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

Numerical Methods for Computational Science and Engineering

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

XI. Numerical Integration

↳ Numerical solution of ODEs

$\dot{y} = f(t) \Rightarrow y(t) = \int_0^t f(\tau)\,d\tau$

11.1 Initial Value Problems (IVP) for ODEs

1st-order ODE in std. form: $\dot{y}(t) = f(t, y(t))$ (ODE)

$f : I \times D \to \mathbb{R}^d$, $I \subset \mathbb{R}$, $D \subset \mathbb{R}^d$ $\hat{=}$ right hand side (rhs)

$t \,\hat{=}$ "time variable"

$y(t) \,\hat{=}$ state $\in \mathbb{R}^d \to D \subset \mathbb{R}^d \,\hat{=}$ state space

Notation: $\dot{y}(t) := \frac{dy}{dt}(t)$

(ODE) $\Leftrightarrow$ $\begin{bmatrix} \dot{y}_1(t) \\ \vdots \\ \dot{y}_d(t) \end{bmatrix} = \begin{bmatrix} f_1(t, y_1(t), \dots, y_d(t)) \\ \vdots \\ f_d(t, y_1(t), \dots, y_d(t)) \end{bmatrix}$

Assume: f continuous

Definition 11.1.3. Solution of an ordinary differential equation

A solution of the ODE $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$ with continuous right hand side function $\mathbf{f}$ is a continuously differentiable *function* "of time t" $\mathbf{y} : J \subset I \to D$, defined on an open interval J, for which $\dot{\mathbf{y}}(t) = \mathbf{f}(t, \mathbf{y}(t))$ holds for all $t \in J$.

" f smooth [in t, y] $\Rightarrow$ y smooth [as a fnct. of t] "

Lemma 11.1.4. Smoothness of solutions of ODEs

Let $\mathbf{y} : I \subset \mathbb{R} \to D$ be a solution of the ODE $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$ on the time interval I.

If $\mathbf{f} : I \times D \to \mathbb{R}^d$ is r-times continuously differentiable with respect to both arguments, $r \in \mathbb{N}_0$, then the trajectory $t \mapsto \mathbf{y}(t)$ is $r+1$-times continuously differentiable in the interior of I.

1.1.1. Examples

→ Population dynamics: growth of population with limited resources

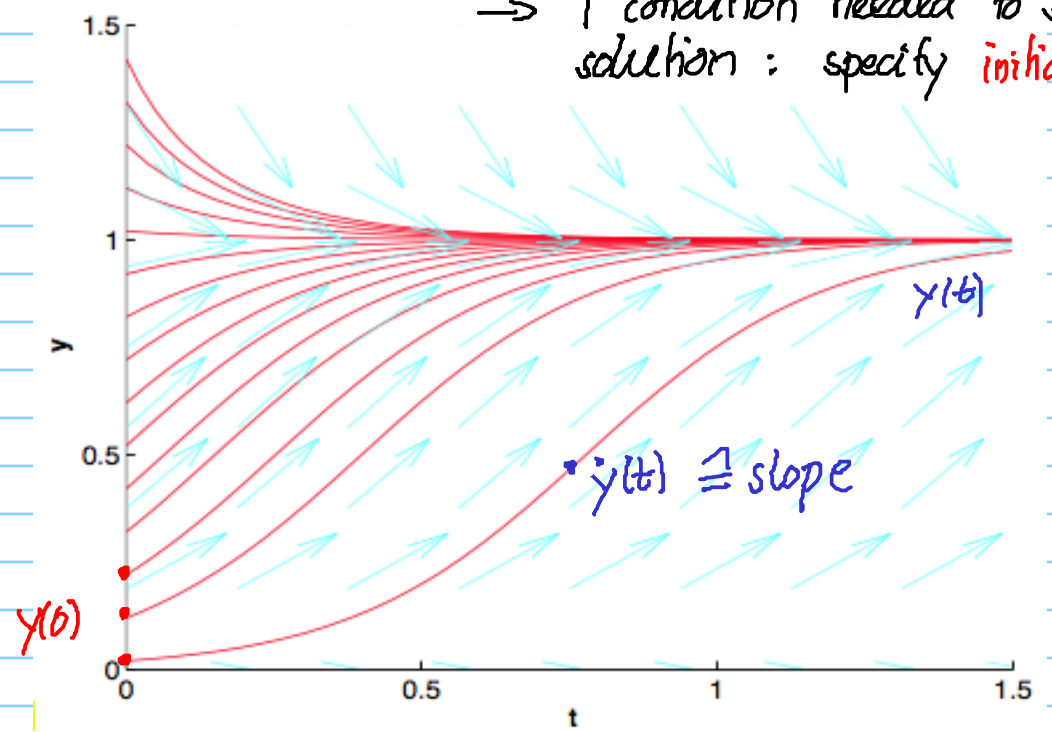
$\dot{y} = (1-y)\,y = f(y)$ [logistic ODE, $d = 1$]

state $y \mathrel{\hat=}$ density of population: State space $D = \mathbb{R}_0^+$

General solution: $y(t) = \dfrac{y(0)}{y(0) + (1-y(0))e^{-t}}$

↑ 1-parameter family of functions

→ 1 condition needed to select a unique solution: specify initial value/state $y(0) = y_0$



log. ODE $\mathrel{\hat=}$ r.h.s does not depend on t

Definition 11.1.7. 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.

Predator - prey model ($d = 2$)

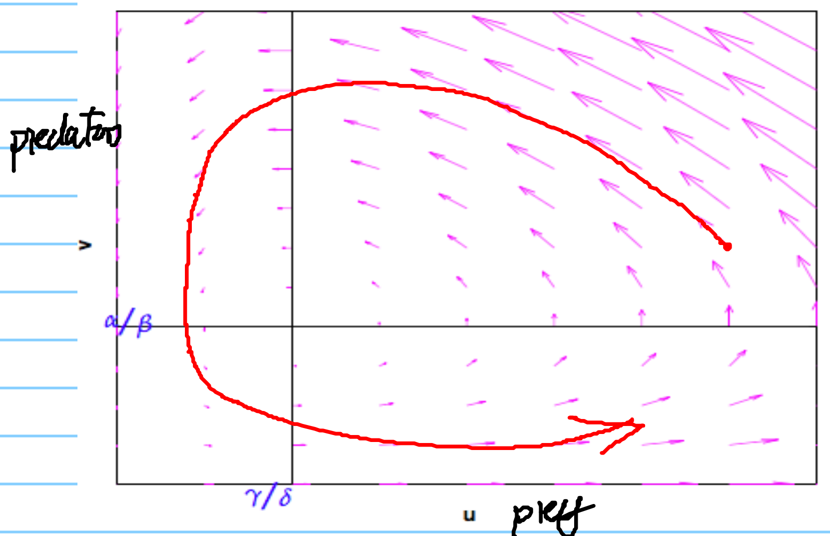
prey $\dot{u} = (1-v)\,u$

predator $\dot{v} = (u-1)\,v$

[Lotka - Volterra - ODE] autonomous

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

↑ vector field ("velocity field")



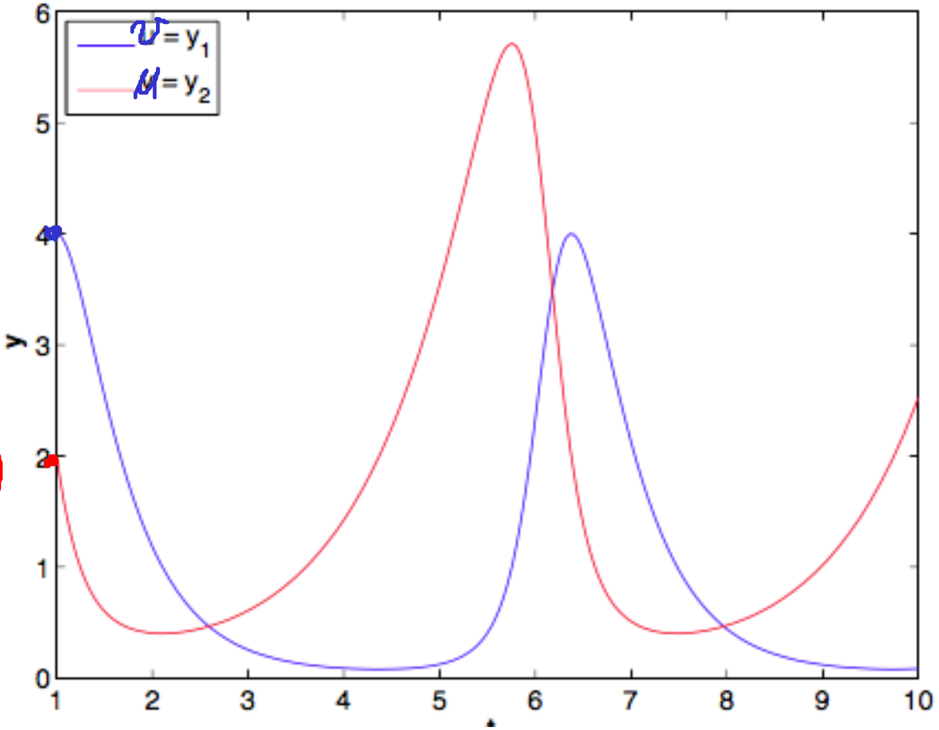
A solution* $t \to y(t)$ (trajectory)

