Numerical Methods for Computational Science and Engineering

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7. Numerical solution of ODEs

ordinary diff. eqns

First order system of ODEs

$$\frac{dy_1}{dt} = f_1(t, y_1, \dots, y_d)$$

$$\frac{dy_2}{dt} = f_2(t, y_1, \dots, y_d)$$

$$\vdots \qquad \vdots$$

$$\frac{dy_d}{dt} = f_d(t, y_1, \dots, y_d)$$

or more compactly

$$\frac{d\underline{y}}{dt} = \underline{f}(t, \underline{y})$$

Unknowns: $y_1, \dots, y_d$: scalar functions of real variable t "time"

Given: RHS $f_1, \dots, f_d$ functions of $d+1$ variables $t, y_1, \dots, y_d$

continuous

$$\underline{f} : I \times D \to \mathbb{R}^d \quad \text{of time } t \text{ and state } \underline{y}$$

$D \subset \mathbb{R}^d$: "state space", $I \subset \mathbb{R}$ finite time interval

Notation: $\frac{d\underline{y}}{dt} = \dot{\underline{y}}$

Definition of solution:

A solution to ODE $\dot{\underline{y}} = \underline{f}(t, \underline{y})$, where $\underline{f}$ is continuous, is a function $\underline{y}: J \subset I \to D$, $\underline{y} \in C^1$ s.t. $\dot{\underline{y}} = \underline{f}(t, \underline{y})$ holds for all $t \in J$.

Smoothness of solutions:

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

Each solution $\underline{y}(t)$ parametrizes a curve $C \subset \mathbb{R}^d$
"trajectory/orbit of the system"

Example: predator – prey model

(simplified ecological model for 2 species, $d=2$)

$u(t)$ ... number of prey at time t

$v(t)$ ... number of predators at time t

Population growth model (Thomas Malthus, 1798)

population of species grows roughly proportional to its size:

$$\dot{u} = \varrho \cdot u$$
$$\dot{v} = \sigma \cdot v$$

growth rates ϱ, σ may depend on the other species

(more prey $\Rightarrow$ predators reproduce faster

more predators $\Rightarrow$ prey are consumed faster)

Simplifying assumption: unlimited resources of prey

Simplest model: Lotka–Volterra model

$\alpha, \beta, \delta, \mu > 0$

$$(*) \quad \begin{aligned} \dot{u} &= \alpha u - \beta u v = (\alpha - \beta v) u \\ \dot{v} &= -\mu v + \delta u v = (-\mu + \delta u) v \end{aligned}$$

growth rates: $\varrho = \alpha - \beta v$

$\sigma = -\mu + \delta u$

$$\underline{y} = \begin{bmatrix} u \\ v \end{bmatrix} \qquad \underline{f}(\underline{y}) = \begin{bmatrix} (\alpha - \beta v) u \\ (-\mu + \delta u) v \end{bmatrix}$$

$$\Leftrightarrow \quad \dot{\underline{y}} = \underline{f}(\underline{y})$$

Note:

① $v = 0 \Rightarrow \dot{u} = \alpha u \Rightarrow u(t) = u(0) e^{\alpha t}$

(no predators → prey increase exp. with growth rate α)

$u = 0 \Rightarrow \dot{v} = -\mu v \Rightarrow v(t) = v(0) e^{-\mu t}$

(no prey ⇒ predators decrease exp. with decrease rate μ)

② (*) is a system of ODEs for which the RHS $\underline{f}$ is independent of the time variable t

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

Such systems are called <u>autonomous</u> ODEs.

(3) Equilibrium points of this system?

