Scientific Computing I

Module 4: Numerical Methods for ODE

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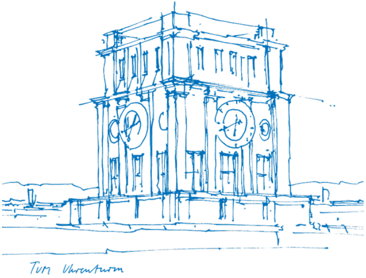


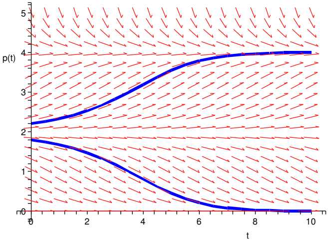
Part I: Basic Numerical Methods

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:

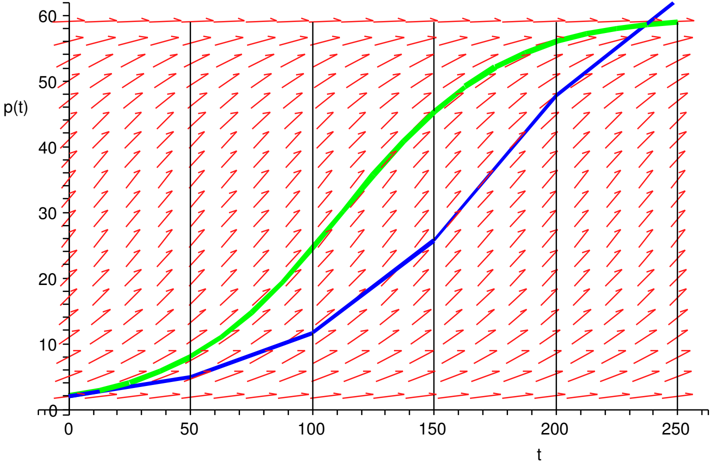
$$\frac{y_{n+1} - y_n}{\tau} \approx \dot{y}_n = f(t_n, y_n)$$

  (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 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:

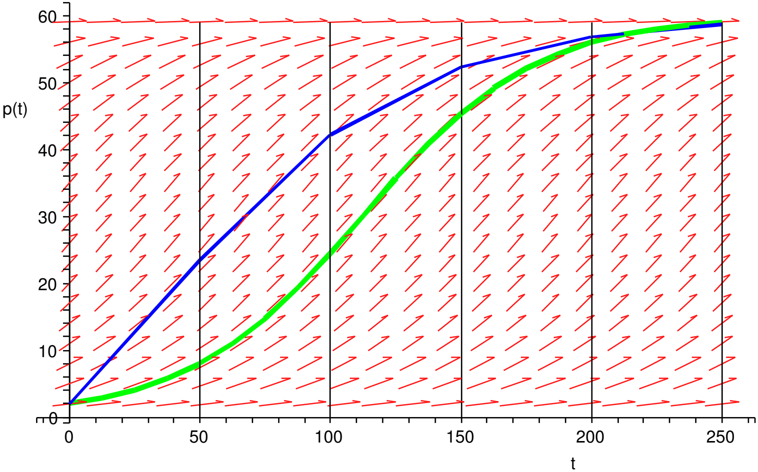
$$y_{n+1} := y_n + \tau f(t_{n+1}, y_{n+1})$$

- 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 often preferred/necessary 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

$$
\begin{aligned}
e_{n+1} &= y_{n+1} - y(t_{n+1}), \\
y_{n+1} &= y_n + \tau f(t_n, y_n), \\
y(t_{n+1}) &= y(t_n) + \tau f(t_n, y(t_n)) + \tau^2 \frac{\ddot{y}(t_n)}{2} + O(\tau^3), \\
\Rightarrow |e_{n+1}| &\dot{\leq} |e_n| + \tau M |e_n| + N\tau^2 \\
&= (1 + M\tau)|e_n| + N\tau^2 \\
&\leq (1 + \tau M)^2 |e_{n-1}| + (1 + \tau M) N\tau^2 + N\tau^2 \\
&\leq \ldots \leq e^{(n+1)\cdot\tau M} \underbrace{|e_0|}_{=0} + N\tau^2 \frac{e^{(n+1)\cdot\tau M} - 1}{\tau M} \\
&= N\tau \frac{e^{(n+1)\cdot\tau M} - 1}{M} = N\tau \frac{e^{(t_{n+1} - t_0)M} - 1}{M} = O(\tau).
\end{aligned}
$$

