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

Numerical Methods for Computational Science and Engineering

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URL: http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE16.pdf

XI. Numerical Integration - Single-Step Methods -

→ Numerical solution of ODEs

11.1. Initial Value Problems for ODEs

"time variable"

ODE: $[\frac{d}{dt}y =] \dot{y} = f(t, y(t))$

right-hand-side function $f: D \subset \mathbb{R}^d \to \mathbb{R}^d$ (continuous)

solution: C^1-function $t \to y(t) \in \mathbb{R}^d$ that satisfies the ODE pointwise $\forall t \in I \subset \mathbb{R}$

$D \subset \mathbb{R}^d \triangleq$ state space

For $d > 1$ $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$ can be viewed as a system of ordinary differential equations:

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}) \iff \begin{bmatrix} \dot{y}_1 \\ \vdots \\ \dot{y}_d \end{bmatrix} = \begin{bmatrix} f_1(t, y_1, \ldots, y_d) \\ \vdots \\ f_d(t, y_1, \ldots, y_d) \end{bmatrix}.$$

$f \in C^m \Rightarrow$ solution $y \in C^{m+1}$

11.1.1. Model with ODEs

Discrete mechanics: $\ddot{y} = f(y)$

transient circuit models

reaction kinetics

.....

Example (population dynamics): Predator-prey model

$d = 2$: $u = u(t)$: prey, $v = v(t)$: predator

ODE-based model: autonomous Lotka-Volterra ODE: $(\alpha, \beta, \gamma, \delta > 0)$

$$\begin{aligned} \dot{u} &= (\alpha - \beta v)u \\ \dot{v} &= (\delta u - \gamma)v \end{aligned} \quad \leftrightarrow \quad \dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}) \quad \text{with} \quad \mathbf{y} = \begin{bmatrix} u \\ v \end{bmatrix}, \quad \mathbf{f}(\mathbf{y}) = \begin{bmatrix} (\alpha - \beta v)u \\ (\delta u - \gamma)v \end{bmatrix}, \qquad (11.1.10)$$

$v = 0$: $\dot{u} = \alpha u \Rightarrow u(t) = u(0)\, e^{\alpha t}$

$u = 0$: $\dot{v} = -\gamma v \Rightarrow$ exponential decay

Definition 11.1.8. Autonomous ODE

An ODE of the from $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$, that is, with a right hand side function that does not depend on time, but only on state, is called autonomous.

$\Rightarrow$ model time-invariant models

(periodic solution)

Solution:

Initial values

Needed to fix a unique solution of an ODE

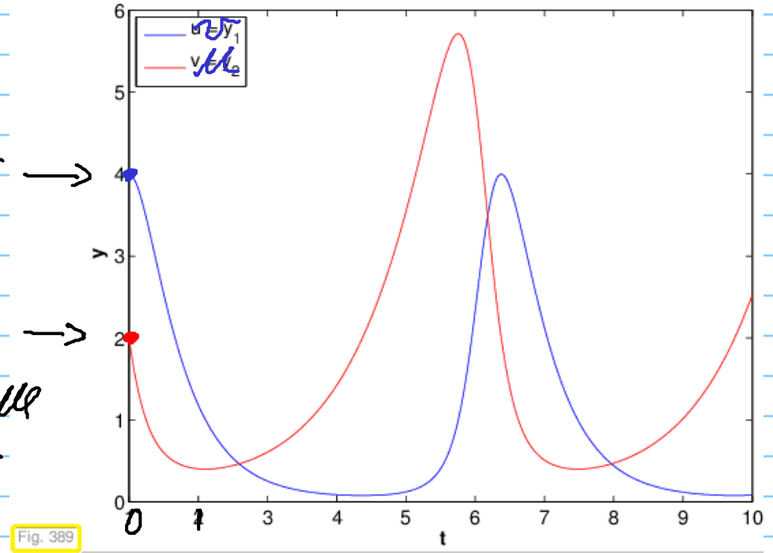


Fig. 389

Solution $\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}$ for $\mathbf{y}_0 := \begin{bmatrix} u(0) \\ v(0) \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$

$\Rightarrow$ In numerical integration we solve initial value problem (IVP) = ODE + initial values

$$\dot{y} = f(t, y), \quad y(t_0) = y_0$$

(t_0: initial time)

$\Rightarrow$ For autonomous ODEs:

If $t \mapsto y(t)$ solution $\Rightarrow$ $t \mapsto y(t - \tau)$ is a solution

$\Rightarrow$ Free choice of t_0: $t_0 := 0$

Solution of IVP → function of time
→ curve in state space: $t \to D$

predator

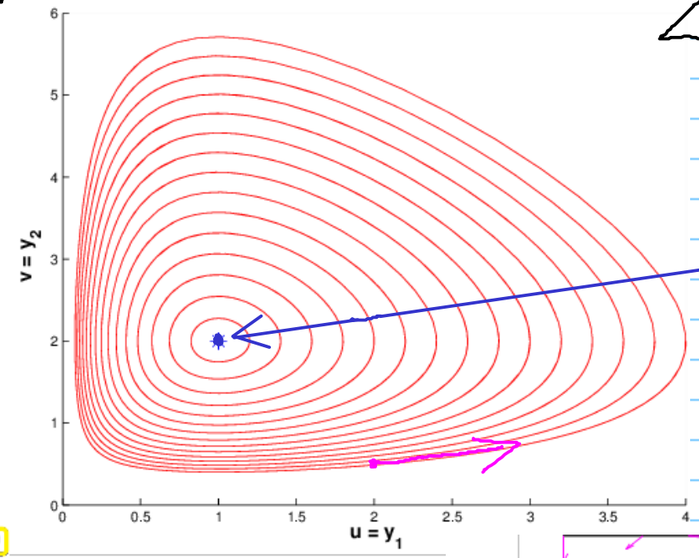


Fig. 390

Solution curves for (11.1.10)

△ trajectories (closed curves)

Stationary point $\bar{y}^*$
$\underline{f}(\bar{y}^*) = 0$

prey

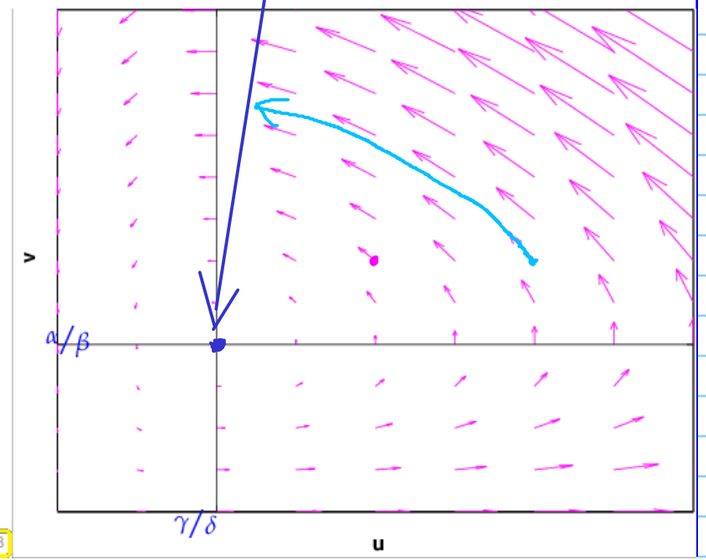


Fig. 388

→ $\hat{=}$ $\underline{f}\left(\begin{bmatrix} u \\ v \end{bmatrix}\right)$

ODE $\hat{=}$ movement of particles in velocity field described by $\underline{f}$