i.e. when is the solution constant $\underline{y}(t) = \underline{y}^*$

$\Rightarrow \quad \underline{f}(\underline{y}^*) = 0$

$\Rightarrow \quad (\alpha - \beta v)\, u = 0$

$(-\mu + \delta u)\, v = 0$

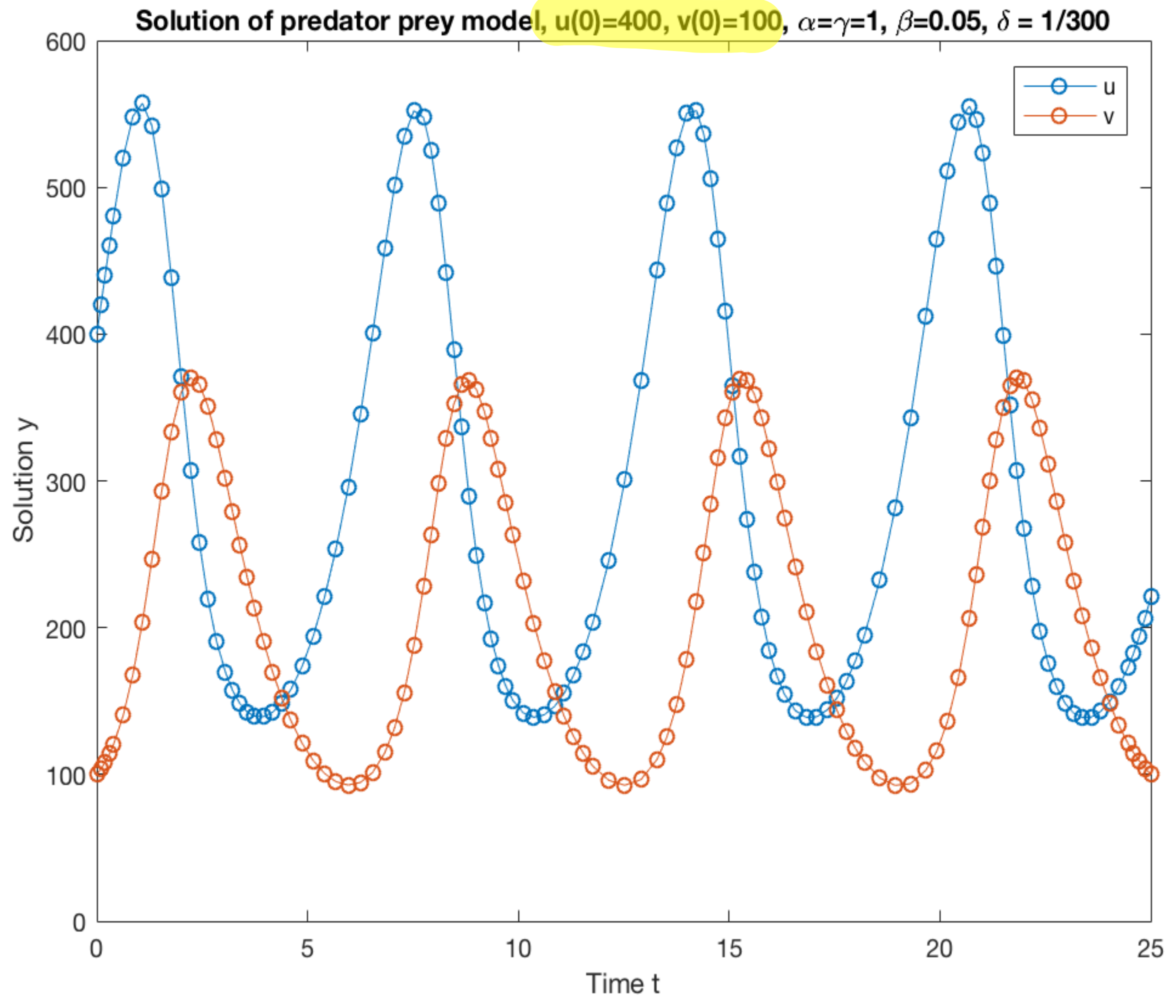
a.) $\alpha = \beta v, \ \mu = \delta u \quad \Leftrightarrow \quad v_2^* = \frac{\alpha}{\beta}, \quad u_2^* = \frac{\mu}{\delta}$

