Numerical Methods for Computational Science and Engineering

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Prof. Rima Alaifari, SAM, ETH Zurich

Higher order Single-Step Methods (Runge Kutta Methods)

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

Fundamental theorem of calculus

$$y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} \dot{y}(t)\,dt = y(t_k) + \int_{t_k}^{t_{k+1}} f(t, y(t))\,dt$$

Idea: Use quadrature to approximate

$$\int_{t_k}^{t_{k+1}} f(t, y(t))\,dt \qquad (*)$$

The Runge-Kutta-2 method (RK-2)

Approximate (*) with the midpoint rule:

$$\int_{t_k}^{t_{k+1}} f(t, y(t))\,dt \approx h \cdot \underbrace{f\left(t_k + \frac{h}{2}, y\left(t_k + \frac{h}{2}\right)\right)}_{\text{approximate by forward Euler}}$$

$$\Rightarrow \quad y\left(t_k + \frac{h}{2}\right) \approx y(t_k) + \frac{h}{2} \cdot f(t_k, y(t_k))$$

Altogether: Calculating solution at time t_{k+1}:

$$\underline{k}_1 = \underline{f}(t_k, \underline{y}_k)$$

$$\underline{k}_2 = \underline{f}\left(t_k + \frac{h}{2}, \underline{y}_k + \frac{h}{2}\underline{k}_1\right)$$

2-stage method

$$\underline{y}_{k+1} = \underline{y}_k + h \cdot \underline{k}_2$$

$$\Rightarrow \underline{y}_{k+1} = \underline{y}_k + h\,\underline{f}\left(t_k + \frac{h}{2}, \underline{y}_k + \frac{h}{2}\underline{f}(t_k, \underline{y}_k)\right)$$

Note:
- RK-2 is a single-step method
- RK-2 is of order 2

Classical Runge-Kutta-4 (RK-4) method

$$\underline{k}_1 = \underline{f}(t_k, \underline{y}_k)$$

$$\underline{k}_2 = \underline{f}\left(t_k + \frac{h}{2}, \underline{y}_k + \frac{h}{2}\underline{k}_1\right)$$

$$\underline{k}_3 = \underline{f}\left(t_k + \frac{h}{2}, \underline{y}_k + \frac{h}{2}\underline{k}_2\right)$$

$$\underline{k}_4 = \underline{f}\left(t_k + h, \underline{y}_k + h\,\underline{k}_3\right)$$

4-stage method

$$\underline{y}_{k+1} = \underline{y}_k + \frac{h}{6}\left(\underline{k}_1 + 2\underline{k}_2 + 2\underline{k}_3 + \underline{k}_4\right)$$

Simpson's rule

Motivation: $$\int_{t_k}^{t_{k+1}} \underline{f}(t, \underline{y}(t))\,dt \approx \frac{h}{6}\Big[\underline{f}(t_k, \underline{y}(t_k)) + 4\,\underline{f}\left(t_k + \frac{h}{2}, \underline{y}\left(t_k + \frac{h}{2}\right)\right) + \underline{f}(t_{k+1}, \underline{y}(t_{k+1}))\Big]$$

$$y(t_k + \tfrac{h}{2}) \approx y(t_k) + \tfrac{h}{2} f(t_k, y(t_k)) \approx y_k + \tfrac{h}{2} k_1$$

forward Euler

$\Rightarrow$ $\underline{k_2}$ is approximation of $\underline{f}(t_k + \frac{h}{2}, y(t_k + \frac{h}{2}))$
(the slope at the midpoint)

Use this approximation to get another estimate of the slope at the midpoint: $\underline{k_3}$

$\underline{k_4}$ estimates slope at the endpoint $\underline{f}(t_k + h, y(t_k + h))$

One can show RK-4 is a fourth-order method

Note: RK-2, RK-4 are explicit methods

<u>General form of Runge-Kutta methods</u>

$$\underline{k_1} = \underline{f}\left(t_k + c_1 h,\ y_k + h \cdot \sum_{j=1}^{s} a_{1j} \underline{k_j}\right)$$

$$\vdots$$

$$\underline{k_s} = \underline{f}\left(t_k + c_s h,\ y_k + h \cdot \sum_{j=1}^{s} a_{sj} \underline{k_j}\right)$$

$$y_{k+1} = y_k + h \cdot \sum_{i=1}^{s} b_i \underline{k_i}$$

where $c_i := \sum_{j=1}^{s} a_{ij}$

A set of coefficients $\{a_{ij}\}_{i,j=1}^{s}$, $\{b_i\}_{i=1}^{s}$, $\{c_i\}_{i=1}^{s}$ specify an s-stage RK method.

For simplicity: presented in tabular format

"Butcher tableau"

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ \vdots & \vdots & & & \vdots \\ c_s & a_{s1} & \cdots & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

Example: RK-2:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$

RK-4

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

Consistency of RK methods:

Discrete evolution of RK methods:

$$\Psi^h \underline{y} = \underline{y} + h \cdot \underbrace{\sum_{i=1}^{s} b_i \, \underline{k}_i(\underline{y})}_{\psi(h,\underline{y})}$$

(Recall:)

Consistency: $\psi(0,\underline{y}) = \underline{f}(\underline{y})$

For RK methods: $\psi(0,\underline{y}) = \left(\sum_{i=1}^{s} b_i\right) \cdot \underline{f}(\underline{y})$

Consistent RK methods:

$$\boxed{\sum_{i=1}^{s} b_i = 1}$$

(this together with $c_i = \sum_{j=1}^{s} a_{ij}$)

Examples:

- Explicit Runge–Kutta methods

$$a_{ij} = 0 \quad \text{if } j \geq i$$

(each k_j is computed only from previous k_i's, $i = 1, \dots, j-1$)

- Diagonally Implicit RK (DIRK) methods

$$a_{ij} = 0 \quad \text{if } j > i$$

and there exists at least one non-zero diagonal entry $a_{ii} \neq 0$.

→ This involves at stage i the solution of a nonlinear system of equations.

Example of DIRK-2: 3-stage, 2nd order

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 \\ 1 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \hline & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array}$$

non-zero diagonal entries

DIRK-2 $\hat{=}$ trapezoidal rule with 2nd order backward difference (TR-BDF2)

<u>Order vs. stages</u>:

<u>Ideally</u>: high order with as few stages as possible

Butcher barriers for explicit RK methods

order p	1	2	3	4	5	6	7	8	≥ 9
minimal no. s of stages	1	2	3	4	6	7	9	11	$\geq p+3$

Convergence / error analysis

Error at time t_k: $\quad e_k := y_k - y(t_k)$

Global error: error at final time: $T = t_N$

$$e_N = y_N - y(t_N)$$

Recall: $\quad y(t_{k+1}) = \Phi^h[y(t_k)]$ evolution (of exact solution at t_k)

$y_{k+1} = \Psi^h y_k$ discrete evolution of our approximation at time t_k

$$\Rightarrow \quad e_{k+1} = y_{k+1} - y(t_{k+1}) = \Psi^h y_k - \Phi^h[y(t_k)]$$

Error splitting:

$$e_{k+1} = \underbrace{\Psi^h y_k - \Psi^h[y(t_k)]}_{\text{propagated error}} + \underbrace{\Psi^h[y(t_k)] - \Phi^h[y(t_k)]}_{\text{one-step error}}$$

propagated error (Error due to using only an approximation y_k of $y(t_k)$ at step $k+1$)

one-step error (Assume true solution at time t_k, what is the error introduced in step $k+1$ through approximating Φ^h by Ψ^h)

