

ETH Lectures 401-0663-00L Numerical Methods for Computer Science
401-2673-00L Numerical Methods for CSE

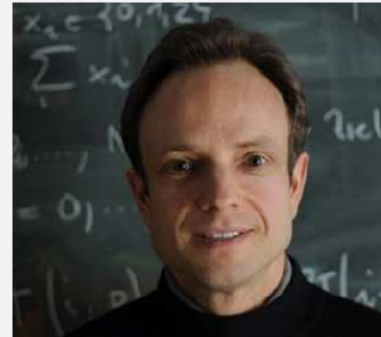
Course Video

Section 12.1: Model Problem Analysis

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(C) Seminar für Angewandte Mathematik, ETH Zürich



Tablet notes may have been corrected and/or extended after the recording of the video!

Prerequisites.

- Complex numbers
- Diagonalization of matrices

Dependencies. Section 11.2.1, Section 11.4, Section 11.5, § 11.5.3.3

Duration: minutes

XII Single-Step Methods for Stiff Initial-Value Problems

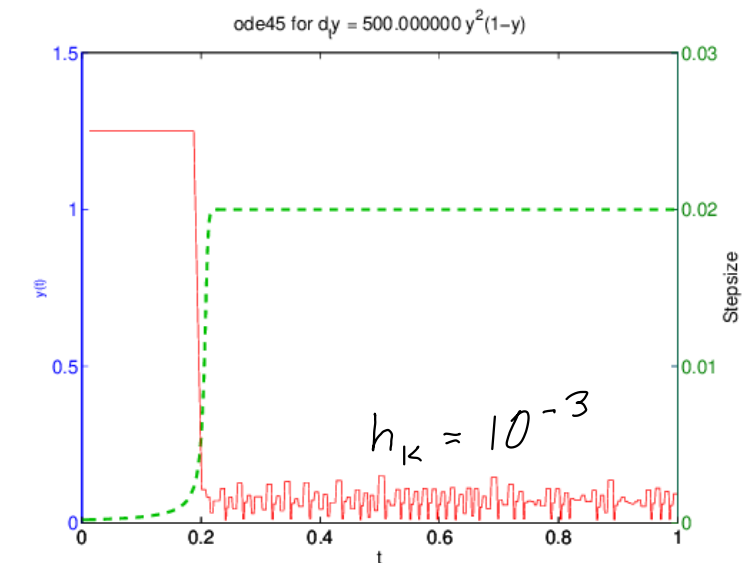
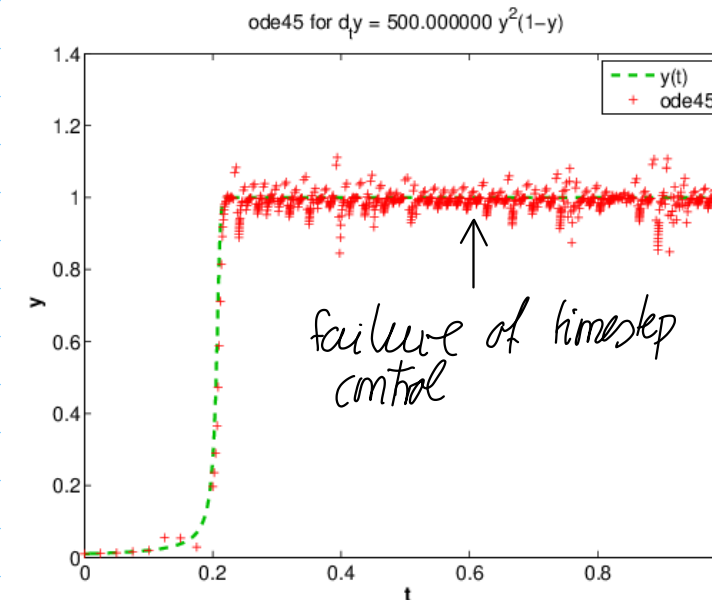
Exp. 12.0.0.1 (Explicit adaptive RK-SSM for stiff IVP)