11.1.2. Theory of IVP

Remark: Autonomization

$$\dot{\bar{y}} = \underline{f}(t, \bar{y}) \quad : \quad \bar{z}(t) = \begin{bmatrix} \bar{y}(t) \\ t \end{bmatrix} \in \mathbb{R}^{d+1}$$

$$\dot{\bar{z}}(t) = \begin{bmatrix} \dot{\bar{y}}(t) \\ 1 \end{bmatrix} = \underbrace{\begin{bmatrix} \underline{f}(z_{d+1}, t), \begin{bmatrix} z_1 \\ \vdots \\ z_d \end{bmatrix} \\ 1 \end{bmatrix}}_{=: \underline{g}(\bar{z})}$$

$$\underbrace{\dot{\bar{z}} = \underline{g}(\bar{z})}_{\text{autonomous ODE}}$$

Remark: Conversion to 1st-order ODE

$$\ddot{\bar{y}} = f(\bar{y}) \qquad [\text{2nd-order ODE}]$$

$$\bar{z}(t) = \begin{bmatrix} \bar{y}(t) \\ \dot{\bar{y}}(t) \end{bmatrix} \in \mathbb{R}^{2d} \Rightarrow \dot{\bar{z}}(t) = \begin{bmatrix} \dot{\bar{y}} \\ \ddot{\bar{y}} \end{bmatrix} = \underbrace{\begin{bmatrix} z_{d+1} \\ \vdots \\ z_{2d} \\ \underline{f}\left(\begin{bmatrix} z_1 \\ \vdots \\ z_d \end{bmatrix}\right) \end{bmatrix}}_{=: \underline{g}(\bar{z})}$$

$$\dot{\bar{z}} = \underline{g}(\bar{z})$$

(4)

Remark : Intrinsic Domain of definition of solutions of IVP

Example : $\dot{y} = y^2$, $y(0) = y_0$

We find the solutions

$$y(t) = \begin{cases} \frac{1}{y_0^{-1} - t} & \text{, if } y_0 \neq 0 \,, \\ 0 & \text{, if } y_0 = 0 \,, \end{cases} \tag{11.1.37}$$

with domains of definition

$$J(y_0) = \begin{cases}]-\infty, y_0^{-1}[& \text{, if } y_0 > 0 \,, \\ \mathbb{R} & \text{, if } y_0 = 0 \,, \\ ]y_0^{-1}, \infty[& \text{, if } y_0 < 0 \,. \end{cases}$$

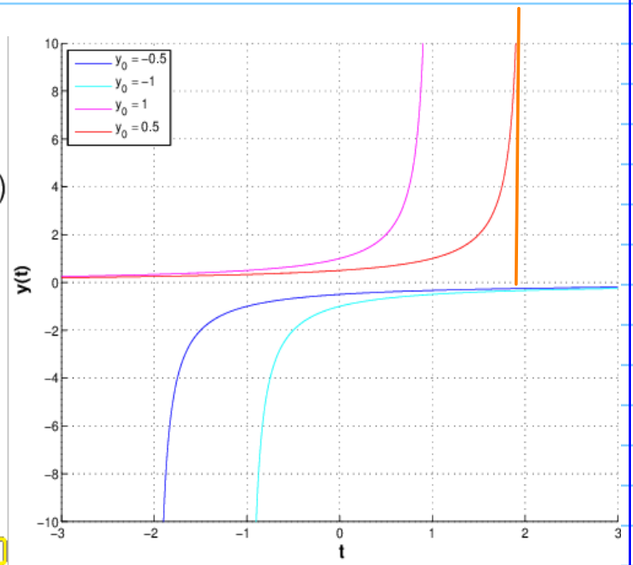


Fig. 396

Blow-up after finite time

"built into the solution"

11.1.3. Evolution operators [for $\dot{y} = f(y)$]

[Assume: Existence $\forall t \in \mathbb{R}$, $\forall y_0 \in D$]

$y_0 \in D \Rightarrow$ Unique solution $\dot{y}(t) = f(y(t))$, $y(0) = y_0$

↳ $\hat{=}$ curve in state space

$t = t^*$ fixed: $y_0 \longrightarrow y(t^*)$

Definition 11.1.39. Evolution operator/mapping

Under Ass. 11.1.38 the mapping

$$\Phi : \begin{cases} \mathbb{R} \times D & \mapsto & D \\ (t, \mathbf{y}_0) & \mapsto & \Phi^t \mathbf{y}_0 := \mathbf{y}(t) \end{cases},$$

where $t \mapsto \mathbf{y}(t) \in C^1(\mathbb{R}, \mathbb{R}^d)$ is the unique (global) solution of the IVP $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{y}_0$, is the evolution operator/mapping for the autonomous ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$.

$t \longrightarrow \Phi^t y_0 \hat{=}$ trajectory : $\frac{d}{dt} \Phi^t y = f(\Phi^t y)$

$y \longrightarrow \Phi^t y \hat{=}$ mapping of state space

Φ encodes the complete set of solutions of the ODE

(5)

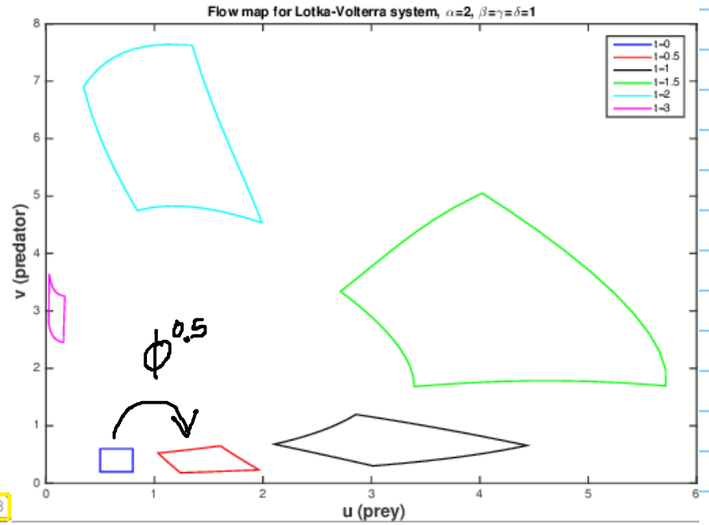


Fig. 398

state mapping $\mathbf{y} \mapsto \Phi^t \mathbf{y}$

11.2. Polygonal Approximation Methods

ODE: $\dot{y} = f(y)$

Goal: Approximate model for evolution operator Φ

Focus on discrete set of times (temporal mesh)

$$\mathcal{M} = \{ 0 = t_0 < t_1 < \dots < t_N = T \}$$

$t_N = T$: final time

11.2.1 Explicit* Euler method

Difference quotient on $\mathcal{M}$

$h_k := t_{k+1} - t_k$

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

"forward difference quotient"

$$\frac{y_{k+1} - y_k}{h_k} = f(y_k)$$

+ set $y_0 = y(0)$ [initial value]

