Scientific Computing I

Module 4: Numerical Methods for ODE

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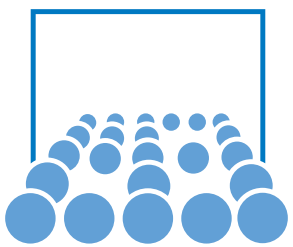


Part I: Basic Numerical Methods

Motivation: Direction Fields

Euler's Method

Discretized Model vs. Discrete Model

Implicit Euler

Analysis of Numerical Schemes for ODE

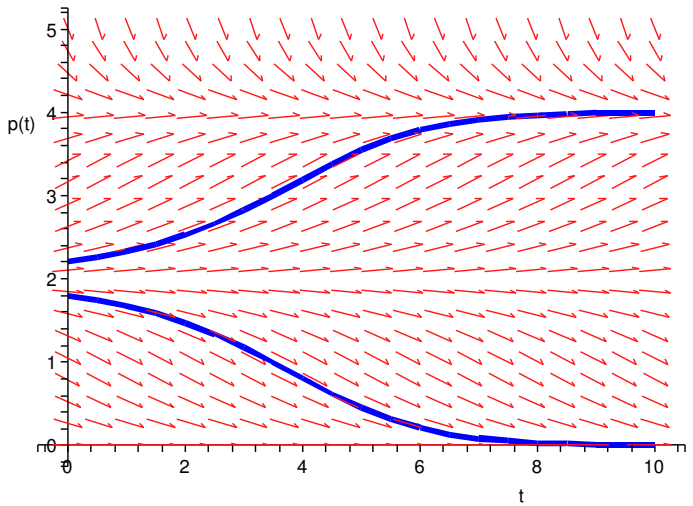
- Local Discretisation Error
- Global Discretisation Error
- Order of Consistency/Convergence

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**:

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

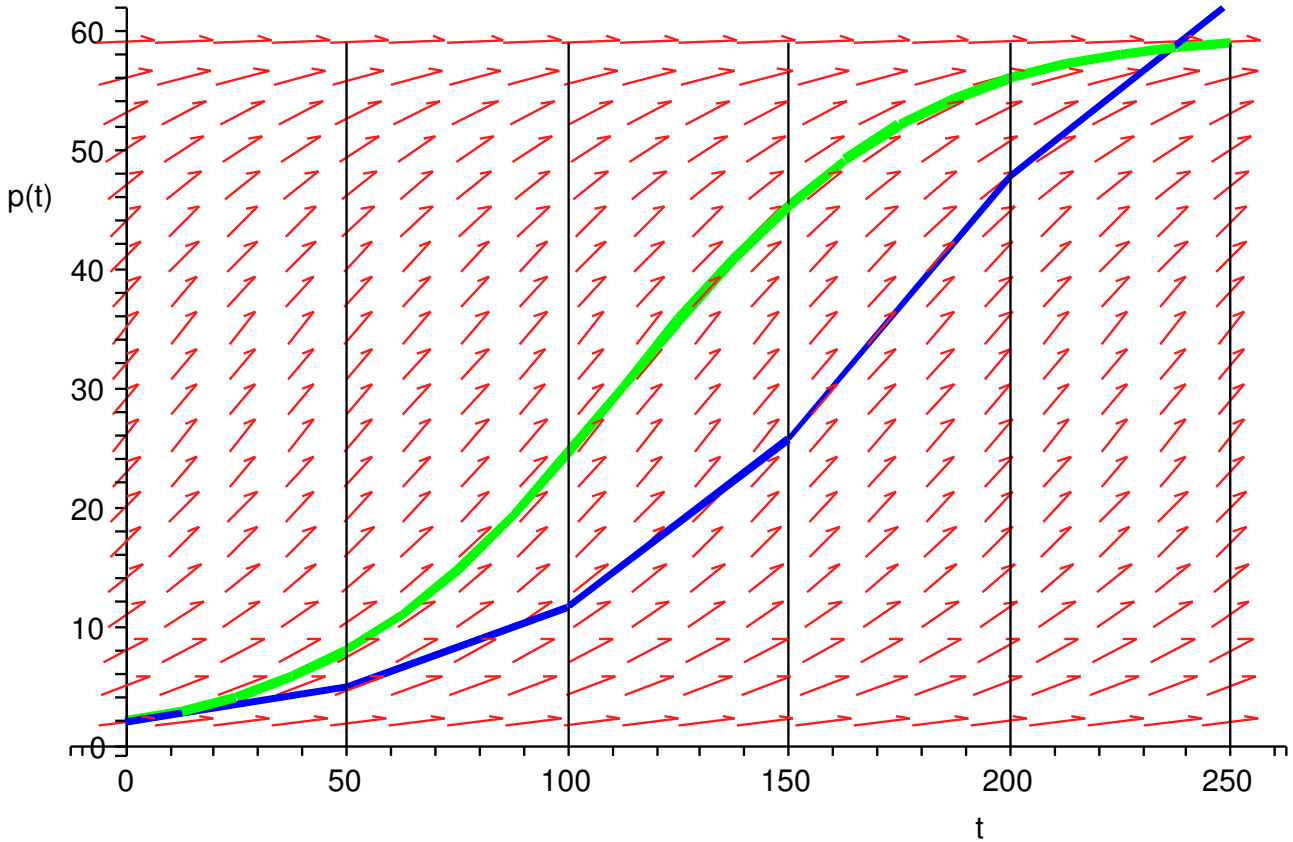
- results from **finite difference** approximation:

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

  (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 and Direction Fields



use direction at the **beginning** of the timestep

Euler's Method – 1D examples

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

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

- 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 extended to systems of ODE $\rightarrow$ use vector notation:

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

- 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:

$$\begin{aligned} p_{n+1} &= p_n + \tau \left(\tfrac{71}{8} - \tfrac{23}{12}p_n - \tfrac{25}{12}q_n\right) p_n \\ q_{n+1} &= q_n + \tau \left(\tfrac{73}{8} - \tfrac{25}{12}p_n - \tfrac{23}{12}q_n\right) q_n \end{aligned}$$

Discretized Model vs. Discrete Model

- example: model of Malthus/radioactive decay ($\dot{p} = -\alpha p$):

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

- 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:

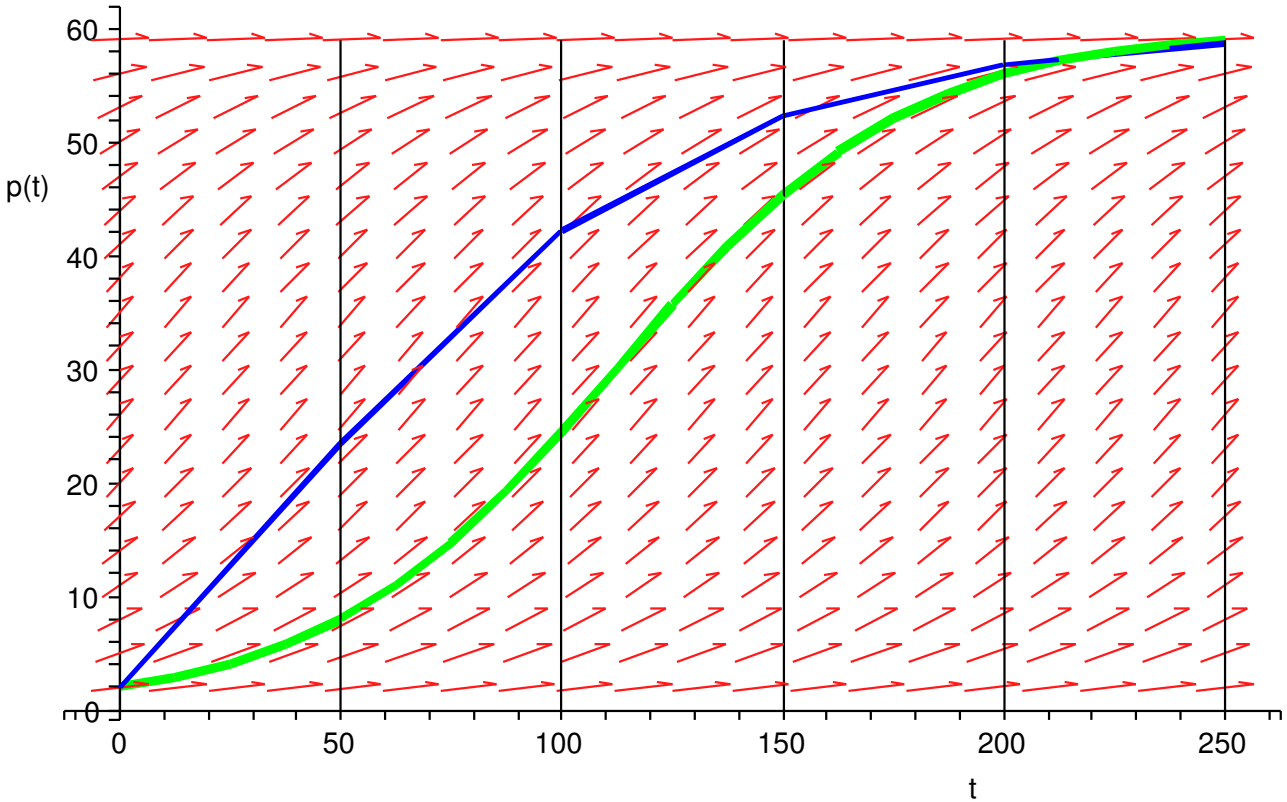
$$y_{n+1} := y_n + \tau f(t_{n+1}, y_{n+1})$$