⇔ path of a floating particle in velocity field f

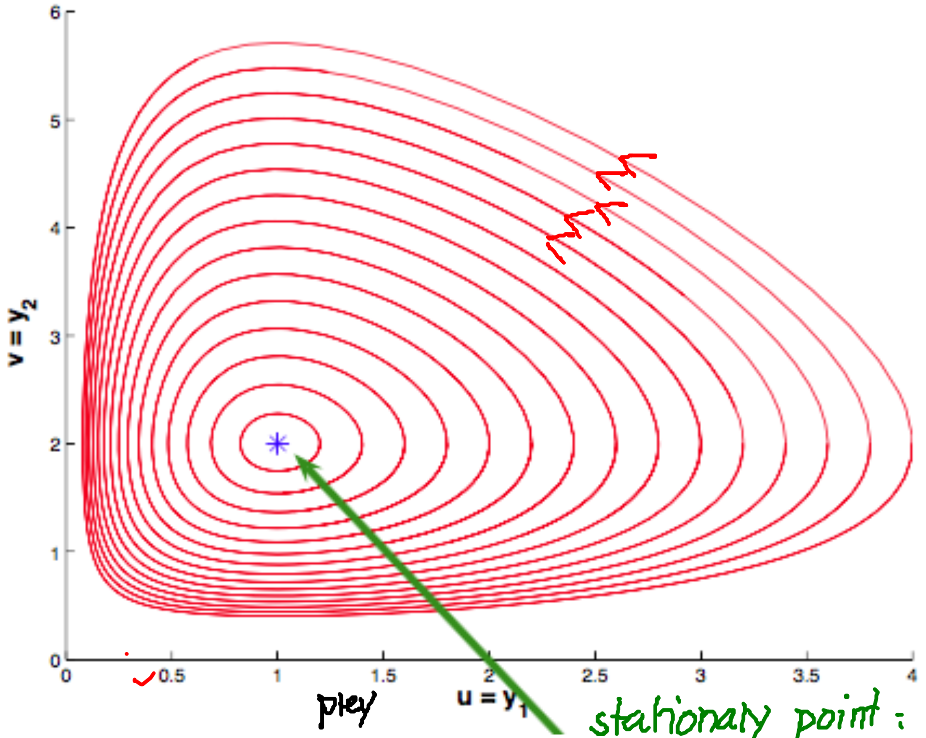
* a curve in state space

$v(0)$

$u(0)$



▷ periodic solutions



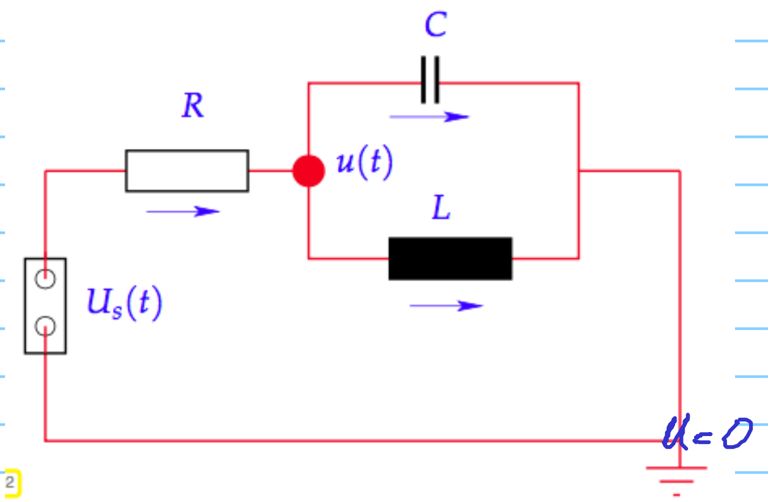
$\underline{y}(t) = \underline{y}^*$

stationary point : $f(\underline{y}^*) = 0$

Example : Transient circuit modeling

Kirchhoff's law

$$i_R(t) - i_C(t) - i_L(t) = 0$$



resistor: $\quad i_R(t) = R^{-1} u_R(t)\,,$

capacitor: $\quad i_C(t) = C\dfrac{du_C}{dt}(t)\,,$

coil: $\quad u_L(t) = L\dfrac{di_L}{dt}(t)\,.$

$\frac{d}{dt}$ →

$$\frac{d}{dt} i_R - \frac{d}{dt} i_C - \frac{d}{dt} i_L = 0$$

$$\frac{1}{R}\frac{d}{dt} u_R - C\frac{d^2}{dt^2} u_C - \frac{1}{L} u_L = 0$$

Introduce time-dependent nodal potentials :

$$\frac{1}{R}\frac{d}{dt}\left(U_s(t) - u(t)\right) - C\frac{d^2}{dt^2} u(t) - \frac{1}{L} u(t) = 0$$

→ 2nd-order ODE

11.1.2. Theory (of IVP)

$$\dot{y} = y \quad \Rightarrow \quad y(t) = Ce^t, \; C \in \mathbb{R}$$

[1-parameter family]

→ Need to fix unique solution: specify initial value

→ IVP: $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$ + $\mathbf{y}(t_0) = \mathbf{y}_0$

r.h.s. $\mathbf{f} : I \times D \to \mathbb{R}^d$

$\mathbf{f}(t, \mathbf{y}) = \mathbf{f}(\mathbf{y})$: autonomous ODE / IVP

Autonomization by introducing t as an additional state component

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}) \; : \quad \mathbf{z}(t) := \begin{bmatrix} \mathbf{y}(t) \\ t \end{bmatrix} \text{ solves } \dot{\mathbf{z}} = \underbrace{\begin{bmatrix} \mathbf{f}(z_{d+1}, z_1, \dots, z_d) \\ 1 \end{bmatrix}}_{\text{equivalent autonomous ODE}}$$

Conversion to 1-st order ODE:

$$\ddot{\mathbf{y}} = \mathbf{f}(\mathbf{y}, \dot{\mathbf{y}}) \; : \quad \mathbf{z}(t) = \begin{bmatrix} \mathbf{y}(t) \\ \dot{\mathbf{y}}(t) \end{bmatrix} \text{ solves } \dot{\mathbf{z}} = \underbrace{\begin{bmatrix} [z_{d+1}, \dots, z_{2d}]^T \\ \mathbf{f}(z_1, \dots, z_d, z_{d+1}, \dots, z_{2d}) \end{bmatrix}}_{\text{equivalent 1st-order ODE}}$$

For 2nd-order ODEs: Initial values required for $\mathbf{y}(t_0)$, $\dot{\mathbf{y}}(t_0)$

$\Omega := I \times D$

Theorem 11.1.30. Theorem of Peano & Picard-Lindelöf [4, Satz II(7.6)], [54, Satz 6.5.1], [10, Thm. 11.10], [32, Thm. 73.1]

If the right hand side function $\mathbf{f} : \hat{\Omega} \mapsto \mathbb{R}^d$ is locally Lipschitz continuous (→ Def. 11.1.27) then for all initial conditions $(t_0, \mathbf{y}_0) \in \hat{\Omega}$ the IVP (11.1.19) has a unique *solution $\mathbf{y} \in C^1(J(t_0, \mathbf{y}_0), \mathbb{R}^d)$ with maximal (temporal) domain of definition $J(t_0, \mathbf{y}_0) \subset \mathbb{R}$.*

$\mathbf{y} \mapsto \mathbf{f}(t, \mathbf{y})$ has finite slope around every point $(t, \mathbf{y}) \in \Omega$

$$\exists L > 0 : \|\mathbf{f}(t, \mathbf{w}) - \mathbf{f}(t, \mathbf{z})\| \leq L \|\mathbf{w} - \mathbf{z}\| \quad \text{locally}$$

Not locally L.C.: $t \to \sqrt{t}$ on $[0, 1]$

Example: Temporal domain of definition

Explosion equation $\dot{y} = y^2$, $y(0) = y_0$

finite-time blow-up ▷

We find the solutions

$$y(t) = \begin{cases} \frac{1}{y_0^{-1} - t} & , \text{ if } y_0 \neq 0 \, , \\ 0 & , \text{ if } y_0 = 0 \, , \end{cases} \tag{11.1.35}$$

with domains of definition

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

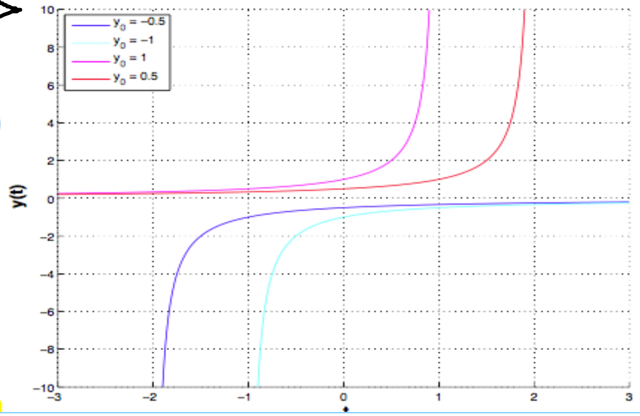


Fig. 293

Remark: Autonomous ODEs: always use $t_0 = 0$

$y(t)$ solution $\Rightarrow$ $y(t-\tau)$ also a solution

11.1.3. Evolution operators

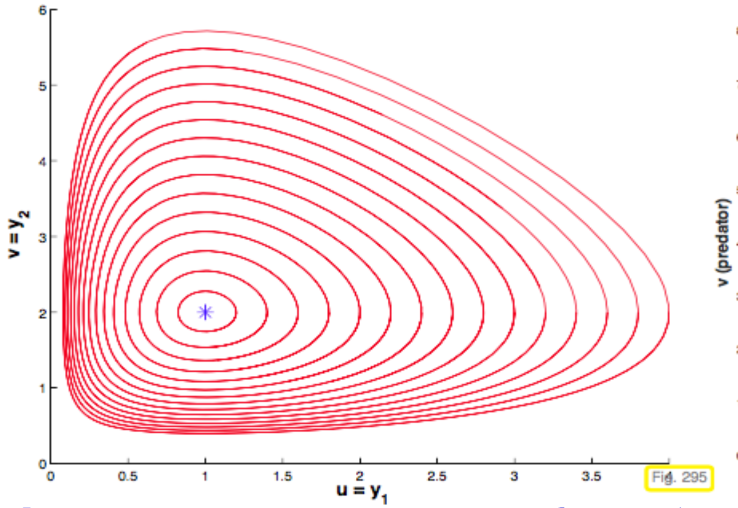
Autonomous ODE: $\dot{y} = f(y)$

[Assume: Global solution: $J(0,y_0) = \mathbb{R}$]
Existence & uniqueness

$y(t;y_0)$ solution of IVP: $\dot{y} = f(y),\ y(0) = y_0$

Evolution map: $\Phi : \begin{cases} \mathbb{R}\times D \to D \\ (t,y_0) \to y(t;y_0) \end{cases}$