Example: explicit Euler

We assume f suff. smooth & Lipschitz continuous, i.e.

$$\exists\, L > 0 \text{ s.t. } \quad \|f(y) - f(z)\| \le L \cdot \|y - z\| \quad \forall y, z \in D$$

$$\boxed{\Psi^h y = y + h \cdot f(y)} \qquad \text{(explicit Euler)}$$

$t_0 = 0, \quad t_N = T$

(1) Propagated error:

$$\| \Phi^h y_k - \Phi^h [y(t_k)] \| = \| y_k + h f(y_k) - y(t_k) - h f(y(t_k)) \|$$

$$\underset{\substack{\uparrow \\ e_k = y_k - y(t_k)}}{=} \| e_k + h \cdot (f(y_k) - f(y(t_k))) \|$$

$$\leq \|e_k\| + h \cdot \| f(y_k) - f(y(t_k)) \|$$

$$\underset{\substack{\uparrow \\ \text{Lipschitz} \\ \text{condition}}}{\leq} \|e_k\| + h \cdot L \cdot \|e_k\| = \underline{\underline{(1+hL)\|e_k\|}}$$

(2) One-step error:

$$\| \Phi^h (y(t_k)) - \underbrace{\Phi^h (y(t_k))}_{y(t_{k+1})} \| = \| \Phi^h (y(t_k)) - y(t_k + h) \|$$

$$= \| y(t_k) + h f(y(t_k)) - y(t_k + h) \|$$

$$= \| y(t_k) + h \dot{y}(t_k) - y(t_k + h) \|$$

$$\underset{\substack{\uparrow \\ \text{First order} \\ \text{Taylor}}}{\leq} \frac{1}{2} h^2 \max_{\tau \in [t_k, t_{k+1}]} \| \ddot{y}(\tau) \|$$

<u>In total:</u>

$$\|e_{k+1}\| \underset{\substack{\uparrow \\ (1)+(2)}}{\leq} (1+hL)\|e_k\| + \overbrace{\frac{1}{2} h^2 \max_{\tau \in [0,T]} \| \ddot{y}(\tau) \|}^{=: \rho}$$

$$\|e_k\| \leq (1+hL)\|e_{k-1}\| + \rho \leq (1+hL)^2 \|e_{k-2}\| + (1+hL)\rho + \rho$$

$$\leq (1+hL)^3 \|e_{k-3}\| + (1+hL)^2 \rho + (1+hL)\rho + \rho$$

$$\leq \dots \underset{\substack{\uparrow \\ \|e_0\|=0}}{\leq} \rho \cdot \left(\sum_{j=0}^{k-1} (1+hL)^j \right)$$

$$1 \leq 1+hL \leq e^{Lh}$$

$$(1+hL)^j \leq e^{jLh} \underset{\substack{\uparrow \\ j\cdot h \leq T}}{\leq} e^{LT}$$

$$\Rightarrow \|e_k\| \leq \rho \cdot \sum_{j=0}^{k-1} e^{LT} = \rho \cdot k \cdot e^{LT}$$

$$\underset{\substack{\uparrow \\ k \leq \frac{T}{h}}}{\leq} \rho \cdot \frac{T}{h} \cdot e^{LT}$$

$$\leq \frac{1}{2} h^2 \cdot \max_{\tau \in [0,T]} \|\ddot{y}(\tau)\| \cdot \frac{T}{h} e^{LT}$$

$$\leq \frac{1}{2} T e^{LT} \max_{\tau \in [0,T]} \|\ddot{y}(\tau)\| \cdot h = \underline{\underline{\mathcal{O}(h)}}$$

$\Rightarrow$ algebraic convergence of order 1.

<u>Note</u>: The constant in the asymptotic convergence grows

- exp. fast in the length of the interval T
- exp. fast in the Lipschitz constant of f
- linearly in $\max_{\tau} \|\ddot{y}(\tau)\|$

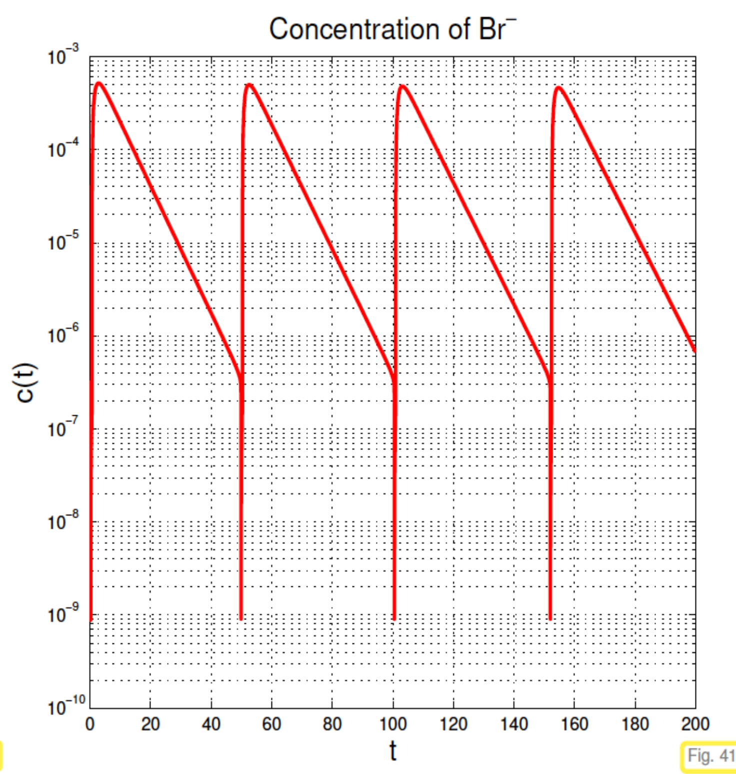
$\rightsquigarrow$ rapidly varying functions require much smaller time steps

In practice: adaptive step size control

- larger step sizes in slowly varying regions
- smaller step sizes in rapidly varying regions

E.g. modelling of chemical reactions

$\rightsquigarrow$ very abrupt dynamics



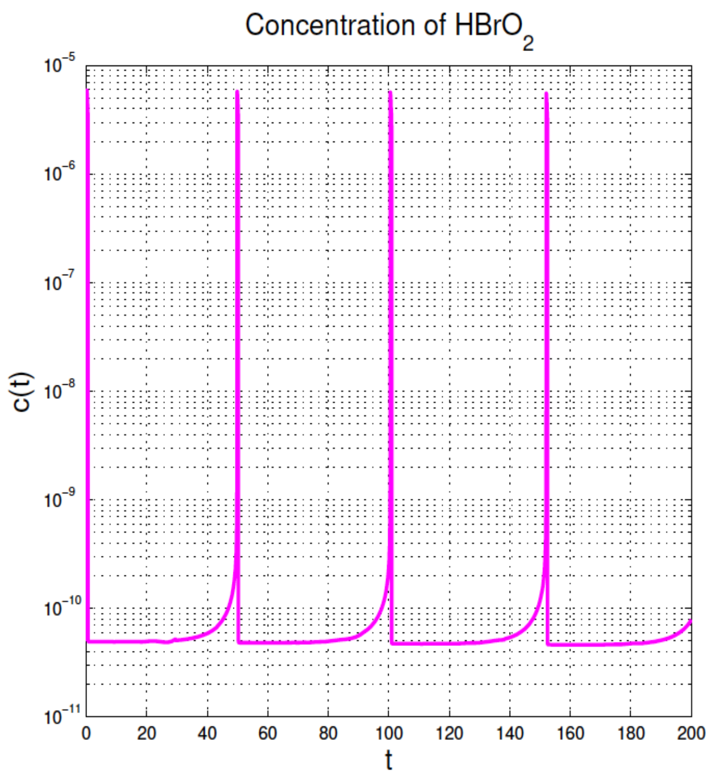


Fig. 415

Stability of Numerical Methods for ODEs

Convergence of the numerical scheme is not enough!

