ETH Lecture 401-0663-00L Numerical Methods for CSE

Numerical Methods for Computational Science and Engineering

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(C) Seminar für Angewandte Mathematik, ETH Zürich

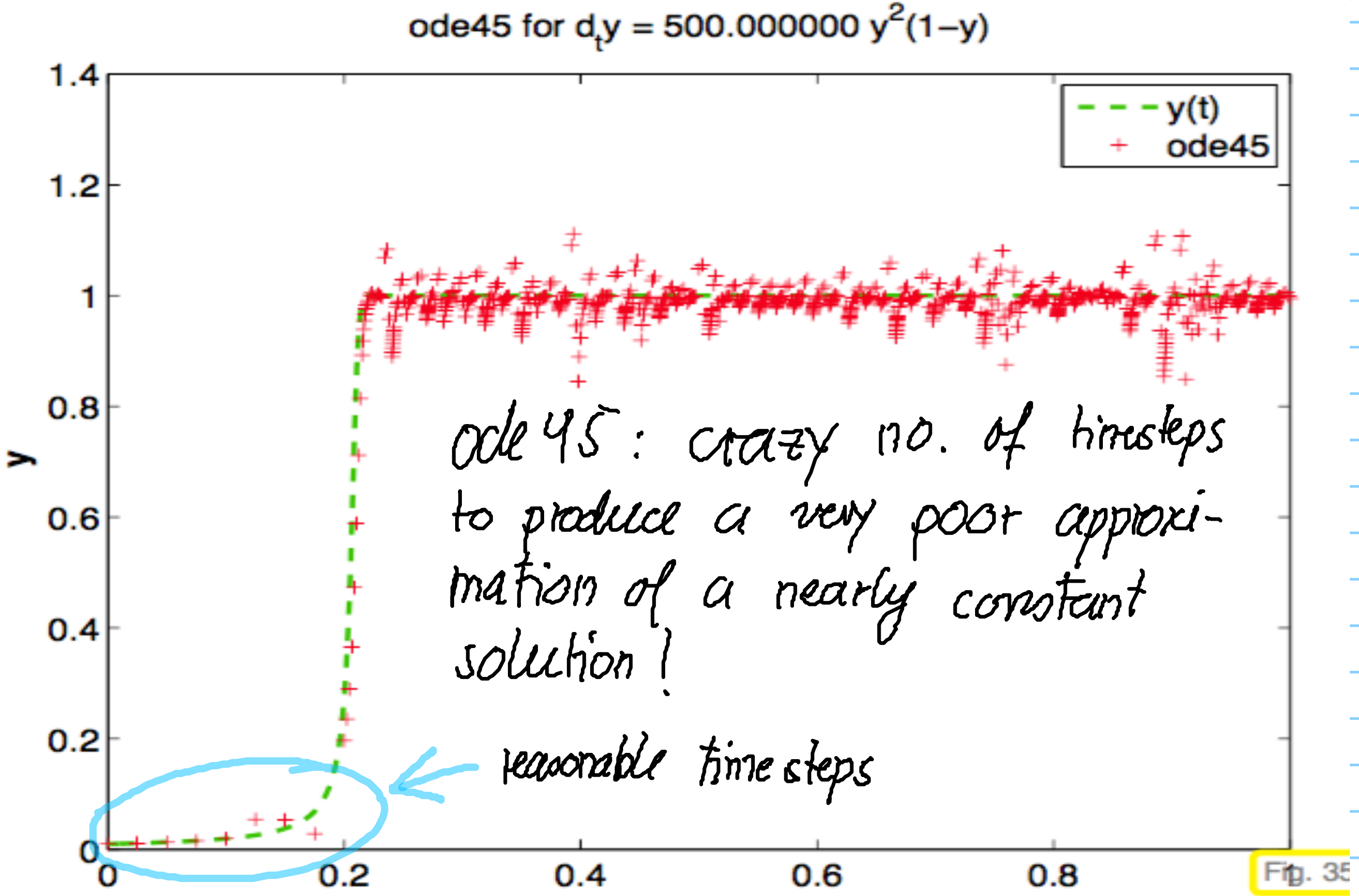
URL: http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE15.pdf

XII. Single step methods for stiff IVPs

MATLAB-script 12.0.2: Use of MATLABintegrator ode45 for a stiff problem

```
fun = @(t,x) 500*x^2*(1-x);
options = odeset('reltol',0.1,'abstol',0.001,'stats','on');
[t,y] = ode45(fun,[0 1],y0,options);
```

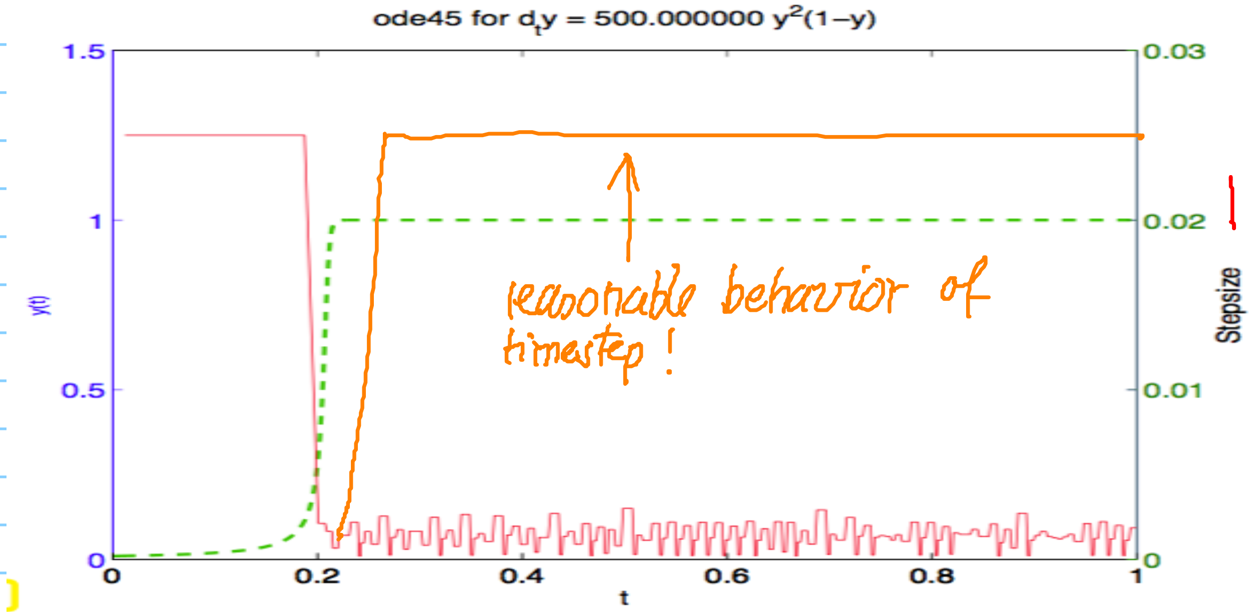
$$\dot{y} = \lambda y^2(1-y^2)$$



ode45: crazy no. of timesteps to produce a very poor approximation of a nearly constant solution!

reasonable timesteps

Fig. 35



reasonable behavior of timestep!

②

What's wrong with RK-SSM underlying ODE45 ?

12.1 Model problem analysis

Example : Explicit Euler method for $\dot{y} = \lambda y$, uniform h
$[\, y(0) = 1 \,,\ \lambda < 0 \,]$ [decay equation]

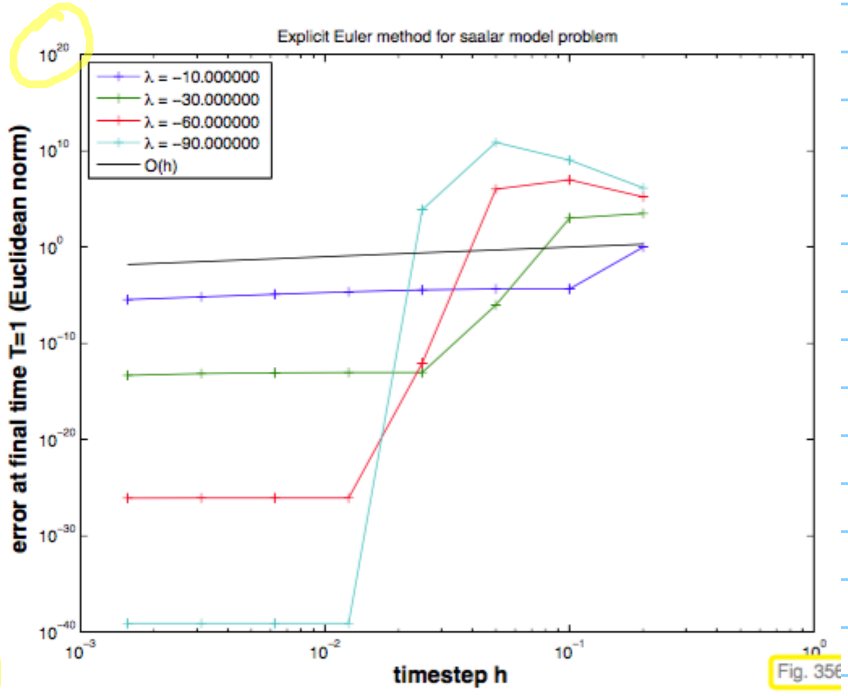


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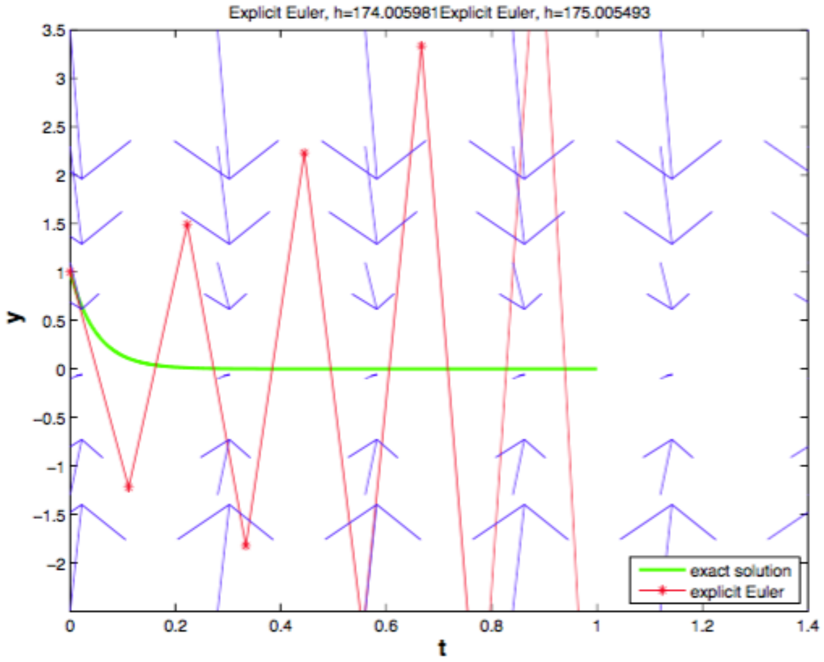
Fig. 356

→ blow-up for large $|\lambda h|$



◁ Exponentially growing oscillations due to overshooting

Analysis : Expl. Eul. $\quad y_{k+1} = y_k + h\lambda y_k$

$$\Rightarrow \quad y_k = (1 + h\lambda)^k y_0 \quad , \; k = 1, \dots, N$$

$$\text{blow-up} \Leftrightarrow \quad |1 + h\lambda| > 1$$

For $\lambda < 0$ we want $y_k \to 0 \Leftrightarrow |1 + h\lambda| < 1$

If $\lambda < 0$, $|h\lambda| > 2 \Rightarrow$ blow-up

Necessary is $|h\lambda| \leq 2 \Rightarrow$ timestep constraint $h < \frac{2}{|\lambda|}$