→ Sect. 11.5.3, § 11.5.3.2: *Ode45*

$$\text{IVP: } \dot{y} = \lambda y^2(1-y), \lambda = 500, y(0) = 0.01$$

Statistics of the integrator run▷

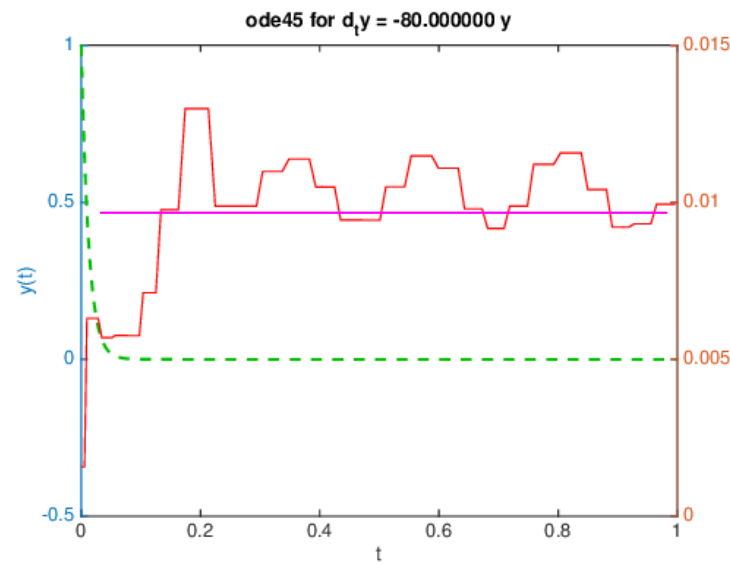
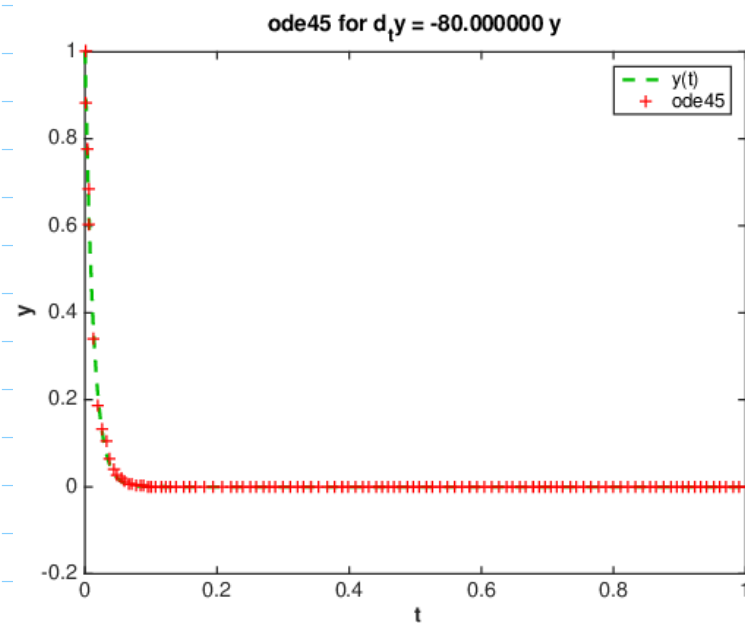
1	— number of steps:	183
2	— number of rejected steps:	185
3	— function calls:	1302



12.1. Model Problem Analysis

Exp. 12.1.0.1. (Adaptive explicit RK-SSM for scalar linear-decay ODE) $\hookrightarrow$ Ode45, § 11.5.3.2

Scalar linear IVP: $\dot{y} = \lambda y$, $\lambda = -80$, $y(0) = 1$



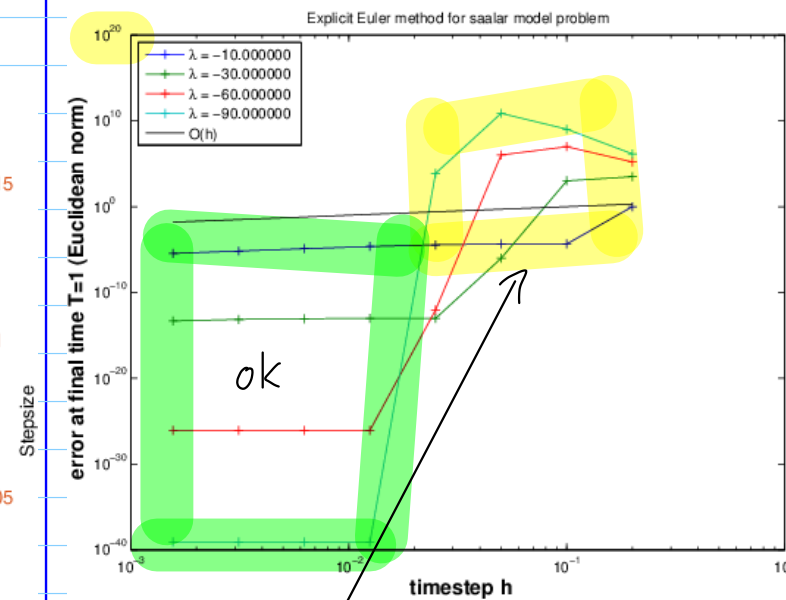
↑
unreasonably small timesteps
though solution is constant ≈ 0

Ex. 12.1.0.3 (Blow-up of explicit Euler method)

