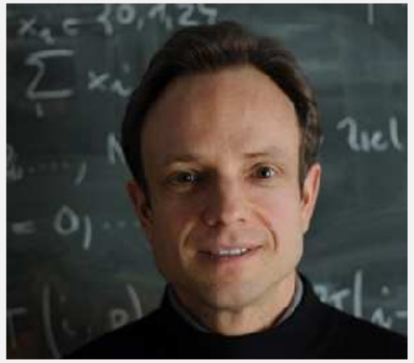
ETH Lecture 401-0674-00L Numerical Methods for ~~Partial~~ Differential Equations

Course Video

Section 7.3: Implicit Runge-Kutta Single-Step Methods



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Prerequisites.
- Polynomial interpolation
- Numerical quadrature

Dependencies. [Lecture → Section 6.3.2], [Lecture → Section 6.4], <[Lecture → Section 4.3]>, [Lecture → Section 7.1]

Duration: minutes

⚠ Video and accompanying tablet notes may not match completely!

[Corrections and updates may have been made in tablet notes.]

VII. Single-Step Methods for Stiff Initial-Value Problems

7.3 Implicit Runge-Kutta Single-Step Methods

Notion 7.2.0.7. 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.

7.3.1 The Implicit Euler Method for stiff IVPs

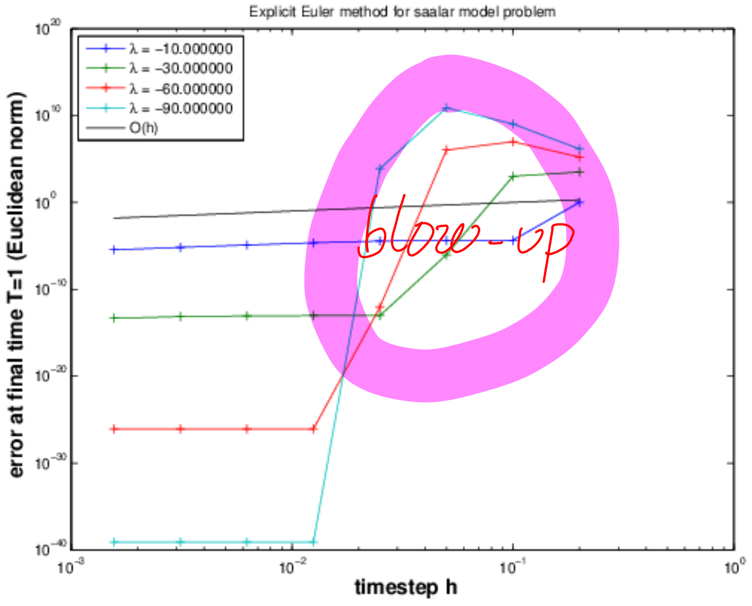
Exp.: 7.3.1.1. (Euler methods for stiff decay IVPs)

IVP: $\dot{y} = \lambda y \,,\; y(0) = 1 \,,\quad \lambda < 0$

Numerical integrator: Explicit Euler method with uniform timestep size $h > 0$

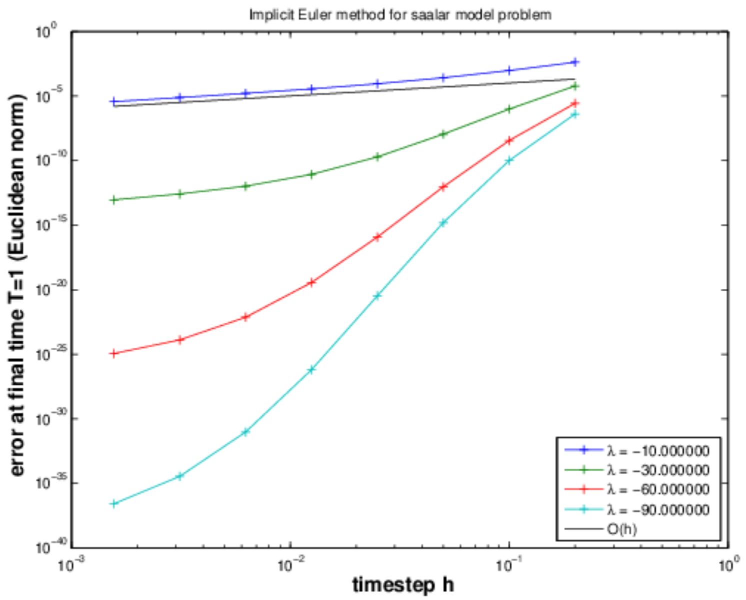
②

Explicit Euler method (6.2.1.4)



λ large: blow-up of y_k for large timestep h

Implicit Euler method (6.2.2.2)



λ large: stable for *all* timesteps $h > 0$!