Experiment : Adaptive timestepping (expl. Euler, expl. trap.)
for decay equation with $\lambda \ll 0$
$[\, \lambda = -100 \,]$

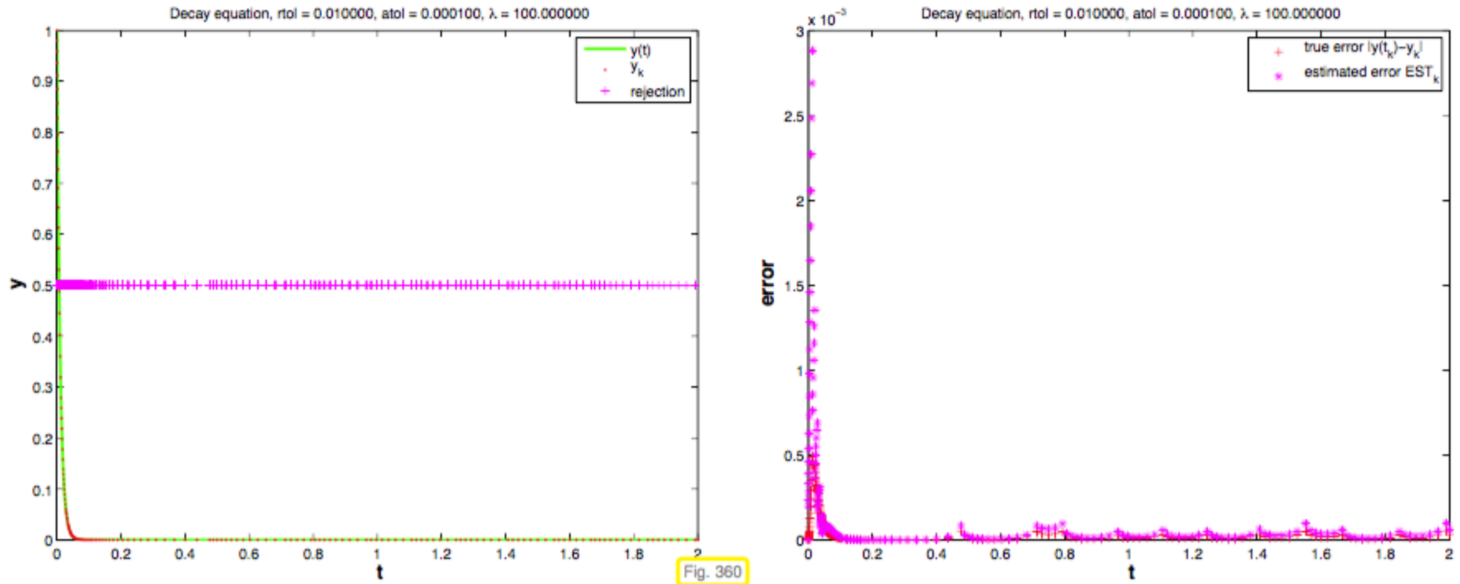


Fig. 360

→ adaptive timestepping detects time step constraints

→ small timesteps throughout (inefficient)

Is this a flaw of explicit Euler ?

Example: Explicit trapezoidal method [2 stage RK-SSM]

$$\dot{y} = \lambda y \quad \Rightarrow \quad y_1 = \underbrace{(1 + \lambda h + \tfrac{1}{2}(\lambda h)^2)}_{=:\, S(\lambda h)} y_0$$

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

No blow-up $\Leftrightarrow$ $|S(\lambda h)| \leq 1$

$[\lambda < 0]$ $\Leftrightarrow$ $-2 < \lambda h < 0$ → timestep constraint

For general explicit RK-SSM : $\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array}$ [Butcher scheme]

applied $\dot{y} = \lambda y$, $\lambda \in \mathbb{R}$

Definition 11.4.9. Explicit Runge-Kutta method

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{i-1} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an s-stage explicit Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h \sum_{j=1}^{i-1} a_{ij} \mathbf{k}_j) \;, \quad i = 1,\dots,s \quad , \quad \mathbf{y}_1 := \mathbf{y}_0 + h \sum_{i=1}^{s} b_i \mathbf{k}_i \,.$$

The vectors $\mathbf{k}_i \in \mathbb{R}^d$, $i = 1,\dots,s$, are called increments, $h > 0$ is the size of the timestep.

$$f(t,y) = \lambda y \quad \Rightarrow \quad \begin{aligned} k_i &= \lambda (y_0 + h \sum_{j=1}^{i-1} a_{ij} k_j) \\ y_1 &= y_0 + h \sum_{i=1}^{s} b_i k_i \end{aligned} \qquad (*)$$

$$(*) \Rightarrow \begin{bmatrix} I - z\mathfrak{A} & 0 \\ -z\underline{b}^T & 1 \end{bmatrix} \begin{bmatrix} \underline{k} \\ y_1 \end{bmatrix} = y_0 \underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{\mathbb{1}}$$

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

$$\Rightarrow \quad y_1 = y_0 + z\underline{b}^T (I - z\mathfrak{A})^{-1} \mathbb{1}\, y_0$$

$$= \underbrace{S(z)}_{\in \mathbb{R}} y_0$$

Theorem 12.1.15. Stability function of explicit Runge-Kutta methods → [32, Thm. 77.2], [45, Sect. 11.8.4]

The discrete evolution Ψ^h_λ *of an explicit* s*-stage Runge-Kutta single step method (→ Def. 11.4.9) with Butcher scheme* $\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array}$ *(see (11.4.11)) for the ODE* $\dot{y} = \lambda y$ *amounts to a multiplication with the number*

$$\Psi^h_\lambda = S(\lambda h) \quad \Leftrightarrow \quad y_1 = S(\lambda h) y_0$$

where S *is the* *stability function*

$$S(z) := 1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1} = \det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T), \quad \mathbf{1} = [1,\dots,1]^T \in \mathbb{R}^s . \qquad (12.1.16)$$

↳ from Cramer's rule

▷ RK-sequence (uniform timestep $h>0$) : $y_k = S(z)^k y_0$

Examples :

- Explicit Euler method (11.2.7): $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$ ➤ $S(z) = 1 + z$
- Explicit trapezoidal method (11.4.6): $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$ ➤ $S(z) = 1 + z + \frac{1}{2}z^2$
- Classical RK4 method: $\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array}$ ➤ $S(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4$

$$\Updownarrow$$

$$e^z = 1 + z + \tfrac{1}{2}z^2 + \tfrac{1}{6}z^3 + \tfrac{1}{24}z^4 + \dots$$

Corollary 12.1.18. Polynomial stability function of explicit RK-SSM

For a consistent (→ Def. 11.3.10) s*-stage explicit Runge-Kutta single step method according to Def. 11.4.9 the stability function* S *defined by* (12.1.16) *is a non-constant polynomial of degree* $\leq s$*:* $S \in \mathcal{P}_s$.

$\Rightarrow \quad |S(z)| \longrightarrow \infty \quad$ as $\quad |z| \longrightarrow \infty$

$\Rightarrow$ Timestep constraint to avoid blow-up for $\dot{y} = \lambda y$

↳ $|\lambda| h$ sufficiently small $\underbrace{\text{to avoid blow-up}}$

$\Leftrightarrow \quad |S(\lambda h)| \leq 1$

Only if one ensures that $|\lambda h|$ is sufficiently small, one can avoid exponentially increasing approximations y_k (qualitatively wrong for $\lambda < 0$) when applying an explicit RK-SSM to the model problem (12.1.3) with uniform timestep $h > 0$,

Model problem analysis for linear systems of ODEs

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

LA : Solved by diagonalization [Note: $\lambda_i \in \mathbb{C}$]

$$\boxed{\mathbf{V}^{-1}\mathbf{M}\mathbf{V} = \mathbf{D} = \mathrm{diag}(\underset{\uparrow}{\lambda_1}, \dots, \underset{\uparrow}{\lambda_d})}$$

eigenvalues

$\mathbf{z} = \mathbf{V}^{-1}\mathbf{y} \quad \Rightarrow \quad \dot{\mathbf{z}} = \mathbf{D}\mathbf{z}$

$\triangleq$ decoupled scalar linear ODEs

⑤ Explicit Euler method for $\dot{y} = My$: diagonalization

$$y_{k+1} = y_k + hMy_k$$

$$z_k = V^{-1}y_k \qquad z_{k+1} = z_k + hV^{-1}MVV^{-1}y_k = (I+hD)z_k$$

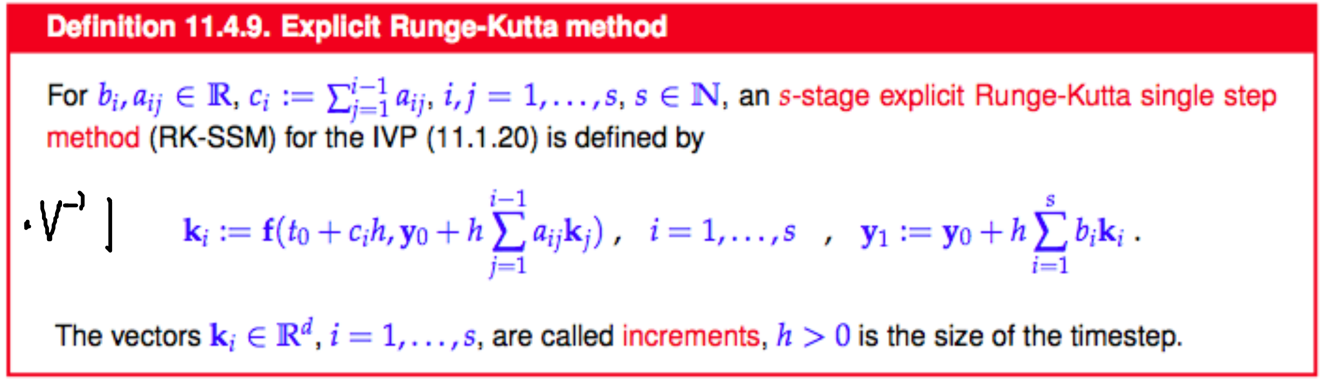
$$\Rightarrow (z_{k+1})_i = (1+h\lambda_i)(z_k)_i \quad [\text{decoupled}]$$

To avoid blow-up ensure $|1+h\lambda_i| \leq 1 \quad \forall i=1,\dots,d$

[also for $\lambda_i \in \mathbb{C}$] $\Leftrightarrow$ $h|\lambda_i| \leq 2$ timestep constraint

General RK-SSM applied to $\dot{y} = My$

$$[\quad V^{-1}MV = D = \text{diag}(\lambda_1,\dots,\lambda_d) \quad]$$



Definition 11.4.9. Explicit Runge-Kutta method

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{i-1} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an s-stage explicit Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

$\cdot V^{-1}$]

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j)\,, \quad i = 1,\dots,s \quad , \quad \mathbf{y}_1 := \mathbf{y}_0 + h\sum_{i=1}^{s} b_i \mathbf{k}_i\,.$$

The vectors $\mathbf{k}_i \in \mathbb{R}^d$, $i = 1,\dots,s$, are called increments, $h > 0$ is the size of the timestep.