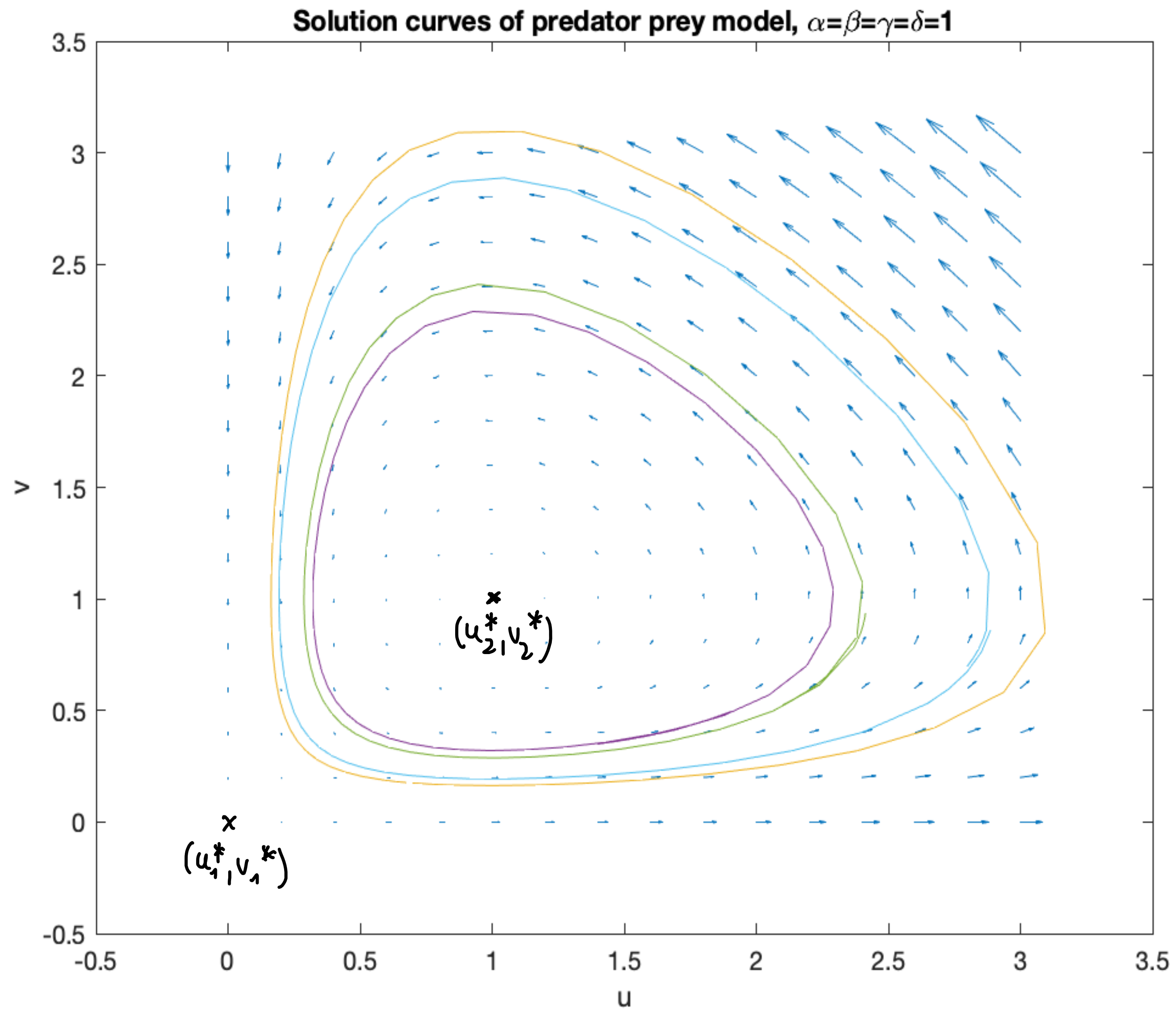
(non-trivial : birth rate of prey is precisely sufficient to continuously feed the predators)

b.) $u_1^* = 0, \quad v_1^* = 0$

(no animals at all)

2 initial values





$(u^*_{1/2}, v^*_{1,2})$ ... stationary points

(f describes movement of particles in this velocity field)

The solution depends on the initial size of the population $u(0), v(0)$

$\rightarrow$ to solve an ODE uniquely, we need additional conditions: Initial value problem (IVP)

i.e. ODE + initial conditions at start time $(t=0)$.

Higher order systems

Example: van der Pol equation

- modeling of electric circuits
- chemical reactions
- wind-induced motions of structures

$$\boxed{\ddot{u}(t) + (u^2 - 1)\dot{u}(t) + u = g(t)}$$

1 eqn
2^{nd} order

Convert this to a system of first orders?

$$y_1 = u$$

$$y_2 = \dot{u}$$

$$\Rightarrow \boxed{\begin{aligned} \dot{y}_1 &= y_2 \\ \dot{y}_2 &= g - (y_1^2 - 1)\, y_2 - y_1 \end{aligned}}$$