§ 7.3.1.2 (Linear model problem analysis of implicit Euler method) $\longrightarrow$ § 7.1.0.44

Linear model problem : $\dot{y} = \lambda y$, $y(0) = y_0$, $\mathrm{Re}\,\lambda < 0$

[solution $y(t) = e^{\lambda t} \longrightarrow 0$ for $t \to \infty$]

Impl. Euler recursion: y_{k+1}: $y_{k+1} = y_k + h\lambda y_{k+1}$

$$\Longleftrightarrow \quad y_{k+1} = \frac{1}{1-\lambda h} y_k$$

$$\triangleright \quad y_k = \left(\frac{1}{1-h\lambda}\right)^k y_0 \xrightarrow{k\to\infty} 0 \quad \forall h > 0$$

$N > 1$: $\dot{y} = My$, $M \in \mathbb{R}^{N,N}$

$y(0) = y_0$

Technique : Diagonalization $\longrightarrow$ § 7.1.0.40

Assume : $\exists\, V \in \mathbb{C}^{N,N}$: $V^{-1}MV = D = \mathrm{diag}(\lambda_1, \dots, \lambda_N)$

Impl. Euler : $\cdot V^{-1} |$ $\quad y_{k+1} = y_k + hMy_{k+1}$

$[z_k := V^{-1}y_k]$ $\quad z_{k+1} = z_k + h\underbrace{V^{-1}MV}_{=D} z_{k+1}$

Decoupling : $(z_{k+1})_\ell = (z_k)_\ell + h\lambda_\ell (z_{k+1})_\ell$, $\ell = 1, \dots, N$

$$\triangleright \quad (z_k)_\ell = \left(\frac{1}{1-h\lambda_\ell}\right)^k (z_0)_\ell \xrightarrow{k\to\infty} 0 \text{ if } \mathrm{Re}\,\lambda_\ell < 0 \quad \forall h > 0$$

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 $\mathbf{M} \in \mathbb{R}^{N,N}$ with eigenvalues $\lambda_1, \dots, \lambda_N$, if $\mathrm{Re}\,\lambda_i < 0$ for all $i = 1, \dots, N$.

No timestep constraint: unconditional stability

7.3.2 Collocation Single-Step Methods

Goal: Unconditionally stable SSMs of higher order

ODE: $\dot{y} = f(t,y)$, $f : I \times D \to \mathbb{R}^N$

§ 7.3.2.1 (Collocation approach)

(Focus of 1st step: $y_0 \to y_1$, time interval $[t_0, t_1]$)

- $t \to y_h(t) \;\hat{=}\;$ approximation of solution $y(t)$

  $y_h \in V \subset C^1([t_0,t_1])$, $\dim V = (s+1)N$

  $\uparrow$ trial space w/ $s \in \mathbb{N}$ fixed

- $N(s+1)$ Collocation conditions:

  $y_h(t_0) = y_0$

  $\dot{y}_h(\tau_j) = f(\tau_j, y_h(\tau_j))$: pointwise satisfaction of ODE

  for $t_0 \le \underbrace{\tau_1 < \tau_2 < \dots < \tau_s}_{\text{collocation points}} \le t_1$

- $y_1 := y_h(t_1)$

§ 7.3.2.4 (Polynomial collocation)

"Standard choice": $V = (\mathcal{P}_s)^N$

$\tau_j := t_0 + c_j h$, $h := t_1 - t_0$, $0 \le c_1 < c_2 < \dots < c_s \le 1$

Recall: Lagrange polynomials L_j

- $L_j \in \mathcal{P}_{s-1}$, $j = 1, \dots, s$
- $L_j(c_\ell) = \delta_{\ell j}$ [cardinal basis] $1 \le j, \ell \le s$

$y_h \in V \Rightarrow \dot{y}_h \in (\mathcal{P}_{s-1})^N$

$$\Rightarrow \dot{y}_h(t_0 + \xi h) = \sum_{j=1}^{s} \dot{y}_h(t_0 + c_j h)\, L_j(\xi), \quad 0 \le \xi \le 1$$

$$= \sum_{j=1}^{s} \underbrace{f(t_0 + c_j h, y_h(t_0 + c_j h))}_{=: k_j \in \mathbb{R}^N} L_j(\xi)$$