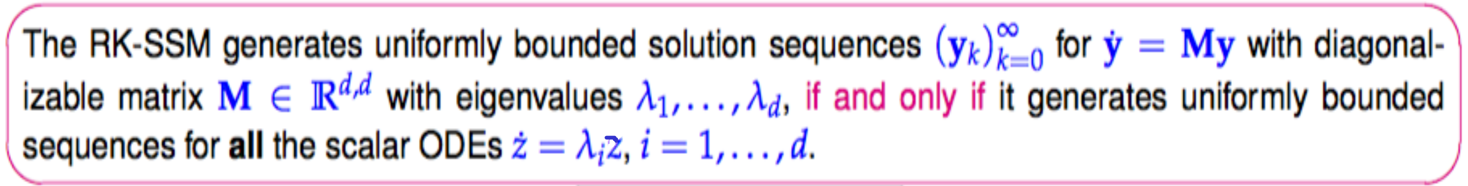
$f(y) = My$, transformed increments : $\hat{k}_i = V^{-1}k_i$

$$z_k = V^{-1}y_k$$

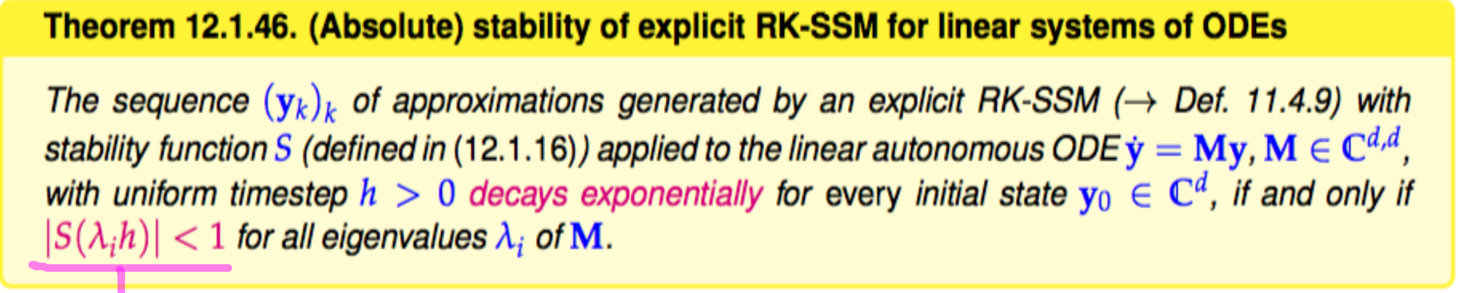
$$\Rightarrow \begin{aligned} \hat{k}_i &= D(z_0 + h\sum_j a_{ij}\hat{k}_j) \\ z_1 &= z_0 + h\sum_{i=1}^{s} b_i \hat{k}_i \end{aligned} \quad \Rightarrow \text{decoupled}$$

$$(\hat{k}_i)_\ell = \lambda_\ell[(z_0)_\ell + h\sum a_{ij}(\hat{k}_j)_\ell]$$

$\hookrightarrow$ Increment equation of RK-SSM applied to $\dot{z} = Dz$.

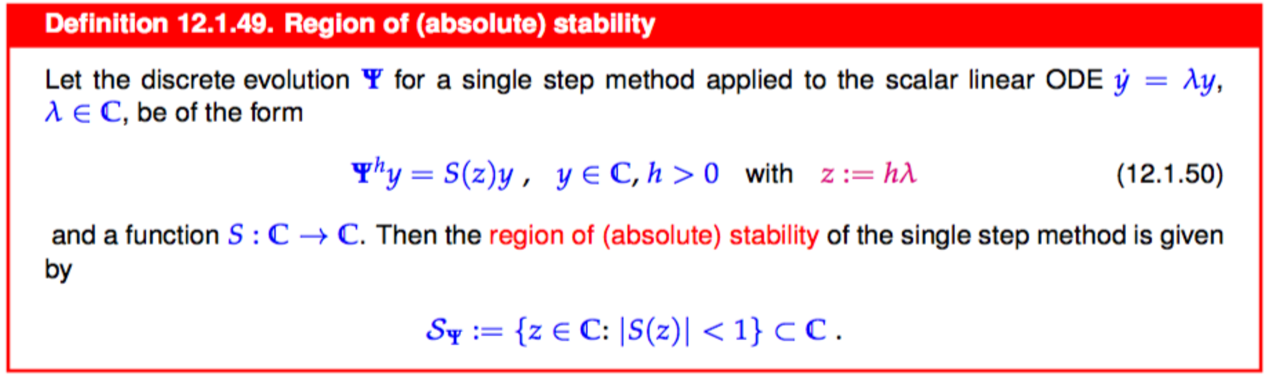


The RK-SSM generates uniformly bounded solution sequences $(\mathbf{y}_k)_{k=0}^{\infty}$ for $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$ with diagonalizable matrix $\mathbf{M} \in \mathbb{R}^{d,d}$ with eigenvalues $\lambda_1,\dots,\lambda_d$, if and only if it generates uniformly bounded sequences for **all** the scalar ODEs $\dot{z} = \lambda_i z$, $i = 1,\dots,d$.



Theorem 12.1.46. (Absolute) stability of explicit RK-SSM for linear systems of ODEs

The sequence $(\mathbf{y}_k)_k$ of approximations generated by an explicit RK-SSM (→ Def. 11.4.9) with stability function S (defined in (12.1.16)) applied to the linear autonomous ODE $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$, $\mathbf{M} \in \mathbb{C}^{d,d}$, with uniform timestep $h > 0$ decays exponentially for every initial state $\mathbf{y}_0 \in \mathbb{C}^d$, if and only if $|S(\lambda_i h)| < 1$ for all eigenvalues λ_i of $\mathbf{M}$.



Definition 12.1.49. Region of (absolute) stability

Let the discrete evolution Ψ for a single step method applied to the scalar linear ODE $\dot{y} = \lambda y$, $\lambda \in \mathbb{C}$, be of the form

$$\Psi^h y = S(z)y\,,\quad y \in \mathbb{C}, h > 0 \quad \text{with} \quad z := h\lambda \tag{12.1.50}$$

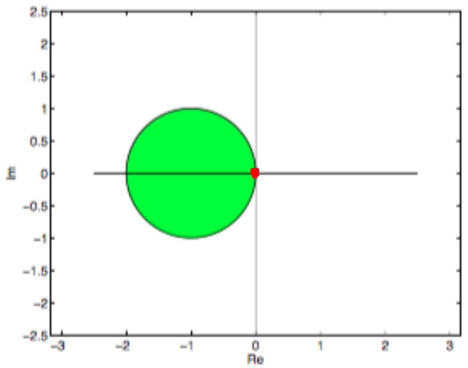
and a function $S : \mathbb{C} \to \mathbb{C}$. Then the region of (absolute) stability of the single step method is given by

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

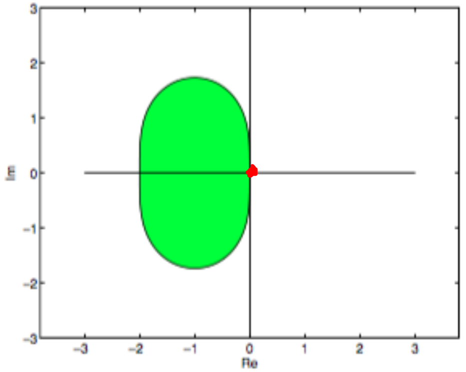
Why $\mathbb{C}$? → because of complex eigenvalues of M

If S_Ψ is bounded $\Rightarrow$ Timestep constraint to avoid blow-up.

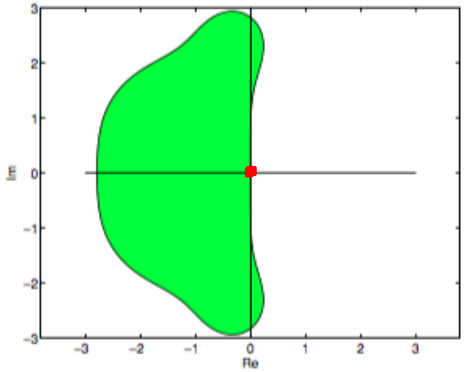
Examples :



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



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



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

$|1+z| < 1$

Remark: $0 \in \partial S_\Psi$, because $S(z) = 1 + z + O(|z|^2)$ for consistent SSM.

boundary

12.2. Stiff IVPs

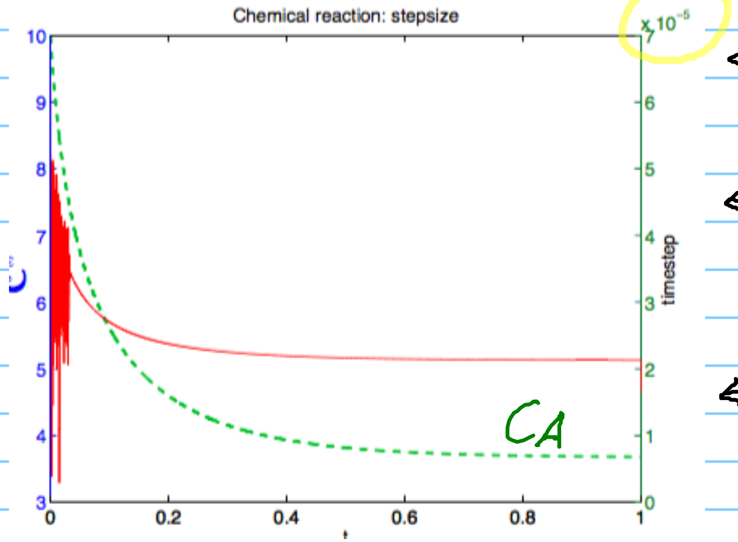
Example : Chemical reaction

reaction: $\underbrace{A + B \underset{k_1}{\overset{k_2}{\rightleftarrows}} C}_{\text{fast reaction}}$, $\underbrace{A + C \underset{k_3}{\overset{k_4}{\rightleftarrows}} D}_{\text{slow reaction}}$

reaction constants: $\boxed{k_1, k_2 \gg k_3, k_4}$

Mathematical model: non-linear ODE involving concentrations $\mathbf{y}(t) = (c_A(t), c_B(t), c_C(t), c_D(t))^T$

$$\dot{\mathbf{y}} := \frac{d}{dt}\begin{bmatrix} c_A \\ c_B \\ c_C \\ c_D \end{bmatrix} = \mathbf{f}(\mathbf{y}) := \begin{bmatrix} -k_1 c_A c_B + k_2 c_C - k_3 c_A c_C + k_4 c_D \\ -k_1 c_A c_B + k_2 c_C \\ k_1 c_A c_B - k_2 c_C - k_3 c_A c_C + k_4 c_D \\ k_3 c_A c_C - k_4 c_D \end{bmatrix} . \qquad (12.2.3)$$



◁ Explicit adaptive RK-SSM

← tiny timesteps though solution does not change much

← Looks like stability induced timestep constraint

Discussion : linear system : $\dot{y} = My$

EVs $\lambda_1, \dots, \lambda_d$:

- There is a λ_j : $\operatorname{Re}\lambda_j \gg 0$ → blow-up of exact solution

[Note: $\operatorname{Re}\lambda$ in $y(t) = e^{\lambda t}$ governs decay/growth :

$$|e^{\lambda t}| = e^{\operatorname{Re}(\lambda t)}$$]

⇒ Blow-up of (y_k) is even desirable

- $\underbrace{\mathrm{Re}\,\lambda_j \leq 0}\ \forall j$ and $|\mathrm{Re}\,\lambda_\ell| \gg 1$

→ Exact solution remains bounded

→ Blow-up of numerical solution disastrous !