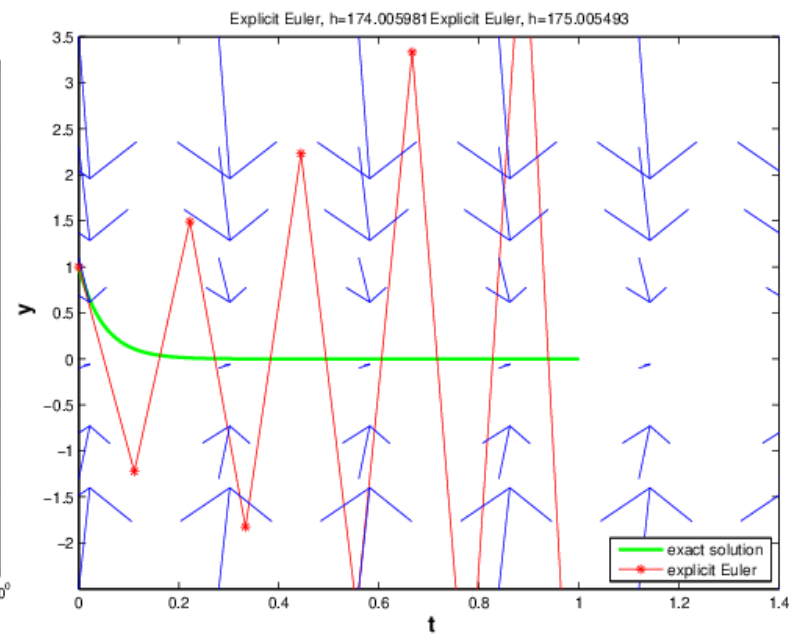
◆ We consider the IVP for the scalar linear decay ODE:

$$\dot{y} = f(y) := \lambda y, \quad \lambda \ll 0, \quad y(0) = 1.$$

◆ We apply the explicit Euler method (11.2.1.5) with uniform timestep $h = 1/M$, $M \in \{5, 10, 20, 40, 80, 160, 320, 640\}$.



$\lambda \ll 0$: blow-up of y_k for large timestep h

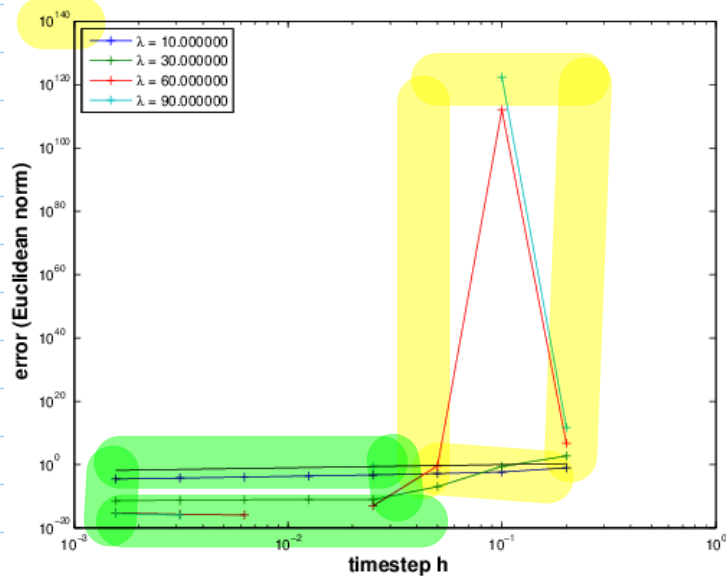


$\lambda = 20$: $\text{---} \hat{=} y(t)$, $\text{---} \hat{=} \text{Euler polygon}$
["overshooting"]

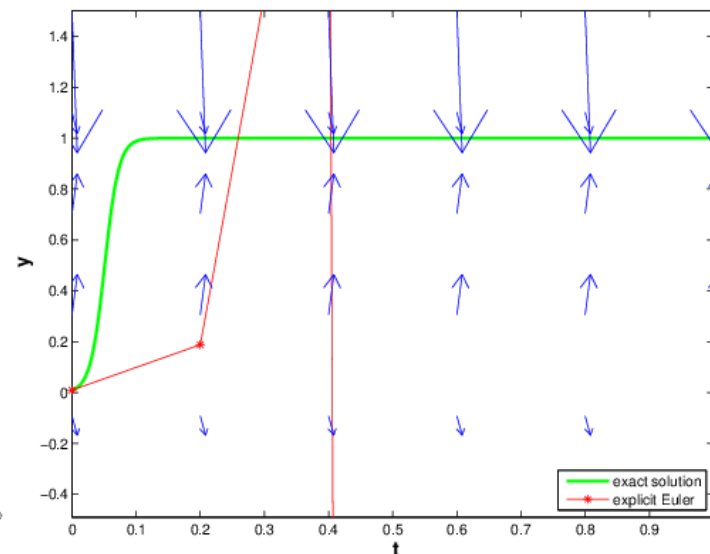
◆ Now we look at an IVP for the logistic ODE, see Ex. 11.1.2.1:

$$\dot{y} = f(y) := \lambda y(1 - y), \quad y(0) = 0.01.$$

◆ As before, we apply the explicit Euler method (11.2.1.5) with uniform timestep $h = 1/M$, $M \in \{5, 10, 20, 40, 80, 160, 320, 640\}$.