- results from **finite difference** approximation:

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

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

Implicit Euler and Direction Fields



use direction at **end** of the timestep

Implicit Euler – Examples

- example: Model of Malthus/radioactive decay

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

- 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

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

- solve linear system of equations:

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

  (for each time step $n \to n+1$)
- in vector notation: $(I - \tau A)\mathbf{y}_{n+1} = \mathbf{y}_n + \tau\mathbf{b}$

Local Discretisation Error

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

$$l(\tau) = \max_{[a,b]} \left\{ \left\| \frac{y(t+\tau) - y(t)}{\tau} - f(t, y(t)) \right\| \right\} = \frac{\tau}{2} ||\ddot{y}_n|| + O(\tau^2)$$

- 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

$$e(\tau) = \max_{k=0,\ldots,k_{max}} \{\|y_k - y(t_k)\|\}$$

$y(t)$ exact solution;
y_k solution of the discretized equations (depends on τ)

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

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

Global Discretisation Error – Explicit Euler

$$
\begin{aligned}
e_n &= y_n - y(t_n), \\
y_{n+1} &= y_n + \tau f(t_n, y_n), \\
y(t_{n+1}) &= y(t_n) + \tau f(t_n, y(t_n)) + \tau^2 \frac{\ddot{y}(t_n)}{2} + O(\tau^3), \\
\Rightarrow |e_{n+1}| &\overset{\cdot}{\leq} |e_n| + \tau M |e_n| + N\tau^2 \\
&= (1 + M\tau)|e_n| + N\tau^2 \\
&\leq (1 + \tau M)^2 |e_{n-1}| + (1 + \tau M) N\tau^2 + N\tau^2 \\
&\leq \ldots \leq e^{n\tau M} \underbrace{|e_0|}_{=0} + N\tau^2 \frac{e^{n\tau M} - 1}{\tau M} \\
&= N\tau \frac{e^{n\tau M} - 1}{M} = O(\tau).
\end{aligned}
$$

Order of Consistency/Convergence

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

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

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

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

We have shown that the explicit Euler method is consistent and convergent of order 1.

For more complicated ODE or numerical schemes
$\rightarrow$ see lecture(s) in Numerical Programming

Part II: Advanced Numerical Methods

Runge-Kutta-Methods

- 2nd-order Runge-Kutta
- 4th-order Runge-Kutta

Multistep Methods

- Adams-Bashforth
- Adams-Moulton
- Leapfrog Scheme

Problems for Numerical Methods for ODE

- Ill-Conditioned Problems
- Stability
- Stiff Equations
- Summary

Runge-Kutta-Methods

- 1st idea: use additional evaluations of f:

$$y_{n+1} = y_n + \tau \sum_{i=1}^{p} \beta_i f(t_n^i, y_n^i) \text{ with } t_n^i \in [t_n; t_{n+1}]$$

  open questions: Where to obtain $y_n^i, i = 1, \ldots, p$? How to choose $\beta_i, i = 1, \ldots, p$?

- 2nd idea: numerical approximations for missing values of y:

$$y_n^i := y_n + \tau \sum_{j=1}^{p} \alpha_{i,j} f(t_n^j, y_n^j)$$

  explicit Runge-Kutta: $\alpha_{i,j} = 0$ if $j \geq i$.

- 3rd idea: choose β_i and $\alpha_{i,j}$ such that order of consistency is maximal (use quadrature rules)

Runge-Kutta-Methods of 2nd Order

- example: 2nd-order Runge-Kutta (“method of Heun”)

$$\begin{aligned} y_n^{\mathrm{I}} &= y_n, \\ y_n^{\mathrm{II}} &= y_n + \tau f(t_n, y_n^1), \\ y_{n+1} &= y_n + \tau \frac{1}{2}(f(t_n, y_n^{\mathrm{I}}) + f(t_{n+1}, y_n^{\mathrm{II}})). \end{aligned}$$

- interpretation of the steps:
  1. $y_n^{\mathrm{II}} = y_n + \tau f(t_n, y_n^{\mathrm{I}})$
     $\rightarrow$ Euler step to obtain estimate y_n^{II} for solution at time t_{n+1}
  2. $y_{n+1} = y_n + \tau \frac{1}{2}(f(t_n, y_n^{\mathrm{I}}) + f(t_{n+1}, y_n^{\mathrm{II}}))$
     $\rightarrow$ Euler step using an averaged direction
     (averages directions obtained from t_n, y_n^{I} and $t_{n+1}, y_n^{\mathrm{II}}$)
- exercise: draw these steps into direction field!