Lotka-Volterra ODE, $d=2$:



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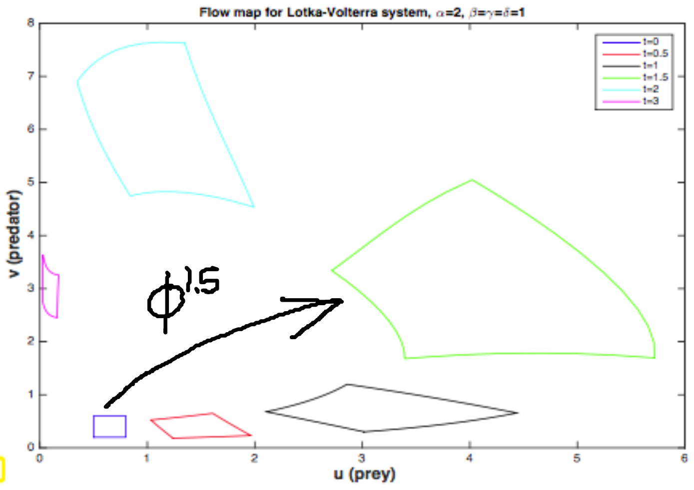


Fig. 295

y_0 fixed: trajectories $t \mapsto \Phi^t y_0 = \Phi(t,y_0)$

Fix t: state mapping $y \mapsto \Phi^t y$

ODE $\Longleftrightarrow$ Evolution map

$$\frac{\partial \Phi}{\partial t}(t,y) = f(\Phi(t,y)) \quad \forall t\in\mathbb{R},\ y\in D$$

$$f(z) = \frac{\partial \Phi}{\partial t}(t,(\Phi^t)^{-1}(z)) \ , \quad \forall z \in D$$

11.2. Polygonal approximation methods

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

We want
- $\to$ $y(T)$ for some "final time" $T > t_0$
- $\to$ approximate trajectory $t \to y_h(t) \approx y(t)$

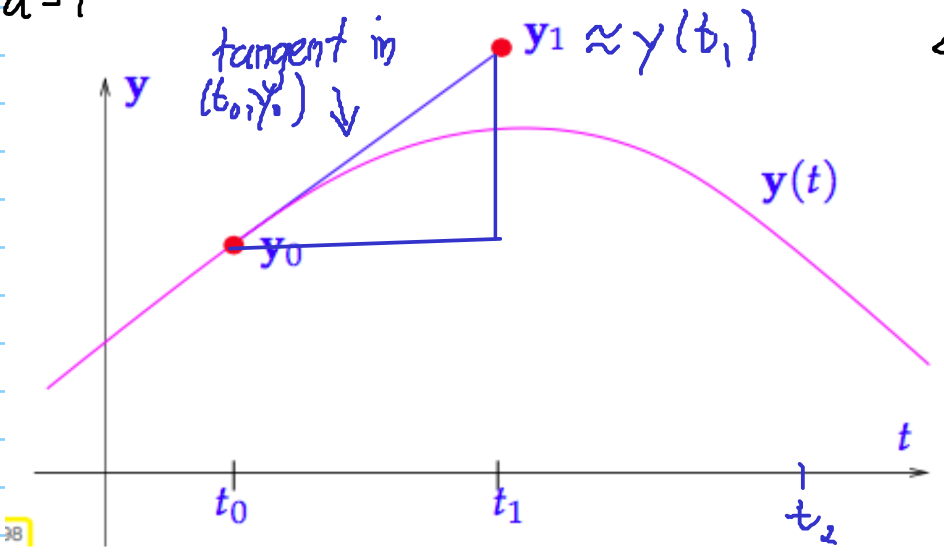
Temporal mesh: $\mathcal{M} = \{t_0 < t_1 < t_2 < \dots < t_N = T\}$

11.2.1. Explicit Euler method

Idea: Follow tangents over short times

$\dot{y} = f(t,y) \Rightarrow f(t,y(t))$ gives slope in t

$d = 1$



$\triangleleft$ 1st step

Then continue with y_1

(timestepping)

$\downarrow$

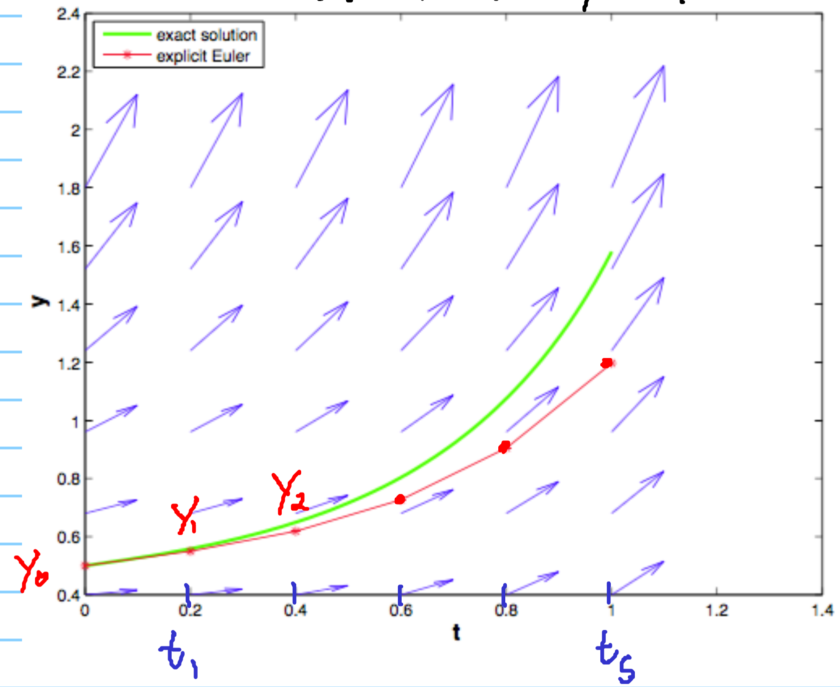
produces a sequence $y_0, y_1, y_2, \dots, y_N$

$y_h(t)$ by p.w. linear interpolation

$\Downarrow$

— $\hat{=}$ polygon

Ricati ODE: $\dot{y} = y^2 + t^2$



Recursion formula $\quad y_{k+1} = y_k + (t_{k+1} - t_k)\, f(t_k, y_k)$

$$\underbrace{\frac{y_{k+1} - y_k}{t_{k+1} - t_k}}_{\text{Difference quotient}} = f(t_k, y_k)$$

$\downarrow$ anchor time

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

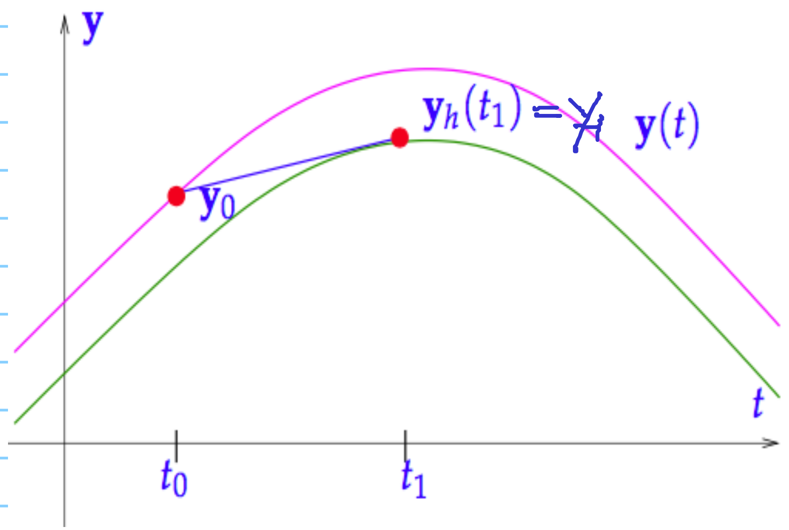
II.2.2. Implicit Euler method

Choose anchor point t_{k+1}

$$\cancel{f(t_{k+1}, y(t_{k+1}))}$$

$$\underbrace{\frac{y_{k+1} - y_k}{t_{k+1} - t_k}}_{\text{Difference quotient}} = f(t_{k+1}, y_{k+1}) \qquad \text{(IE)}$$

$\to$ $d \times d$ (non-linear) system of equations for y_{k+1}



Geometry of implicit Euler method:

Approximate solution through (t_0, y_0)

- straight line through (t_0, y_0)
- with slope $f(t_1, y_1)$

$\triangleleft$ — $\hat{=}$ trajectory through (t_0, y_0),

— $\hat{=}$ trajectory through (t_1, y_1),

— $\hat{=}$ tangent at — in (t_1, y_1).

⑦ Can we solve for y_{k+1}? $\quad h_k := t_{k+1} - t_k$

(IE) $\Rightarrow \quad y_{k+1} = y_k + h_k f(t_{k+1}, y_{k+1})$

y_{k+1} solves: $G(h_k, y_{k+1}) = 0$, $\quad G(h,y) = y - y_k - h f(y)$

[For autonomous ODE, $f \in C^1$]

Does $y \to G(h_k, y)$ have a unique zero?

- $G(0, y_k) = 0$
- $D_y G(0, y) = I \to$ invertible

Implicit function theorem: for small $|h|$: $G(h,y) = 0$ defines a function $h \mapsto y(h)$: $G(h, y(h)) = 0$

$\to$ y_{k+1} exists for sufficiently small h.