Order of Consistency/Convergence

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

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

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

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

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
- Explicit Midpoint Rule

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 $y_n^i, i = 1, \dots, p$? How to choose $\beta_i, i = 1, \dots, p$?
- 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”)

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

- 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)

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

- 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. $y_{n+1} = y_n + \tau\, f\big(t_n + \frac{\tau}{2}, y_n^{\mathrm{II}}\big)$
     $\rightarrow$ 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:

$$
\begin{aligned}
t_n^{\mathrm{I}} &= t_n, & y_n^{\mathrm{I}} &= y_n, && (1)\\
t_n^{\mathrm{II}} &= t_n + \frac{\tau}{2}, & y_n^{\mathrm{II}} &= y_n + \frac{\tau}{2} f(t_n^{\mathrm{I}}, y_n^{\mathrm{I}}), && (2)\\
t_n^{\mathrm{III}} &= t_n + \frac{\tau}{2}, & y_n^{\mathrm{III}} &= y_n + \frac{\tau}{2} f(t_n^{\mathrm{II}}, y_n^{\mathrm{II}}), && (3)\\
t_n^{\mathrm{IV}} &= t_{n+1}, & y_n^{\mathrm{IV}} &= y_n + \tau f(t_n^{\mathrm{III}}, y_n^{\mathrm{III}}). && (4)
\end{aligned}
$$

- 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

Runge-Kutta Methods – Butcher Tableau

Generic notation for p-step Runge-Kutta schemes ($i = 1, \ldots, p$):

- use intermediate time steps $t_n^i := t_n + \gamma_i \tau$, with $\gamma_i \in [0, 1]$
- intermediate directions $k^i := f(t_n^i, y_n + \tau \sum_{j=1}^{i-1} \alpha_{ij} k^j)$ with weights α_{ij}
- "final" step $y_{n+1} = y_n + \tau \sum_{i=1}^{p} \beta_i k^i$ with suitable β_i

Leads to "Butcher" tableau of parameters γ_i, β_i and α_{ij}:

$$
\begin{array}{c|cccc}
\gamma_1 & \alpha_{11} & \alpha_{12} & \ldots & \alpha_{1p} \\
\gamma_2 & \alpha_{21} & \alpha_{22} & \ldots & \alpha_{2p} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\gamma_p & \alpha_{p1} & \alpha_{p2} & \ldots & \alpha_{pp} \\
\hline
 & \beta_1 & \beta_2 & \ldots & \beta_p
\end{array}
$$

with $\alpha_{ij} = 0$ if $j \geq i$ (for explicit schemes)

Multistep Methods

- 1st idea: use previous steps for computation:

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

- 2nd idea: use integral form of ODE

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

Multistep and Numerical Quadrature

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

$$y(t_{n+s}) - y(t_{n+s-1}) = \int_{t_{n+s-1}}^{t_{n+s}} f(\theta, y(\theta)) d\theta \approx \int_{t_{n+s-1}}^{t_{n+s}} p(\theta) d\theta$$

  where

$$p(t_{n+j}) = f(t_{n+j}, y(t_{n+j})) \qquad \text{for } j = 0, \ldots, s-1.$$

- compute integral and obtain quadrature rule:

$$y_{n+s} = y_{n+s-1} + \tau \sum_{j=0}^{s-1} \beta_j f(t_{n+j}, y(t_{n+j}))$$

Adams-Bashforth

- $s = 1 \Rightarrow$ use y_n only to compute y_{n+1} (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 and y_{n+1} to compute y_{n+2}:

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

- 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+s} in polynomial p $\Rightarrow$ **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 (trapezoidal rule)

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

- how to obtain y_{n+s}?
  - solve (nonlinear) equation $\Rightarrow$ difficult!
  - easier and more common: **predictor-corrector** approach
    (e.g.: explicit predictor plus fixpoint iteration on implicit scheme)

Explicit Midpoint Rule

- formally a multi-step scheme: $y_{n+2} = g(y_n, y_{n+1})$
- 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:

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

- 2nd-order accurate with low computational effort, but tends to be instable (see below)

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 for explicit single-step methods required for non-oscillatory behaviour of 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 explicitLMM2.py

Example:

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

- exact solution: $y(t) = (e^t)$
- well-conditioned: $y_\varepsilon(0) = 1 + \varepsilon \Rightarrow y_\varepsilon(t) - y(t) = \varepsilon e^t$
- use following explicit multistep scheme ($s = 2$):

$$y_{n+2} = -4y_{n+1} + 5y_n + \tau \cdot [4 \cdot f(t_{n+1}, y_{n+1}) + 2 \cdot f(t_n, y_n)]$$