Example :
$$\dot{y}(t) = \lambda\,(y(t) - \sin t) + \cos t$$
$$y(0) = 0 \qquad \lambda \in \mathbb{R}$$

$$\boxed{y(t) = \sin t \quad \text{unique solution}}$$

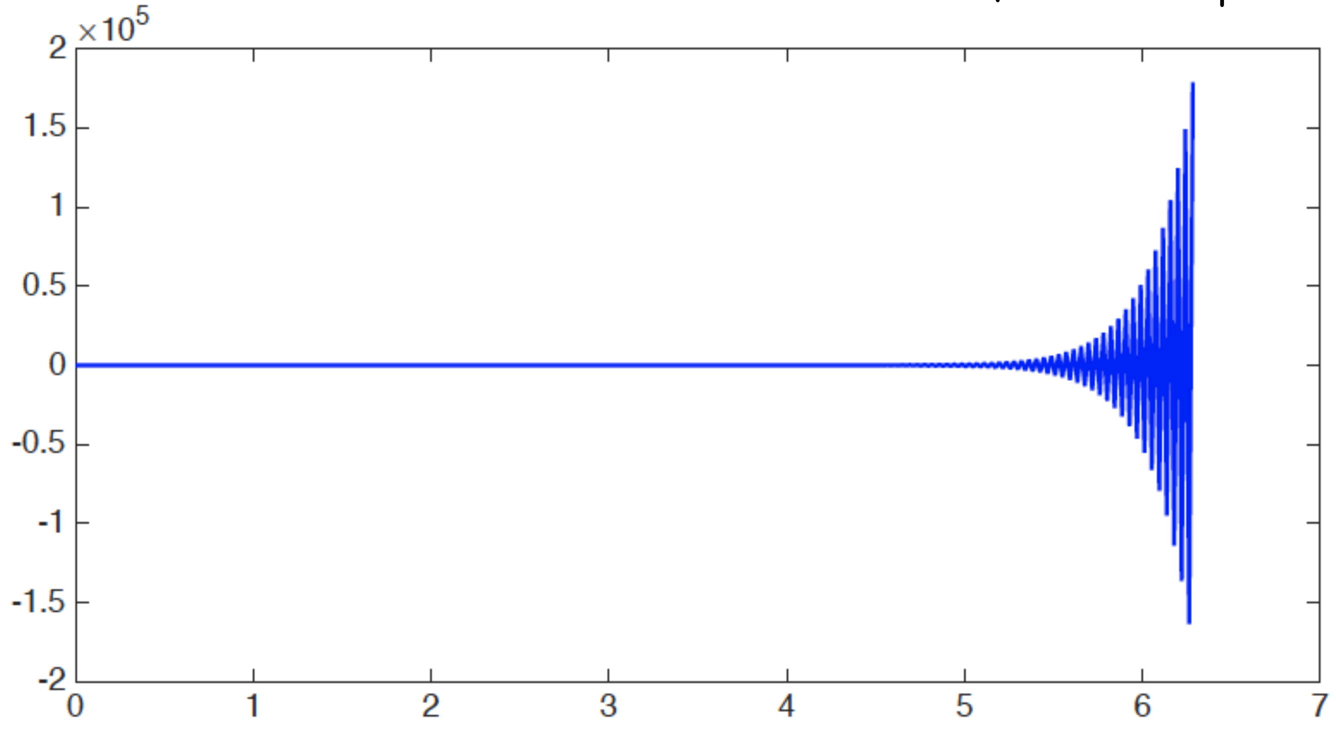
Explicit Euler for solving numerically :