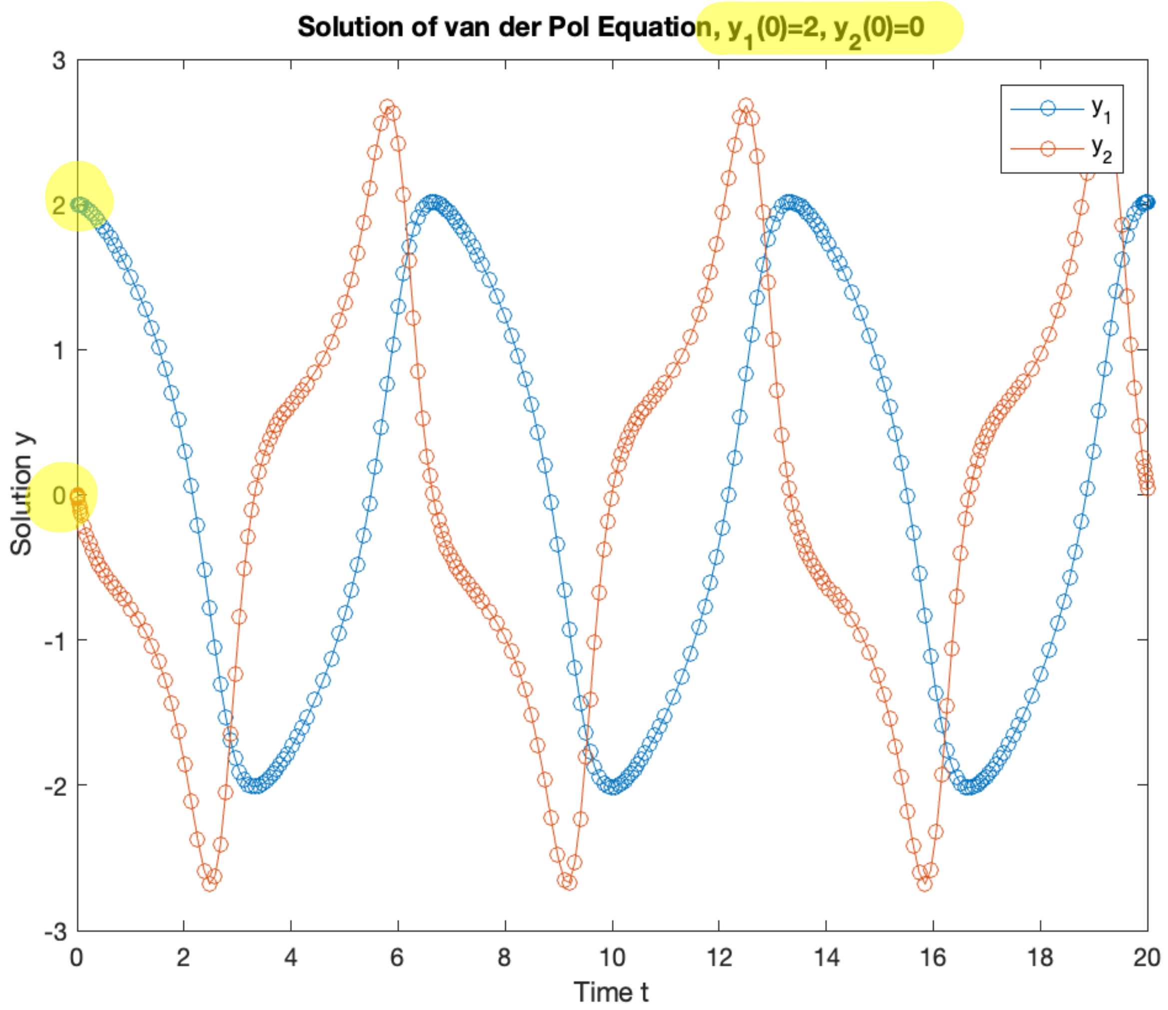
2 eqns
1^{st} order

and we can define $f_1(t, y_1, y_2) = y_2$

$$f_2(t, y_1, y_2) = g - (y_1^2 - 1)\, y_2 - y_1$$

If g is not constant, then this system is non-autonomous.

Solution example $(g(t) = 0)$ of an IVP



$\rightarrow$ 2 initial conditions!