$\Rightarrow$ sequence: $\{ y_0, y_1, \dots, y_N \}$ with $y_k \approx y(t_k)$

* created by f-eval above

Geometry: polygonal approximation of trajectories ▷

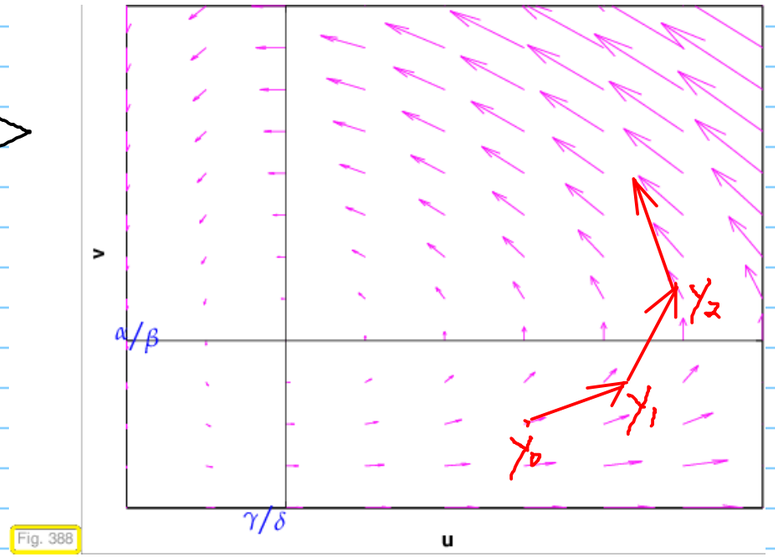


Fig. 388

11.2.2. Implicit Euler method

$$\dot{y} = f(y) \quad \Longrightarrow \quad \frac{y_{k+1} - y_k}{h_k} = f(y_{k+1}) \quad [1]$$

↑ "backward difference quotient"

to build sequence $(y_0, y_1, \ldots, y_N)$ ← given initial value

⇒ solve system of d equ. in each step for d unknowns

11.2.3. Implicit midpoint method

$$\dot{y} = f(y) \quad \Longrightarrow \quad \frac{y_{k+1} - y_k}{h_k} = \left[f\left(y\left(\frac{t_k + t_{(k+1)}}{2} \right) \right) \right]$$

↑ d.q.

↑ not available

polygonal approx: $y\left(\frac{t_k + t_{(k+1)}}{2}\right) \approx \frac{1}{2} y_k + \frac{1}{2} y_{k+1}$

▷

$$\frac{y_{k+1} - y_k}{h_k} = f\left(\frac{1}{2} (y_k + y_{k+1}) \right) \quad [2]$$

Remark: Implicit methods ⇒ for small h_k [1], [2] can be solved for y_{k+1},

III.3. General Single-Step Methods

Expl. Euler: $y_{k+1} = y_k + h_k f(y_k)$ $\longrightarrow$ $\Psi^h y = y + hf(y)$

Impl. Euler: $y_{k+1} = y_k + h_k f(y_{k+1})$ $\longrightarrow$ "$\Psi^h y := z : z = y + hf(z)$"

$$y_{k+1} = \Psi(h_{k+1}, y_k) =: \Psi^h y_k$$

What makes a good Ψ?

$$y(t_1) = \Phi^{h_1} y_0 \quad \Longleftrightarrow \quad y_1 = \Psi^{h_1} y_0$$

$$\Psi : I \times D \to \mathbb{R}^d \approx \Phi : I \times D \to \mathbb{R}^d$$

must approximate the evolution operator

At least the direction of $h \to \Psi^h y$ in $h = 0$ should be $f(y)$:

Definition 11.3.5. Single step method (for autonomous ODE) → [?, Def. 11.2]

Given a discrete evolution $\Psi : \Omega \subset \mathbb{R} \times D \mapsto \mathbb{R}^d$, an initial state $\mathbf{y}_0$, and a temporal mesh $\mathcal{M} := \{0 =: t_0 < t_1 < \cdots < t_N := T\}$ the recursion

$$\mathbf{y}_{k+1} := \Psi(t_{k+1} - t_k, \mathbf{y}_k) , \quad k = 0, \ldots, N-1 , \tag{11.3.6}$$

defines a single step method (SSM) for the autonomous IVP $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{y}_0$ on the interval $[0, T]$.

Consistent discrete evolution → Minimal requirement

The discrete evolution Ψ defining a single step method according to Def. 11.3.5 and (11.3.6) for the autonomous ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ invariably is of the form

$$\Psi^h \mathbf{y} = \mathbf{y} + h\psi(h, \mathbf{y}) \quad \text{with} \quad \psi : I \times D \to \mathbb{R}^d \text{ continuous}, \ \psi(0, \mathbf{y}) = \mathbf{f}(\mathbf{y}) . \tag{11.3.9}$$

$$\frac{d}{dh} \Psi^h \Big|_{h=0} = 0 + \psi(0, y) + 0 \cdot \dot{\psi}(h, y) = f(y)$$

11.3.2. Asymptotic Convergence of SSM

IVP + SSM : | study $\max_k \|y_k - y(t_k)\|$ [$\|y_N - y(T)\|$]

↓

for family of meshes $(\mathcal{M}_\ell)$ [e.g. equid. meshes]

$h_\ell := \max_k |t_{k+1}^\ell - t_k^\ell| \to 0$ for $\ell \to \infty$

Example: $\dot{y} = \lambda(1-y)y$ [logistic ODE]

$y_0 \in [0,1] \Rightarrow$ solution exists on $\mathbb{R}$

Error at final time $T = 1$, equid. meshes

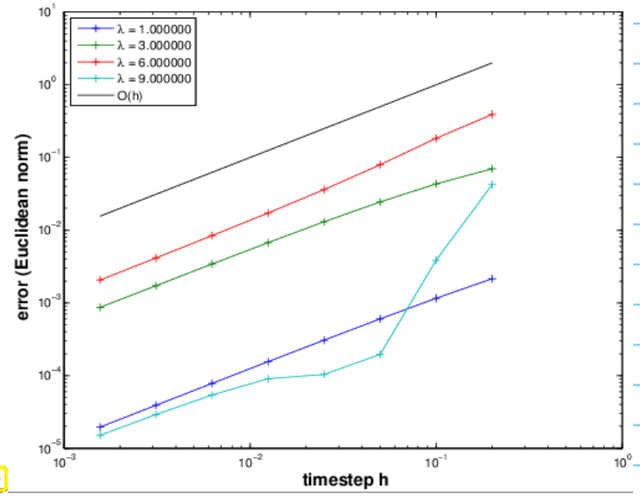


Fig. 405

explicit Euler method

△ Alg. cvg.

$err = O(h^\alpha)$

$\alpha = 1$

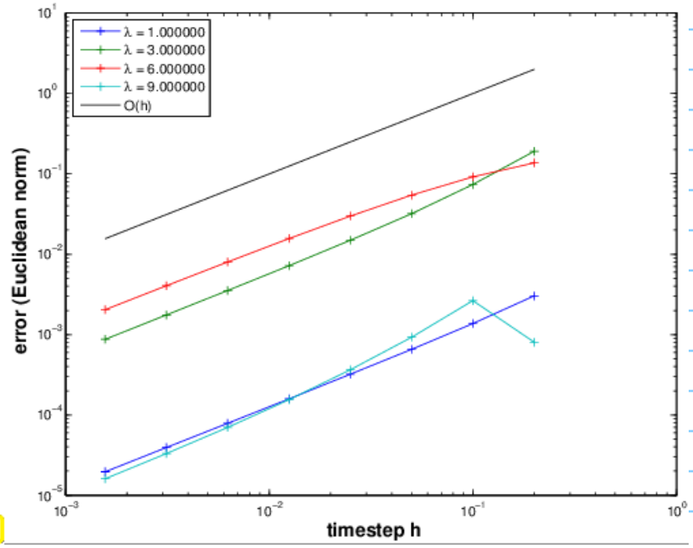


Fig. 406

implicit Euler method

△ Alg. cvg.