→ Avoid blow-up ! → time step constraint ! $\lrcorner$

Example : Strongly attractive limit cycle

ODE : $\dot{\mathbf{y}} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \mathbf{y} + \lambda(1-\|\mathbf{y}\|^2)\,\mathbf{y}$

$\|\mathbf{y}(0)\|_2 = 1 \Rightarrow \|\mathbf{y}(t)\|_1 = 1 \quad \forall t$

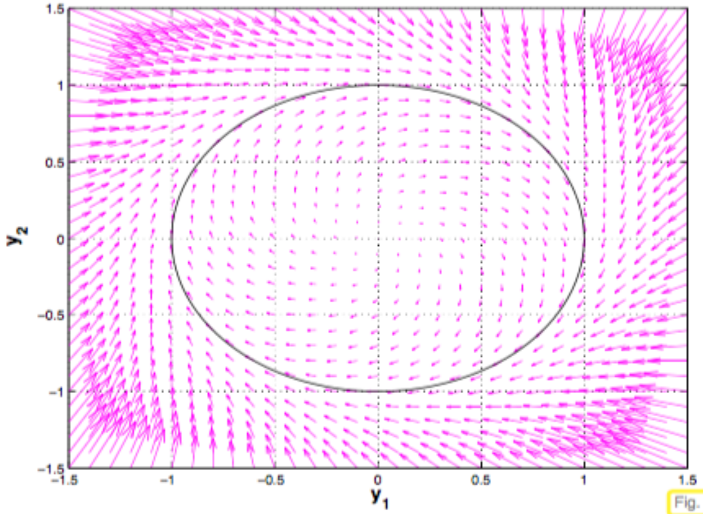


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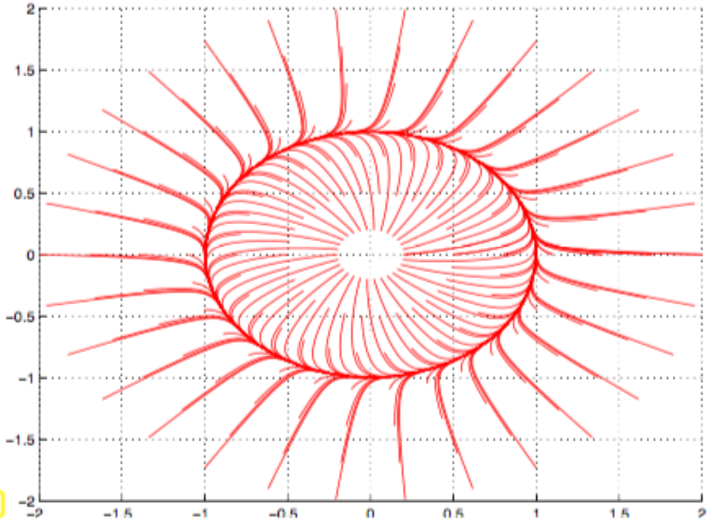
Fig. 369

vectorfield $\mathbf{f}$ ($\lambda = 1$)



solution trajectories ($\lambda = 10$)

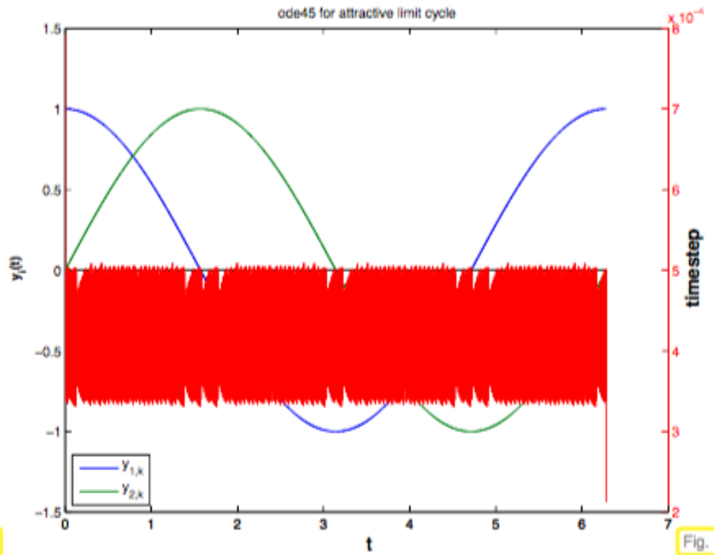


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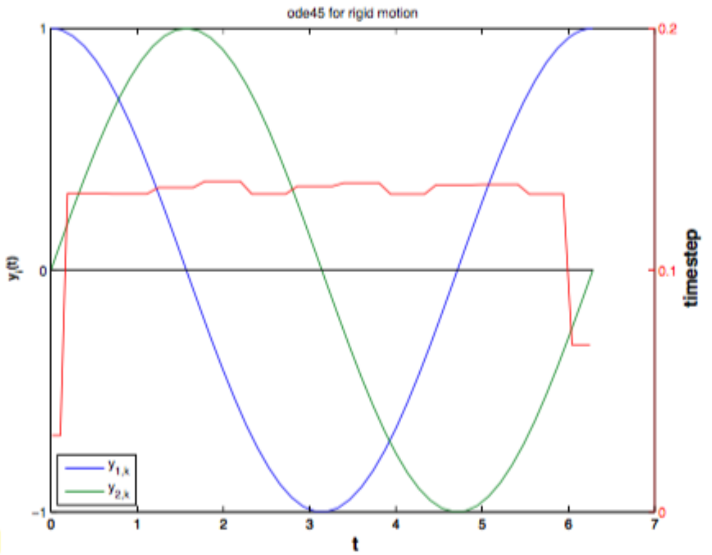
Fig. 371

many (3794) steps ($\lambda = 1000$)



accurate solution with few steps ($\lambda = 0$)

Notion 12.2.9. Stiff IVP

An initial value problem is called stiff, if stability imposes much tighter timestep constraints on *explicit single step methods* than the accuracy requirements.

Heuristic considerations for predicting stiffness :

- Linear ODEs $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$: ✓
- General ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$, stiffness state dependent

Stiff at state $\mathbf{y}^* \in \mathbf{y}(t)$?

Tool : Linearization $\mathbf{f}(\mathbf{y}) \approx \mathbf{f}(\mathbf{y}^*) + D\mathbf{f}(\mathbf{y}^*)(\mathbf{y}-\mathbf{y}^*)$

▷ "Close" to $\mathbf{y}^*$ solutions of $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ will behave like solutions of the linearized ODE

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{y}^*) + D\mathbf{f}(\mathbf{y}^*)(\mathbf{z}-\mathbf{y}^*) \qquad (L)$$

⑧ (L) ≙ affine linear ODE

Linearization of explicit RK-SSM

Definition 11.4.9. Explicit Runge-Kutta method

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{i-1} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an s-stage explicit Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

$$\mathbf{k}_i := \mathbf{f}(\cancel{t_0 + c_i h}, \mathbf{y}_0 + h\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j)\ , \quad i = 1,\dots,s \quad , \quad \mathbf{y}_1 := \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\ .$$

The vectors $\mathbf{k}_i \in \mathbb{R}^d$, $i = 1,\dots,s$, are called increments, $h > 0$ is the size of the timestep.

$y_0 := y^*$: $\quad k_i \doteq f(y^*) + Df(y^*)\, h \sum_{j=1}^{i-1} a_{ij} k_j$

≙ increment equ. for RK-SSM applied to (L) !

→ For small h RK-SSM at state y^* will behave like the same $\underbrace{\text{RK-SSM applied to (L)}}_{\text{amenable to linear model problem analysis}}$ at y^*.

for small timestep the behavior of an explicit RK-SSM applied to $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ close to the state $\mathbf{y}^*$ is determined by the eigenvalues of the Jacobian $D\,\mathbf{f}(\mathbf{y}^*)$.

How to distinguish stiff initial value problems

An initial value problem for an autonomous ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ will probably be stiff, if, for substantial periods of time,

$$\min\{\operatorname{Re}\lambda :\ \lambda \in \sigma(D\,\mathbf{f}(\mathbf{y}(t)))\} \ll 0\,, \tag{12.2.15}$$

$$\max\{\operatorname{Re}\lambda, 0 :\lambda \in \sigma(D\,\mathbf{f}(\mathbf{y}(t)))\} \approx 0\,, \tag{12.2.16}$$

where $t \mapsto \mathbf{y}(t)$ is the solution trajectory and $\sigma(\mathbf{M})$ is the spectrum of the matrix $\mathbf{M}$, see Def. 7.1.1.

Examples :

- $\dot{y} = f(y) := \lambda y^2(1-y)\ , \quad \lambda \gg 1$

$$Df(y) = 2\lambda y(1-y) - \lambda y^2 \begin{cases} \ll 0 & \text{if } y \approx 1 \\ \approx 0 & \text{for } y \approx 0 \end{cases}$$

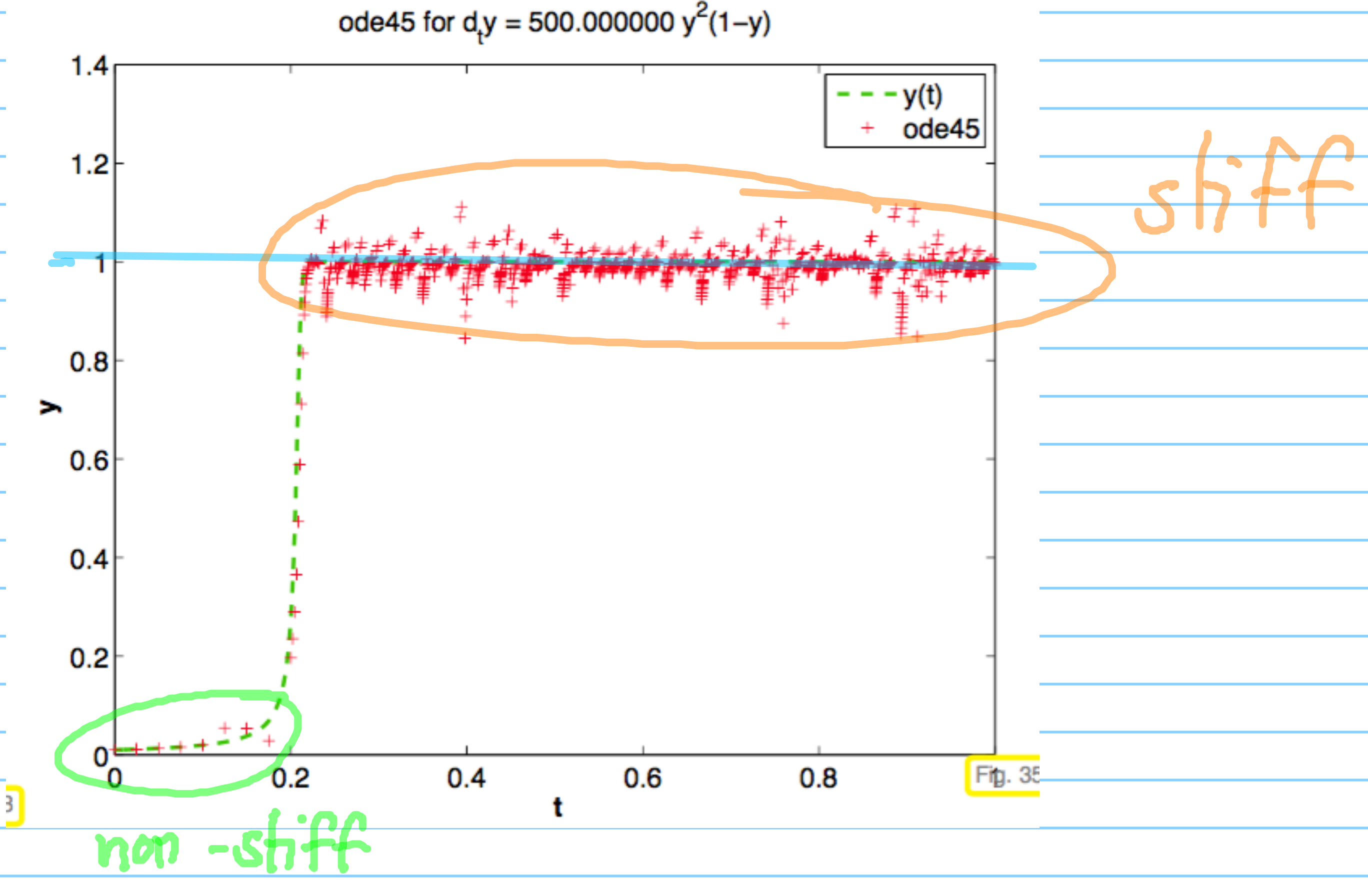


Fig. 35

- $\mathbf{f}(\mathbf{y}) := \begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\mathbf{y} + \lambda(1 - \|\mathbf{y}\|_2^2)\,\mathbf{y}\ , \quad \lambda \gg 1$

$$Df(y) = \begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix} + \lambda\{-2yy^T + (1 - \|y\|_2^2)I\}$$

$$\|y\|_2 = 1 \Rightarrow \sigma(Df(y)) = -\lambda \pm \sqrt{\lambda^2 - 1}$$

[$\dot{y} = \lambda y(1-y)$, stiffness conditional on y_0]
$\lambda \gg 1$

12.3. Implicit Runge-Kutta single step methods

12.3.1. The implicit Euler method for stiff IVPs

Imp. Eul.: $\quad y_{k+1} = y_k + hf(y_{k+1})$

Linear model problem analysis: apply to $\dot{y} = \lambda y$

$\rightarrow \quad y_{k+1} = \frac{1}{(1-h\lambda)} y_k \quad$ [uniform timestep h]

