned} (1-a_{11})p_{n+1} - a_{12}q_{n+1} &= b_1 \\ -a_{21}p_{n+1} + (1-a_{22})q_{n+1} &= b_2 \end{aligned}$$

  (for each time step n)

Local Discretisation Error

- local influence of using differences instead of derivatives
- example: Euler's method

$$l(\tau) = \max_{[a,b]}\left\{\left\|\frac{y_{t+\tau} - y(t)}{\tau} - f(t, y(t))\right\|\right\}$$

- memory hook: insert exact solution $y(t)$ into

$$\frac{y_{n+1} - y_n}{\tau} - \dot{y}_n$$

A numerical scheme is called **consistent**, if

$$l(\tau) \to 0 \qquad \text{for } \tau \to 0$$

Global Discretisation Error

- compare numerical solution with exact solution
- example: Euler's method

$$e(\tau) = \max_{[a,b]} \{\|y_k - y(t_k)\|\}$$

($y(t)$ the exact solution; y_k the solution of the discretized equation)

A numerical scheme is called **convergent**, if

$$e(\tau) \to 0 \qquad \text{for } \tau \to 0$$

Order of Consistency/Convergence

A numerical scheme is called **consistent** of order p (p-th order consistent), if

$$l(\tau) = \mathcal{O}(\tau^p)$$

A numerical scheme is called **convergent** of order p (p-th order convergent), if

$$e(\tau) = \mathcal{O}(\tau^p)$$

Part II

Advanced Numerical Methods

Runge-Kutta-Methods

- 1st idea: use additional evaluations of f, e.g.:

$$y_{n+1} = g(y_n, f(t_n, y_n), f(t_{n+1}, y_{n+1}))$$

  open question: where to obtain y_{n+1}), how to choose g
- 2nd idea: numerical approximations for missing values of y:

$$\begin{aligned} y_{n+1} &\approx y_n + \tau f(t_n, y_n) \\ \Rightarrow y_{n+1} &= g\big(y_n, f(t_n, y_n), f(t_{n+1}, y_n + \tau f(t_n, y_n))\big) \end{aligned}$$

Runge-Kutta-Methods of 2nd order

- 3rd idea: choose g such that order of consistency is maximal
- example: 2nd-order Runge-Kutta:

$$y_{n+1} = y_n + \frac{\tau}{2}\left(f(t_n, y_n) + f(t_{n+1}, y_n + \tau f(t_n, y_n))\right)$$

  ("method of Heun")
- further example: modified Euler (also 2nd order)

$$y_{n+1} = y_n + \tau f\left(t_n + \frac{\tau}{2}, y_n + \frac{\tau}{2} f(t_n, y_n)\right)$$

Runge-Kutta-Method of 4th order

classical 4th-order Runge-Kutta:

- intermediate steps:

$$\begin{aligned} k_1 &= f(t_n, y_n) \\ k_2 &= f\left(t_n + \frac{\tau}{2}, y_n + \frac{\tau}{2} k_1\right) \\ k_3 &= f\left(t_n + \frac{\tau}{2}, y_n + \frac{\tau}{2} k_2\right) \\ k_3 &= f(t_n + \tau, y_n + \tau k_3) \end{aligned}$$

- explicit scheme:

$$y_{n+1} = y_n + \frac{\tau}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Multistep Methods

- 1st idea: use previous steps for computation:

$$y_{n+1} = g(y_n, y_{n-1}, \dots, y_{n-q+1})$$

- 2nd idea: use integral form of ODE

$$\begin{aligned} \dot{y}(t) &= f(t, y(t)) \\ \int_{t_n}^{t_{n+1}} \dot{y}(t)dt &= \int_{t_n}^{t_{n+1}} f(t, y(t))dt \\ y(t_{n+1}) - y(t_n) &= \int_{t_n}^{t_{n+1}} f(t, y(t))dt = ? \end{aligned}$$

Multistep and Numerical Quadrature

- 3rd idea: use numerical method for integration
  $\rightarrow$ interpolate f using a polynomial p:

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} f(t, y(t))dt \approx \int_{t_n}^{t_{n+1}} p(t)dt$$

  where

$$p(t_j) = f(t_j, y(t_j)) \qquad \text{for } j = n-s+1, \dots, n.$$

- compute integral and obtain quadrature rule:

$$y_{n+1} = y_n + \sum_{j=n-s+1}^{n} \alpha_j f(t_j, y_j)$$

Adams-Bashforth

- $s = 1 \Rightarrow$ use y_n only (leads to Euler's method):

$$p(t) = f(t_n, y_n), \qquad y_{n+1} = y_n + \tau f(t_n, y_n)$$

- $s = 2 \Rightarrow$ use y_{n-1} and y_n:

$$\begin{aligned} p(t) &= \frac{t_n - t}{\tau} f(t_{n-1}, y_{n-1}) + \frac{t - t_{n-1}}{\tau} f(t_n, y_n), \\ y_{n+1} &= y_n + \frac{\tau}{2}(3f(t_n, y_n) - f(t_{n-1}, y_{n-1})) \end{aligned}$$