order = 1

impl. midp. method

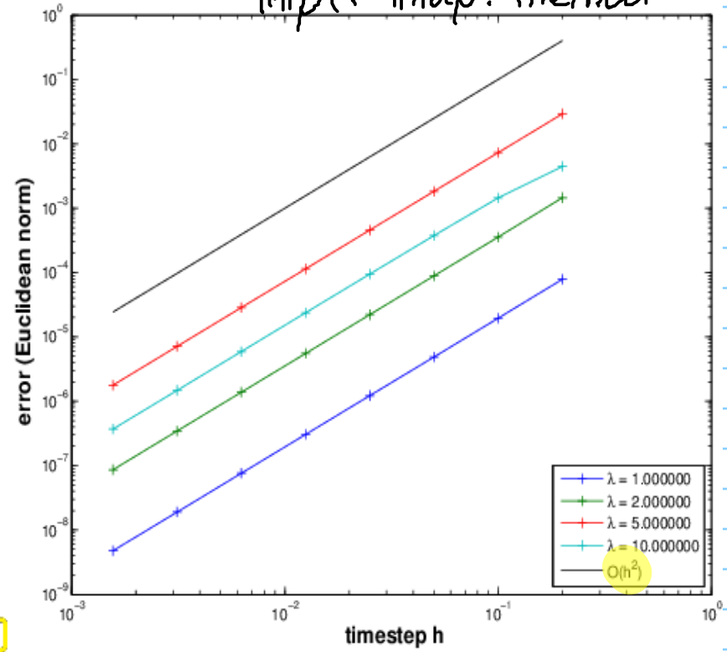


Fig. 407

△ Alg. cvg.

order = 2

All SSM converge algebraically in meshwidth h with some order $p \in \mathbb{N}$: $\text{err} = O(h^p)$

an important characteristic of the method

Repetition:

$$\dot{y} = f(y) \quad , \quad f : D \subset \mathbb{R}^d \to \mathbb{R}^d$$

Evolution operator $\Phi : \mathbb{R} \times D \to \mathbb{R}^d$

Numerical integrators $\Rightarrow$ Discrete evolution $\Psi : \mathbb{R} \times D \to \mathbb{R}^d$

$\Downarrow$

Single-step method on temporal mesh $\mathcal{M} = \{0 = t_0 < t_1 < \dots < t_N = T\}$

$\hookrightarrow$ $y_{k+1} = \Psi^{h_{k+1}} y_k$, $h_{k+1} := t_{k+1} - t_k$

Goal: $y_k \approx y(t_k)$, where $t \to y(t)$ solves IVP: $\dot{y} = f(y), y(0) = y_0$

How to get a function $y_h : [0,T] \to \mathbb{R}^d$ from $(y_k)_k$?

$\to$ by interpolation: Euler method $\to$ p.w. linear interpolation

better: piece cubic interpolation based on $y_k, f(y_k) \approx \dot{y}(t_k)$

11.4. Explicit Runge-Kutta-Methods

IVP: $\dot{\mathbf{y}}(t) = \mathbf{f}(t, \mathbf{y}(t))$, $\mathbf{y}(t_0) = \mathbf{y}_0$ $\Rightarrow$ $\mathbf{y}(t_1) = \mathbf{y}_0 + \int_{t_0}^{t_1} \mathbf{f}(\tau, \mathbf{y}(\tau))\, d\tau$

Apply num. quad!

Idea: approximate the integral by means of s-point quadrature formula ($\to$ Section 7.1, defined on the reference interval $[0,1]$) with nodes $c_1, \dots, c_s$, weights $b_1, \dots, b_s$.

$$\mathbf{y}(t_1) \approx \mathbf{y}_1 = \mathbf{y}_0 + h \sum_{i=1}^{s} b_i \mathbf{f}(t_0 + c_i h, \mathbf{y}(t_0 + c_i h)) \quad , \quad h := t_1 - t_0 \, . \tag{11.4.3}$$

Obtain these values by bootstrapping

approximate by some other "lower-order" discrete evolution

Quadrature formula = trapezoidal rule (7.2.5):

$$Q(f) = \tfrac{1}{2}(f(0) + f(1)) \quad \leftrightarrow \quad s = 2: \; c_1 = 0, c_2 = 1 \, , \; b_1 = b_2 = \frac{1}{2} \, , \tag{11.4.5}$$

and $\mathbf{y}(t_1)$ approximated by explicit Euler step (11.2.7)

$$\mathbf{k}_1 = \mathbf{f}(t_0, \mathbf{y}_0) \, , \quad \mathbf{k}_2 = \mathbf{f}(t_0 + h, \mathbf{y}_0 + h\mathbf{k}_1) \, , \quad \mathbf{y}_1 = \mathbf{y}_0 + \tfrac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2) \, . \tag{11.4.6}$$

(11.4.6) = explicit trapezoidal method (for numerical integration of ODEs).

$$y_1 = y_0 + h\left[\tfrac{1}{2} f(y_0) + \tfrac{1}{2} f(y_1)\right] = y_0 + \tfrac{1}{2} h \left(f(y_0) + f(y_0 + h f(y_0))\right)$$

(10)

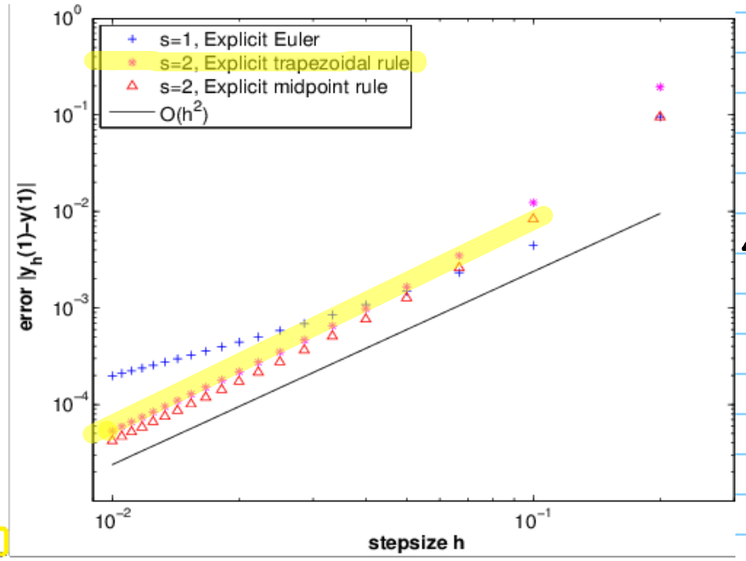


Fig. 413

Errors at final time $y_h(1) - y(1)$

(Logistic ODE)

◁ Alg. conv. order = 2

↳ f-eval enough to compute Ψ^h !

Definition 11.4.9. Explicit Runge-Kutta method

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{i-1} a_{ij}$, $i,j = 1,\ldots,s$, $s \in \mathbb{N}$, 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 ($\mathbf{y}_0 \in D$)

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

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

≙ coefficient

Impl.: $k_1 = f(t_0 + c_1 h, y_0)$ → k_2 → k_3 → .. → k_s

Notation: Butcher scheme

Butcher scheme notation for explicit RK-SSM

Shorthand notation for (explicit) Runge-Kutta methods [?, (11.75)]

Butcher scheme ▷

(Note: $\mathfrak{A}$ is strictly lower triangular $s \times s$-matrix)

$$\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccccc} c_1 & 0 & & \cdots & & 0 \\ c_2 & a_{21} & \ddots & & & \vdots \\ \vdots & \vdots & & & \ddots & \vdots \\ c_s & a_{s1} & & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & & \cdots & b_{s-1} & b_s \end{array} \qquad (11.4.11)$$

$$y(t) \approx \sum_{i=1}^{s} w_i(t)\, k_i \quad \text{"dense output"}$$

RK-SSM consistent ?