Two general remarks:

① Any higher order equation/system can be transformed to a system of first order ODEs.

$$(**) \quad \underline{y}^{(n)} = \underline{f}(t, \underline{y}, \dot{\underline{y}}, \dots, \underline{y}^{(n-1)}) \qquad \underline{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_d \end{pmatrix}$$

Extend the system by adding additional components: all the derivatives up to order $n-1$

$$\underline{z}(t) := \begin{bmatrix} \underline{y}(t) \\ \underline{y}^{(1)}(t) \\ \vdots \\ \underline{y}^{(n-1)}(t) \end{bmatrix} = \begin{bmatrix} \underline{z}_1 \\ \underline{z}_2 \\ \vdots \\ \underline{z}_n \end{bmatrix} \qquad \underline{z}(t) \in \mathbb{R}^{n \cdot d}$$

$$(**) \iff \dot{\underline{z}} = \underline{g}(\underline{z}) \quad \text{with } \underline{g}(\underline{z}) = \begin{bmatrix} \underline{z}_2 \\ \underline{z}_3 \\ \vdots \\ \underline{z}_n \\ \underline{f}(t, \underline{z}_1, \dots, \underline{z}_n) \end{bmatrix}$$

Note: This extended system requires that we specify initial conditions for the first $n-1$ derivatives:

$$\underline{y}(t_0), \dot{\underline{y}}(t_0), \dots, \underline{y}^{(n-1)}(t_0)$$

$\Rightarrow$ $n \cdot d$ initial values

② Autonomization

Recall: $\dot{\underline{y}} = \underline{f}(\underline{y})$ (as in predator-prey model)

is called an autonomous ODE

Any non-autonomous ODE can be transformed to an equivalent autonomous ODE.

How? By extending the system by one more variable

→ introduce an extra coordinate $y_0 = t$ to represent time

y_0 satisfies:
- $\dot{y}_0(t) \left(= \frac{dy_0}{dt} \right) = 1$
- initial condition $y_0(t_0) = t_0$

Thus we can write

$$\boxed{\begin{aligned} \dot{y}_1(t) &= f_1(t, y_1, \dots, y_d) \\ \dot{y}_2(t) &= f_2(t, y_1, \dots, y_d) \\ &\vdots \\ \dot{y}_d(t) &= f_d(t, y_1, \dots, y_d) \end{aligned}} \iff \boxed{\begin{aligned} \dot{y}_0(t) &= 1 \\ \dot{y}_1(t) &= f_1(y_0, y_1, \dots, y_d) \\ \dot{y}_2(t) &= f_2(y_0, y_1, \dots, y_d) \\ &\vdots \\ \dot{y}_d(t) &= f_d(y_0, y_1, \dots, y_d) \end{aligned}}$$

non-autonomous system — equivalent auton. system

Example: Autonomous form of the van der Pol equation:

original:
$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = g(t) - (y_1^2 - 1)y_2 - y_1$$

autonomous form:

Introduce $y_0 = t$ (linear function in t)

$\dot{y}_0 = 1$

$\dot{y}_1 = y_2$

$\dot{y}_2 = \underbrace{g(y_0) - (y_1^2 - 1)y_2 - y_1}_{\text{function in } y_0, y_1, y_2}$

<u>Altogether</u>: It suffices to consider <u>autonomous first order</u> IVPs.

Remark: IVPs for autonomous ODEs:

initial time does not play a role

canonical choice $t = 0$.

Existence & uniqueness of solutions:

Recall from Analysis:

If $\underline{f}(t, \underline{y})$ is a differentiable function, then the IVP

$$\dot{\underline{y}} = \underline{f}(t, \underline{y}), \quad \underline{y}(t_0) = \underline{y}_0$$

admits a unique solution $\underline{y}$ defined on a <u>maximal</u> domain J, $t_0 \in J$.