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



$\lambda = 90$: — $\hat{=}$ $y(t)$, — $\hat{=}$ Euler polygon

$\triangleright$ Blow-up, unless $h \leq \frac{2}{|\lambda|}$

$\hat{=}$ Stability-induced timestep constraint

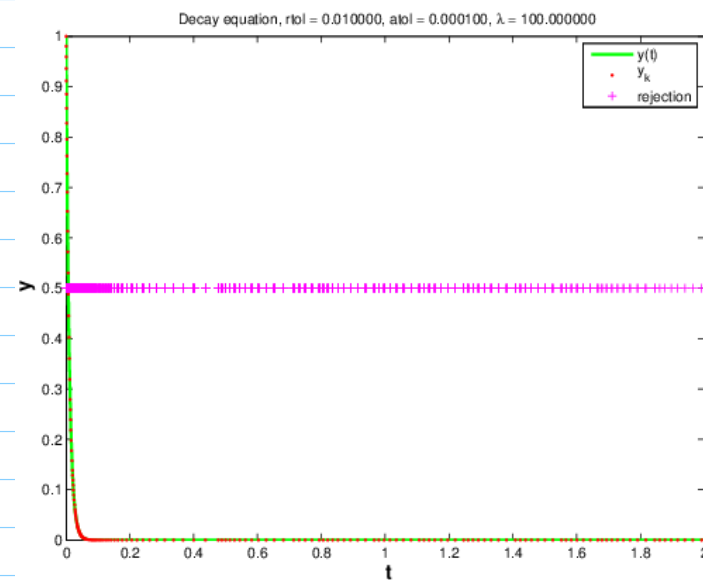
Exp. 12.1.0.8 (Simple adaptive himestepping for fast decay)

◆ "Linear model problem IVP": $\dot{y} = \lambda y$, $y(0) = 1$, $\lambda = -100$

◆ Simple adaptive timestepping method as in Exp. 11.5.2.8, see Code 11.5.2.6. Timestep control based on the pair of 1st-order explicit Euler method and 2nd-order explicit trapezoidal method.

↓
Timestep control based on

- explicit Euler method
- explicit trapezoidal method



△ Step size control maintains timestep below stability-induced threshold.

§ 12.1.0.4 (Linear model problem analysis: explicit Euler method)

Linear model problem IVP: $\dot{y} = f(y) := \lambda y$, $y(0) = y_0$, $\lambda \ll 0$

$\triangleright$ Solution $y(t) = y_0 e^{\lambda t} \rightarrow 0$ for $t \rightarrow \infty$

Expl. Euler (stepsize $h > 0$): $y_{k+1} = y_k + h f(y_k) = (1 + h\lambda) y_k$

$|y_k| = |(1 + h\lambda)^k y_0| \xrightarrow{k \rightarrow \infty} \begin{cases} \infty, & \text{if } |1 + h\lambda| > 1 \Leftrightarrow h > \frac{2}{|\lambda|} \\ 0, & \text{if } |1 + h\lambda| < 1 \Leftrightarrow h < \frac{2}{|\lambda|} \end{cases}$

correct behavior $\rightarrow$

4) Ex. 12.1.0.9 (Explicit trapezoidal method for decay equation)