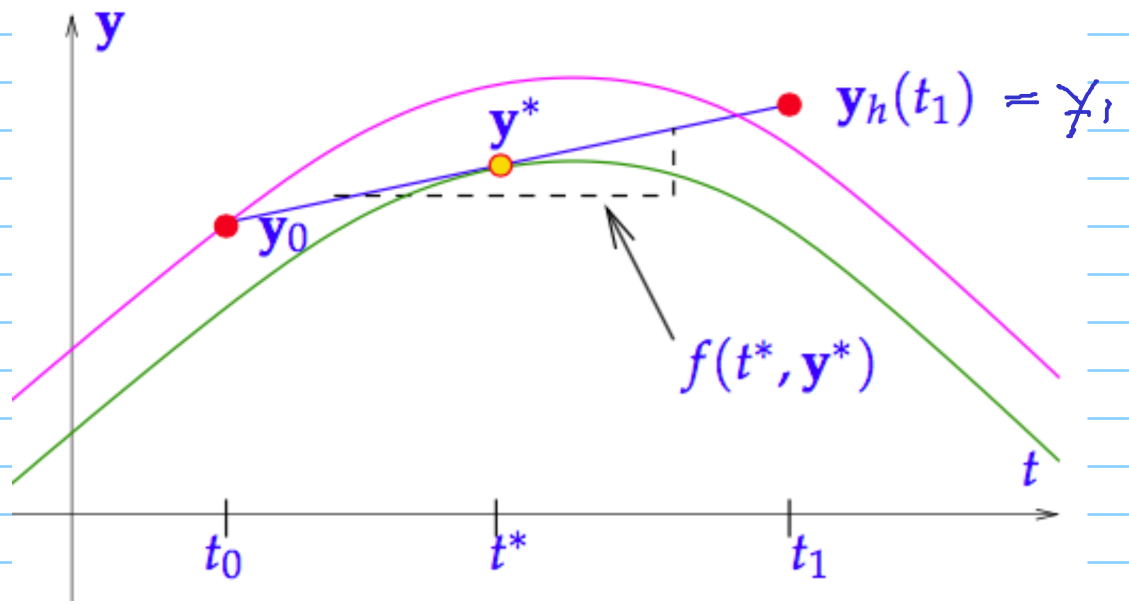
$\to$ $y_0, y_1, \dots, y_N$ well defined on sufficiently fine meshes.

II.2.3. Implicit midpoint method

$$\cancel{f\left(\frac{t_{k+1}+t_k}{2}, y\left(\frac{t_{k+1}+t_k}{2}\right)\right)}$$

$$\approx$$

$$\underbrace{\frac{y_{k+1} - y_k}{t_{k+1} - t_k}}_{\text{Difference quotient}} = \underbrace{f\left(\frac{t_{k+1}+t_k}{2}, \frac{y_{k+1}+y_k}{2}\right)}_{\text{polygonal approximation}}$$



(IMP) $\quad y_{k+1} = y_k + h_k f\left(\frac{t_k + t_{k+1}}{2}, \frac{y_k + y_{k+1}}{2}\right)$

All three polygonal methods (for sufficiently small h_k) define recursions

$$y_{k+1} = \Psi(h_k, y_k)$$

$\to$ Sequence $y_0, y_1, \dots, y_N$ (timestepping)

Hope: $\quad y_k \approx y(t_k)$

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

$\hookrightarrow$ evolution map

11.3. General Single Step Methods (SSM)

Euler methods / implicit midpoint method for IVP $\dot{y} = f(y)$, $y(0) = y_0$:

→ recursion $\quad y_{k+1} = \Psi(h_k, y_k)$ ↳ discrete evolution

$\approx \updownarrow$

$y(t_{k+1}) = \Phi(h, y(t_k))$ ← ↳ evolution map

Goal: $\Psi \approx \Phi$

Definition 11.3.5. Single step method (for autonomous ODE) → [45, Def. 11.2]

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

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

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

Notation: $\quad y_{k+1} = \Psi^{h_k} y_k \quad , \quad h_k := t_{k+1} - t_k$

SSM can also be defined through first step: $y_1 = \Psi^h y_0$

Consistent discrete evolution

The discrete evolution $\boldsymbol{\Psi}$ 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

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

Consistent SSM look like explicit Euler

Expl. Euler: $\Psi^h y = y + h f(y)$

Impl. midpoint method:

$$\Psi^h y_0 := y_1 = y_0 + h f(\tfrac{1}{2}(y_0 + y_1))$$
$$= y_0 + h \underbrace{f(y_0 + \tfrac{1}{2} h f(\ldots))}_{=: \psi(h,y)}$$

Impl. fct. thm: $y_1(h, y_0)$ is continuous ⇒ ψ continuous

$\psi(0, y_0) = f(y_0)$

Convergence *

Setting: $\dot{y} = f(y)$, $y(0) = y_0$

Assume: $\|f(z) - f(w)\| \le L\|z - w\| \quad \forall z, w \in D$

Error measure: $\max_j \|y_j - y(t_j)\|$

sequence produced by SSM $\qquad$ exact solution

* need family of meshes $(\mathcal{M}_\ell)_\ell$: $h_\ell := \max_j |t^\ell_{j+1} - t^\ell_j| \to 0$ as $\ell \to \infty$

h-refinement $\qquad$ meshwidth

(9)

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

Final time $T = 1 \to h = \frac{1}{N}$, $N = \#\mathcal{M}$

Measured: $|y_N - y(T)|$

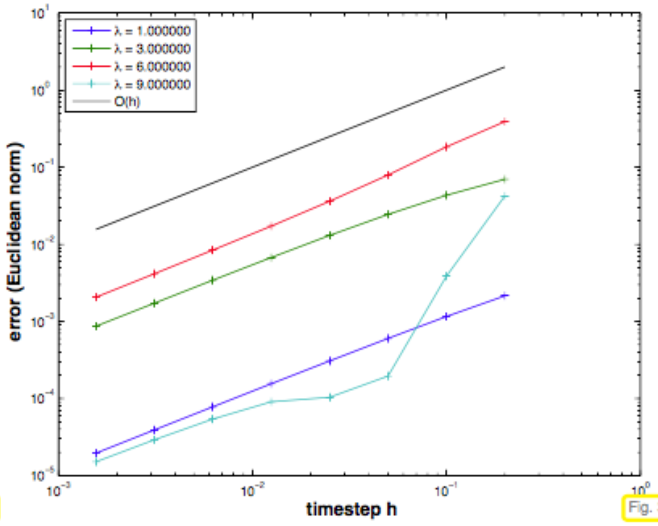
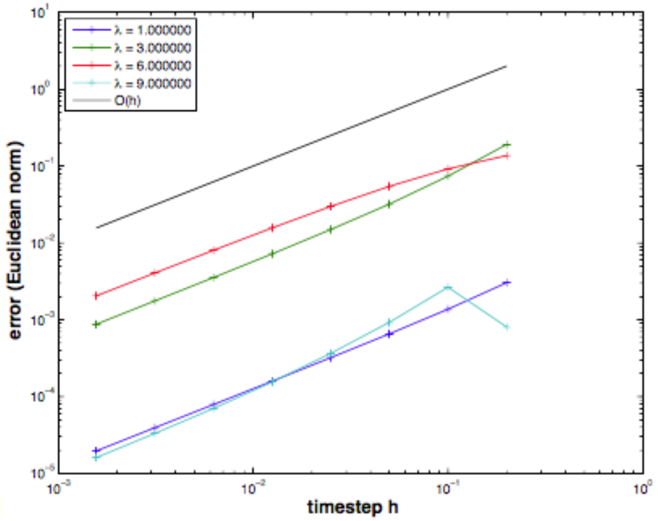


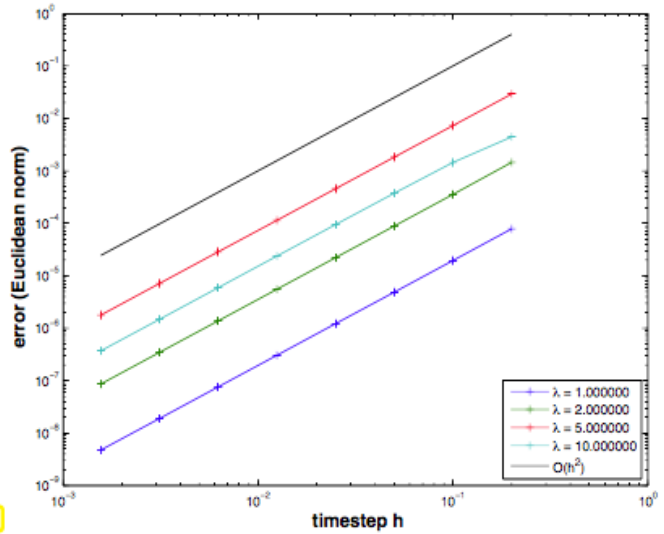
Fig. 335

explicit Euler method



implicit Euler method

$\to$ algebraic cvg. for $h \to 0$: $O(h)$ "first order"



◁ Implicit midpoint method $O(h^2)$

In general* consistent SSM converge algebraically for meshwidth $h \to 0$: error $= O(h^p)$, $p \in \mathbb{N}$

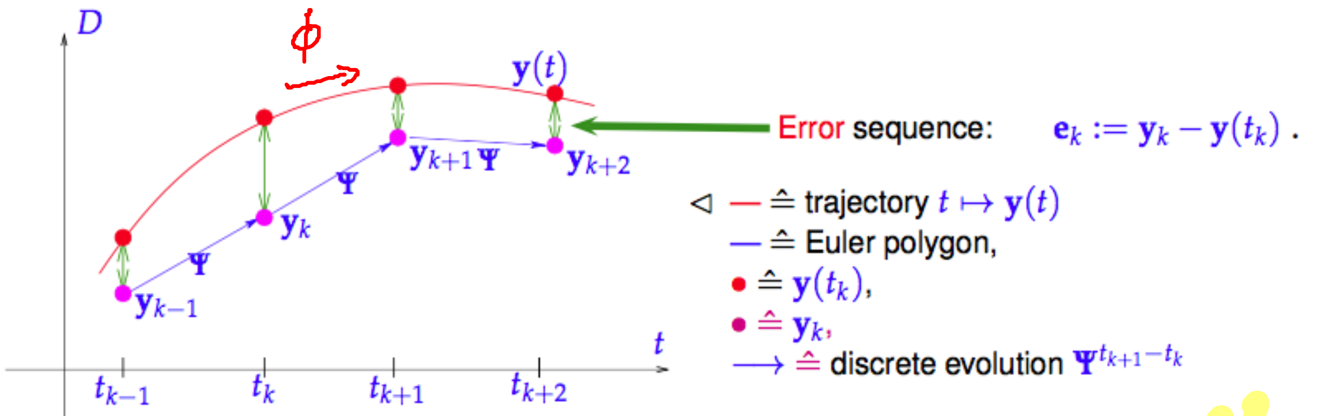
$p \mathrel{\hat{=}}$ order of SSM

* for smooth trajectories

Analysis for expl. Euler (for smooth $f \to$ smooth $y(t)$)