$\Rightarrow \quad y_{k+1} = \left[\frac{1}{1-h\lambda}\right]^k y_0$

If $\lambda < 0 \Rightarrow \left|\frac{1}{1-h\lambda}\right| < 1 \Rightarrow \lim\limits_{k\to 0} y_k = 0$ for all $h > 0$!

$\rightarrow$ No stability induced timestep constraint

Same result for linear ODEs: $\dot{y} = My$, $M \in \mathbb{R}^{d,d}$
[by diagonalization]

For any timestep, the implicit Euler method generates exponentially decaying solution sequences $(\mathbf{y}_k)_{k=0}^{\infty}$ for $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$ with diagonalizable matrix $\mathbf{M} \in \mathbb{R}^{d,d}$ with eigenvalues $\lambda_1, \dots, \lambda_d$, if $\operatorname{Re}\lambda_i < 0$ for all $i = 1, \dots, d$.

Implicit Euler: order 1

12.3.2. Collocation SSM

First step of SSM for IVP: $\dot{y} = f(y)$, $y(0) = y_0$

$\rightarrow y_1$, stepsize h

(i) On $[0,h]$ approximate $y(t) \approx y_h(t) \in V$

$V \hat{=}$ finite-dim. space of functions $[0,h] \rightarrow \mathbb{R}^d$

Standard choice: $V = (\mathcal{P}_s)^d$, $\dim V = s+1$

(ii) Selection of y_h through collocation conditions

$$\left\{\begin{array}{l} y_h(0) = y_0 \;,\quad \dot{y}_h(\tau_j) = f(y_h(\tau_j)) \\ \text{for collocation points } 0 \leq \tau_1 \leq \ldots \leq \tau_s \leq h \end{array}\right.$$

$\rightarrow$ $s+1$ equations

(iii) $y_1 = y_h(h)$

Collocation points from reference interval $[0,1]$: $\tau_j = c_j h$

$$0 \leq c_1 \leq c_2 \leq \ldots \leq c_s \leq 1$$

$$\dot{y}_h \in (\mathcal{P}_{s-1})^d \Rightarrow \dot{y}_h(\tau h) = \sum_{j=1}^{s} \dot{y}_h(hc_j) L_j(\tau) \,,\quad 0 \leq \tau \leq 1$$

$\{L_j\}_{j=1}^{s} \hat{=}$ Lagrange polynomials of degree $s-1$ for node set $\{c_j\}_{j=1}^{s}$: $L_j(c_i) = \delta_{ij}$

from coll. cond.

$$\Rightarrow \quad \dot{y}_h(\tau h) = \sum_{j=1}^{s} f(y_h(c_j h)) L_j(\tau)$$

$\int_0^\xi \ldots d\tau$

$$\Rightarrow \quad y_h(\xi h) - \underbrace{y_h(0)}_{y_0} = h \sum_{j=1}^{s} \underbrace{f(y_h(c_j h))}_{=:\, k_j} \int_0^\xi L_j(\tau)\, d\tau$$

$\xi = c_i$ $\quad y_h(c_i h)$

$\xi = 1$

$$\mathbf{k}_i = f(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j) \,, \qquad a_{ij} := \int_0^{c_i} L_j(\tau)\,\mathrm{d}\tau \,,$$

$$\mathbf{y}_1 := \mathbf{y}_h(t_1) = \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i \,. \quad \text{where} \quad b_i := \int_0^1 L_i(\tau)\,\mathrm{d}\tau \,. \qquad (12.3.11)$$

Collocation single step method (CL-SSM)

$\rightarrow$ $s > 1$: k_i to be determined by solving a system of equations $\rightarrow$ implicit method

CL-SSM applied to $\dot{y} = f(t)$, $y(0) = 0$

$$y_1 = h \sum_{i=1}^{s} b_i f(c_i h) \quad , \quad b_i = \int_0 L_i(\tau)\,d\tau$$

$\hat{=}$ a polynomial quadrature formulas $\downarrow$ weights

Convergence of CL-SSM:

$\dot{y} = 10y(1-y)$, $y_0 = 0.01$, $T = 1$

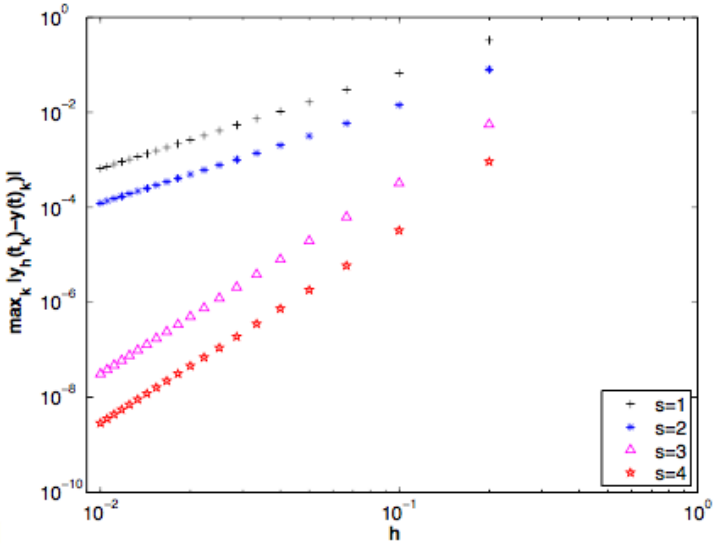
❶ Equidistant collocation points, $c_j = \frac{j}{s+1}$, $j = 1,\cdots,s$.

We observe algebraic convergence with the empiric rates

$s = 1 \;:\; p = 1.96$
$s = 2 \;:\; p = 2.03$
$s = 3 \;:\; p = 4.00$
$s = 4 \;:\; p = 4.04$

} same as orders of polynomial quad. rules with nodes c_j.

Fig. 374



❶ Gauss points in $[0,1]$ as normalized collocations points c_j , $j = 1,\ldots,s$.

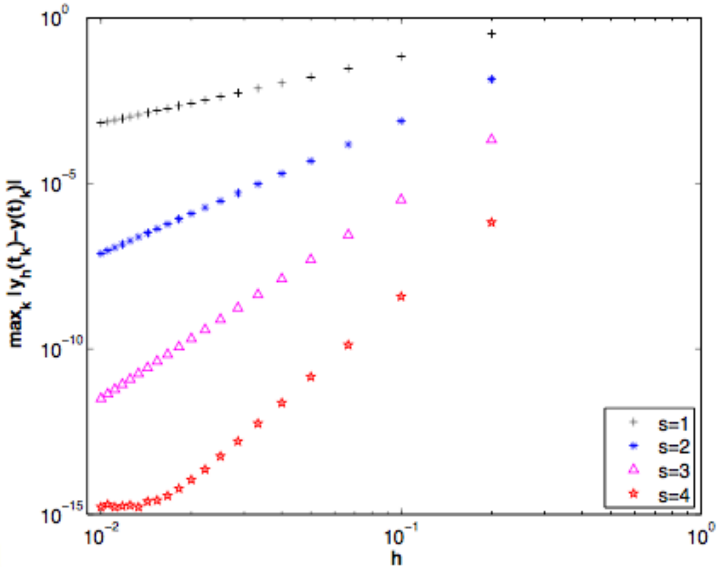
We observe algebraic convergence with the empiric rates

$s = 1 \;:\; p = 1.96$
$s = 2 \;:\; p = 4.01$
$s = 3 \;:\; p = 6.00$
$s = 4 \;:\; p = 8.02$

} order $2s$ = order of s-pt. Gauss quad.

Gauss collocation SSM

Fig. 375



Theorem 12.3.17. Order of collocation single step method [13, Satz .6.40]

Provided that $\mathbf{f} \in C^p(I \times D)$, *the order (→ Def. 11.3.21) of an* s*-stage collocation single step method according to* (12.3.11) *agrees with the order (→ Def. 5.3.1) of the quadrature formula on* $[0,1]$ *with nodes* c_j *and weights* b_j, $j = 1,\ldots,s$.

$$\mathbf{k}_i = f(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,, \quad \text{where} \quad a_{ij} := \int_0^{c_i} L_j(\tau)\,\mathrm{d}\tau\,, \qquad (12.3.11)$$

$$\mathbf{y}_1 := \mathbf{y}_h(t_1) = \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\,. \qquad b_i := \int_0^{1} L_i(\tau)\,\mathrm{d}\tau\,.$$

Definition 11.4.9. Explicit Runge-Kutta method

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{i-1} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an s-stage explicit Runge-Kutta single step method (RK-SSM) for the ODE $\dot{\mathbf{y}} = \mathbf{f}(t,\mathbf{y})$, $\mathbf{f}: \Omega \to \mathbb{R}^d$, is defined by ($\mathbf{y}_0 \in D$)

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j)\,, \quad i = 1,\dots,s \quad , \quad \mathbf{y}_1 := \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\,.$$

The vectors $\mathbf{k}_i \in \mathbb{R}^d$, $i = 1,\dots,s$, are called increments, $h > 0$ is the size of the timestep.

Definition 12.3.18. General Runge-Kutta single step method (*cf.* Def. 11.4.9)

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{s} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an s-stage Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,, \quad i = 1,\dots,s \quad , \quad \mathbf{y}_1 := \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\,.$$

As before, the $\mathbf{k}_i \in \mathbb{R}^d$ are called increments.

General Butcher scheme notation for RK-SSM

Shorthand notation for Runge-Kutta methods

Butcher scheme ▷

$$\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}\,. \qquad (12.3.20)$$

Note: now $\mathfrak{A}$ can be a general $s \times s$-matrix.