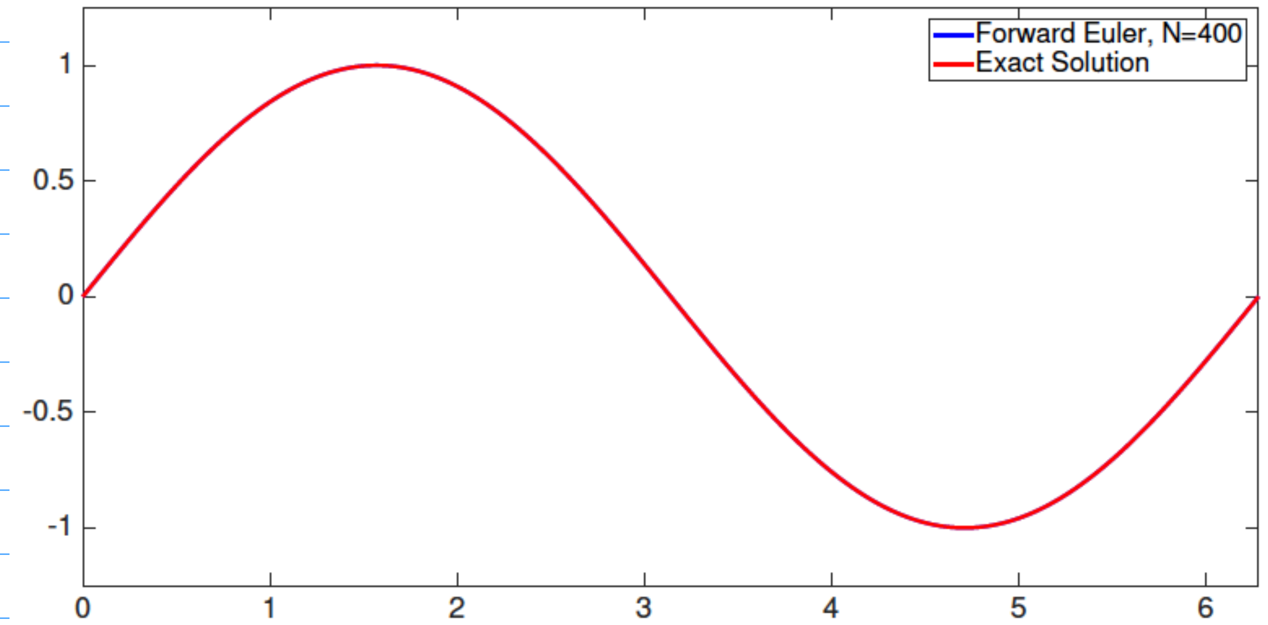
$[0, 10]$

$\lambda = -100$

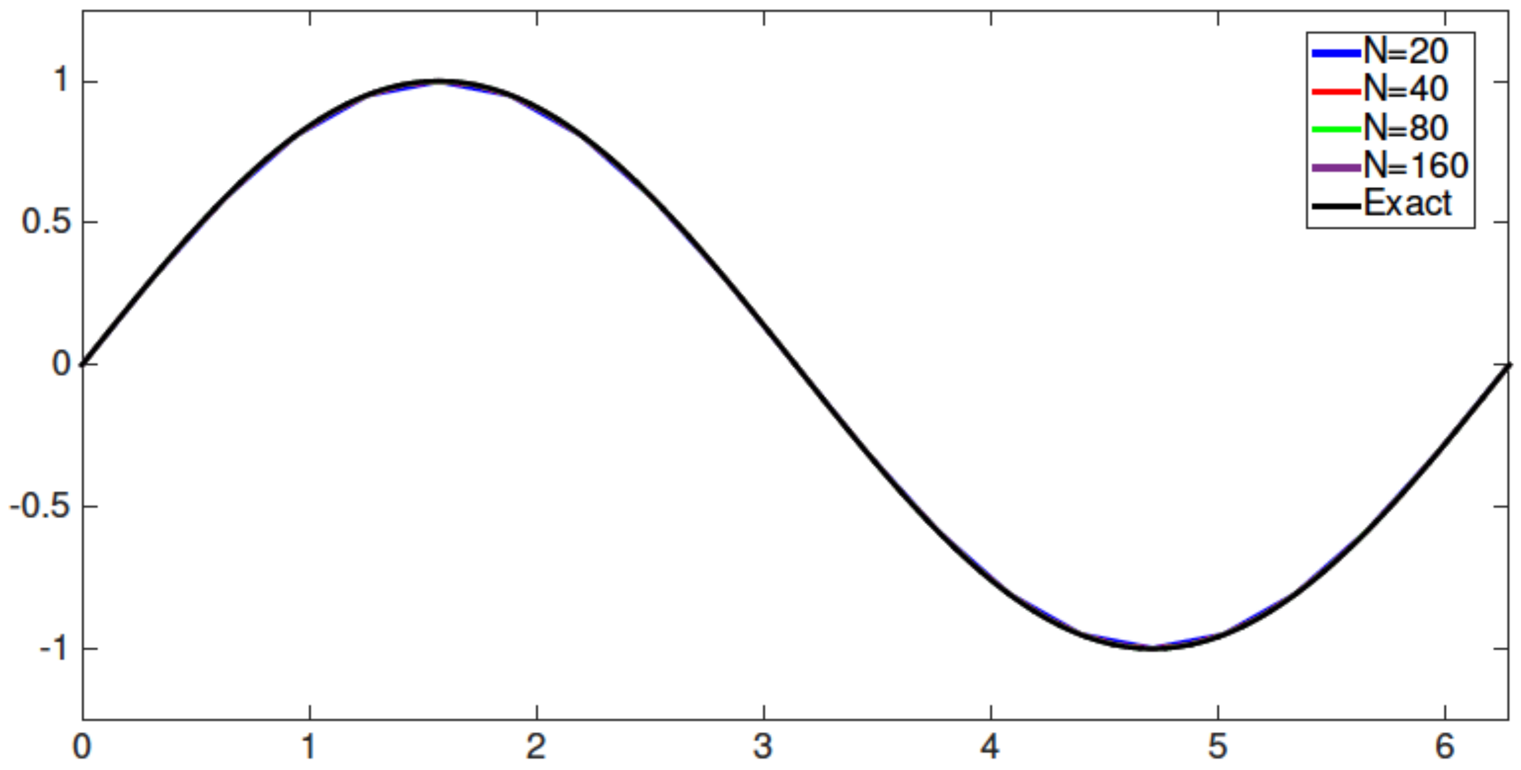
N	Error	$\lvert 1 + \lambda h \rvert$
100	6.70×10^{66}	5.283
200	1.04×10^{59}	2.141
300	1.79×10^{5}	1.094
320	2.29×10^{-6}	0.964
400	3.74×10^{-7}	0.571

Expl. Euler, N=300





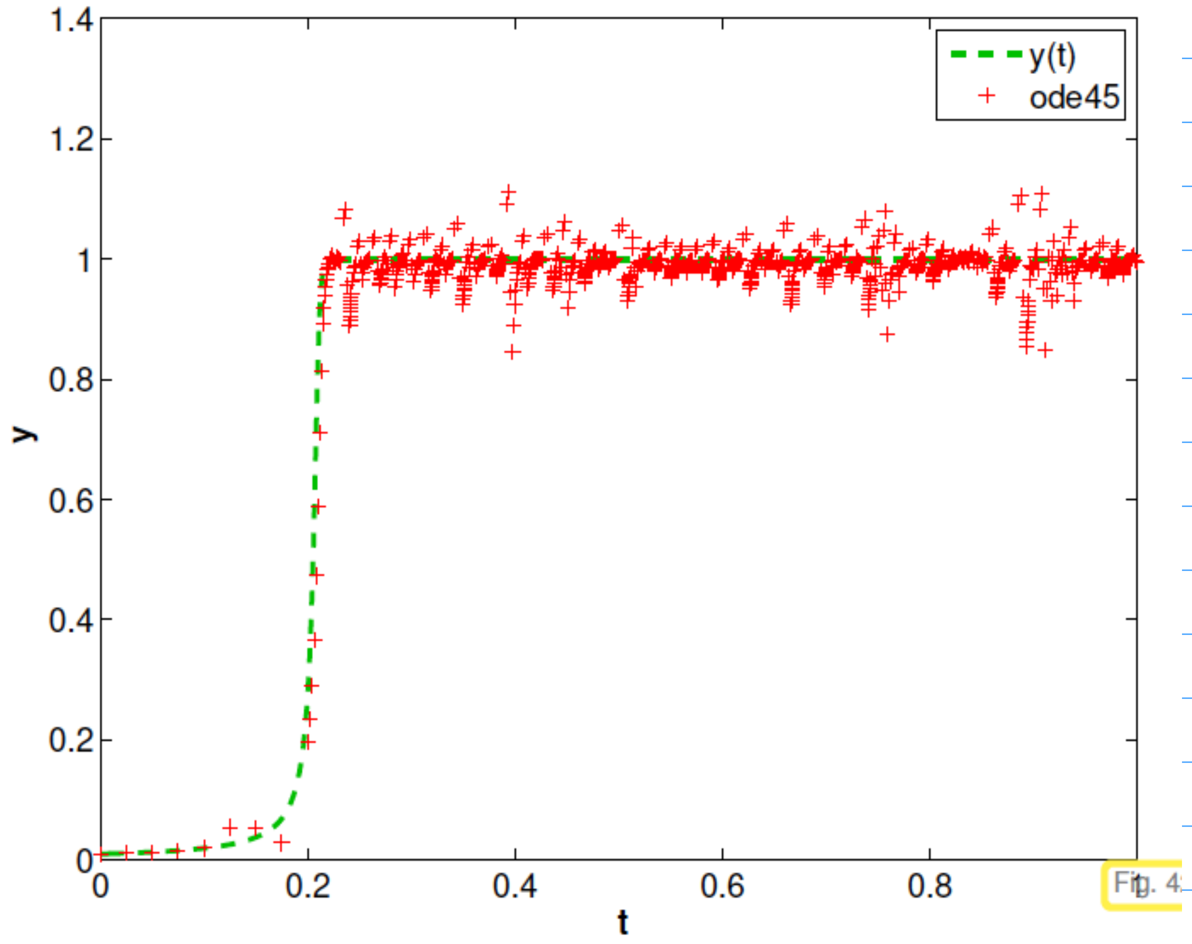
Comparison: Implicit Euler does not suffer from this phenomenon!