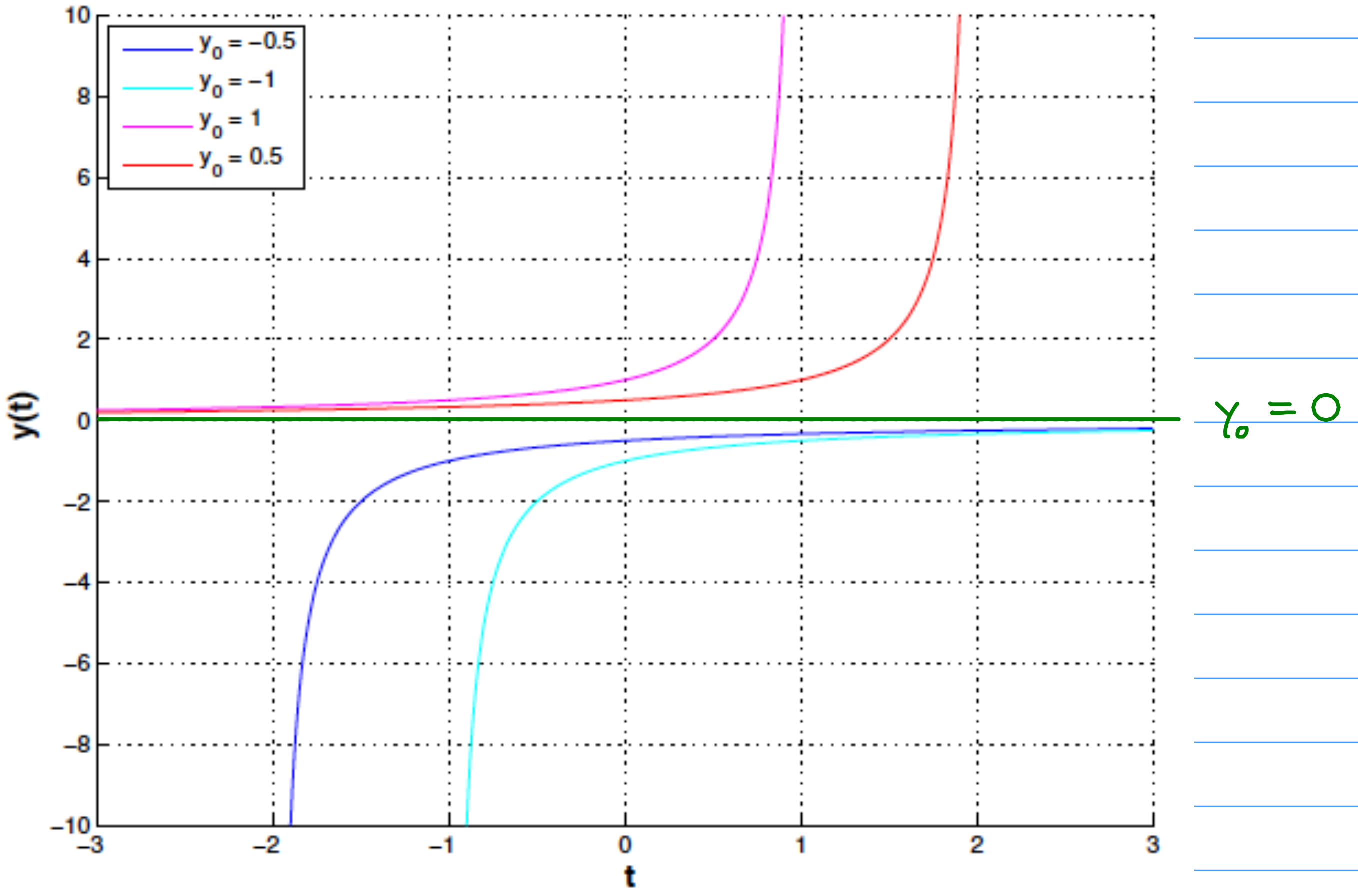
J depends on $(t_0, \underline{y}_0)$, i.e. $J = J(t_0, \underline{y}_0)$

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

(autonomous)

has the solution

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



$$J(0, Y_0) = J(Y_0) = \begin{cases} \mathbb{R} & \text{if } Y_0 = 0 \\ (-\infty, Y_0^{-1}) & \text{if } Y_0 > 0 \\ (Y_0^{-1}, \infty) & \text{if } Y_0 < 0 \end{cases}$$

(Maximal domain of definition of the solution depends on initial value Y_0)

Evolution operator

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

and assume that $\forall\, \underline{y}_0 \in D$ the unique solution $\underline{y}$ is global, i.e. exists $\forall\, t \in \mathbb{R}$.

Definition 8.1.5 (Evolution operator/mapping). Under assumption 8.1.1 the mapping