Explicit trapezoidal method for $\dot{y} = f(t, y)$

$$k_1 = f(t_0, y_0), \quad k_2 = f(t_0 + h, y_0 + h k_1)$$

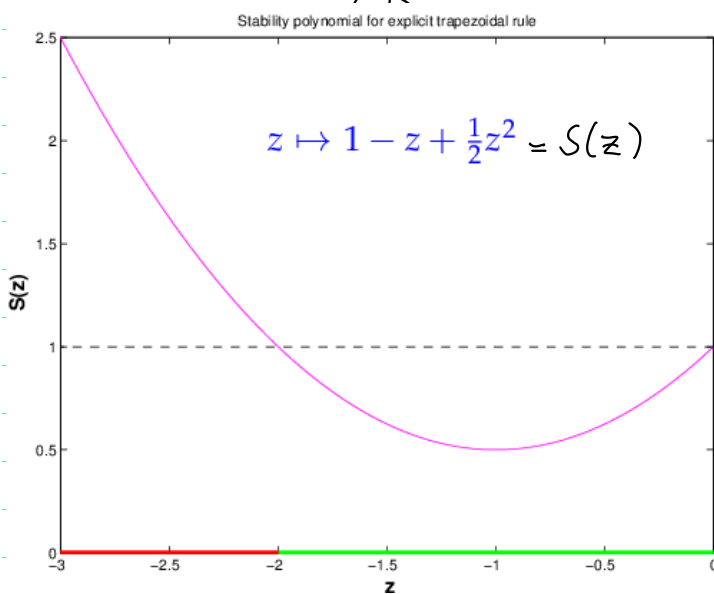
$$y_1 = y_0 + \frac{1}{2}h(k_1 + k_2)$$

For $f(t, y) := \lambda y, \quad \lambda < 0$:

$$k_1 = \lambda y_0, \quad k_2 = \lambda(y_0 + h\lambda y_0)$$

$$\Rightarrow y_1 = \underbrace{(1 + \lambda h + \frac{1}{2}(\lambda h)^2)}_{=: S(\lambda h)} y_0$$

$$\Rightarrow y_k = S(\lambda h)^k y_0, \quad k \in \mathbb{N}$$



Clearly, blow-up can be avoided only if $|S(h\lambda)| \leq 1$:

$$|S(h\lambda)| < 1 \Leftrightarrow -2 < h\lambda < 0.$$

Qualitatively correct decay behavior of $(y_k)_k$ only under **timestep constraint**

$$h \leq |2/\lambda|. \quad (12.1.0.12)$$

◁ the **stability function** for the explicit trapezoidal method

§ 12.1.0.13 (Model problem analysis for general explicit RK-SSMs)

s -stage RK-SSM $\leftrightarrow \begin{array}{c|c} \underline{c} & \underline{A} \\ \hline & \underline{b}^T \end{array}, \quad \underline{A} \in \mathbb{R}^{s,s}, \quad \underline{c}, \underline{b} \in \mathbb{R}^s$

Definition 11.4.0.11. Explicit Runge-Kutta single-step 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 $\dot{y} = f(t, y), f: \Omega \rightarrow \mathbb{R}^N$, is defined by $(y_0 \in D)$

$$\mathbf{k}_i := f(t_0 + c_i h, y_0 + h \sum_{j=1}^{i-1} a_{ij} \mathbf{k}_j), \quad i = 1, \dots, s, \quad y_1 := y_0 + h \sum_{i=1}^s b_i \mathbf{k}_i.$$

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

For $N=1, f(t, y) := \lambda y, \lambda \in \mathbb{R}$:

$$\begin{aligned} k_i &= \lambda(y_0 + h \sum_{j=1}^{i-1} a_{ij} k_j), \\ y_1 &= y_0 + h \sum_{i=1}^s b_i k_i \end{aligned} \Rightarrow \begin{bmatrix} \mathbf{I} - z\mathbf{A} & 0 \\ -z\mathbf{b}^T & 1 \end{bmatrix} \begin{bmatrix} \mathbf{k} \\ y_1 \end{bmatrix} = y_0 \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad (12.1.0.14)$$

$$\underline{1} := [1, \dots, 1]^T \in \mathbb{R}^s$$

$$z := \lambda h$$

$$\underline{k} = \frac{1}{\lambda} [k_1, \dots, k_s]^T \in \mathbb{R}^s$$

⑤ By Cramer's rule: $y_1 = S(z) y_0$

$$y_1 = y_0 \frac{\det \begin{bmatrix} \mathbf{I} - z\mathbf{A} & \mathbf{1} \\ -z\mathbf{b}^T & 1 \end{bmatrix}}{\det \begin{bmatrix} \mathbf{I} - z\mathbf{A} & 0 \\ -z\mathbf{b}^T & 1 \end{bmatrix}} \Rightarrow S(z) = \det(\mathbf{I} - z\mathbf{A} + z\mathbf{1}\mathbf{b}^T), \quad (12.1.0.16)$$

Theorem 12.1.0.17. Stability function of some explicit Runge-Kutta methods $\rightarrow$,

The discrete evolution Ψ_λ^h of an explicit s -stage Runge-Kutta single step method ($\rightarrow$ Def. 11.4.0.11) with Butcher scheme $\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array}$ (see (11.4.0.13)) for the ODE $\dot{y} = \lambda y$ amounts to a multiplication with the number

$$\Psi_\lambda^h = S(\lambda h) \Leftrightarrow y_1 = S(\lambda h) y_0,$$

where S is the **stability function** (SF)

$$S(z) := 1 + z\mathbf{b}^T(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{1} = \det(\mathbf{I} - z\mathbf{A} + z\mathbf{1}\mathbf{b}^T), \quad \mathbf{1} := [1, \dots, 1]^T \in \mathbb{R}^s. \quad (12.1.0.18)$$