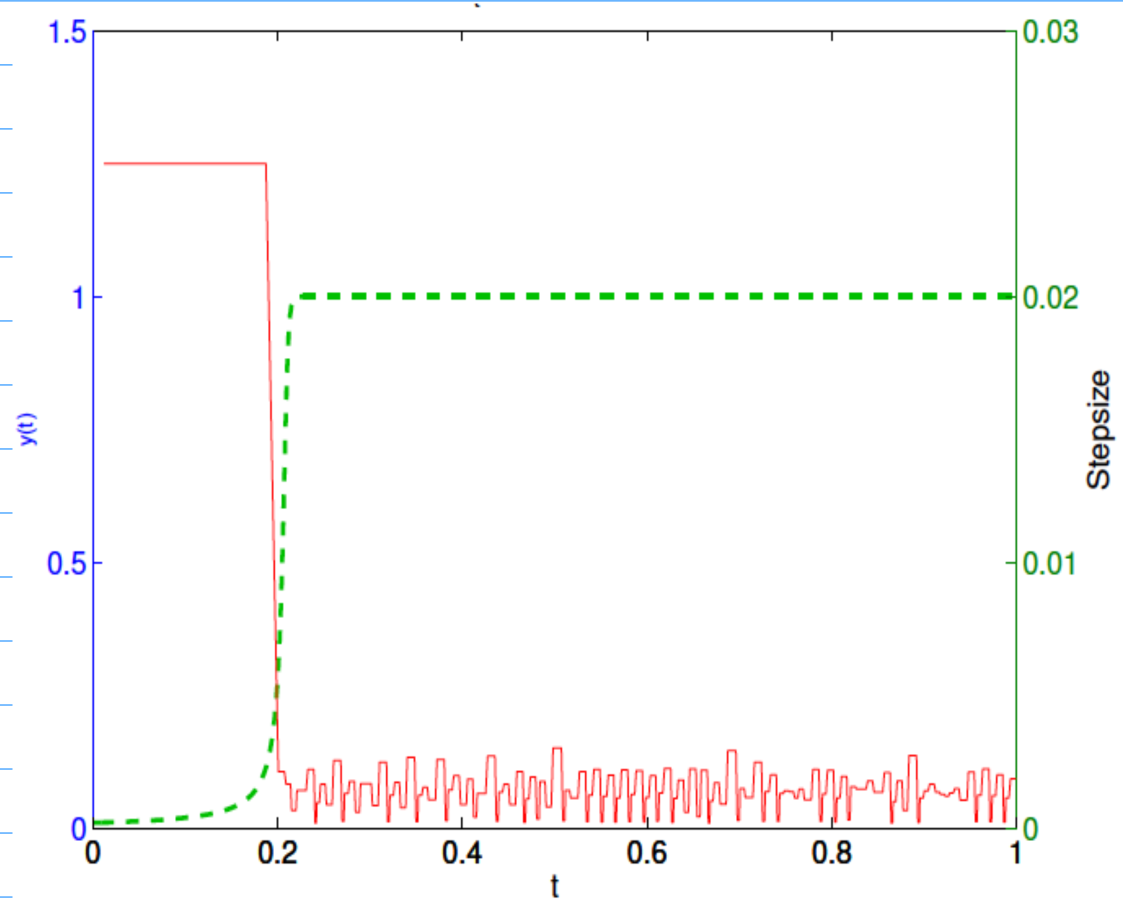


Example: $\dot{y} = \lambda y^2 (1-y)$ $\quad y(0) = \frac{1}{100}$

logistic ODE $\quad \lambda = 500$

Solve with standard RK solver (ode45)





Here: Use of tiny step sizes on region where the solution is practically constant.

Absolute stability

The phenomena we have seen before are referred to as stiffness of the IVP.

Note: This is not always necessarily a property of the solution itself, but of the system

[Example: $y(t) = \sin t$ is a solution both to

stiff: $\dot{y}(t) = \lambda(y(t) - \sin t) + \cos t$ and

non-stiff: $\dot{y}(t) = \cos t$]

Consider the following model problem:

$$\dot{y} = \lambda y, \quad y(0) = y_0, \quad \lambda \in \mathbb{R}^-$$

Exact solution: $y(t) = y_0 e^{\lambda t}$

$\rightarrow$ rapidly decaying to zero $(\lambda < 0)$

Solve with explicit Euler:

$$y_{k+1} = y_k + h f(y_k) = y_k + h\lambda y_k = (1 + \lambda h) y_k$$

for stability we need: $|y_{k+1}| < |y_k|$

$\Leftrightarrow \quad |1 + \lambda h| < 1$ "absolutely stable"

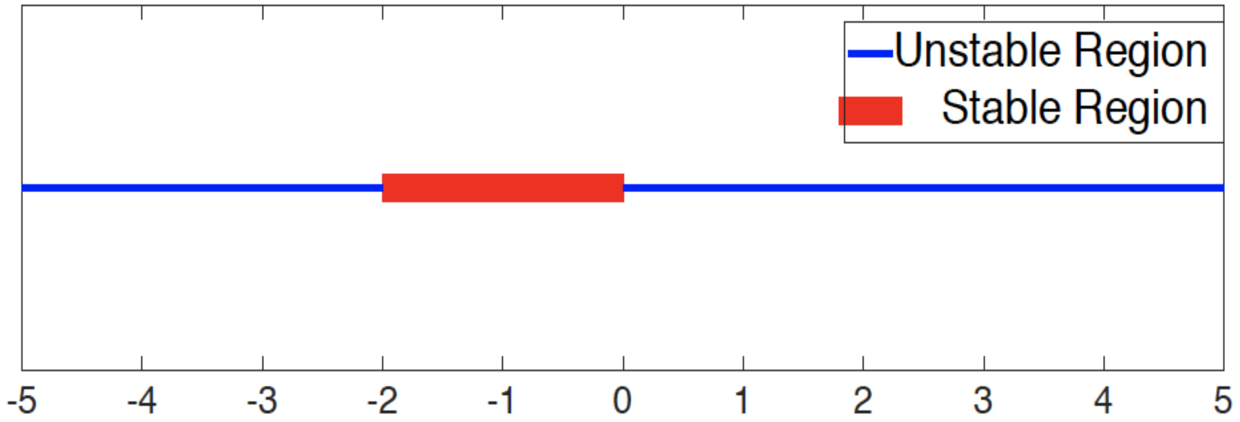
Recall $\lambda < 0 \quad \Rightarrow \quad -2 < \lambda h < 0$