Consistent discrete evolution

The discrete evolution Ψ defining a single step method according to Def. 11.3.5 and (11.3.6) for the autonomous ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ invariably is of the form

$$\Psi^h \mathbf{y} = \mathbf{y} + h\psi(h,\mathbf{y}) \quad \text{with} \quad \begin{array}{l} \psi : I \times D \to \mathbb{R}^d \text{ continuous,} \\ \psi(0,\mathbf{y}) = \mathbf{f}(\mathbf{y})\,. \end{array} \qquad (11.3.9)$$

Discr. Evol.: $\Psi^h y = y + h \underbrace{\sum_{i=1}^{s} b_i K_i(y)}_{\psi(h,y)}$

for $h = 0$: $K_i = f(y_0)$

$$\Rightarrow \quad \Psi(0,y) = \sum_{i=1}^{s} b_i f(y) \overset{!}{=} f(y) \Leftrightarrow \sum_{i=1}^{s} b_i = 1$$

an order condition — Consistency conditions for RK-SSM

Examples :

Explicit Euler method (11.2.7): $s = 1$

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \quad \rightarrow \quad \text{order} = 1$$

explicit trapezoidal rule (11.4.6): $s = 2$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad \rightarrow \quad \text{order} = 2$$

Classical 4th-order RK-SSM:

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array} \quad \rightarrow \quad \text{order} = 4$$

Goal : High order few stages

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

Why is high order desirable ?

→ For the sake of efficiency !

$s \hat{=}$ no. of stages

Order-p method : assume $\text{err}(h) \approx Ch^p$

Cost: $W \approx s/h \approx$ no. of equidistant timesteps

to achieve error reduction by factor $\rho > 1$

$$\frac{C h_{old}^p}{C h_{new}^p} \overset{!}{=} \rho$$

$$\Rightarrow \quad h_{new} = \rho^{-1/p} \cdot h_{old}$$

$$W_{new} = \rho^{1/p} \cdot W_{old}$$

The larger p, the less effort is needed for prescribed error reduction.

$\sim$ # f-evaluations

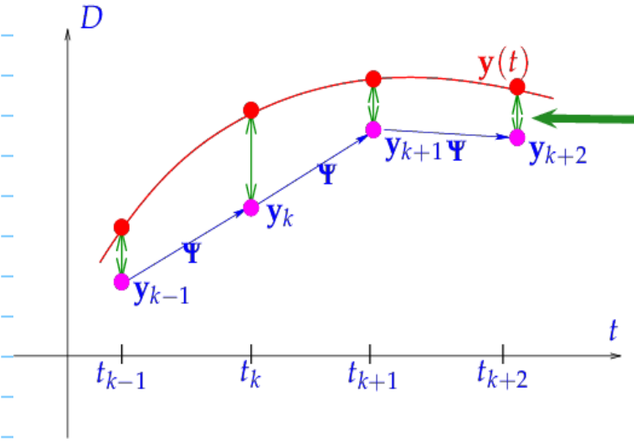
Convergence analysis: explicit Euler (equid. timestep)

Assume: • f smooth

• $\| f(x) - f(z) \| \leq L \| x - z \|$ (*)

Error: $e_k := y_k - y(t_k) \Rightarrow \Psi^h y = y + h f(y)$

$$\mathbf{y}_{k+1} = \mathbf{y}_k + h_k \mathbf{f}(\mathbf{y}_k) , \quad k = 1, \ldots, N-1 . \tag{11.2.7}$$



Error sequence: $\mathbf{e}_k := \mathbf{y}_k - \mathbf{y}(t_k)$.

◁ — ≙ trajectory $t \mapsto \mathbf{y}(t)$

— ≙ Euler polygon,

• ≙ $\mathbf{y}(t_k)$,

• ≙ $\mathbf{y}_k$,

⟶ ≙ discrete evolution $\Psi^{t_{k+1}-t_k}$

$y_{k+1} = \Psi^{h_k} y_k$

Fundamental error splitting

$$\begin{aligned} \mathbf{e}_{k+1} &= \Psi^{h_k}\mathbf{y}_k - \Phi^{h_k}\mathbf{y}(t_k) \\ &= \underbrace{\Psi^{h_k}\mathbf{y}_k - \Psi^{h_k}\mathbf{y}(t_k)}_{\text{propagated error}} \\ &\quad + \underbrace{\Psi^{h_k}\mathbf{y}(t_k) - \Phi^{h_k}\mathbf{y}(t_k)}_{\text{one-step error}} . \end{aligned} \tag{11.3.25}$$

$y(t_{k+1}) = \Phi^{h_k} y(t_k)$

↑ exact solution

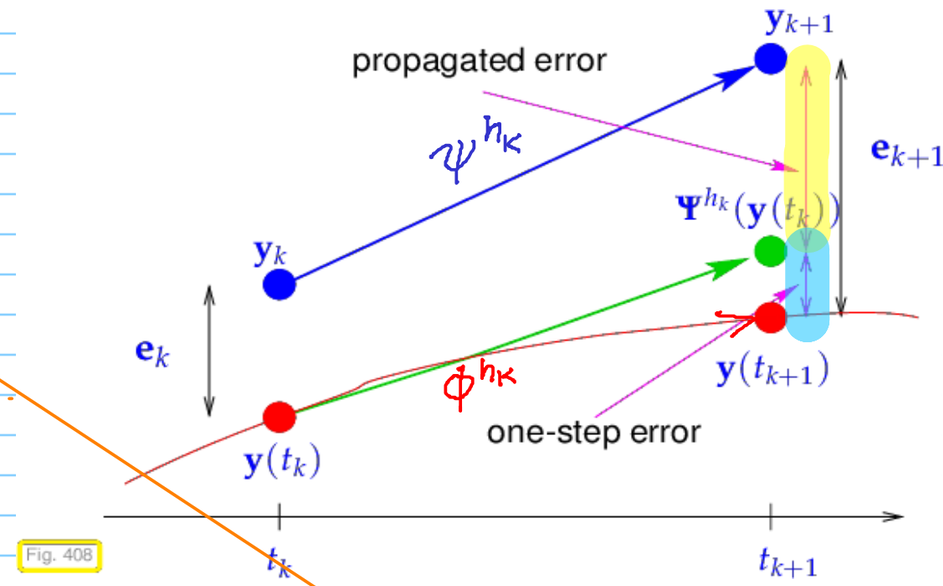


Fig. 408

Propagated error:

$$\begin{aligned} \| \Psi^h y_k - \Psi^h y(t_k) \| &= \| y_k + h f(y_k) - y(t_k) - h f(y(t_k)) \| \\ &= \| e_k + h (f(y_k) - f(y(t_k)) \| \\ &\overset{(*)}{\leq} (1 + hL) \| e_k \| \end{aligned}$$

One step error:

$$\begin{aligned} \Psi^h y(t_k) - y(t_k + h) &= y(t_k) + h f(y(t_k)) - y(t_k + h) \\ \text{Use ODE:} &= y(t_k) + h \dot{y}(t_k) - y(t_k + h) \\ \text{Taylor} &= \tfrac{1}{2} h^2 \ddot{y}(\tau) , \quad t_k \leq \tau \leq t_{k+1} \end{aligned}$$

③ Obtain *recursion* for error norms $\epsilon_k := \|\mathbf{e}_k\|$ by $\triangle$-inequality:

(13)

$$\epsilon_{k+1} \le (1+h_k L)\epsilon_k + \rho_k\,, \quad \rho_k := \tfrac{1}{2}h_k^2 \max_{t_k\le\tau\le t_{k+1}} \|\ddot{\mathbf{y}}(\tau)\| \,. \tag{11.3.30}$$

↳ bound for one-step error

Taking into account $\epsilon_0 = 0$, this leads to

$$\epsilon_k \le \sum_{l=1}^{k}\prod_{j=1}^{l-1}(1+Lh_j)\,\rho_l\,, \quad k=1,\ldots,N\,. \tag{11.3.31}$$