Runge-Kutta-Methods of 2nd Order (2)

- further example: “modified Euler” (also 2nd order)

$$\begin{aligned} y_n^{\mathrm{I}} &= y_n, \\ y_n^{\mathrm{II}} &= y_n + \frac{\tau}{2} f(t_n, y_n^{\mathrm{I}}), \\ y_{n+1} &= y_n + \tau\, f\left(t_n + \frac{\tau}{2}, y_n^{\mathrm{II}}\right) \end{aligned}$$

- interpretation of the steps:
  1. $y_n^{\mathrm{II}} = y_n + \frac{\tau}{2} f(t_n, y_n^{\mathrm{I}})$
     $\rightarrow$ Euler step with step size $\tau/2$
     to obtain estimate y_n^{II} for solution at time $t_{n+\frac{1}{2}}$
  2. $y_{n+1} = y_n + \tau\, f\left(t_n + \frac{\tau}{2}, y_n^{\mathrm{II}}\right)$
     $\rightarrow$ Euler step using direction obtained from $t_{n+\frac{1}{2}}, y_n^{\mathrm{II}}$
- exercise: draw these steps into direction field!

Runge-Kutta-Method of 4th order

classical 4th-order Runge-Kutta:

- intermediate steps:

$$t_n^{\mathrm{I}} = t_n, \qquad y_n^{\mathrm{I}} = y_n, \tag{1}$$

$$t_n^{\mathrm{II}} = t_n + \frac{\tau}{2}, \qquad y_n^{\mathrm{II}} = y_n + \frac{\tau}{2} f(t_n^{\mathrm{I}}, y_n^{\mathrm{I}}), \tag{2}$$

$$t_n^{\mathrm{III}} = t_n + \frac{\tau}{2}, \qquad y_n^{\mathrm{III}} = y_n + \frac{\tau}{2} f(t_n^{\mathrm{II}}, y_n^{\mathrm{II}}), \tag{3}$$

$$t_n^{\mathrm{IV}} = t_{n+1}, \qquad y_n^{\mathrm{IV}} = y_n + \tau f(t_n^{\mathrm{III}}, y_n^{\mathrm{III}}). \tag{4}$$

- explicit scheme:

$$y_{n+1} = y_n + \frac{\tau}{6}\left(f(t_n^{\mathrm{I}}, y_n^{\mathrm{I}}) + 2f(t_n^{\mathrm{II}}, y_n^{\mathrm{II}}) + 2f(t_n^{\mathrm{III}}, y_n^{\mathrm{III}}) + f(t_n^{\mathrm{IV}}, y_n^{\mathrm{IV}}) \right)$$

- How would you translate this method into efficient pseudo-code? Remember that unnecessary evaluations of f can be very costly!

Pseudo-Code Runge-Kutta-Method of 4th order

```
f[1] = f(t,y[n]);
dt2 = dt/2;
t2 = t + dt2;
f[2] = f(t2, y[n] + dt2*f[1]);
f[3] = f(t2, y[n] + dt2*f[2]);
t = t + dt;
f[4] = f(t, y[n] + dt*f[3]);
y[n+1] = y[n] + dt * (f[1] + 2*f[2] + 2*f[3] + f[4]);
```

Note: each `f[..]` will be a vector (1D array) for systems of ODE

Multistep Methods

- 1st idea: use previous steps for computation:

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

- 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

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

- 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:

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

- 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: Crank-Nicolson method

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

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

Leapfrog Scheme

- formally a multi-step scheme: $y_{n+1} = g(y_n, y_{n-1})$
- derive from symmetric difference quotient:

$$\begin{aligned} \dot{y}(t) &= f(t, y(t)) \\ \frac{y(t+\tau) - y(t-\tau)}{2\tau} &= f(t, y(t)) \end{aligned}$$

- leads to the following time-stepping scheme:

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

- 2nd-order accurate with low computational effort, but tends to be instable

Problems for Numerical Methods for ODE

Short overview on possible problems:

- **Ill-Conditioned Problems:**
  small changes in the input $\Rightarrow$ big changes in the exact solution of the ODE

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- **Instability:**
  big errors in the numerical solution compared to the exact solution (for arbitrarily small time steps although the method is consistent)

Problems for Numerical Methods for ODE

Short overview on 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

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  - only at critical points?
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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: $y_\varepsilon(0) = 1 + \varepsilon \Rightarrow y_\varepsilon(t) - y(t) = \varepsilon e^{-2t}$

Stability

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- 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 few 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