K_i obtained by solving increment equations iteratively (simplified Newton method)

↳ freeze Jacobian

Stages : $g_i = h\sum_{j=1}^{s} a_{ij} k_j \Leftrightarrow k_i = f(y_0 + g_i)$

Focus on d=1: $= h\sum a_{ij} f(y_0 + g_j)$

$$\Updownarrow$$

$$\vec{g} = \begin{bmatrix} g_1 \\ \vdots \\ g_s \end{bmatrix} \in \mathbb{R}^s \; : \quad F(\vec{g}) = 0$$

$$F(\vec{g}) = \vec{g} - h\mathcal{A}\begin{bmatrix} f(y_0 + g_1) \\ \vdots \\ f(y_0 + g_s) \end{bmatrix}$$

Initial guess for simplified Newton: (h is small)

$$\vec{g}^{(0)} = 0$$

$$DF(0) = I - h\mathcal{A}\begin{bmatrix} \frac{\partial f}{\partial y}(y_0 + 0) & & \\ & \ddots & \\ & & \frac{\partial f}{\partial y}(y_0 + 0) \end{bmatrix}$$

$$= I - h\frac{\partial f}{\partial y}(y_0)\mathcal{A}$$

▷ Iteration: $$\vec{g}^{(\ell+1)} = \vec{g}^{(\ell)} - \underset{\substack{\uparrow \\ \text{invertible for } h \text{ small enough}}}{DF(\underline{0})^{-1}} F(\vec{g}^{(\ell)})$$

17.12.15 : Recap

- Stiffness
- Implicit Euler methods is unconditionally stable for $\dot{y} = \lambda y$, $\lambda < 0$
- Collocation RK-SSM (includes implicit Euler: $s = 1$, $c_s = 1$)

$$\mathbf{k}_i = f(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,, \qquad \text{where} \quad a_{ij} := \int_0^{c_i} L_j(\tau)\,\mathrm{d}\tau\,,$$
$$\mathbf{y}_1 := \mathbf{y}_h(t_1) = \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\,. \qquad b_i := \int_0^1 L_i(\tau)\,\mathrm{d}\tau\,. \tag{12.3.11}$$

$$s = 1,\ c_1 = 1 \Rightarrow a_{11} = b_1 = \int_0^1 L_1(\tau)d\tau = \int_0^1 1 d\tau = 1$$

12.3.4. Model problem analysis for implicit RK-SSM

Apply RK-SSM to $\dot{y} = \lambda y \Rightarrow y_1 = S(z)\, y_0$

$z := \lambda h$

Definition 12.3.18. General Runge-Kutta single step method (*cf.* Def. 11.4.9)

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{s} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an *s*-stage Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,,\quad i = 1,\dots,s \quad,\quad \mathbf{y}_1 := \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\,.$$

As before, the $\mathbf{k}_i \in \mathbb{R}^d$ are called increments.

$f(t,y) := \lambda y$:

▶ $$k_i = \lambda(y_0 + h\sum_{j=1}^{i-1} a_{ij}k_j)\,, \qquad \Rightarrow \quad \begin{bmatrix} \mathbf{I} - z\mathfrak{A} & 0 \\ -z\mathbf{b}^\top & 1 \end{bmatrix} \begin{bmatrix} \mathbf{k} \\ y_1 \end{bmatrix} = y_0 \begin{bmatrix} \mathbf{1} \\ 1 \end{bmatrix}$$
$$y_1 = y_0 + h\sum_{i=1}^{s} b_i k_i$$

▷ $$S(z) := \underbrace{1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1}}_{\text{stability function}} = \frac{\det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T)}{\det(\mathbf{I} - z\mathfrak{A})}\,, \quad z := \lambda h$$

$\uparrow$ $\Downarrow$

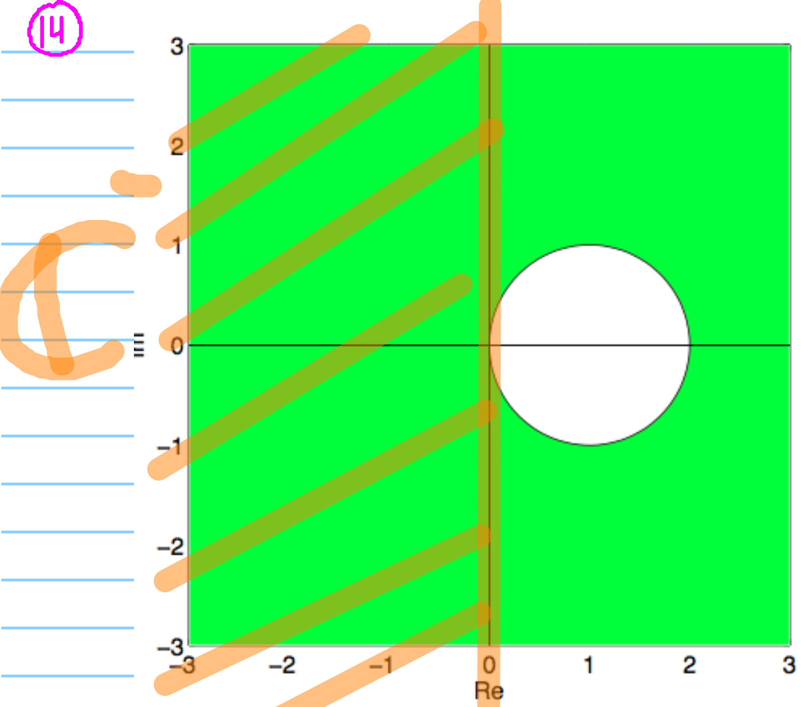
rational function : $S(z) = \dfrac{P(z)}{Q(z)}$, $P, Q \in \mathcal{P}_s$

Example:

- Impl. Euler: $\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \Rightarrow S(z) = \dfrac{1}{1-z}$

Region of stability: $\lim_{|z|\to\infty} S(z) = 0$

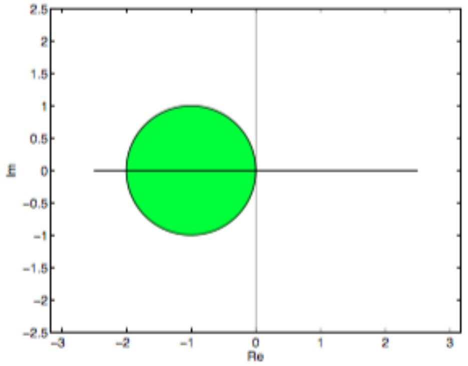
$$S_\Psi := \{z \in \mathbb{C} : |S(z)| < 1\} = \{z \in \mathbb{C} : |z-1| > 1\}$$



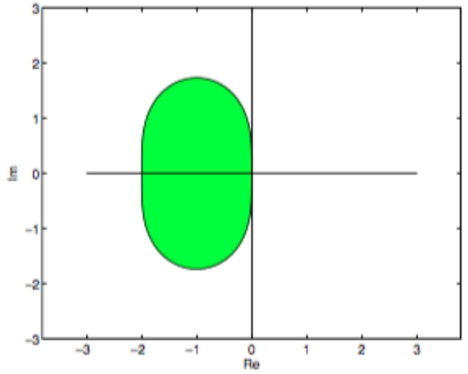
$\mathcal{S}_\Psi$: implicit Euler method (??)

▷ A-stable

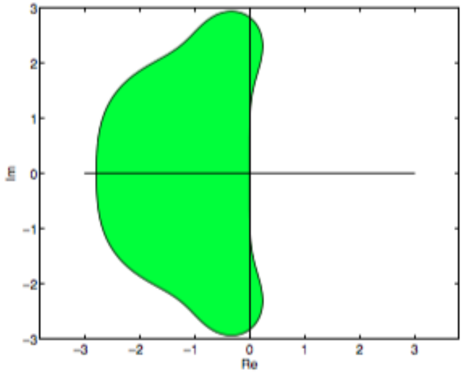
$\Updownarrow$



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



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



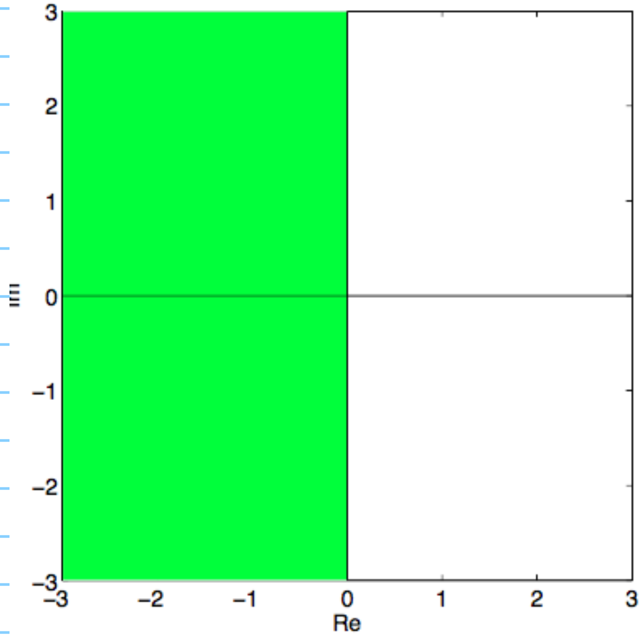
$\mathcal{S}_\Psi$: classical RK4 method

order 2s !

- Implicit midpoint rule: $[\, s = 1,\ c_1 = \frac12,\ b_1 = 1,\ a_{11} = \frac12 \,]$

= Gauss collocation RK-SSM

$$\begin{array}{c|c} \frac12 & \frac12 \\ \hline & 1 \end{array} \Rightarrow S(z) = \frac{1+\frac12 z}{1-\frac12 z}$$



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

$\mathcal{S}_\Psi = \mathbb{C}^-$

→ unconditional stability

→ ideal region of stability :

$\operatorname{Re}\lambda < 0 \Rightarrow h\lambda \in \mathcal{S}_\Psi$

$\Rightarrow$ decaying (y_k)

$\operatorname{Re}\lambda > 0 \Rightarrow |S(h\lambda)| > 1$

$\Rightarrow$ growing (y_k)

$\Updownarrow$

exact match for growth/decay of exact solution $y(t) = Ce^{\lambda t}$

Theorem 12.3.35. Region of stability of Gauss collocation single step methods [13, Satz 6.44]

s-stage Gauss collocation single step methods defined by (12.3.11) with the nodes c_s given by the s Gauss points on $[0,1]$, feature the "ideal" stability domain:

$$\mathcal{S}_\Psi = \mathbb{C}^- . \tag{12.3.34}$$

In particular, all Gauss collocation single step methods are A-stable.

⑮ A-stable = unconditionally stable for decay equ.

Definition 12.3.32. A-stability of a Runge-Kutta single step method

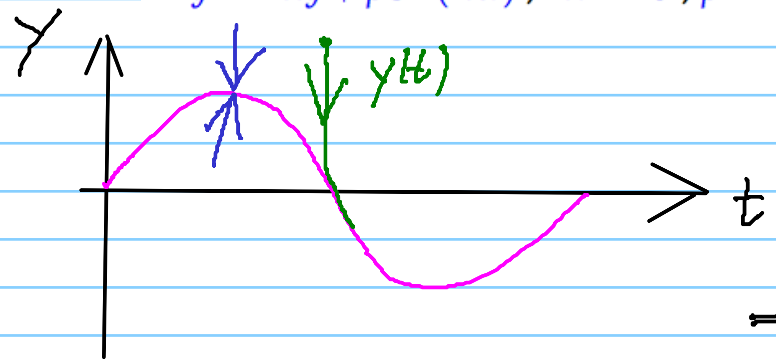
A Runge-Kutta single step method with stability function S is A-stable, if

$$\mathbb{C}^- := \{z \in \mathbb{C}\colon \mathrm{Re}\, z < 0\} \subset \mathcal{S}_\Psi . \quad (\mathcal{S}_\Psi \mathrel{\hat{=}} \text{region of stability Def. 12.1.49})$$

A-stable Runge-Kutta single step methods will not be affected by stability induced timestep constraints when applied to stiff IVP (→ Notion 12.2.9).