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

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

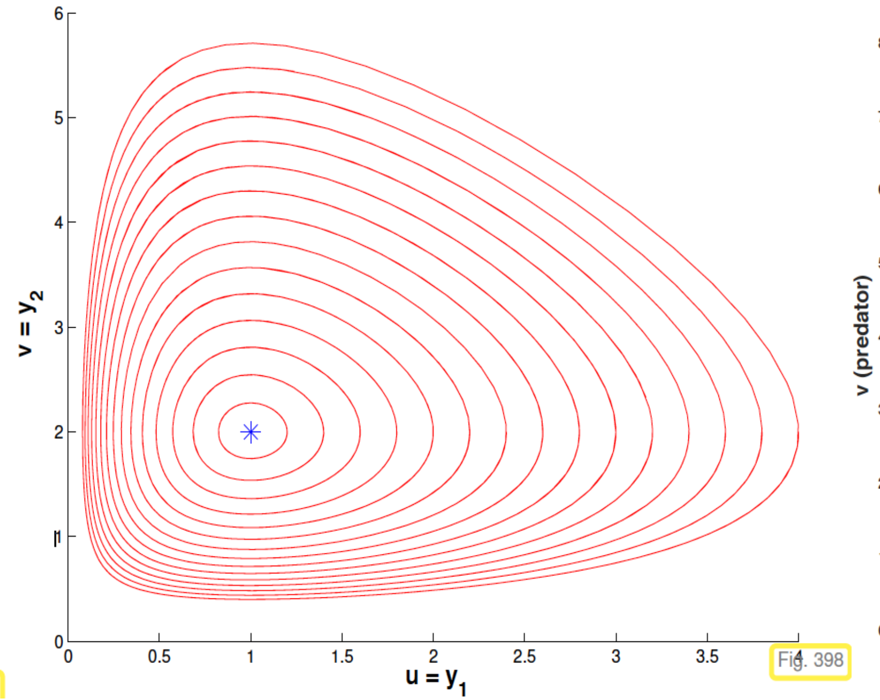
Note: • By definition $\frac{\partial \Phi}{\partial t}(t, \underline{y}_0) = \underline{f}(\Phi^t \underline{y}_0)$

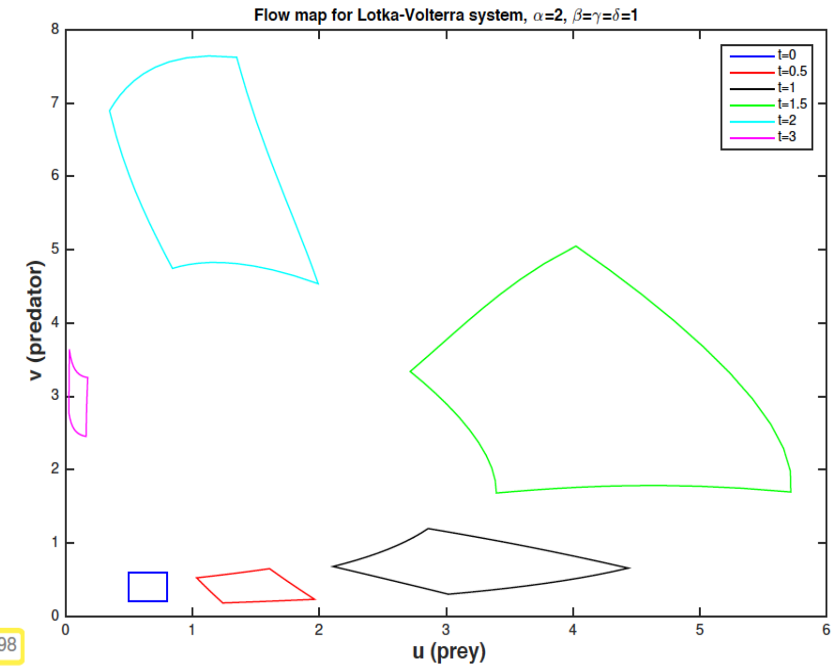
• Φ encodes the complete set of solutions of

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

$t \mapsto \Phi^t y_0$ trajectory

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





trajectories

$t \mapsto \Phi^t y_0$

state mapping

$y \mapsto \Phi^t y$

Each curve corresponds to one choice y_0

In practice: ODEs very often do not have a closed form solution

Next: Find a numerical / approximate solution

Polygonal Approximation Methods

For the ODE $\dot{y} = f(y)$ we want an approximate model for Φ (evolution operator)

on a temporal mesh $\mathcal{M} = \{0 = t_0 < t_1 < t_2 < \ldots < t_N = T\}$

We start with a simple idea: Taylor approximation

$$y(t) \approx y(t_k) + (t - t_k)\,\dot{y}(t_k) = y(t_k) + (t - t_k)\, f(y(t_k))$$