$\rightarrow$ polynomial of degree $\leq s$

Corollary 12.1.0.20. Polynomial stability function of explicit RK-SSM

For a consistent ($\rightarrow$ Def. 11.3.1.12) s -stage explicit Runge-Kutta single step method according to Def. 11.4.0.11 the stability function S defined by (12.1.0.18) is a non-constant **polynomial** of degree $\leq s$, that is, $S \in \mathcal{P}_s$.

Ex. 12.1.0.19 (Stability functions of some explicit RK-SSMs)

Explicit Euler method (11.2.1.5): $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \Rightarrow S(z) = 1 + z.$

Expl. trapezoidal method (11.4.0.8): $\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 1 & 1 & 0 \\ & \frac{1}{2} & \frac{1}{2} \end{array} \Rightarrow S(z) = 1 + z + \frac{1}{2}z^2.$

Classical RK4 method: $\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array} \Rightarrow S(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4.$

Rem. 12.1.0.21 (Stability function and exponential function)

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

• RK-SSM: $y_1 = S(h\lambda) y_0$

• Exact: $y(h) = e^{\lambda h} y_0$

$\Rightarrow$ Expect $S(\lambda h) \approx e^{\lambda h} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} (\lambda h)^\ell$

$\Rightarrow$ Order q : $S(z) = \sum_{\ell=0}^q \frac{1}{\ell!} z^\ell + z^{q+1} p(z)$

Lemma 12.1.0.23. Stability function as approximation of exp for small arguments

Let S denote the stability function of an s -stage explicit Runge-Kutta single step method of order $q \in \mathbb{N}$. Then

$$|S(z) - \exp(z)| = O(|z|^{q+1}) \quad \text{for } |z| \rightarrow 0. \quad (12.1.0.24)$$

↑ one-step error

Corollary 12.1.0.25. Stages limit order of explicit RK-SSM

An explicit s -stage RK-SSM has maximal order $q \leq s$.

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 (12.1.0.5) with uniform timestep $h > 0$,

→ stability induced timestep constraint

For $\lambda < 0$, $|\lambda| \gg 1$ enforces timesteps way smaller than required by accuracy: inefficient!

§ 12.1.0.30 (Systems of linear ODEs)

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

Ex. 12.1.0.35 (Transient simulation of RLC circuit)

§ 12.1.0.26 (Stability-induced timestep constraint)

$|S(h\lambda)| > 1 \Rightarrow$ Exp. blow-up of $(y_k)_k$ for $k \rightarrow \infty$

$$S \in \mathcal{P}_s, S \neq \text{const} \Rightarrow \lim_{|z| \rightarrow \infty} |S(z)| = \infty$$

▷ $\{z \in \mathbb{R} : |S(z)| \leq 1\}$ bounded

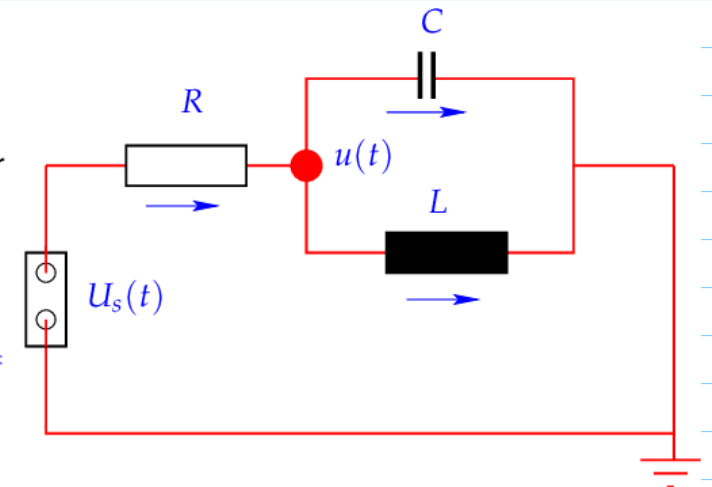
$\Leftrightarrow |S(\lambda h)| \leq 1$ only if h sufficiently small

Consider circuit from Ex. 11.1.2.11

Transient nodal analysis leads to the second-order linear ODE

$$\ddot{u} + \alpha \dot{u} + \beta u = g(t),$$

with coefficients $\alpha := (RC)^{-1}$, $\beta = (LC)^{-1}$, $g(t) = \alpha \dot{U}_s(t)$.