Use the elementary estimate $(1+Lh_j) \le \exp(Lh_j)$ (by convexity of exponential function):

$$(11.3.31) \;\Rightarrow\; \epsilon_k \le \sum_{l=1}^{k}\prod_{j=1}^{l-1}\exp(Lh_j)\cdot\rho_l = \sum_{l=1}^{k}\exp(L\textstyle\sum_{j=1}^{l-1}h_j)\rho_l\,.$$

Note: $\sum_{j=1}^{l-1} h_j \le T$ for final time T and conclude

$y \in C^2$ required

$$\epsilon_k \le \exp(LT)\sum_{l=1}^{k}\rho_l \le \exp(LT)\max_k\frac{\rho_k}{h_k}\sum_{l=1}^{k}h_l \le T\exp(LT)\max_{l=1,\ldots,k}h_l\cdot\max_{t_0\le\tau\le t_k}\|\ddot{\mathbf{y}}(\tau)\|\,.$$

$$\|\mathbf{y}_k - \mathbf{y}(t_k)\| \le T\exp(LT)\max_{l=1,\ldots,k}h_l\cdot\max_{t_0\le\tau\le t_k}\|\ddot{\mathbf{y}}(\tau)\|\,. \tag{11.3.32}$$

$\|\mathbf{y}_k - \mathbf{y}(t_k)\| = e_k$

1st-order alg. conv. $O(h)$

11.5. Adaptive Stepsize Control

Example:

This is a special case of an "oscillating" Zhabotinski-Belousov reaction [?]:

$$\begin{aligned} \mathrm{BrO_3^-} + \mathrm{Br^-} &\mapsto \mathrm{HBrO_2} \\ \mathrm{HBrO_2} + \mathrm{Br^-} &\mapsto \mathrm{Org} \\ \mathrm{BrO_3^-} + \mathrm{HBrO_2} &\mapsto 2\,\mathrm{HBrO_2} + \mathrm{Ce(IV)} \\ 2\,\mathrm{HBrO_2} &\mapsto \mathrm{Org} \\ \mathrm{Ce(IV)} &\mapsto \mathrm{Br^-} \end{aligned} \tag{11.5.2}$$

ODE

$$\begin{aligned} y_1 := c(\mathrm{BrO_3^-}): &\quad \dot{y}_1 = -k_1y_1y_2 - k_3y_1y_3\,, \\ y_2 := c(\mathrm{Br^-}): &\quad \dot{y}_2 = -k_1y_1y_2 - k_2y_2y_3 + k_5y_5\,, \\ y_3 := c(\mathrm{HBrO_2}): &\quad \dot{y}_3 = k_1y_1y_2 - k_2y_2y_3 + k_3y_1y_3 - 2k_4y_3^2\,, \\ y_4 := c(\mathrm{Org}): &\quad \dot{y}_4 = k_2y_2y_3 + k_4y_3^2\,, \\ y_5 := c(\mathrm{Ce(IV)}): &\quad \dot{y}_5 = k_3y_1y_3 - k_5y_5\,, \end{aligned} \tag{11.5.3}$$

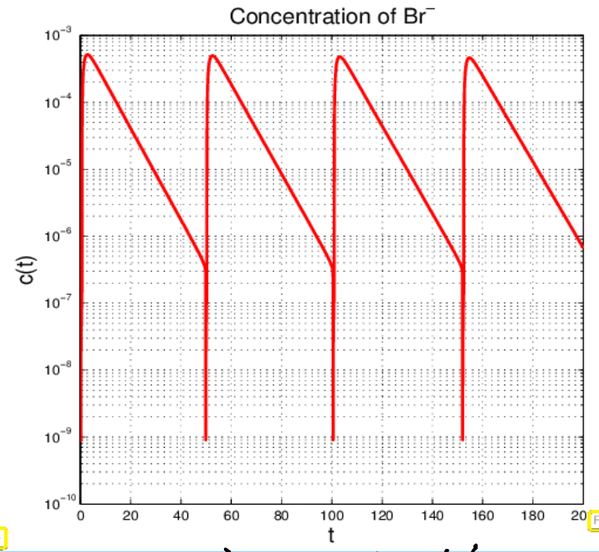


Fig. 414

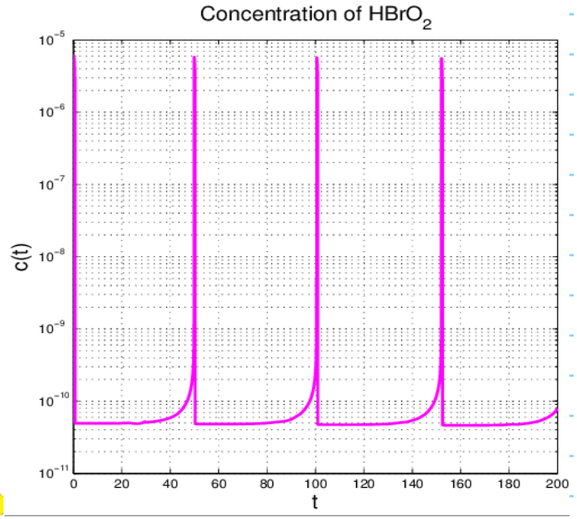


Fig. 415

$y(t)$ = highly non-uniform in time

(4)

→ suggest use of highly non-uniform temporal meshes

Example: Blow-up

We return to the "explosion ODE" of Ex. 11.1.35 and consider the scalar autonomous IVP:

$$\dot{y} = y^2 , \quad y(0) = y_0 > 0 .$$

$$\blacktriangleright \quad y(t) = \frac{y_0}{1 - y_0 t} , \quad t < 1/y_0 .$$

As we have seen a solution exists only for finite time and then suffers a Blow-up, that is, $\lim_{t \to 1/y_0} y(t) = \infty$

: $J(y_0) =]-\infty, 1/y_0]$!

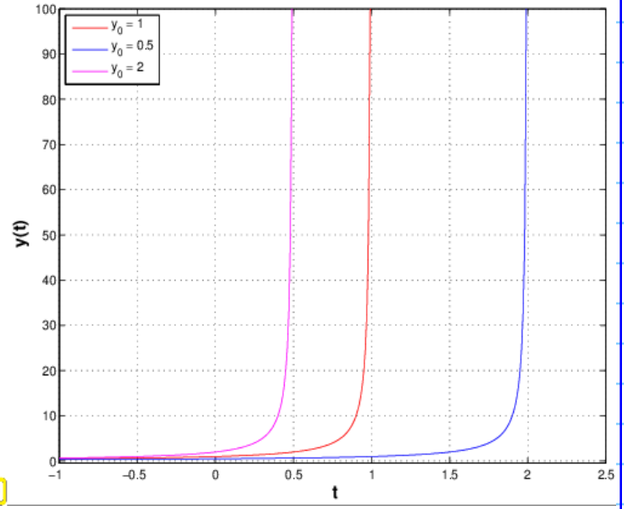


Fig. 416

Expl. Euler & uniform time step → no "numerical blow-up"

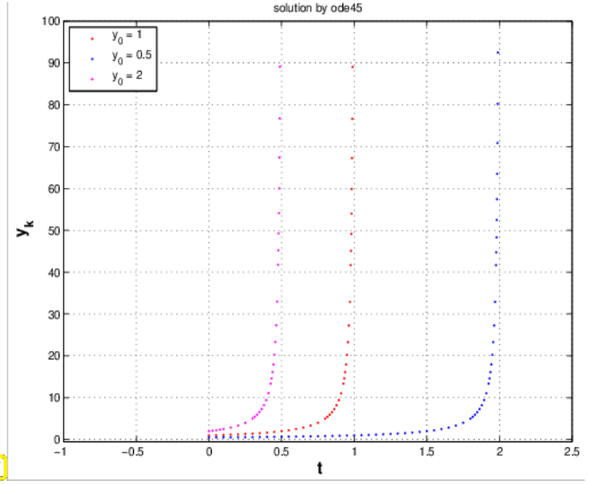


Fig. 417

Simulation with MATLAB's `ode45`:

MATLAB-code 11.5.5:

```
1 fun = @(t,y) y.^2;
2 t1,y1] = ode45(fun,[0 2],1);
3 [t2,y2] = ode45(fun,[0
    2],0.5);
4 [t3,y3] = ode45(fun,[0 2],2);
```

Adaptive stepsize selection

Stepsize adaptation for single step methods

Objective: N as small as possible & $\max_{k=1,\ldots,N} \|\mathbf{y}(t_k) - \mathbf{y}_k\| < \mathtt{TOL}$ or $\|\mathbf{y}(T) - \mathbf{y}_N\| < \mathtt{TOL}$, TOL = tolerance

Policy: Try to curb/balance one-step error by

- ✦ adjusting *current* stepsize h_k,
- ✦ predicting suitable *next* timestep h_{k+1}

} local-in-time stepsize control

Tool: Local-in-time one-step error estimator (*a posteriori*, based on $\mathbf{y}_k, h_{k-1}$)

use merely y_k & h_k → cheap

(I)

by comparing two SSM of different order

Idea: *Estimation of one-step error*

Compare results for two discrete evolutions Ψ^h, $\widetilde{\Psi}^h$ of different order over *current timestep* h:

If $\mathrm{Order}(\widetilde{\Psi}) > \mathrm{Order}(\Psi)$, then we expect

$$\underbrace{\Phi^h \mathbf{y}(t_k) - \Psi^h \mathbf{y}(t_k)}_{\text{one-step error}} \approx \mathrm{EST}_k := \underbrace{\widetilde{\Psi}^h \mathbf{y}(t_k) - \Psi^h \mathbf{y}(t_k)}_{\text{computable}} . \qquad (11.5.8)$$

$= y(t_{k+1})$

replaces exact solution

Heuristics for concrete h

(II) Stepsize adaptation based on EST_k

(I)

$$EST_k \lesssim \max\{ATOL, RTOL \cdot \|y_k\|\}$$

absolute tol. relative tol.

- YES → Step accepted
  - $h_{k+1} = \alpha \cdot h_k$ ($\alpha \approx 1.1$)
  - ↓ next step
- NO → Step rejected : repeat
  - $h_k := \frac{1}{2} \cdot h_k$ → (I)

Algorithm: Embedded RK-SSM

$\Psi, \widetilde{\Psi}$ ↔ same increments

0					
$\frac{1}{3}$	$\frac{1}{3}$				
$\frac{1}{3}$	$\frac{1}{6}$	$\frac{1}{6}$			
$\frac{1}{2}$	$\frac{1}{8}$	0	$\frac{3}{8}$		
1	$\frac{1}{2}$	0	$-\frac{3}{2}$	2	
y_1	$\frac{1}{6}$	0	0	$\frac{2}{3}$	$\frac{1}{6}$
$\widehat{y}_1$	$\frac{1}{10}$	0	$\frac{3}{10}$	$\frac{2}{5}$	$\frac{1}{5}$

→ $\widetilde{\Psi}$ (order 5)

→ Ψ (order 4)

Merson's embedded RK-SSM

Remark: $y_{k+1} = \widetilde{\Psi}^{h_k} y_k$

→ Estimate error of Ψ but use $\widetilde{\Psi}$ for timestepping } works!

Example: $\dot{y} = \cos(\alpha y)$ → arctan solution

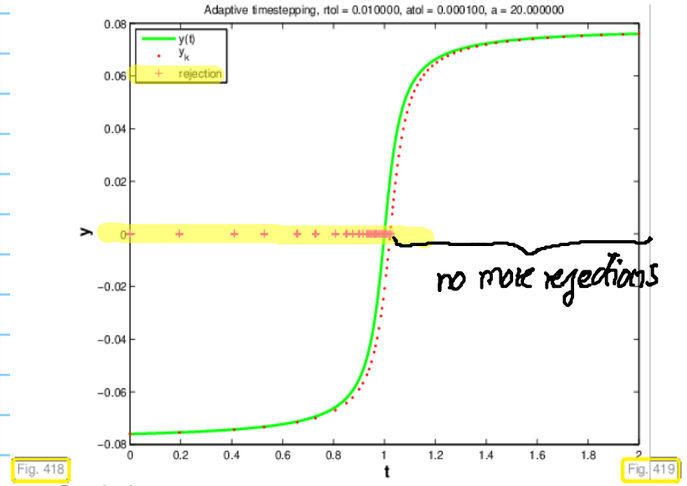


Fig. 418

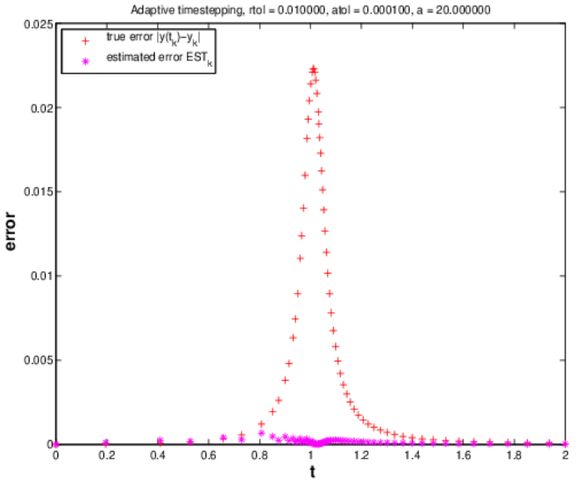


Fig. 419

Statistics: 66 timesteps, 131 rejected timesteps

EST_k are not related to total error!

C++11 code 11.5.11: Simple local stepsize control for single step methods

```
// Auxiliary function:  default norm for an EIGEN vector type
template <class State>
double _norm(const State &y) { return y.norm(); }

template <class DiscEvolOp, class State, class NormFunc =
    decltype(_norm<State>)>
std::vector<std::pair<double, State> >
odeintadapt(DiscEvolOp &Psilow, DiscEvolOp &Psihigh,
            State& y0,double T, double h0,
            double reltol, double abstol, double hmin,
            NormFunc &norm = _norm<State>) {
  double t = 0; // initial time
  State y = y0; // initial state
  double h = h0; // timestep to start with
  std::vector<std::pair<double,State>> states; // for output
  states.push_back({t, y});

  while ((states.back().first < T) && (h >= hmin))  { //
    State yh = Psihigh(h, y0); // high order discrete evolution Ψ̃^h
    State yH = Psilow(h, y0); // low order discrete evolution Ψ^h
    double est = norm(yH-yh); // local error estimate EST_k

    if (est < max(reltol*norm(y0), abstol)) { // step accepted
      y0 = yh; // use high order approximation
      t = t+min(T-t,h); // next time t_k
      states.push_back({t,y0}); //
      h = 1.1*h;  // try with increased stepsize
    }
    else // step rejected
      h = h/2; // try with half the stepsize
  }
  // Numerical integration has ground to a halt !
  if (h < hmin)  {
    cerr << "Warning: Failure at t=" << states.back().first
      << ". Unable to meet integration tolerances without reducing
         the step "
      << "size below the smallest value allowed ("<< hmin <<") at
         time t." << endl;
  }
  return states;
}
```