Integrate [$y_h(t_0) = y_0$]

$$y_h(t_0 + \xi h) = y_0 + h \sum_{j=1}^{s} k_j \int_0^{\xi} L_j(\zeta)\, d\zeta \qquad (*)$$

[$\xi \leftarrow c_j$]

$$\triangleright\; k_i = f\Big(t_0 + c_j h,\; y_0 + h \sum_{j=1}^{s} k_j \int_0^{c_j} L_j(\zeta)\, d\zeta\Big), \quad 1 \le i \le N$$

Rem. 7.3.2.7 (Implicit collocation SSM)

$\to$ $N \cdot s$ non-linear equs. for k_j

("implicit")

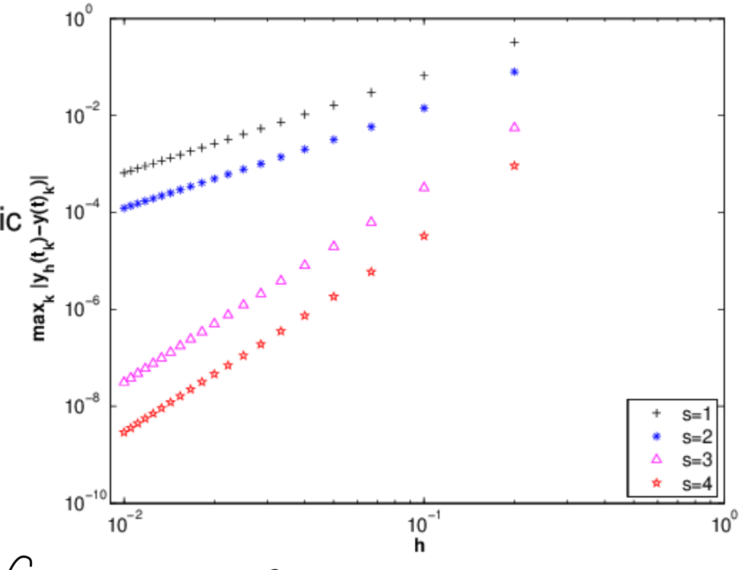
Exp. 7.3.2.10. (Convergence of collocation SSMs)

- IVP: $\dot{y} = \lambda y(1-y)$, $y(0) = 0.01$, $\lambda = 100$
- Collocation SSM on $[0,1]$ w/ uniform timestep $h>0$

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

We observe algebraic convergence with the empiric rates

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



$\triangleright$ Order $= \begin{cases} s & \text{for even } s \\ s+1 & \text{for odd } s \end{cases}$

§ 7.3.2.8 (Collocation SSM and quadrature)

$$\left.\begin{aligned} \dot{y} &= f(t) \\ y(0) &= 0 \end{aligned}\right\} \Rightarrow \quad y_1 = h \sum_{i=1}^{s} \int_0^1 L_i(\tau)\,d\tau \cdot f(t_0 + c_j h)$$

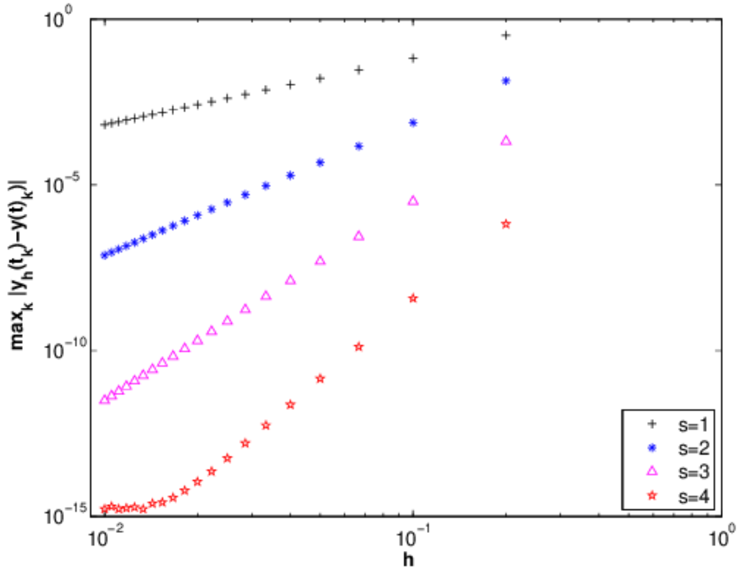
$\hat{=}$ s-pt. quadrature formula on $[t_0, t_1]$ nodes c_j

Exp. 7.3.2.10 cont'd :

❶ Gauss points in $[0,1]$ as normalized collocation 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 $= 2s$!