The catch :

Example : $\dot{y} = -\lambda y + \beta \sin(2\pi t)$, $\lambda = 10^6, \beta = 10^6$, $y(0) = 1$,



◁ $t \to \sin(2\pi t)$ will strongly attract solution

⇒ stiff problem

$$\dot{\underline{z}} = \begin{bmatrix} -\lambda z_1 + \beta \sin(2\pi z_2) \\ 1 \end{bmatrix} \underline{z} \quad , \underline{z}(t) = \begin{bmatrix} y(t) \\ t \end{bmatrix}$$

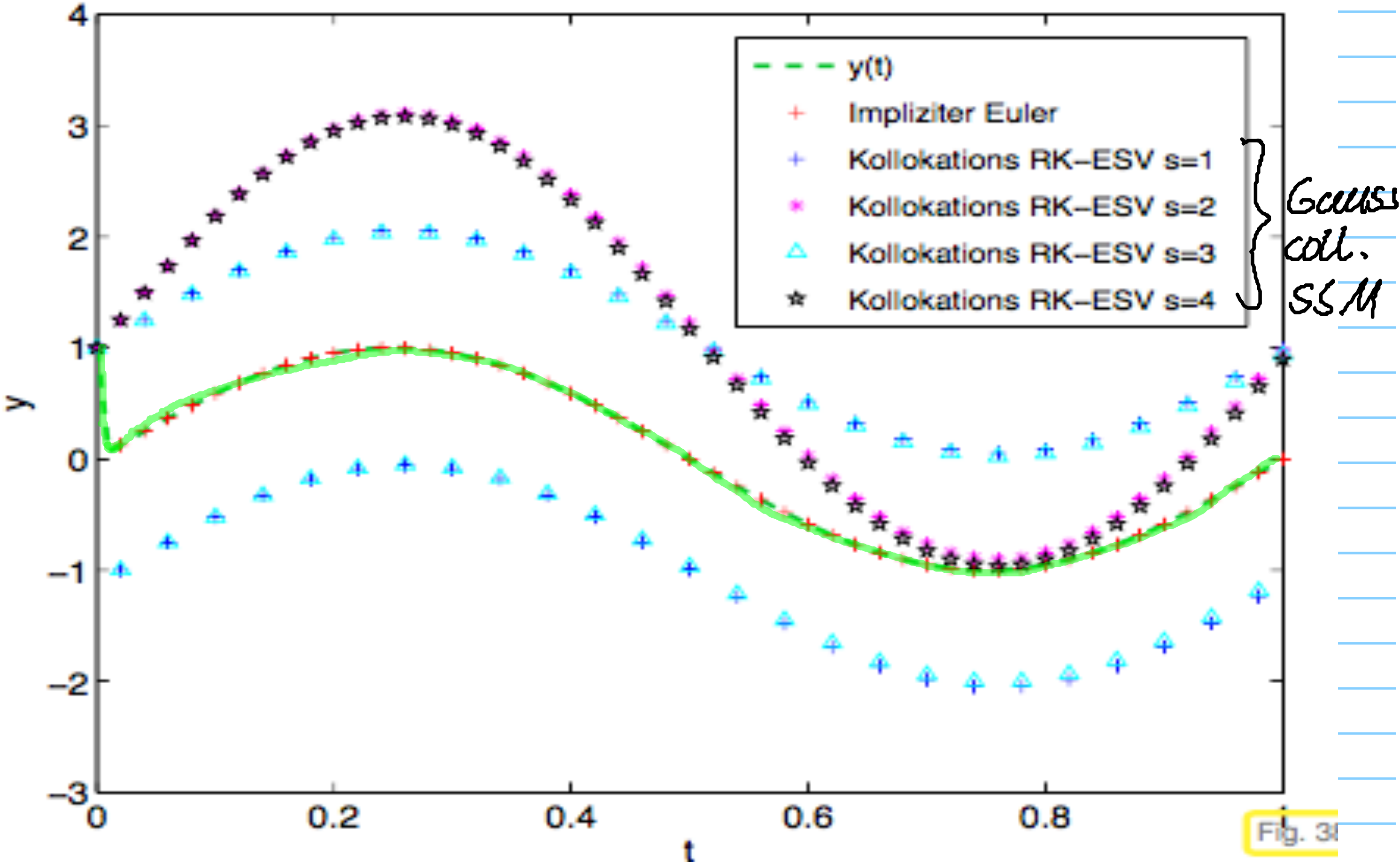


Fig. 3

For Gauss coll. SSM : $\lim_{|z| \to \infty} |S(z)| = 1$

$|\lambda h| \gg 1 \Rightarrow |S(\lambda h)| \approx 1$: $\underbrace{y_k = (S(z))^k y_0}_{\text{for } \dot{y} = \lambda y}$

⇒ Very slow decay of the SSM solution

⇕

Very fast decay of $t \to y(t)$

We want $S(``\infty") = 0$ → GC-SSM $|S(``\infty")| = 1$

↑ ↳ Satisfied for impl. Euler

desirable for very stiff problems

Definition 12.3.38. L-stable Runge-Kutta method → [32, Ch. 77]

A Runge-Kutta method (→ Def. 12.3.18) is L-stable/asymptotically stable, if its stability function (→ Thm. 12.3.27) satisfies

A-stability →

$$(i)\quad \operatorname{Re} z < 0 \;\Rightarrow\; |S(z)| < 1\,, \tag{12.3.39}$$

$$(ii)\quad \lim_{\operatorname{Re} z \to -\infty} S(z) = 0\,. \tag{12.3.40}$$

$$L\text{-stability} = A\text{-stability} + S(``\infty") = 0$$

Construction of L-stable methods:

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

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

$$\Rightarrow S(\infty) = 1 - \underline{b}^T\mathcal{A}^{-1}\mathbf{1} \overset{!}{=} 0$$

$$\underline{b} = (\mathcal{A})_{j,:} \quad [\,j\text{-th row of } \mathcal{A}\,]$$

$$\Rightarrow \underline{b}^T\mathcal{A}^{-1} = \underline{e}_j^T \Rightarrow \underline{b}^T\mathcal{A}^{-1}\mathbf{1} = 1$$

$S(\infty) = 0$ for all RK-SSM with Butcher scheme

$$\triangleright \quad \begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_{s-1} & a_{s-1,1} & \cdots & a_{s-1,s} \\ 1 & b_1 & \cdots & b_s \\ \hline & b_1 & \cdots & b_s \end{array}$$

Satisfied for collocation RK-SSM with $c_s = 1$!

$$\mathbf{k}_i = f(t_0 + c_i h, \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,, \qquad \text{where} \quad a_{ij} := \int_0^{c_i} L_j(\tau)\,d\tau\,,$$

$$\mathbf{y}_1 := \mathbf{y}_h(t_1) = \mathbf{y}_0 + h\sum_{i=1}^{s} b_i\mathbf{k}_i\,. \qquad b_i := \int_0^1 L_i(\tau)\,d\tau\,. \tag{12.3.11}$$

= s-stage Gauss-Radau collocation SSM of order 2s-1, L-stable

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

Implicit Euler method

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

Radau RK-SSM, order 3

$$\begin{array}{c|ccc} \frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\ \frac{4+\sqrt{6}}{10} & \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\ 1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\ \hline & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{array}$$

Radau RK-SSM, order 5

12.4. Semi-implicit RK-SSM

Idea: Fixed small number of Newton steps to compute increments

⇔ Linearize increment equation

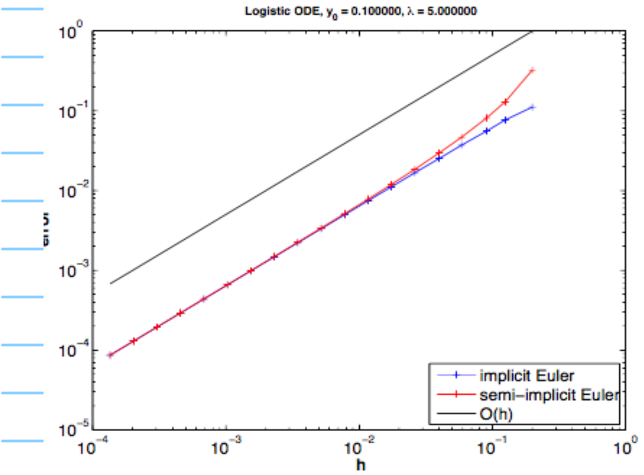
Example: Impl. Euler for $\dot{y} = f(y)$ $y_1 = y_0 + hf(y_1)$

Linearization (around y_0): $y_1 \doteq y_0 + h[f(y_0) + Df(y_0)(y_1 - y_0)]$

$$y_1 = y_0 + \underbrace{(I - hDf(y_0))}_{\text{invertible for sufficiently small } h}{}^{-1} hf(y_0) \qquad (*)$$

(*) = Semi-implicit Euler SSM

$[\ \sigma(I - hDf(y_0)) = 1 - h\sigma(Df(y_0))\ ]$



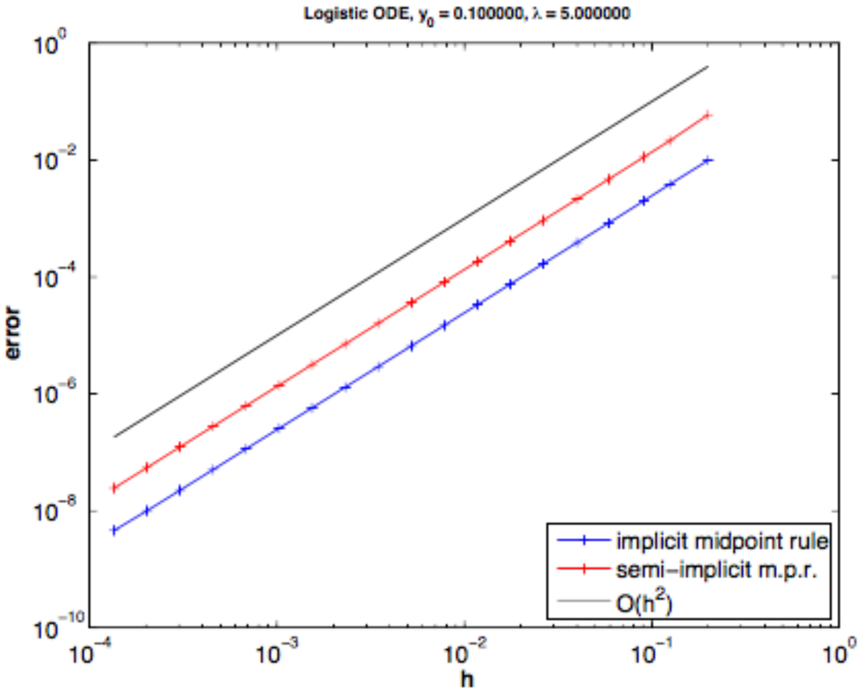
$\dot{y} = 5y(1-y)$

(*) $\hat{=}$ order 1

Semi-implicit midpoint method

Linearization $\left[\begin{array}{l} y_1 = y_0 + hf(\tfrac{1}{2}(y_0 + y_1)) \\ \hookrightarrow y_1 \doteq y_0 + h[f(y_0) + \tfrac{1}{2}Df(y_0)(y_1 - y_0)] \end{array}\right.$