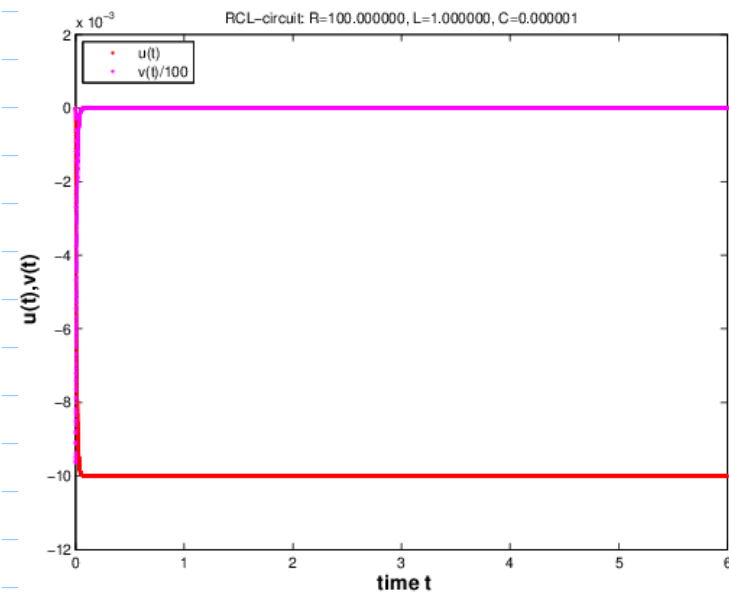


⑦ Equivalent linear (non-autonomous) first-order ODE

$$\underbrace{\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix}}_{=: \dot{\mathbf{y}}} = \underbrace{\begin{bmatrix} 0 & 1 \\ -\beta & -\alpha \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} - \begin{bmatrix} 0 \\ g(t) \end{bmatrix}}_{=: \mathbf{f}(t, \mathbf{y})}, \quad \text{with } \beta \gg \alpha \gg 1 \text{ in usual settings.}$$

$\Leftrightarrow$ Affine linear ODE : $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y} + \mathbf{b}(t)$

Apply adaptive embedded RK-SSM Ode45 :



$R = 100\Omega$, $L = 1\text{H}$, $C = 1\mu\text{F}$, $U_s(t) = 1\text{V}$,
 $u(0) = v(0) = 0$ ("switch on")

ode45 statistics:

17901 successful steps
 1210 failed attempts
 114667 function evaluations

Tiny timesteps despite virtually constant solution!

Recalled : **Diagonalization** of $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$

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

$$\dot{\mathbf{y}} = \mathbf{M}\mathbf{y} \quad [z(t) = V^{-1}\mathbf{y}(t)] \Rightarrow \dot{\mathbf{z}} = D\mathbf{z}$$

Decoupled scalar ODEs

$$\dot{z}_m = \lambda_m z_m, \quad m=1, \dots, N$$

$$z_m(t) = e^{\lambda_m t} z_m(0)$$

$$\Rightarrow \mathbf{y}(t) = V \mathbf{z}(t) = V \text{diag}(e^{\lambda_m t})_{m=1}^N V^{-1} \mathbf{y}(0)$$

§ 12.1.0.40 ("Diagonalization" of explicit Euler method)

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}) := \mathbf{M}\mathbf{y} \Rightarrow \mathbf{y}_{k+1} = \mathbf{y}_k + h \mathbf{M}\mathbf{y}_k$$

$$[\exists V \in \mathbb{C}^{N,N} : V^{-1} M V = D = \text{diag}(\lambda_1, \dots, \lambda_N)]$$

$$\Rightarrow V^{-1} \mathbf{y}_{k+1} = V^{-1} \mathbf{y}_k + h V^{-1} M V (V^{-1} \mathbf{y}_k)$$

$$[\mathbf{z}_k = V^{-1} \mathbf{y}_k] : \mathbf{z}_{k+1} = \mathbf{z}_k + h D \mathbf{z}_k$$

⑧ $\Rightarrow \underbrace{(\underline{z}_{k+1})_e = (\underline{z}_k)_e + h \lambda_e (\underline{z}_k)_e}_{\leftrightarrow \text{expl. Euler for } \dot{y} = \lambda_e y}$

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

$\hookrightarrow$ if $|1 + h\lambda_i| \leq 1$

Also applies to $\lambda_i \in \mathbb{C}$, Rem. 12.1.0.42

§ 12.1.0.43 (Extended model problem analysis for explicit RK-SSMs)

Definition 11.4.0.11. Explicit Runge-Kutta single-step 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 $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}), \mathbf{f}: \Omega \rightarrow \mathbb{R}^N$, is defined by $(\mathbf{y}_0 \in D)$