No instability observed

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Theorem 7.3.2.12. Order of collocation single step method

Provided that $\mathbf{f} \in C^p(I \times D)$, *the order* ($\to$ *Def. 6.3.2.8*) *of an* s*-stage collocation single step method according to* (9.2.6.26) *agrees with the order* ($\to$ *Def. 2.7.5.29*) *of the quadrature formula on* $[0,1]$ *with nodes* c_j *and weights* b_j, $j = 1, \dots, s$.

7.3.3 General Implicit RK-SSMs

Summary : Collocation SSM for $\dot{y} = f(t, y)$

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

$$\mathbf{y}_1 := \mathbf{y}_h(t_1) = \mathbf{y}_0 + h \sum_{i=1}^{s} b_i \mathbf{k}_i . \qquad b_i := \int_0^1 L_i(\tau)\, \mathrm{d}\tau . \tag{7.3.2.6}$$

Lagrange polynomial

Compare :

Definition 6.4.0.9. 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 $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$, $\mathbf{f} : \Omega \to \mathbb{R}^N$, 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 $\mathbf{k}_i \in \mathbb{R}^N$, $i = 1, \dots, s$, are called **increments**, $h > 0$ is the size of the timestep.

Definition 7.3.3.1. General Runge-Kutta single step method (*cf.* Def. 6.4.0.9)

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 (6.1.3.2) 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 vectors $\mathbf{k}_i \in \mathbb{R}^N$ are called **increments**.

Notation :

General Butcher scheme notation for RK-SSM

Shorthand notation for Runge-Kutta methods

Butcher scheme $\triangleright$

$$\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} . \tag{7.3.3.3}$$

Note that now, in contrast to (6.4.0.11), $\mathfrak{A}$ can be a general $s \times s$-matrix.

Rem 7.3.3.6 (Stage-form equations for increments)

(for autonomous ODE $\dot{y} = f(y)$)

$$\underset{\substack{\uparrow \\ \text{stage}}}{g_i} := h\sum_{j=1}^{s} a_{ij} k_j \longleftrightarrow k_i = f(y_0 + g_i)$$

▷ Stage equations:

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

$$\Updownarrow$$

$$g_i = h\sum_{j=1}^{s} a_{ij} f(y_0 + g_j)$$

& $$y_1 = y_0 + h\sum_{i=1}^{s} b_i f(y_0 + g_i)$$

Note: $|h| \ll 1 \Rightarrow g_i \approx 0$

Good initial guess: $g_i = 0$
(for Newton's method)

Rem 7.3.3.9 (Solving the stage equations)

$$g_i = h\sum_{j=1}^{s} a_{ij} f(y_0 + g_j)$$

$$\Updownarrow \qquad \vec{g} = \begin{bmatrix} g_1 \\ \vdots \\ g_s \end{bmatrix} \in \mathbb{R}^{N\cdot s}$$

$$F(\vec{g}) = \vec{g} - h\,(\underset{\substack{\uparrow \\ \text{Kronecker product}}}{A \otimes I_N})\begin{bmatrix} f(y_0+g_1) \\ \vdots \\ f(y_0+g_s) \end{bmatrix} = 0$$

Apply simplified Newton method w/ $\vec{g}^{(0)} = 0$

$$\vec{g}^{(m+1)} = \vec{g}^{(m)} - DF(0)^{-1}\vec{g}^{(m)}, \quad m = 0,1,2,\dots$$

$$DF(0) = I_{Ns} - h(A \otimes Df(y_0))$$

$$\downarrow$$

I_{Ns} for $h = 0$ $\Rightarrow$ Invertible for small $|h|$

(7)

7.3.4. Model Problem Analysis for IRK-SSMs

Scalar linear ODE : $\dot{y} = \lambda y \quad , \lambda \in \mathbb{C}$

$\downarrow$ RK-SSM

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

Theorem 7.3.4.4. Stability function of Runge-Kutta methods, *cf.* Section 11.4.3

The discrete evolution Ψ^h_λ of an s-stage Runge-Kutta single step method ($\rightarrow$ Def. 9.2.6.31) with Butcher scheme $\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array}$ *(see (9.2.6.33)) for the ODE $\dot{y} = \lambda y$ is given by a multiplication with*

$$S(z) := \underbrace{1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1}}_{\text{stability function}} = \frac{\det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T)}{\det(\mathbf{I} - z\mathfrak{A})} , \quad z := \lambda h , \quad \mathbf{1} = [1, \dots, 1]^T \in \mathbb{R}^s .$$

by block GE $\qquad$ by Cramer's rule $\qquad$ $S(z)$ is a rational function

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

Ex. 7.3.4.5 (Stability functions of simple IRK-SSMs)