Explicit Euler is absolutely stable only if

$$h < \frac{2}{|\lambda|}$$

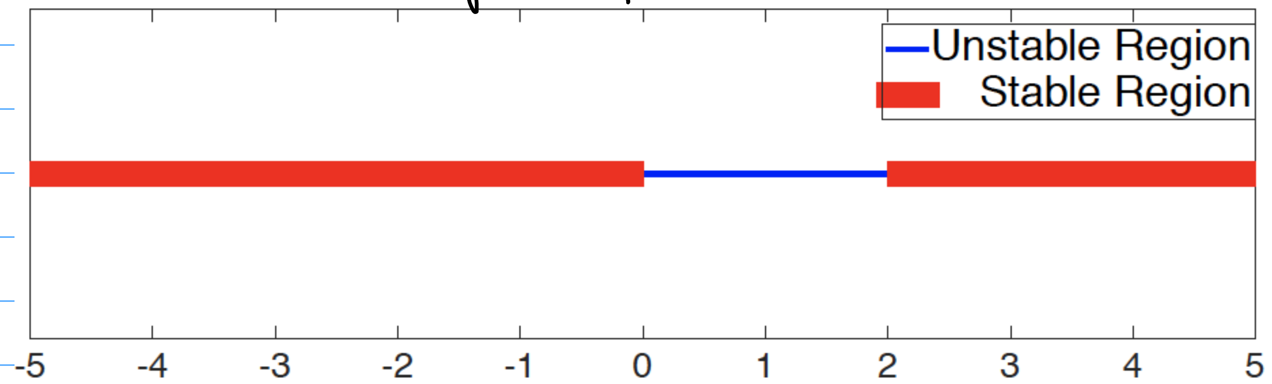
$\Rightarrow$ h has to be small relative to the constant λ.

Stability region for expl. Euler



λh

Stability region for implicit Euler



λh

$\lambda < 0, \; h > 0 \Rightarrow \lambda h < 0$

$\Rightarrow$ Any choice of h remains in the stability region

Absolute stability for explicit RK methods:

Example: Explicit trapezoidal method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

for $\dot{y} = \lambda y, \quad y(0) = y_0, \quad \lambda < 0$

$$k_1 = f(y_0) = \lambda y_0$$

$$k_2 = f(y_0 + hk_1) = \lambda (y_0 + hk_1)$$

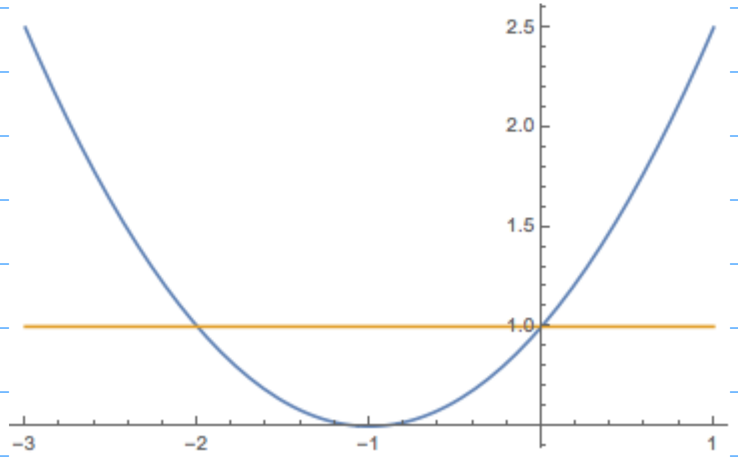
$$y_1 = y_0 + \frac{h}{2}(k_1 + k_2) = y_0 + \frac{h}{2}\left(\lambda y_0 + \lambda y_0 + \lambda^2 h y_0\right)$$

$$= y_0 \left(1 + h\lambda + \frac{1}{2}(\lambda h)^2\right)$$

$S(\lambda h) := 1 + h\lambda + \frac{1}{2}(h\lambda)^2$ stability function

$y_k = S(\lambda h)^k y_0$

for absolute stability: $|S(\lambda h)| < 1$



$-2 < \lambda h < 0$: stability region

General explicit RK methods:

$\dot{y} = \lambda y$ scalar eqn.

$$\boxed{\begin{aligned} k_i &= \lambda\Big(y_0 + h\sum_{j=1}^{i-1} a_{ij} k_j\Big) \\ y_1 &= y_0 + h\sum_{i=1}^{s} b_i k_i \end{aligned}} \qquad (*)$$

$$\begin{array}{c|cccc} c_1 & 0 & & & 0 \\ \vdots & a_{21} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ c_s & a_{s1} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & \cdots & \cdots & b_s \end{array} \quad =: \mathcal{A}$$

$\underline{b} := \begin{pmatrix} b_1 \\ \vdots \\ b_s \end{pmatrix}$ $\quad \underline{c} := \begin{pmatrix} c_1 \\ \vdots \\ c_s \end{pmatrix}$

$\underline{k} := \frac{1}{\lambda}\begin{pmatrix} k_1 \\ \vdots \\ k_s \end{pmatrix}$ $\qquad z := \lambda h$

$$\Rightarrow \boxed{\begin{aligned} \underline{k} &= y_0 \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} + z \mathcal{A} \underline{k} \\ y_1 &= y_0 + z \underline{b}^T \underline{k} \end{aligned}} \qquad (**)$$

$(*) \Leftrightarrow (**)$

$$\Rightarrow \begin{bmatrix} I - z\mathcal{A} & 0 \\ -z\underline{b}^T & 1 \end{bmatrix} \begin{bmatrix} \underline{k} \\ y_1 \end{bmatrix} = y_0 \begin{bmatrix} 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}$$

Recall Schur complement & block Gauss elimination:

$$y_1 = y_0 + z \underline{b}^T (I - z\mathcal{A})^{-1} y_0 \cdot \underline{1}$$

$$= y_0 \left(1 + z \underline{b}^T (I - z\mathcal{A})^{-1} \underline{1} \right)$$

$$\Rightarrow S(z) := 1 + z \underline{b}^T (I - z\mathcal{A})^{-1} \underline{1} \qquad \text{stability function}$$

$$y_1 = S(\lambda h)\, y_0$$

Alternative formula:

$$y_1 = \frac{\det \begin{bmatrix} I - z\mathcal{A} & y_0 \underline{1} \\ -z\underline{b}^T & y_0 \end{bmatrix}}{\det \begin{bmatrix} I - z\mathcal{A} & \underline{0} \\ -z\underline{b}^T & 1 \end{bmatrix}} \qquad \text{Cramer's rule}$$

$$= y_0 \cdot \frac{\det \begin{bmatrix} I - z\mathcal{A} & \underline{1} \\ -z\underline{b}^T & 1 \end{bmatrix}}{\det \begin{bmatrix} I - z\mathcal{A} & \underline{0} \\ -z\underline{b}^T & 1 \end{bmatrix}}$$

Schur's determinant identity:

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det D \cdot \det (A - BD^{-1}C)$$

$$\Rightarrow \quad Y_1 = Y_0 \cdot \frac{\det(I - z\mathcal{A} + z\underline{1}\,\underline{b}^T)}{\det(I - z\mathcal{A})}$$

Note: $\mathcal{A}$ strictly lower triangular

$\Rightarrow$ $I - z\mathcal{A}$ lower triangular with all diagonal entries $= 1$

$\Rightarrow$ $\det(I - z\mathcal{A}) = 1$

$$\Rightarrow \quad Y_1 = Y_0 \cdot \det(I - z\mathcal{A} + z\underline{1}\,\underline{b}^T)$$

$$\Rightarrow \quad S(z) = 1 + z\underline{b}^T (I - z\mathcal{A})^{-1}\underline{1}$$

$$= \det(I - z\mathcal{A} + z\underline{1}\,\underline{b}^T)$$

$$Y_k = S(\lambda h)^k Y_0 \qquad \Phi_\lambda^h = S(\lambda h)$$

Examples: • Explicit Euler: $S(z) = 1 + z$

• Explicit trapezoidal:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array} \qquad S(z) = 1 + z + \frac{z^2}{2}$$

• Classical RK-4:

$$S(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4$$

The stability function S of a consistent s-stage RK method is a <u>non-constant</u> polynomial of degree $\leq s$: $\quad S \in \mathcal{P}_s$

$$\Rightarrow \quad \lim_{|z|\to\infty} |S(z)| = \infty$$

Define region of absolute stability:

$$\mathcal{S}_{\Phi} := \{ z \in \mathbb{C} : |S(z)| < 1 \} \subset \mathbb{C}$$

$$\left(\text{Here: } \Phi^h y = S(z) y \ , \quad \lambda h = z \right)$$

$\Rightarrow$ For explicit RK methods one always needs to ensure $|\lambda h|$ is suff. small.