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

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

$\leftrightarrow$ Butcher scheme $\begin{array}{c|c} \mathcal{A} \\ \hline \mathbf{b}^T \end{array}, \mathcal{A} \in \mathbb{R}^{s,s}$

Apply to ODE $\dot{y} = \mathbf{f}(y) := \mathbf{M}y$

$$\mathbf{k}_\ell = \mathbf{M}(\mathbf{y}_0 + h \sum_{j=1}^{\ell-1} a_{\ell j} \mathbf{k}_j), \quad \ell = 1, \dots, s, \quad \mathbf{y}_1 = \mathbf{y}_0 + h \sum_{\ell=1}^s b_\ell \mathbf{k}_\ell. \quad (12.1.0.44)$$

Diagonalization:

$$[\exists V \in \mathbb{C}^{N,N}: V^{-1} M V = D = \text{diag}(\lambda_1, \dots, \lambda_N)]$$

$$\begin{aligned} V^{-1} \mathbf{k}_\ell &= V^{-1} M V (V^{-1} \mathbf{y}_0 + h \sum_{j=1}^{\ell-1} a_{\ell j} V^{-1} \mathbf{k}_j) \\ V^{-1} \mathbf{y}_1 &= V^{-1} \mathbf{y}_0 + h \sum_{i=1}^s b_i V^{-1} \mathbf{k}_i \end{aligned}$$

$$[\hat{\mathbf{k}}_\ell := V^{-1} \mathbf{k}_\ell, \quad \underline{\mathbf{z}}_k := V^{-1} \mathbf{y}_k]$$

$$\begin{aligned} \hat{\mathbf{k}}_\ell &= D (\underline{\mathbf{z}}_0 + h \sum_{j=1}^{\ell-1} a_{\ell j} \hat{\mathbf{k}}_j) \\ \underline{\mathbf{z}}_1 &= \underline{\mathbf{z}}_0 + h \sum_{i=1}^s b_i \hat{\mathbf{k}}_i \end{aligned}$$

Decoupled:

$$\begin{aligned} (\hat{\mathbf{k}}_\ell)_m &= \lambda_m ((\underline{\mathbf{z}}_0)_m + h \sum_{j=1}^{\ell-1} a_{\ell j} (\hat{\mathbf{k}}_j)_m) \\ (\underline{\mathbf{z}}_1)_m &= (\underline{\mathbf{z}}_0)_m + h \sum_{i=1}^s b_i (\hat{\mathbf{k}}_i)_m, \quad m = 1, \dots, N \end{aligned}$$

$$\hat{=} \text{RK-SSM for } \dot{y} = \lambda_m y$$

§ 12.1.0.49 (Region of stability for explicit RK-SSM)

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

Stability analysis: reduction to scalar case

Understanding the behavior of RK-SSM for autonomous scalar linear ODEs $\dot{y} = \lambda y$ with $\lambda \in \mathbb{C}$ is enough to predict their behavior for general autonomous linear systems of ODEs.

$$\|\mathbf{y}_k\| \xrightarrow{k \rightarrow \infty} \infty \iff |(z_k)_m| \xrightarrow{k \rightarrow \infty} \infty \text{ for one } m$$

Theorem 12.1.0.48. (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 ($\rightarrow$ Def. 11.4.0.11) with stability function S (defined in (12.1.0.18)) applied to the linear autonomous ODE $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$, $\mathbf{M} \in \mathbb{C}^{N,N}$, with uniform timestep $h > 0$ decays exponentially for every initial state $\mathbf{y}_0 \in \mathbb{C}^N$, if and only if $|S(\lambda_i h)| < 1$ for all eigenvalues λ_i of $\mathbf{M}$.

↑ stability function

Definition 12.1.0.51. 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

$$\Psi^h y = S(z)y, \quad y \in \mathbb{C}, h > 0 \quad \text{with} \quad z := h\lambda \quad (12.1.0.52)$$

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

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

$\lambda h \in S_\Psi \Rightarrow$ No blow-up of RK-SSM solutions for ODE $\dot{y} = \lambda y$ can occur

Explicit s -stage RK-SSMs : $S \in \mathcal{P}_s$

$\Rightarrow S_\Psi$ bounded

$\Rightarrow$ **Timestep constraint** : $\lambda_m h \in S_\Psi \quad \forall m=1, \dots, N$

$\forall$ eigenvalues λ_m of $M \in \mathbb{R}^{N,N}$, $\dot{\mathbf{y}} = M\mathbf{y}$

$\rightarrow$ to avoid blow-up

▷ Please answer review questions 12.1.0.54
without relying on these notes or the lecture
document.