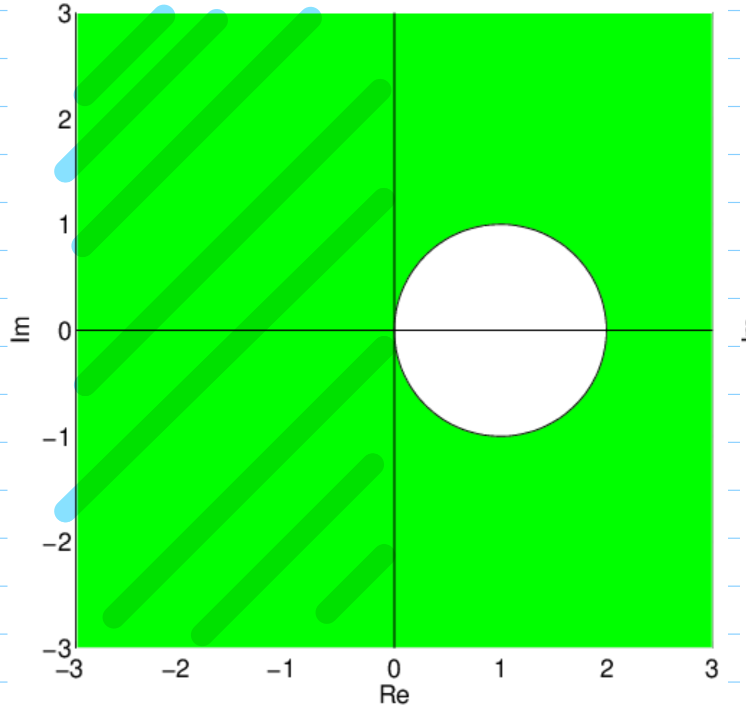
Implicit Euler method: $\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$ ➤ $S(z) = \dfrac{1}{1-z}$.

Implicit midpoint method: $\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$ ➤ $S(z) = \dfrac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z}$.

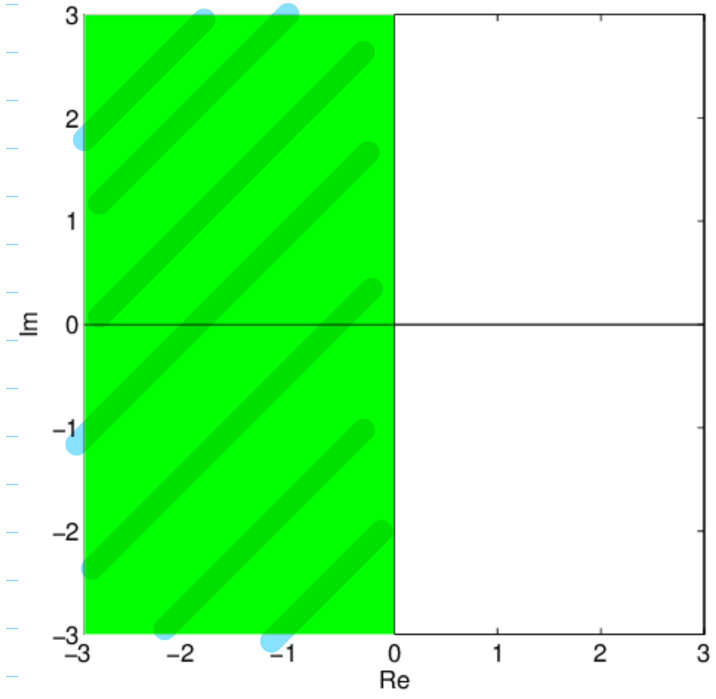
↳ 1-pt Gauss collocation SSM

Regions of stability

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



$\mathcal{S}_\Psi$: implicit Euler method (6.2.2.2)



$\mathcal{S}_\Psi$: implicit midpoint method (6.2.3.3)

$\mathrm{Re}\,\lambda < 0 \implies h\lambda \in S_\Psi \quad \forall h > 0$

$\implies$ unconditional stability

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§ 7.3.4.4 (A-stability)