For $\lambda \in \mathbb{R}^-$, $\lambda \ll 0$ $\Rightarrow$ can lead to unreasonably small choices of h.

Systems of linear ODEs

$$\dot{y} = M y \qquad M \in \mathbb{R}^{d,d}$$

where M is assumed to be diagonalizable:

$$M = V D V^{-1} \qquad \left(V^{-1} M = D V^{-1} \right)$$

$$D = \operatorname{diag}(\lambda_1, \dots, \lambda_d)$$

$$V = \begin{bmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_d \\ | & | & & | \end{bmatrix} \qquad M v_i = \lambda_i v_i$$

Runge-Kutta scheme:

$$V^{-1}\underline{k}_\ell = V^{-1} M\Big(\underline{y}_0 + h\sum_{j=1}^{\ell-1} a_{\ell j}\,\underline{k}_j\Big) \qquad \ell = 1,\dots,s$$

(S1)

$$V^{-1}\underline{y}_1 = V^{-1}\Big(\underline{y}_0 + h\sum_{\ell=1}^{s} b_\ell\,\underline{k}_\ell\Big)$$

$$\Rightarrow\quad V^{-1}\underline{k}_\ell = D\Big(V^{-1}\underline{y}_0 + h\sum_{j=1}^{\ell-1} a_{\ell j}\,V^{-1}\underline{k}_j\Big)$$

$$V^{-1}\underline{y}_1 = V^{-1}\underline{y}_0 + h\sum_{\ell=1}^{s} b_\ell\,V^{-1}\underline{k}_\ell$$

Define $\underline{\hat{k}}_\ell := V^{-1}\underline{k}_\ell$

$\underline{\hat{y}}_k := V^{-1}\underline{y}_k$

$$\Rightarrow\quad \underline{\hat{k}}_\ell = D\Big(\underline{\hat{y}}_0 + h\sum_{j=1}^{\ell-1} a_{\ell j}\,\underline{\hat{k}}_j\Big)$$

$$\underline{\hat{y}}_1 = \underline{\hat{y}}_0 + h\sum_{\ell=1}^{s} b_\ell\,\underline{\hat{k}}_\ell \qquad \text{(S2)}$$

Componentwise:

$$(\underline{\hat{k}}_\ell)_i = \lambda_i\Big((\underline{\hat{y}}_0)_i + h\sum_{j=1}^{\ell-1} a_{\ell j}(\underline{\hat{k}}_j)_i\Big)$$

$$(\underline{\hat{y}}_1)_i = (\underline{\hat{y}}_0)_i + h\sum_{\ell=1}^{s} b_\ell\,(\underline{\hat{k}}_\ell)_i$$

For each component $i = 1,\dots,d$ (S2) is the Runge-Kutta method (from before) applied to the scalar IVP

$$\dot{y} = \lambda_i y \qquad y(0) = (V^{-1}\underline{y}_0)_i$$

$\Rightarrow$ stability for $\dot{y} = My$ can be verified componentwise:

<u>Theorem</u>: The sequence $(y_k)_{k=1}^{N}$ of approximations obtained from an explicit RK method with stability function S applied to

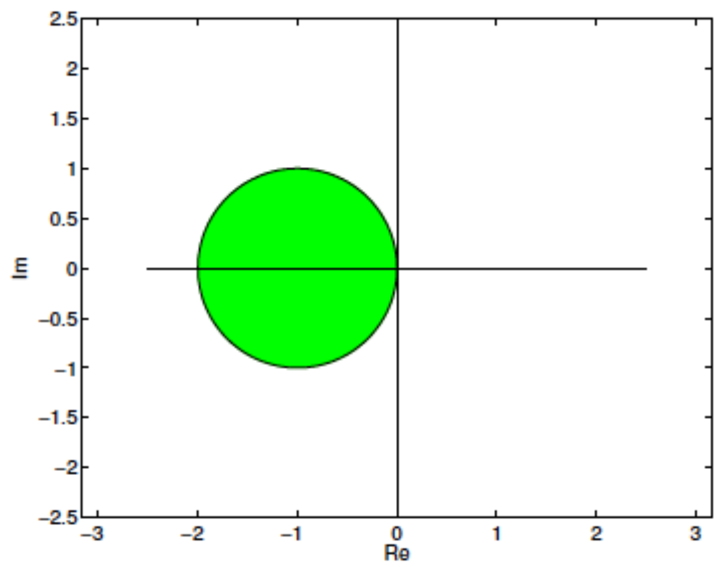
$$\dot{y} = My$$

decays exponentially for any y_0 if the step size h fulfills

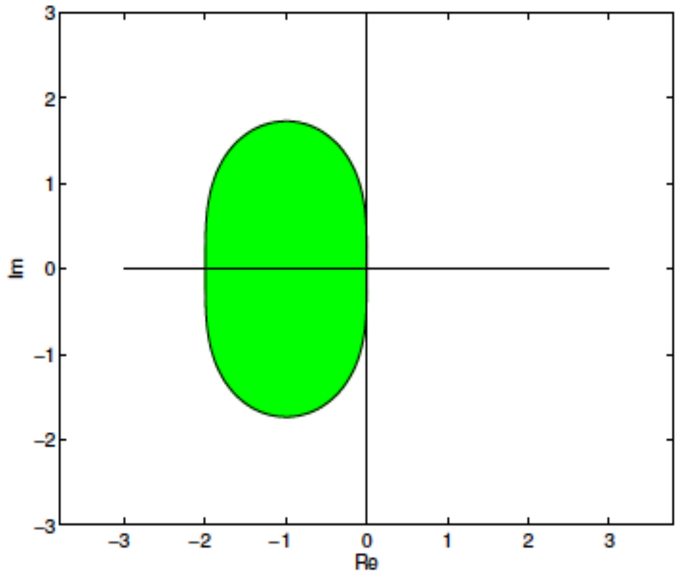
$$|S(\lambda_i h)| < 1$$

for all eigenvalues λ_i of M.