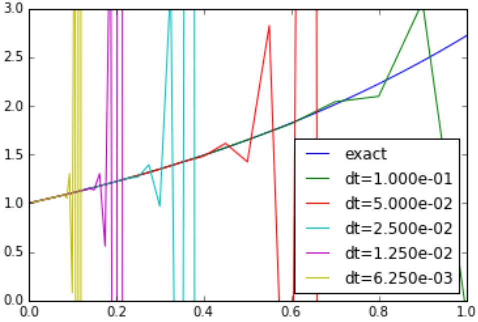
- leads to numerical scheme:

$$y_{n+2} = -4y_{n+1} + 5y_n + \tau \cdot [4y_{n+1} + 2y_n]$$

- consistency of the method: order 3

Stability: Example explicitLMM2.py (2)

Observation:
for start with exact initial values: $y_0 = y(0)$ and $y_1 = y(\tau)$



$\Rightarrow$ multistep method explLMM2 is 3rd-order consistent, but does not converge here: instable behaviour

Stability

- reason: difference equation generates spurious solutions
- analysis: roots μ_i of characteristic polynomial – are all $|\mu_i| < 1$?

Stability of ODE schemes:

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

Stability: Example Explicit Midpoint Rule

Example ODE (Dahlquist):

$$\dot{y}(t) = -10y(t), \qquad y(0) = 1$$

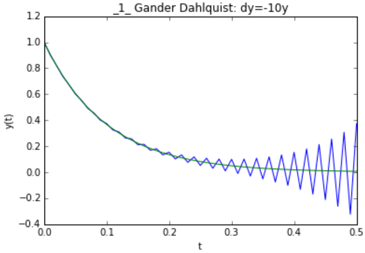
- exact solution: $y(t) = (e^{-10t})$
- use explicit midpoint rule ($s = 2$):

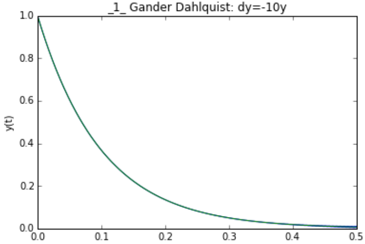
$$y_{n+2} = y_n + 2\tau f(t_{n+1}, y_{n+1})$$

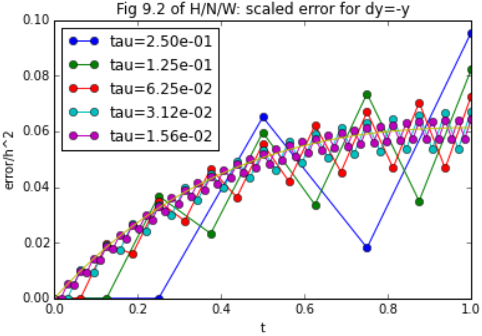
- starting steps: $y_0 = y(0) = 1, \quad y_1 = y(\tau) = e^{-10\tau}$
- method is zero-stable

Stability: Example Explicit Midpoint Rule (2)

python demo: different $\tau = 0.01, 0.001 \quad \Rightarrow \quad$ Martini glass effect

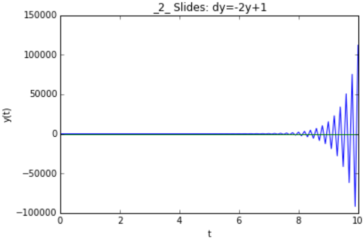


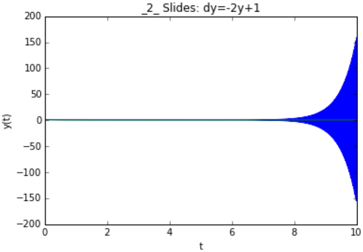


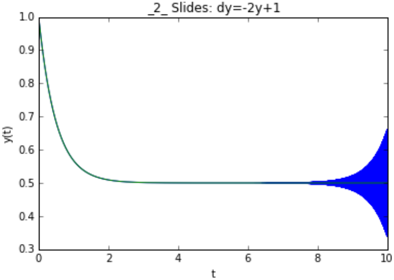


Stability: Martini Glass Effect

slightly different problem: different $\tau = 0.1, 0.01, 0.001$







Stiff Equations

Example:

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

- exact solution: $y(t) = e^{-1000t} + 1$
- explicit Euler (i.e., a **stable scheme**):

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

- 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 explicit time step
- but does not contribute much to the accuracy of 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: attention with non-smooth r.h.s.
  do not use uniform τ and s

Implicit methods:

- for stiff equations
- most often used as corrector scheme

(Extrapolation methods:)

- for very long runtimes
- for very high accuracy