Definition 7.3.4.9. A-stability of a Runge-Kutta single step method

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

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

($\mathcal{S}_\Psi \hat{=}$ region of stability Def. 7.1.0.51)

A-stable Runge-Kutta single step methods will not be affected by stability induced timestep constraints when applied to stiff IVP (→ Notion 9.2.7.16). ; unconditional stability

§ 7.3.4.10 ("Ideal" region of stability*)

Remember : $S(z) \approx \exp(z)$

$*$ $\quad S_\Psi^* := \{ z \in \mathbb{C} : |\exp(z)| < 1 \}$

$\quad\quad = \mathbb{C}^-$

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

$$\operatorname{Re}\lambda < 0 \Rightarrow \begin{cases} (y_k) \xrightarrow{k\to\infty} 0 \\ y(t) \xrightarrow{t\to\infty} 0 \end{cases}$$

$$S_\Psi = \mathbb{C}^- \Rightarrow$$

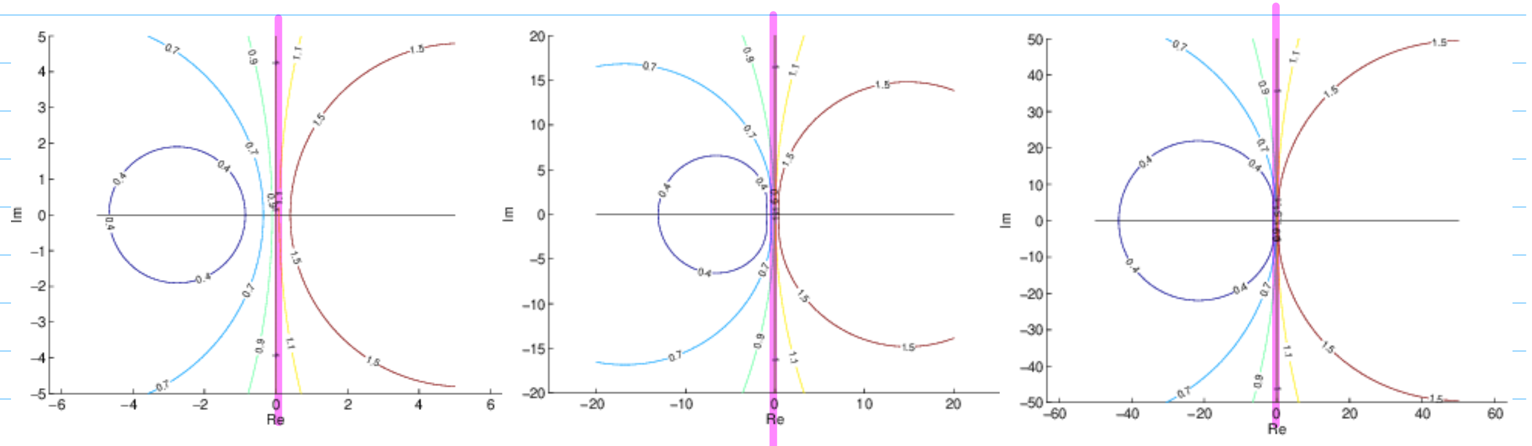
$$\operatorname{Re}\lambda > 0 \Rightarrow \begin{cases} (y_k) \xrightarrow{k\to\infty} \infty \\ y(t) \xrightarrow{t\to\infty} \infty \end{cases}$$

RK-SSMs with $S_\Psi = \mathbb{C}^-$?

→ implicit midpoint method

Implicit midpoint method: $\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$ ➤ $S(z) = \dfrac{1+\frac{1}{2}z}{1-\frac{1}{2}z}$.

Level lines of $|S(z)|$ for Gauss collocation SSMs :



Implicit midpoint method $\quad$ $s = 2$ (order 4) $\quad$ $s = 4$ (order 8)

Theorem 7.3.4.12. Region of stability of Gauss collocation single step methods

s-stage Gauss collocation single step methods defined by (9.2.6.26) with the nodes c_s given by the s Gauss points on $[0,1]$, feature the "ideal" stability domain:

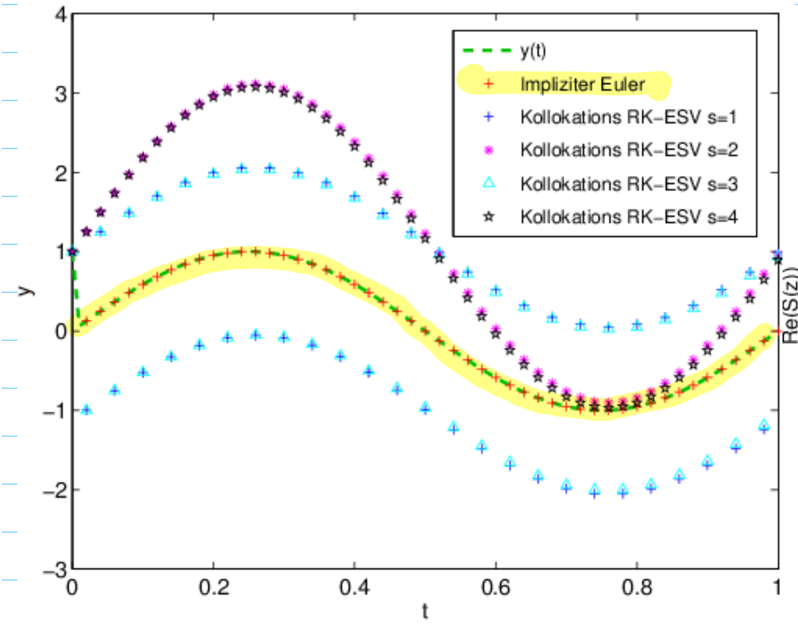
$$\mathcal{S}_\Psi = \mathbb{C}^- \,. \tag{7.3.4.11}$$

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

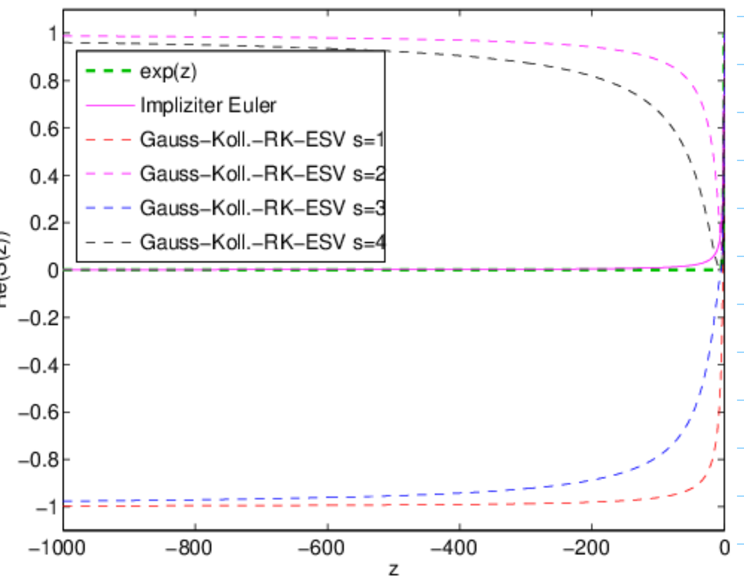
Exp. 7.3.4.13 (IRK-SSMs for stiff IVP)

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

▷ $y(t) \approx \sin(2\pi t)$ after very short time



Solutions by RK-SSMs



Stability functions on $\mathbb{R}^-$

↓

For GC-SSM

Hardly any decay $\Leftarrow$ $|S(z)| \to 1$ for $z \to -\infty$

vs. $e^z \to 0$ for $z \to -\infty$

Impl. Eul.: $S(z) = \dfrac{1}{1-z} \to 0$ as $z \to -\infty$

§ 7.3.4.14 (L-stability)

Definition 7.3.4.15. L-stable Runge-Kutta method →

A Runge-Kutta method (→ Def. 9.2.6.31) is L-stable/asymptotically stable, if its stability function (→ Thm. 7.3.4.4) satisfies

A-stable: (i) $\operatorname{Re} z < 0 \Rightarrow |S(z)| < 1$, (7.3.4.16)

(ii) $\lim\limits_{\operatorname{Re} z \to -\infty} S(z) = 0$. (7.3.4.17)

Rem. 7.3.4.18 (Necessary condition for L-stability of RK-SSM)

RK-SSM by Butcher scheme $\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array}$

Thm 7.3.4.4

▷ Stability function $S(z) = 1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1}$