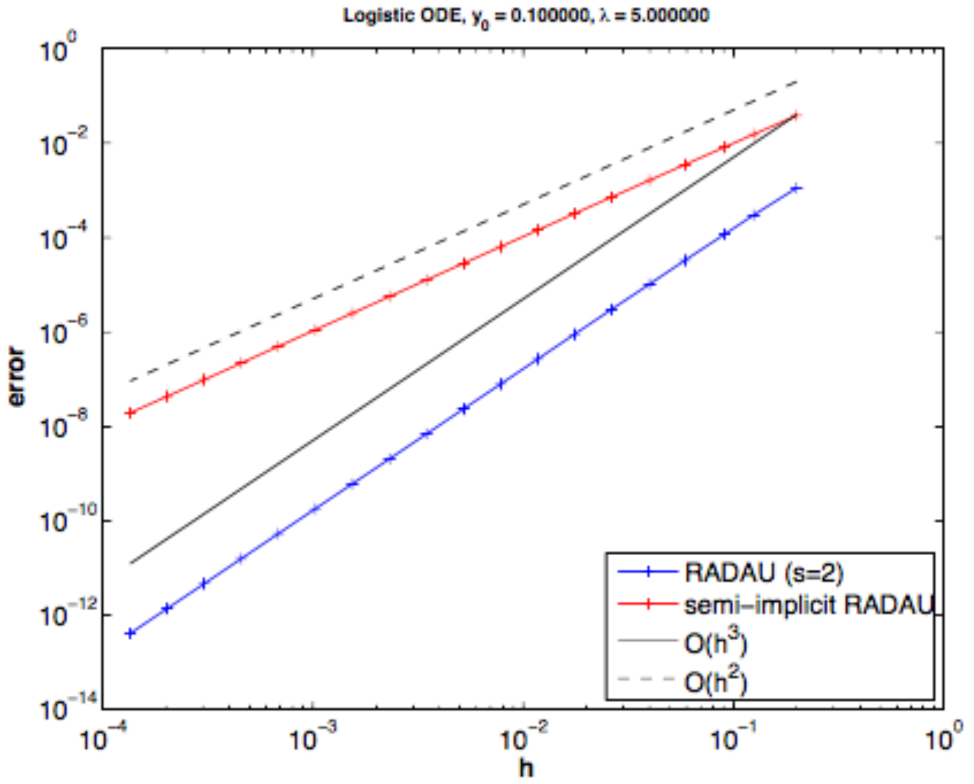
$$(1 - \tfrac{1}{2}hDf(y_0))(y_1 - y_0) = hf(y_0)$$



▷ Order 2 preserved

Is one Newton step enough for all implicit RK-SSM?

NO!



▷ Loss of order

Good news: Fixed number of Newton steps is enough

Class of s-stage semi-implicit (linearly implicit) Runge-Kutta methods (Rosenbrock-Wanner (ROW) methods):

$$(\mathbf{I} - ha_{ii}\mathbf{J})\mathbf{k}_i = \mathbf{f}(\mathbf{y}_0 + h\sum_{j=1}^{i-1}(a_{ij}+d_{ij})\mathbf{k}_j) - h\mathbf{J}\sum_{j=1}^{i-1} d_{ij}\mathbf{k}_j\,, \quad \mathbf{J} = D\,\mathbf{f}(\mathbf{y}_0)\,, \tag{12.4.6}$$

$$\mathbf{y}_1 := \mathbf{y}_0 + \sum_{j=1}^{s} b_j \mathbf{k}_j\,.$$

Practice: Determine a_{ij}, d_{ij}, b_j from order conditions

From a 2015 paper:

$$\dot{\mathbf{u}} = \mathbf{F}(t, \mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0.$$

A Rosenbrock–Wanner (ROW) method with s internal stages can be formulated by

$$\mathbf{k}_i = \mathbf{F}\left(t_m + \alpha_i\tau_m, \tilde{\mathbf{U}}_i\right) + \tau_m J\sum_{j=1}^{i}\gamma_{ij}\mathbf{k}_j + \tau_m\gamma_i\partial_t\mathbf{F}(t_m, \mathbf{u}_m),$$

$$\tilde{\mathbf{U}}_i = \mathbf{u}_m + \tau_m\sum_{j=1}^{i-1}\alpha_{ij}\mathbf{k}_j, \quad i = 1, \ldots, s,$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau_m\sum_{i=1}^{s} b_i\mathbf{k}_i,$$

where $J := \partial_{\mathbf{u}}\mathbf{F}(t_m, \mathbf{u}_m)$ is the Jacobian of $\mathbf{F}$ w.r.t. $\mathbf{u}$, α_{ij}, γ_{ij}, b_i are the parameters of the method, and

$$\alpha_i := \sum_{j=1}^{i-1}\alpha_{ij}, \qquad \gamma_i := \sum_{j=1}^{i-1}\gamma_{ij}, \qquad \gamma := \gamma_{ii} > 0, \quad i = 1, \ldots, s.$$

$$\text{(A1)} \quad \sum_{i=1}^{s} b_i = 1$$

$$\text{(A2)} \quad \sum_{i=1}^{s} b_i\beta_i = \frac{1}{2} - \gamma$$

$$\text{(A3a)} \quad \sum_{i=1}^{s} b_i\alpha_i^2 = \frac{1}{3}$$

$$\text{(A3b)} \quad \sum_{i,j=1}^{s} b_i\beta_{ij}\beta_j = \frac{1}{6} - \gamma + \gamma^2$$

$$\text{(A4a)} \quad \sum_{i=1}^{s} b_i\alpha_i^3 = \frac{1}{4}$$

$$\text{(A4b)} \quad \sum_{i,j=1}^{s} b_i\alpha_i\alpha_{ij}\beta_j = \frac{1}{8} - \gamma/3$$

$$\text{(A4c)} \quad \sum_{i,j=1}^{s} b_i\beta_{ij}\alpha_j^2 = \frac{1}{12} - \gamma/3$$

$$\text{(A4d)} \quad \sum_{i,j,k=1}^{s} b_i\beta_{ij}\beta_{jk}\beta_k = \frac{1}{24} - \frac{1}{2}\gamma + \frac{3}{2}\gamma^2 - \gamma^3,$$

where we use the abbreviations $\beta_{ij} := \alpha_{ij} + \gamma_{ij}$ and $\beta_i := \sum_{j=1}^{i-1}\beta_{ij}$.

◁ Conditions for order 4

Table 3
Set of coefficients for ROS3PRL2 method.

γ = 4.3586652150845900e−01	
α_{21} = 1.3075995645253771e+00	γ_{21} = −1.3075995645253771e+00
α_{31} = 5.0000000000000000e−01	γ_{31} = −7.0988575860972170e−01
α_{32} = 5.0000000000000000e−01	γ_{32} = −5.5996735960277766e−01
α_{41} = 5.0000000000000000e−01	γ_{41} = −1.5550856807552085e−01
α_{42} = 5.0000000000000000e−01	γ_{42} = −9.5388516575112225e−01
α_{43} = 0.0000000000000000e+00	γ_{43} = 6.7352721231818413e−01
b_1 = 3.4449143192447917e−01	$\hat{b}_1$ = 5.0000000000000000e−01
b_2 = −4.5388516575112231e−01	$\hat{b}_2$ = −2.5738812086522078e−01
b_3 = 6.7352721231818413e−01	$\hat{b}_3$ = 4.3542008724775044e−01
b_4 = 4.3586652150845900e−01	$\hat{b}_4$ = 3.2196803361747034e−01

Order 3 ROW method, L-stable

How to explore L-stability of a ROW method ?

(i) Apply SSM to $\dot{y} = \lambda y$ [$f(y) = \lambda y$]

(ii) We get $y_1 = S(\lambda h) y_0$

[More general $Q(\lambda h) y_1 = P(\lambda h) y_0$, P, Q polynomials]

(iii) Verify $\lim_{z \to \infty} S(z) = 0$

(iv) Show $\mathrm{Re}\, z < 0 \Rightarrow |S(z)| < 1$

Use Thm : If S rational, defined on $\mathbb{C}^- \cup i\mathbb{R}$, $\lim_{z \to \infty} S(z) = 0$

$$\Rightarrow |S(z)| < \sup_{\tau \in \mathbb{R}} |S(i\tau)| \quad \text{for all } z \in \mathbb{C}^-$$

Remark:

"ideal stability function"

$$\dot{y} = \lambda y$$

$$y(h) = e^{\lambda h} y(0)$$

$$\Updownarrow \qquad y_0 = y(0)$$

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

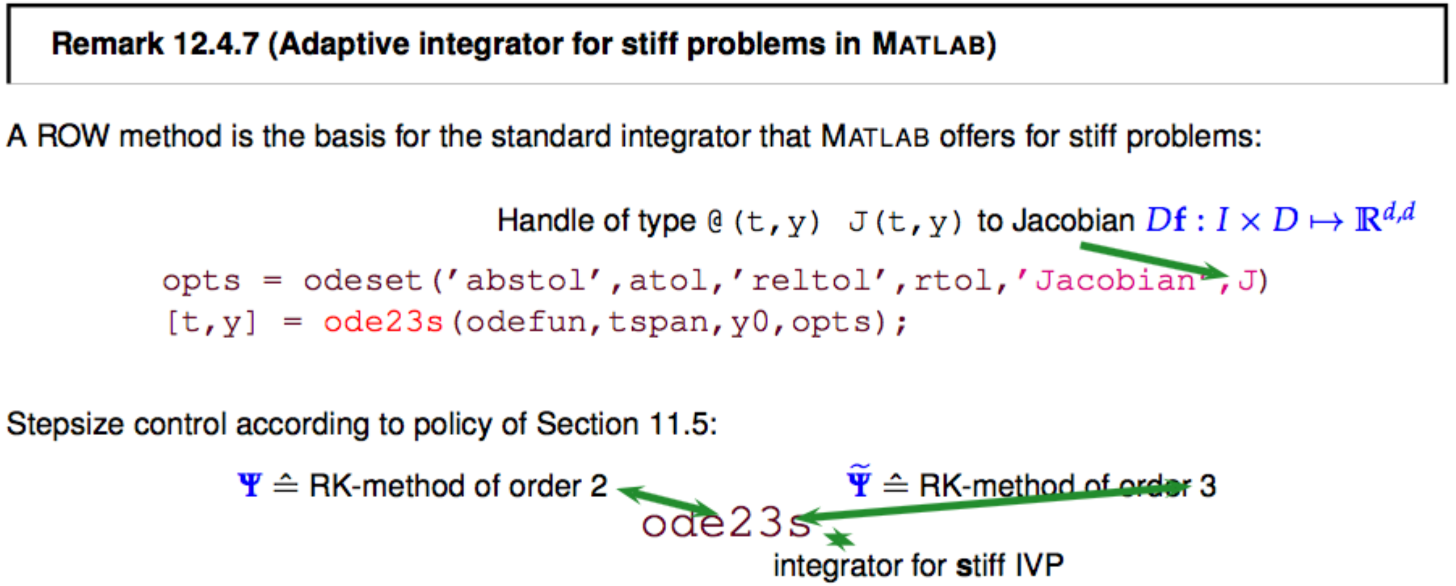
For SSM : $S(z) \sim e^z$ for $|z| \ll 1$

SSM of order p

$$\Rightarrow \quad S(z) - e^z = O(|z|^{p+1}) \quad \text{for } z \to 0$$

Summary :

- Stiff IVP
- Stability induced timestep constraint
- A-stability & L-stability
- Methods : (semi-) implicit RK-SSM usually in embedded form



Remark 12.4.7 (Adaptive integrator for stiff problems in MATLAB)

A ROW method is the basis for the standard integrator that MATLAB offers for stiff problems:

Handle of type `@(t,y) J(t,y)` to Jacobian $\mathbf{D}f : I \times D \mapsto \mathbb{R}^{d,d}$

```
opts = odeset('abstol',atol,'reltol',rtol,'Jacobian',J)
[t,y] = ode23s(odefun,tspan,y0,opts);
```

Stepsize control according to policy of Section 11.5:

$\Psi \hat{=}$ RK-method of order 2 $\qquad \widetilde{\Psi} \hat{=}$ RK-method of order 3

`ode23s`

integrator for stiff IVP