Assume L.C.: $\|f(z) - f(w)\| \le L \|z - w\| \quad \forall z, w \in D$

Expl. Euler: $\mathbf{y}_{k+1} = \mathbf{y}_k + h_k \mathbf{f}(\mathbf{y}_k)$, $k = 1, \dots, N-1$. (11.2.7)

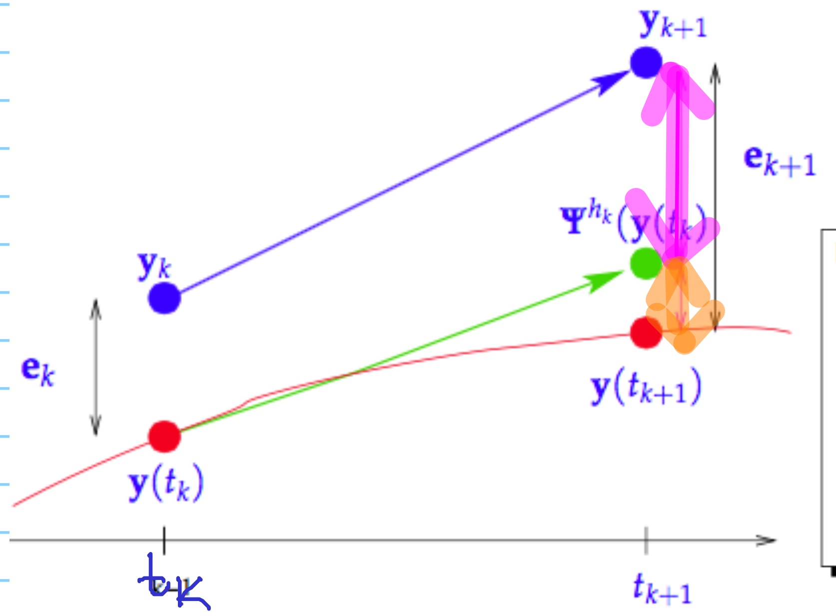


Discrete evol. $\Psi^h y = y + h f(y)$

Key idea: Error splitting

$e_{k+1} = \Psi^{h_k} y_k - \Phi^{h_k} y(t_k)$

$= \left(\Psi^{h_k} y_k - \Psi^{h_k} y(t_k)\right) + \left(\Psi^{h_k} y(t_k) - \Phi^{h_k} y(t_k)\right)$



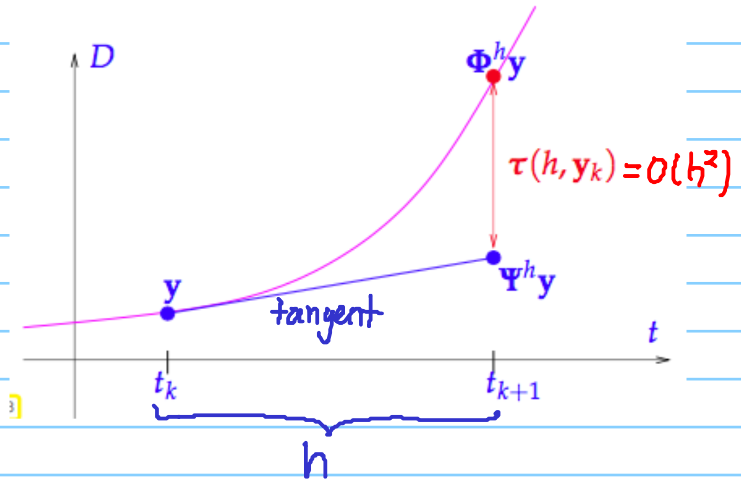
$\hat{=}$ propagated error

$\hat{=}$ one-step error

Fundamental error splitting

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

- One-step error :



Taylor :

$$y(t_k+h) =$$

$$= y(t_k) + \dot{y}(t_k)h + \tfrac{1}{2}h^2\ddot{y}(\xi)$$

$$= \Psi^h y(t_k) + \tfrac{1}{2}h^2 \ddot{y}(\xi)$$

$$t_k < \xi < t_{k+1}$$

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

- Propagated error :

$$\| \Psi^h(y(t_k)) - \Psi^h y_k \| = \| e_k + h(f(y(t_k)) - f(y_k)) \|$$

+ Lipschitz cont. $\leq \|e_k\| + hL\|e_k\|$

Combined $\Longrightarrow$ error recursion for $\varepsilon_k := \|e_k\|$

$$\varepsilon_{k+1} \leq (1+h_k L)\varepsilon_k + \delta_k \;, \quad \delta_k := \tfrac{1}{2}h_k^2 \ddot{y}(\xi_k)$$

$$\varepsilon_0 = 0$$

$$\longrightarrow \quad \varepsilon_k \leq \sum_{\ell=1}^{k} \prod_{j=1}^{\ell-1} (1+h_j L)\, \delta_\ell$$

$[\, 1+x \leq e^x \,]$ $\quad \leq \sum_{\ell=1}^{k} \left(\prod_{j=1}^{\ell-1} e^{h_j L} \right) \delta_\ell$

$$\leq \sum_{\ell=1}^{k} e^{(\underbrace{\sum_{j=1}^{\ell-1} h_j}_{\leq T})L} \cdot \delta_\ell$$

$$\leq e^{TL} \|\ddot{y}\|_{L^\infty([0,T])} \sum_{\ell=1}^{k} h_\ell \,(\tfrac{1}{2}\underbrace{h_\ell}_{\leq h})$$

for all $k=1,..,N$: $\leq \underbrace{e^{TL} \|\ddot{y}\|_{L^\infty([0,T])}\, h\, T}_{O(h)}$

Note: One-step-error $O(h^2)$ $\longleftrightarrow$ Total error $O(h)$

For SSM : One-step-error $O(h^{p+1})$ $\longrightarrow$ Order p

11.4. Explicit Runge-Kutta SSM

Goal: Explicit SSM with order $p > 1$

Rationale for high order: unknown constant

Discretization error $\approx C h^p$ [assume sharp]

Goal: error reduction by factor $\rho > 1$ by h-refinement

$$\frac{C h_0^p}{C h_1^p} = \rho \Rightarrow h_1 = \rho^{-1/p} \cdot h_0$$

Effort $\sim$ #{timesteps} $\sim h^{-1}$:

$$W_1 = \rho^{1/p} \cdot W_0$$

effort after refinement — effort before refinement

Less additional effort to achieve prescribed error reduction the larger p.

Construction

$$\left.\begin{array}{l} \dot{y} = f(y) \\ y(0) = y_0 \end{array}\right\} \Rightarrow y(h) = y_0 + \int_0^h f(y(\tau))\,d\tau$$

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

Idea: Quadrature! s-pt. Q.F. on [0,1], weights b_i, nodes c_i

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

Idea: approximate the integral by means of s-point quadrature formula (→ Section 5.1, defined on the reference interval $[0,1]$) with nodes $c_1, \dots, c_s$, weights $b_1, \dots, b_s$.

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

Obtain these values by bootstrapping

Goal: One-step-error $O(h^{p+1})$

→ sufficient to approximate $y(t_0 + c_i h)$ with error $O(h^p)$, because of multiplication w/ h!

⇒ $y(t_0 + c_i h)$ approximate by SSM of order $p-1$ [Start with expl. Euler]

Examples:

- Quadrature formula = trapezoidal rule (5.2.5):

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

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

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

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

- Quadrature formula → simplest Gauss quadrature formula = midpoint rule (→ Ex. 5.2.3) & $\mathbf{y}(\frac{1}{2}(t_1+t_0))$ approximated by explicit Euler step (11.2.7)

$$\mathbf{k}_1 = \mathbf{f}(t_0, \mathbf{y}_0)\,, \quad \mathbf{k}_2 = \mathbf{f}(t_0 + \tfrac{h}{2}, \mathbf{y}_0 + \tfrac{h}{2}\mathbf{k}_1)\,, \quad \mathbf{y}_1 = \mathbf{y}_0 + h\mathbf{k}_2\,. \qquad (11.4.7)$$

(11.4.7) = explicit midpoint method (for numerical integration of ODEs) [10, Alg. 11.18].

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.

Effort for one step : s f-eval.

Butcher scheme

Shorthand notation for (explicit) Runge-Kutta methods [10, (11.75)]

Butcher scheme ▷

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

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

$b_i \triangleq$ quadrature weights *

* Apply RK-SSM to $\dot{y} = f(t)$

Remark: RK-SSM consistent, if $\sum_{i=1}^{s} b_i = 1$

Examples

- Explicit Euler method (11.2.7): $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$ ➤ order = 1
- explicit trapezoidal rule (11.4.6): $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$ ➤ order = 2
- explicit midpoint rule (11.4.7): $\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$ ➤ order = 2
- Classical 4th-order RK-SSM: $\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array}$ ➤ order = 4

Construction high-order RK-SSM by solving order conditions

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

Theory : $p \leq s$

```
[t,y] = ode45(odefun,tspan,y0);
```

- `odefun` : Handle to a function of type `@(t,y)` $\leftrightarrow$ r.h.s. $\mathbf{f}(t,\mathbf{y})$
- `tspan` : vector $(t_0, T)^T$, initial and final time for numerical integration
- `y0` : (vector) passing initial state $\mathbf{y}_0 \in \mathbb{R}^d$

:

- `t` : temporal mesh $\{t_0 < t_1 < t_2 < \cdots < t_{N-1} = t_N = T\}$
- `y` : sequence $(\mathbf{y}_k)_{k=0}^N$ (column vectors)

```
function varargout = ode45(ode,tspan,y0,options,varargin)
% Processing of input parameters omitted
% :
% Initialize method parameters, c.f. Butcher scheme (11.4.11)
pow = 1/5;
A = [1/5, 3/10, 4/5, 8/9, 1, 1];
B = [
    1/5         3/40     44/45     19372/6561     9017/3168        35/384
    0           9/40     -56/15    -25360/2187    -355/33          0
    0           0        32/9      64448/6561     46732/5247
        500/1113
    0           0        0         -212/729       49/176           125/192
    0           0        0         0              -5103/18656
        -2187/6784
    0           0        0         0              0                11/84
    0           0        0         0              0                0
    ];
E = [71/57600; 0; -71/16695; 71/1920; -17253/339200; 22/525; -1/40];
% : (choice of stepsize and main loop omitted)
% ADVANCING ONE STEP.
hA = h * A;
hB = h * B;
f(:,2) = feval(odeFcn,t+hA(1),y+f*hB(:,1),odeArgs{:});
f(:,3) = feval(odeFcn,t+hA(2),y+f*hB(:,2),odeArgs{:});
f(:,4) = feval(odeFcn,t+hA(3),y+f*hB(:,3),odeArgs{:});
f(:,5) = feval(odeFcn,t+hA(4),y+f*hB(:,4),odeArgs{:});
f(:,6) = feval(odeFcn,t+hA(5),y+f*hB(:,5),odeArgs{:});

tnew = t + hA(6);
if done, tnew = tfinal; end    % Hit end point exactly.
h = tnew - t;          % Purify h.
ynew = y + f*hB(:,6);
% : (stepsize control, see Sect. 11.5 dropped
```

Butcher scheme

Compute k_i

$\Rightarrow$ Linear comb. of k_i

11.5. Adaptive Stepsize Control

Example: Oscillatory chemical reaction

BZ-reaction

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

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

Abrupt changes in concentrations over many orders of magnitude

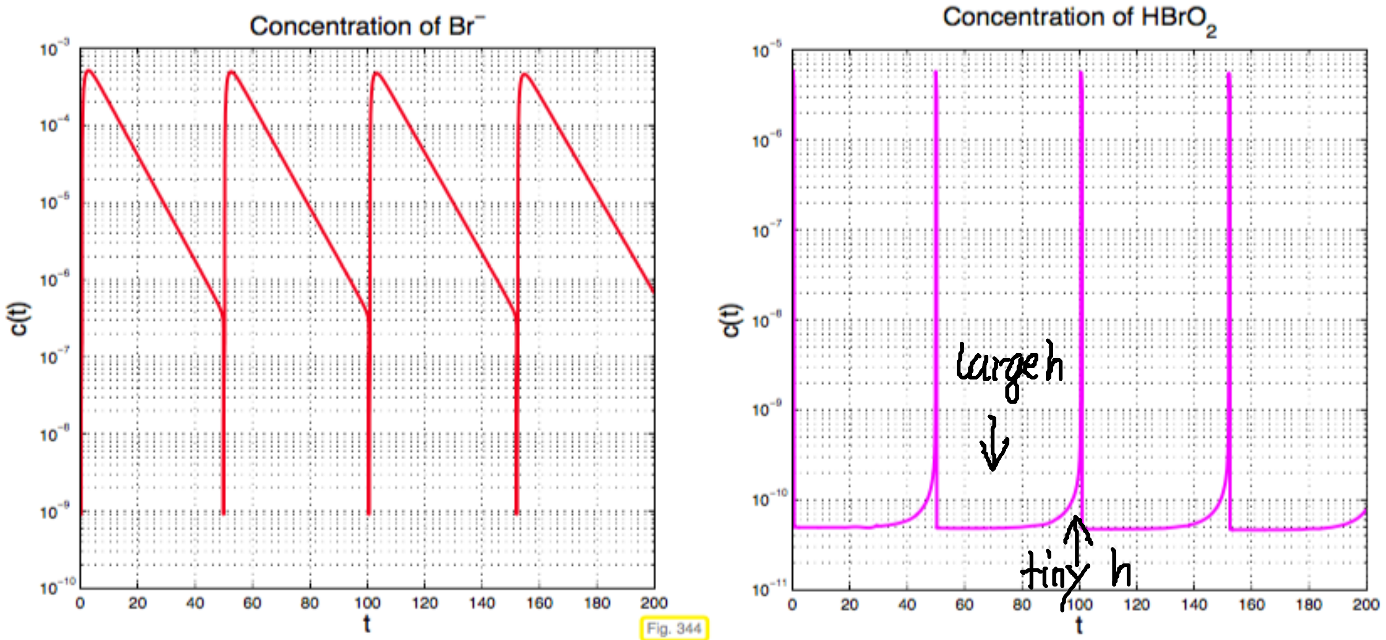


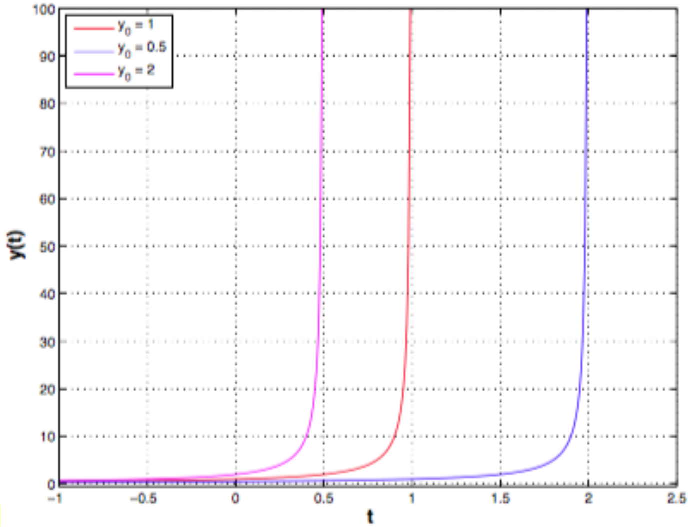
Fig. 344

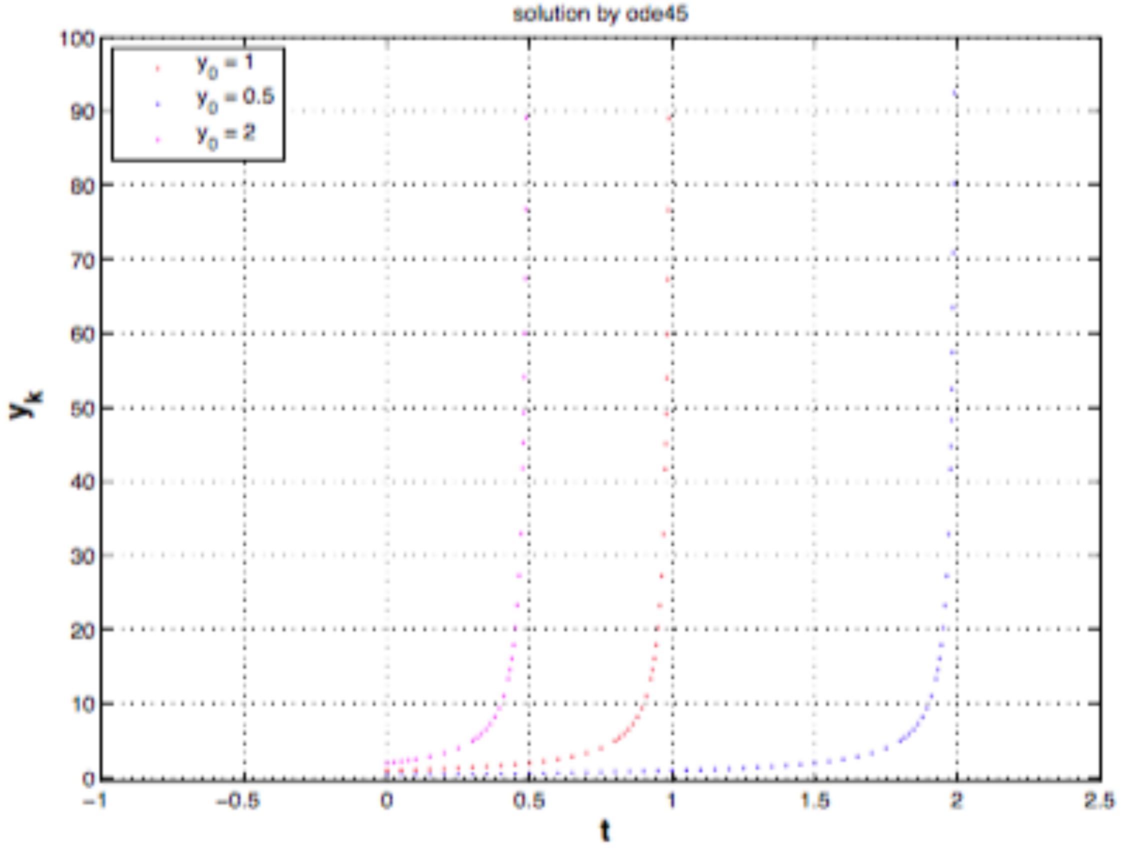
Example: blow-up

$$\dot{y} = y^2$$

blow-up after finite time ▷

impossible to solve with fixed timestep





◁ adaptive timestepping detects blow-up

Policy: (cmp. adaptive composite quadrature)

Be efficient! Be accurate!

Stepsize adaptation for single step methods

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

[Dream]

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})

Choose h_k based on y_{k-1} and h_{k-1} alone

Cheap & easy to implement

(I) ESTIMATE of one-step error

Idea: *Estimation of one-step error*

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

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

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

Heuristics for concrete h

(II) REFINE

$\mathrm{EST}_k \le \max(\mathrm{atol}, \mathrm{rtol}\cdot\|y_k\|)$?