- usually consistent of s-th order
- modified at start (no previous values available)

Adams-Moulton

- use idea of Adams-Bashforth, but:
  include value $y_{n+1} \Rightarrow$ **implicit scheme**
- first order: implicit Euler

$$p(t) = f(t_{n+1}, y_{n+1}), \qquad y_{n+1} = y_n + \tau f(t_{n+1}, y_{n+1})$$

- second order:

$$y_{n+1} = y_n + \frac{\tau}{2}(f(t_n, y_n) + f(t_{n+1}, y_{n+1}))$$

- how to obtain y_{k+1}?
  - solve (nonlinear) equation $\Rightarrow$ difficult!
  - easier and more common: *predictor-corrector* approach

Problems for Numerical Methods for ODE

Possible problems:

- **Ill-Conditioned Problems:**
  small changes in the input $\Rightarrow$ big changes in the exact solution of the ODE
- **Instability:**
  big errors in the numerical solution compared to the exact solution (for arbitrarily small time steps although the method is consistent)
- **Stiffness:**
  small time steps required for acceptable errors in the approximate solution (although the exact solution is smooth)

Ill-Conditioned Problems

- small changes in input entail completely different results
- Numerical treatment of such problems is always difficult!
- discriminate:
  - only at critical points?
  - everywhere?
- possible risks:
  - non-precise input
  - round-off errors,...
- question: what are you interested in?
  - really the solution for specific initial condition?
  - statistical info on the solution?
  - general behaviour (patterns)?

Stability

Example:

$$\dot{y}(t) = -2y(t) + 1, \qquad y(0) = 1$$

- exact solution: $y(t) = \frac{1}{2}(e^{-2t} + 1)$
- well-conditioned: $y_\varepsilon(0) = 1 + \varepsilon \Rightarrow y_\varepsilon(t) - y(t) = \varepsilon e^{-2t}$
- use **midpoint** rule (multistep scheme):

$$y_{n+1} = y_{n-1} + 2\tau \cdot f(x_n, y_n)$$

- leads to numerical scheme:

$$y_{n+1} = y_{n-1} + 2\tau(1 - 2y_n)$$

Stability (2)

Observation:

- 2-step rule:

$$y_{n+1} = y_{n-1} + 2\tau(1 - 2y_n)$$

  start with exact initial values: $y_0 = y(0)$ and $y_1 = y(\tau)$
- numerical results for different sizes of τ:
  - $\tau = 1.0 \Rightarrow y_9 = -4945.5,\ y_{10} = 20953.9$
  - $\tau = 0.1 \Rightarrow y_{79} = -1725.3,\ y_{80} = 2105.7$
  - $\tau = 0.01 \Rightarrow y_{999} = -154.6,\ y_{1000} = 158.7$
- midpoint rule is 2nd-order consistent, but does not converge here: oscillations or instable behaviour

Stability (3)

- reason: difference equation generates spurious solutions
- analysis: roots μ_i of characteristic polynomial $y^2 = y^0 + 4\tau(1 - y)$; all $|\mu_i| < 1$?

Stability of ODE schemes:

- single step schemes: always stable
- multistep schemes: additional stability conditions
- in general:
  consistency + stability = convergence

Stiff Equations

Example:

$$\dot{y}(t) = -1000y(t) + 1000, \qquad y(0) = y_0 = 2$$

- exact solution: $y(t) = e^{-1000t} + 1$
- explicit Euler (stable):

$$\begin{aligned} y_{k+1} &= y_k + \tau(-1000y_k + 1000) \\ &= (1 - 1000\tau)y_k + 1000\tau \\ &= (1 - 1000\tau)^{k+1} + 1 \end{aligned}$$

- oscillations and divergence for $\delta t > 0.002$
- Why that? Consistency and stability are **asymptotic** terms!

Stiff Equations – Summary

Typical situation:

- one term in the ODE demands very small time step
- but does not contribute much to the solution

Remedy: use implicit (or semi-implicit) methods

Summary

Runge-Kutta-methods:

- multiple evaluations of f (expensive, if f is expensive to compute)
- stable, well-behaved, easy to implement

Multistep methods:

- higher order, but only evaluations of f (interesting, if f is expensive to compute)
- stability problems; behave “like wild horses”
- in practice: do not use uniform τ and s

Implicit methods:

- for stiff equations
- most often used as corrector scheme