$= 1 + \mathbf{b}^T(\tfrac{1}{z}\mathbf{I} - \mathfrak{A})^{-1}\mathbf{1}$

▷ $S(-\infty) = 1 - \mathbf{b}^T\mathfrak{A}^{-1}\mathbf{1} \overset{!}{=} 0$

▷ If $\mathbf{b} = (\mathfrak{A})_{s,:}$ $\Longrightarrow$ $S(-\infty) = 0$

Butcher scheme (9.2.6.33) for L-stable RK-methods, see Def. 9.2.7.48 $\triangleright$
$$\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_{s-1} & a_{s-1,1} & \cdots & a_{s-1,s} \\ 1 & b_1 & \cdots & b_s \\ \hline & b_1 & \cdots & b_s \end{array}.$$

Ex. 7.3.4.21 (L-stable IRK-SSMs)

s-stage Gauss-Radau methods (collocation SSMs)

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

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

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

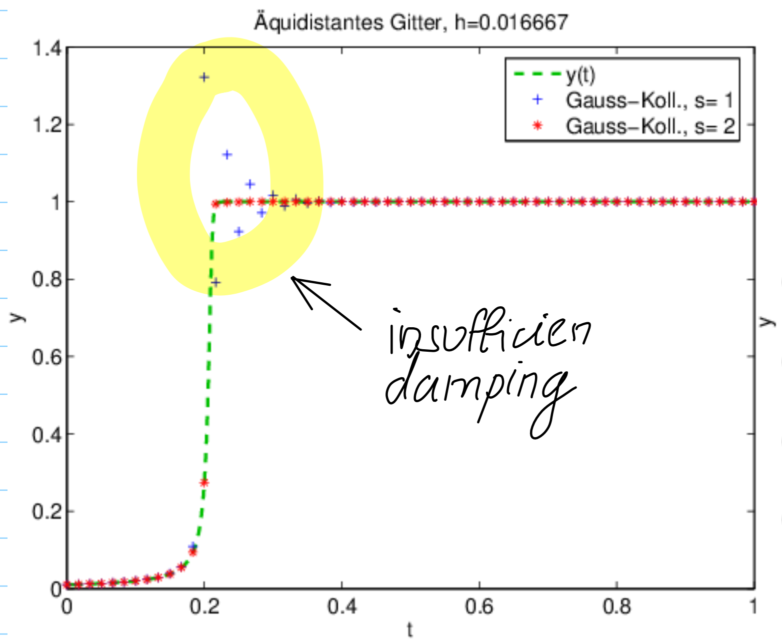
Radau RK-SSM, order 5

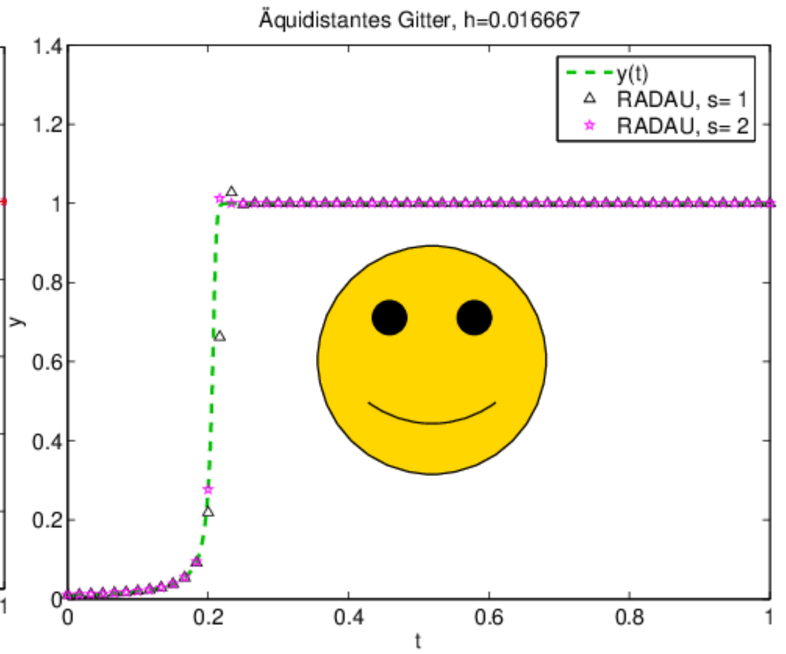
Order $= 2s-1$, L-stable

Exp. 7.3.4.22 (Gauss-Radau SSMs for stiff IVP)

IVP: $\dot{y}(t) = \lambda y^2(1-y)$, $\lambda = 500$, $y(0) = \frac{1}{100}$.

- Uniform timesteps on $[0,1]$





Please answer review questions

After you have watched the video take a short break and then try to answer the

review questions 7.3.4.23

You should do this without consulting other parts of the lecture document or tablet notes.