Accept step, goto next step with $h_{k+1} = \alpha h_k$ for some $\alpha > 1$

Reject step, repeat with $h_k \leftarrow \frac{1}{2} h_k$

MATLAB-code 11.5.11: Simple local stepsize control for single step methods

```
function [t,y] =
  odeintadapt(Psilow,Psihigh,T,y0,h0,reltol,abstol,hmin)
t = 0; y = y0; h = h0;                %
while ((t(end) < T) && (h > hmin)) %
  yh = Psihigh(h,y0);    % high order discrete evolution Ψ̃^h
  yH = Psilow(h,y0);     % low order discrete evolution Ψ^h
  est = norm(yH-yh);     % ↔ EST_k

  if (est < max(reltol*norm(y0),abstol))                %
    y0 = yh; y = [y,y0]; t = [t,t(end) + min(T-t(end),h)]; %
    h = 1.1*h;  % step accepted, try with increased stepsize
  else, h = h/2; end   % step rejected, try with half the stepsize
end
```

ESTIMATE

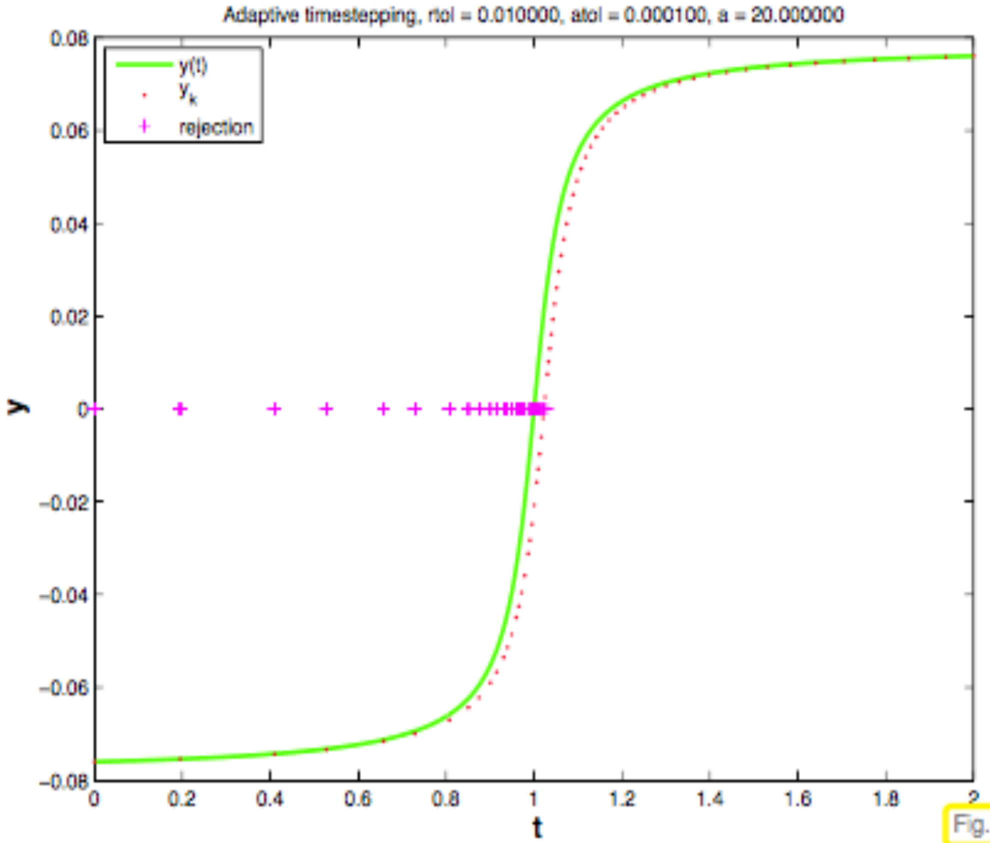
EST_k has next to nothing to do with $y(t_k) - y_k$!

$\hookrightarrow$ only $\approx$ one-step error

No global error control through local-in-time adaptive timestepping

The absolute/relative tolerances imposed for local-in-time adaptive timestepping do *not* allow to predict accuracy of solution!

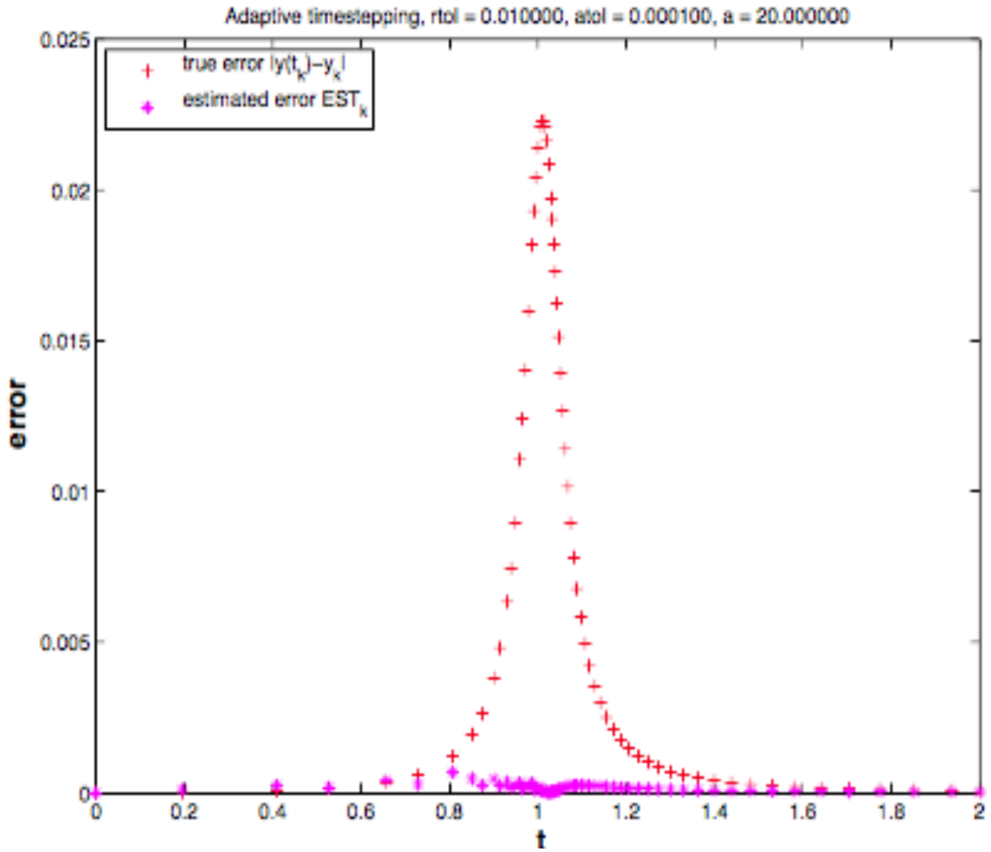
Example: $\dot{y} = \cos(\alpha y)$, Code 11.5.11 w/ expl. Eul. (order 1) & expl. trp. meth. (order 2)



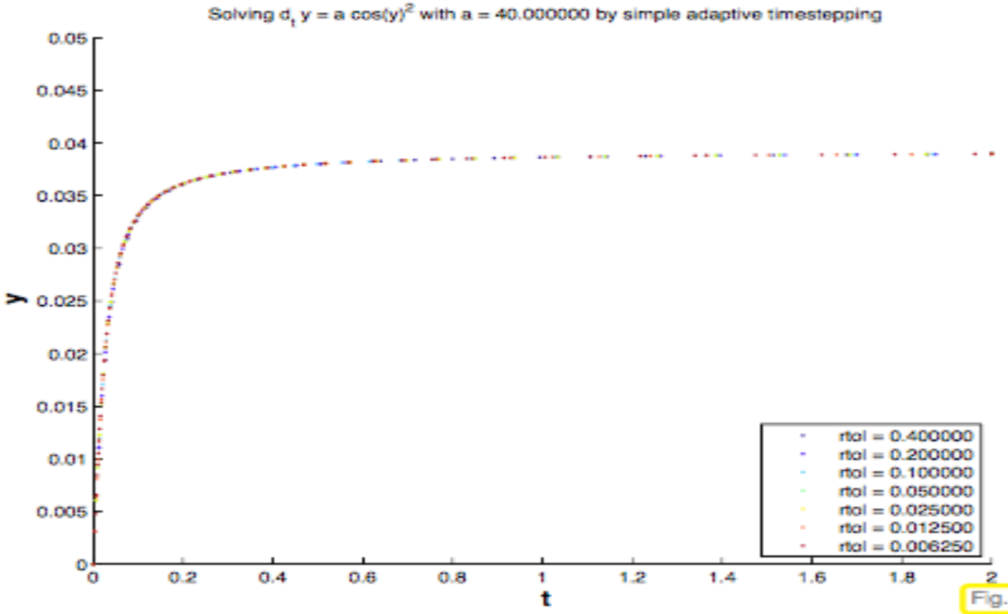
7

Fig. 3

$\lhd$ ASC works !