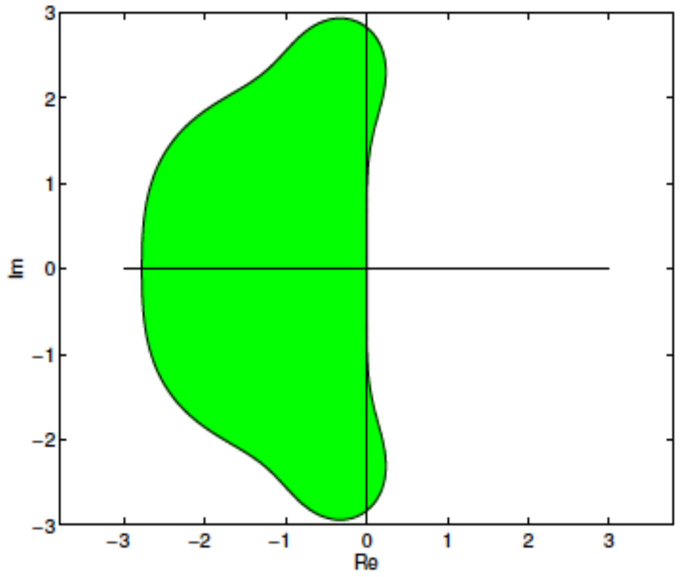
Note: $\mathrm{Re}\,\lambda_i < 0 \quad \forall\, i = 1, \dots, d \Rightarrow \|y(t)\| \to 0$ as $t \to \infty$



$\mathcal{S}_\Psi$: explicit Euler (11.2.7)



$\mathcal{S}_\Psi$: explicit trapezoidal method



$\mathcal{S}_\Psi$: classical RK4 method

Stability function of implicit RK methods:

Recall:

$$y_1 = y_0 \cdot \underbrace{\frac{\det(I - z\mathfrak{A} + z\,\mathbf{1}\,\mathbf{b}^T)}{\det(I - z\mathfrak{A})}}_{= S(z)}$$

For implicit methods: $\mathfrak{A}$ is no longer strictly lower diagonal

$$S(z) = \frac{p(z)}{q(z)} \qquad p, q \in \mathcal{P}_s$$

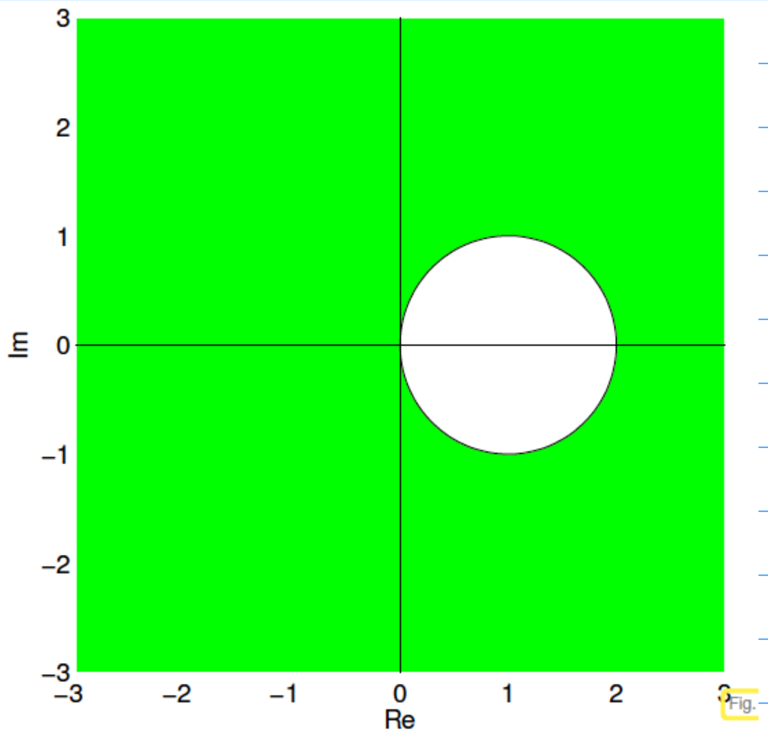
↑ rational function

$\Rightarrow$ stability region $\mathcal{S}_\Psi = \{ z \in \mathbb{C} : |S(z)| < 1 \}$

is no longer necessarily a bounded region!

Example: Implicit Euler

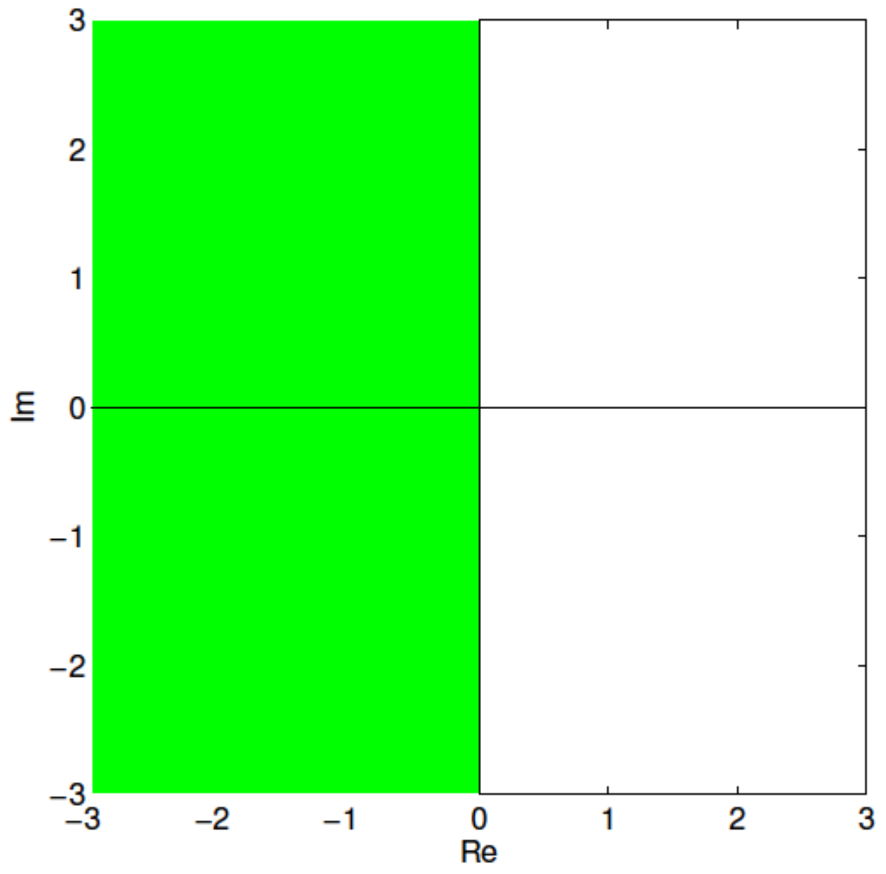
$$S(z) = \frac{1}{1-z} \qquad \lim_{|z| \to \infty} |S(z)| = 0$$



$\mathcal{S}_\Psi$: implicit Euler method (11.2.13)

Implicit midpoint method:

$$S(z) = \frac{1 + z/2}{1 - z/2}$$



$\mathcal{S}_\Psi$: implicit midpoint method (11.2.18)

Definition [A-stability]

An RK method with stability function S is A-stable if

$$\mathbb{C}^- := \{ z \in \mathbb{C} : \operatorname{Re} z < 0 \} \subset \mathcal{S}_\Phi$$

stability region

Note: An A-stable method is necessarily implicit.

Family of A-stable RK methods:

Gauss-Legendre (or Gauss collocation methods)

s-stage, order $2s$

Example: Gauss – Legendre order 2 $\hat{=}$ midpoint rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

Gauss – Legendre of order 4:

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \sqrt{3}/6 & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$S_{\Phi} = \mathbb{C}^-$ for G – L methods

High order G – L methods are rarely used (due to high comp. cost)