y(0) = 0

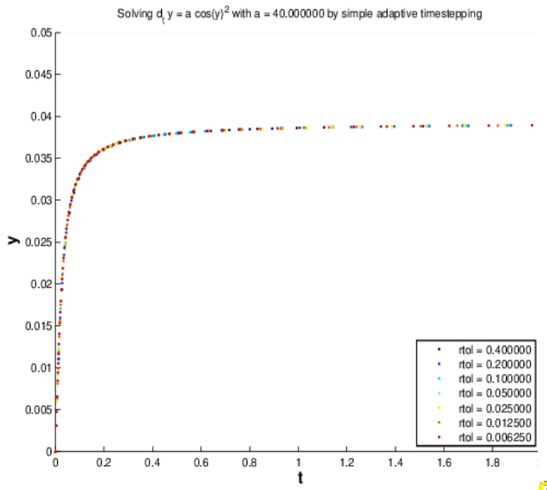


Fig. 420

Solutions $(y_k)_k$ for different values of `rtol`

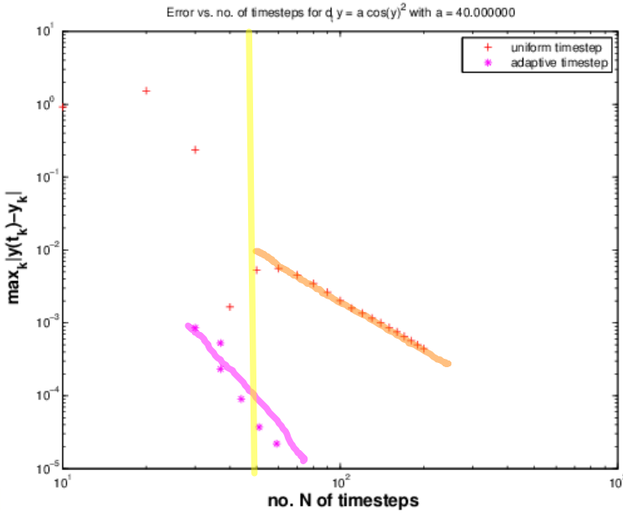


Fig. 421

Error vs. computational effort

∇ atol, rtol ✗ true size of error

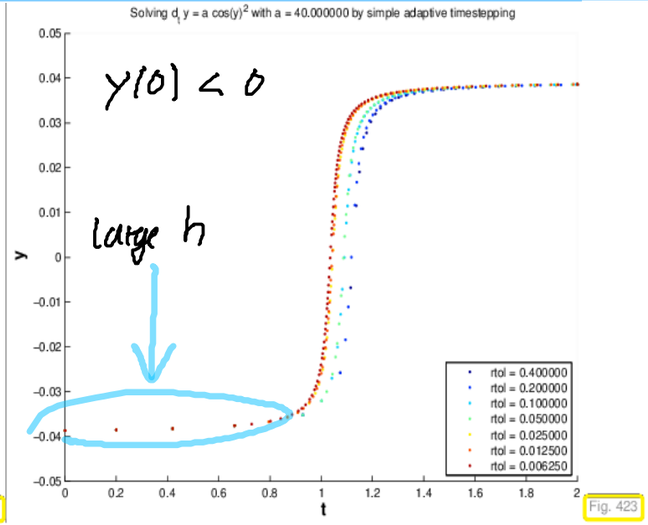


Fig. 422

Solutions $(y_k)_k$ for different values of `rtol`

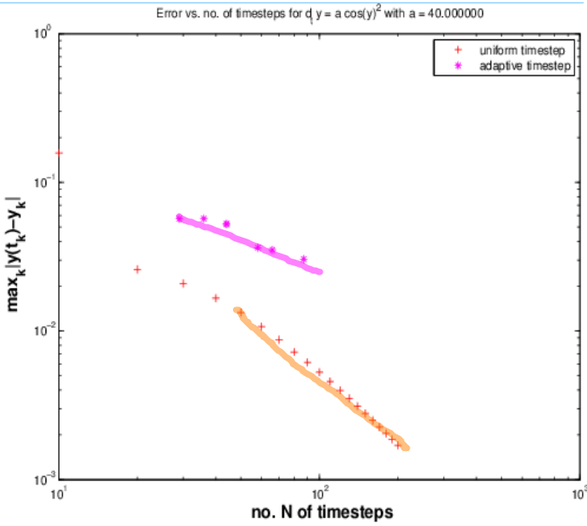


Fig. 423

Error vs. computational effort

Here: Position of step has sensitive dependence on $y(0)$

☺ "Wrong result" is still acceptable!
[→ Backward error analysis]

Stepsize prediction:

More ambitious goal! When $\mathrm{EST}_k > \mathrm{TOL}$: stepsize adjustment better $h_k = ?$
When $\mathrm{EST}_k < \mathrm{TOL}$: stepsize prediction good $h_{k+1} = ?$

$\Psi \hat{=}$ order p $\qquad \widetilde{\Psi} \hat{=}$ order $p+1$

$$\mathrm{EST}_k := \widetilde{\Psi}^h y_k - \Psi^h y_k$$

$$\begin{aligned} \Psi^{h_k}\mathbf{y}(t_k) - \Phi^{h_k}\mathbf{y}(t_k) &\doteq ch_k^{p+1} + O(h_k^{p+2}), \\ \widetilde{\Psi}^{h_k}\mathbf{y}(t_k) - \Phi^{h_k}\mathbf{y}(t_k) &\doteq O(h_k^{p+2}). \end{aligned} \quad \Rightarrow \quad \boxed{\mathrm{EST}_k \doteq ch_k^{p+1}} \,. \qquad (11.5.18)$$

Efficient timestep h^*:

$$C = \left(\frac{h_k^{p+1}}{\mathrm{EST}_k}\right)^{-1} \Rightarrow \quad \begin{aligned} \mathrm{EST}_k^* &= \mathrm{TOL} \quad \text{(Goal)} \\ c(h^*)^{p+1} &= \mathrm{TOL} \end{aligned}$$

"Optimal timestep": (stepsize prediction)

$$h_* = h_k \sqrt[p+1]{\frac{\mathrm{TOL}}{\mathrm{EST}_k}} \,. \qquad (11.5.21)$$

C++11 code 11.5.22: Refined local stepsize control for single step methods

```
// Auxiliary function:  default norm for an EIGEN vector type
template <class State>
double _norm(const State &y) { return y.norm(); }

template <class DiscEvolOp, class State, class NormFunc =
    decltype(_norm<State>)>
std::vector<std::pair<double, State> >
odeintssctrl(DiscEvolOp &Psilow, unsigned int p, DiscEvolOp &Psihigh,
             State& y0,double T, double h0,
             double reltol, double abstol, double hmin,
             NormFunc &norm = _norm<State>) {
  double t = 0; // initial time
  State y = y0; // initial state
  double h = h0; // timestep to start with
  std::vector<std::pair<double,State>> states; // for output
  states.push_back({t, y});

  // Main timestepping loop
  while ((states.back().first < T) && (h >= hmin)) { //
    State yh = Psihigh(h, y0); // high order discrete evolution Ψ̃^h
    State yH = Psilow(h, y0); // low order discrete evolution Ψ^h
    double est = norm(yH-yh); // ↔ EST_k
    double tol = max(reltol*norm(y0), abstol); // effective tolerance

    // Optimal stepsize according to (11.5.21)
    h = h*max(0.5,min(2.,pow(tol/est,1./(p+1)))); //
    if (est < tol)  // step accepted
      states.push_back({t = t+min(T-t,h),y0 = yh}); // store next
         approximate state
  }
  if (h < hmin) {
    cerr << "Warning: Failure at t="
      << states.back().first
      << ". Unable to meet integration tolerances without reducing
         the step"
      << " size below the smallest value allowed ("<< hmin <<") at
         time t." << endl;
  }
  return states;
}
```