◁ $EST_k \not\approx$ true error at t_k

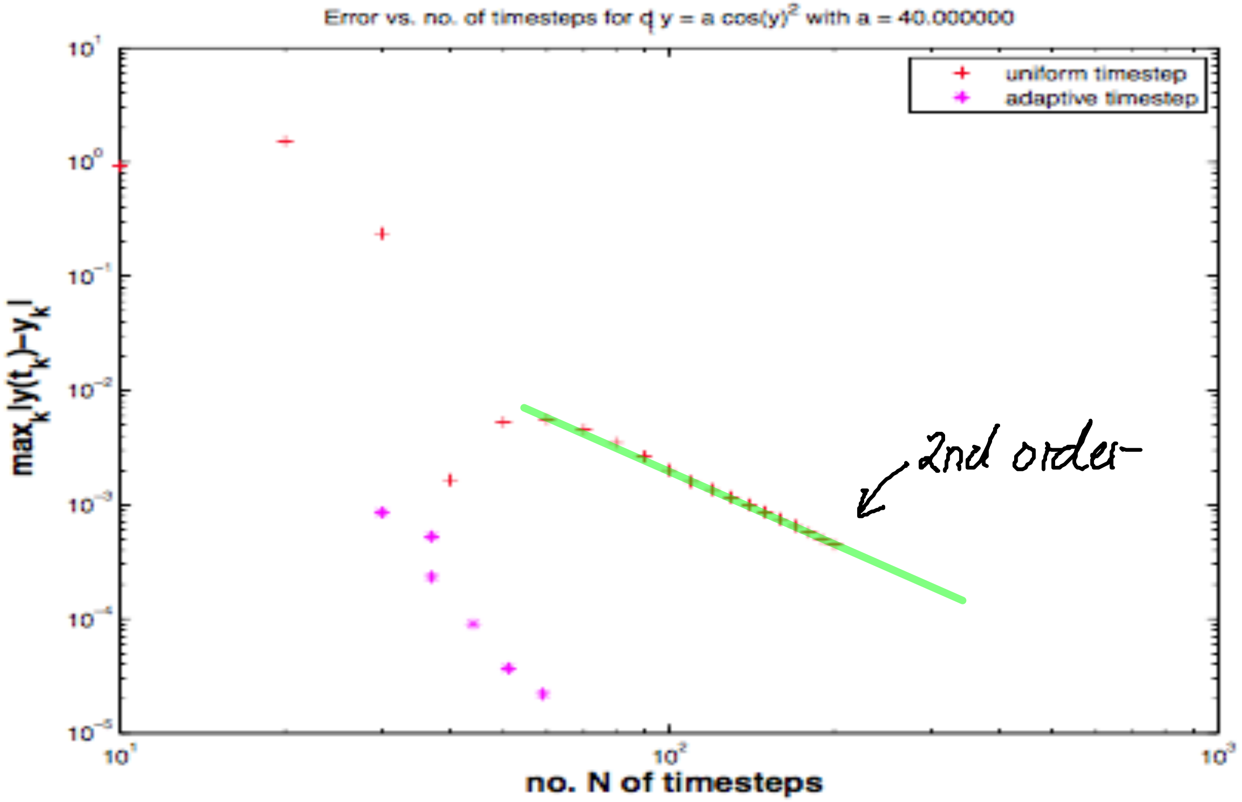


$y_0 = 0$
→ no step

349 Fig. 350

Solutions $(\mathbf{y}_k)_k$ for different values of `rtol`

Gain through adaptivity



Error vs. computational effort

→ Adaptivity efficient !

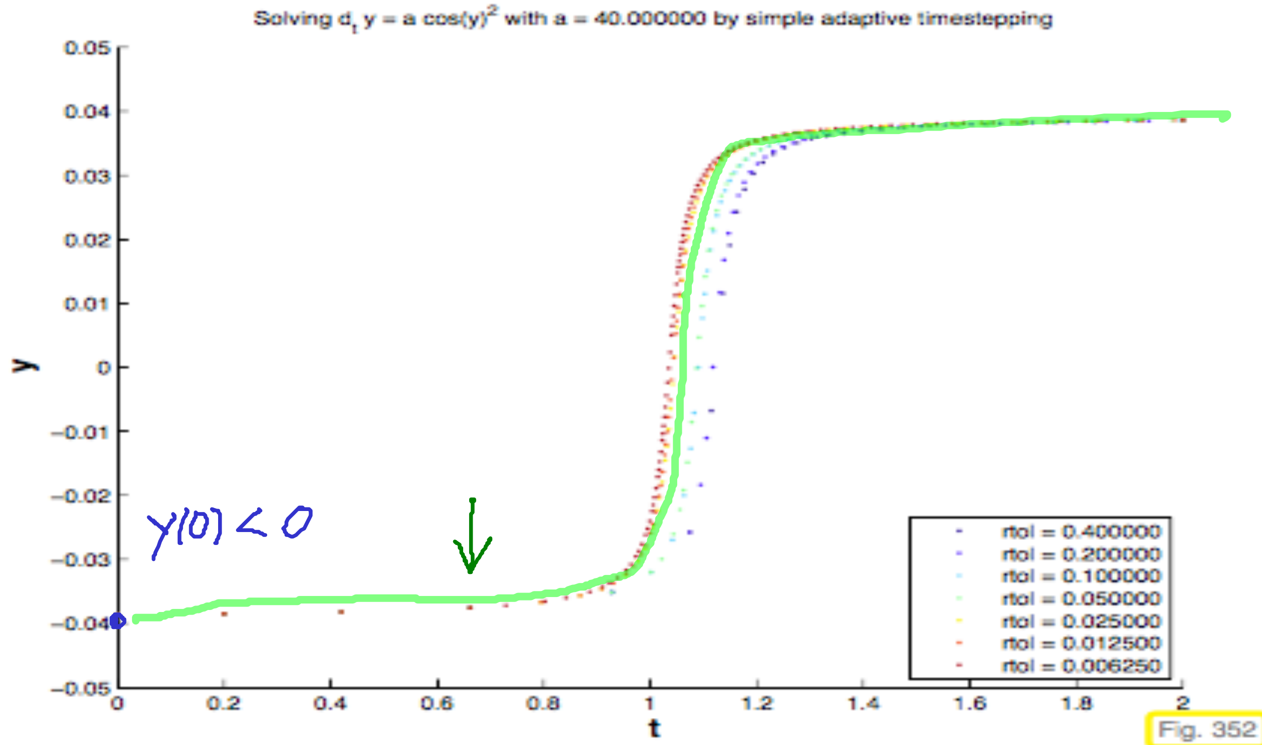
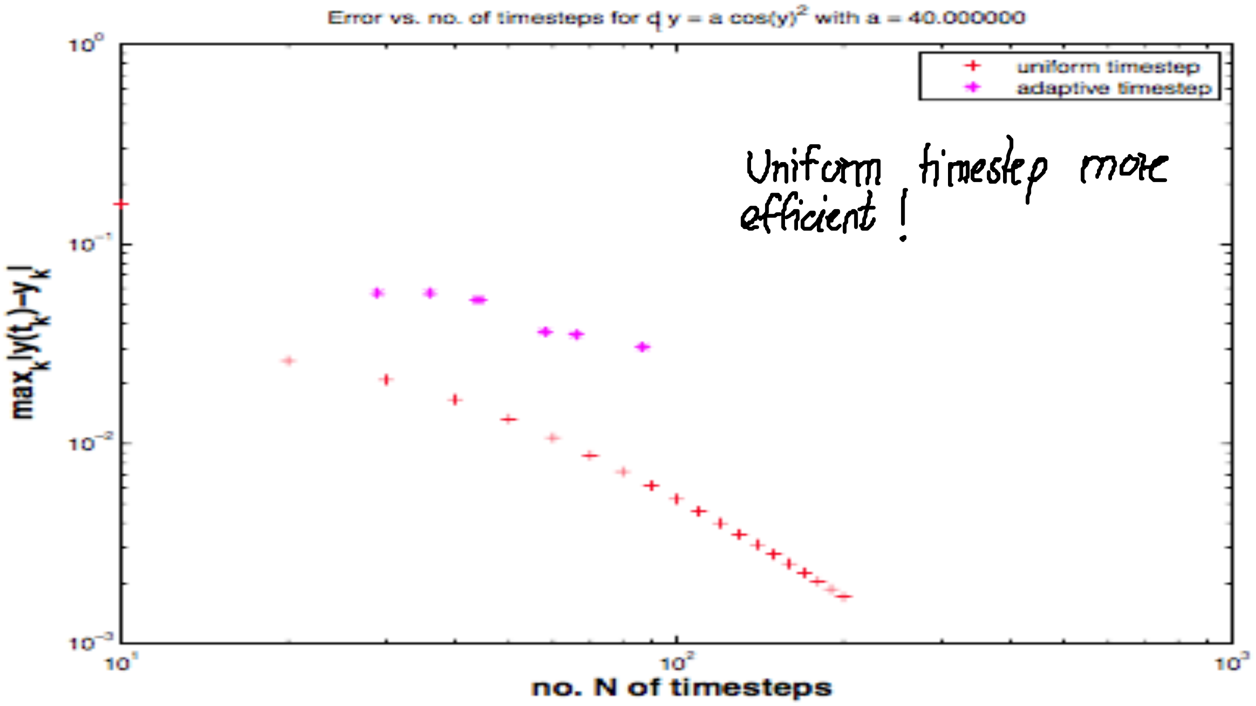


Fig. 352



Error vs. computational effort

Here: sensitive dependence of step position on $y(t)$ for small times

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 $h_{k+1} = ?$

$$\mathrm{EST}_k := \| \tilde{\Psi}^h y_k - \Psi^h y_k \| , \quad h := h_k$$

order p+1   order p

One-step errors:

$$\Rightarrow \quad \| \Psi^h y_k - \Phi^h y_k \| = c h^{p+1} + O(h^{p+2})$$
$$\| \tilde{\Psi}^h y_k - \Phi^h y_k \| = O(h^{p+2})$$

known   exact solution

$$\Rightarrow \quad \mathrm{EST}_k \approx c h^{p+1} \quad \text{for small } h$$

Goal (efficiency!) $\quad \mathrm{EST}_k = \mathrm{TOL}$

$$h_{new} : \quad c h_{new}^{p+1} = \mathrm{TOL} \qquad (*)$$

$$EST_k \approx c h^{p+1} \Longrightarrow c \approx \frac{EST}{h^{p+1}}$$

$$(*) \Longrightarrow \boxed{h_{new} = h \cdot \sqrt[p+1]{\frac{TOL}{EST}}}$$

recommended new timestep

MATLAB-code 11.5.22: Refined local stepsize control for single step methods

```
function [t,y] =
   odeintssctrl(Psilow,p,Psihigh,T,y0,h0,reltol,abstol,hmin)
t = 0; y = y0; h = h0;                    %
while ((t(end) < T) && (h > hmin)) %
  yh = Psihigh(h,y0);   % high order discrete evolution Ψ̃^h  ⎫
  yH = Psilow(h,y0);    % low order discrete evolution Ψ^h   ⎬ ESTIMATE
  est = norm(yH-yh);    % ↔ EST_k                             ⎭

  tol = max(reltol*norm(y(:,end)),abstol); %
  h = h*max(0.5,*min(2,*(tol/est)^(1/(p+1)))); % Optimal stepsize
     according to (11.5.21)
  if (est < tol)                                          %
    y0 = yh; y = [y,y0]; t = [t,t(end) + min(T-t(end),h)]; % step
      accepted
  end
end
```

* safeguard against oscillating timesteps

Implementation $\hat{=}$ embedded RK methods (same coeffs. a_{ij}, different b_i for different orders)