$$\Rightarrow y(t_{k+1}) \approx y(t_k) + (t_{k+1} - t_k) f(y(t_k))$$

Starting from initial condition

$$y(0) = y_0$$

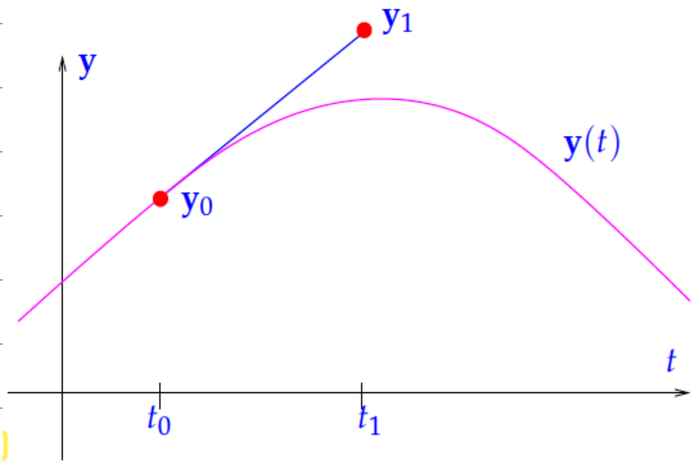
we can define y_k, the approximation of $y(t_k)$, iteratively as:

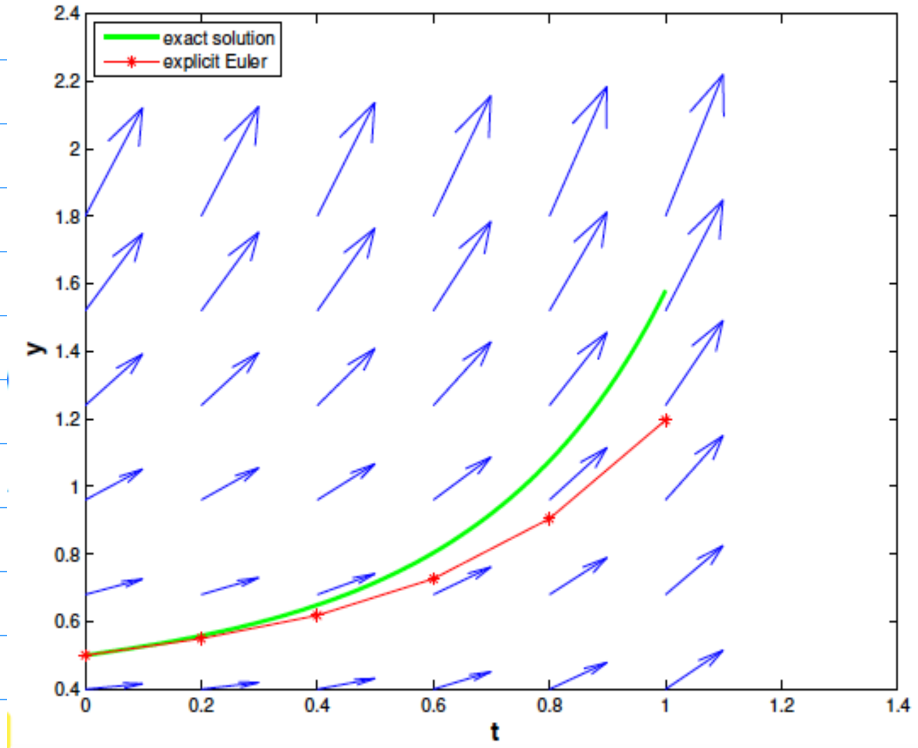
$$\boxed{y_{k+1} = y_k + \underbrace{(t_{k+1} - t_k)}_{=: h_k} f(y_k)}$$

Explicit Euler method

With equidistant mesh:

$$y_{k+1} = y_k + h f(y_k)$$





Example: $\dot{y} = y \qquad y(0) = 1 \qquad (*)$

(We know the explicit solution: $y(t) = \exp(t)$)

Explicit Euler with uniform step size h:

$$\begin{aligned} y_{k+1} &= y_k + h \cdot y_k = (1+h) y_k = (1+h)^2 y_{k-1} \\ &= \dots = (1+h)^{k+1} y(0) \\ &= (1+h)^{k+1} \end{aligned}$$

$\Rightarrow \quad Y_k = (1+h)^k$

$t_k = hk \qquad y(t_k) = \exp(t_k) = \exp(hk)$

$$\approx (1+h)^k = Y_k$$

$$(1+h)^{t_k/h} = Y_k$$

Formula from calculus:

$$\exp(t) = \lim_{h \to 0} (1+h)^{t/h}$$

So indeed: for small h, the explicit Euler scheme approximates the solution of (*).

Error $\quad e_{t_k} := Y_k - y(t_k) = (1+h)^{t_k/h} - \exp(t_k)$

h	$\lvert e_1\rvert$	$\lvert e_2\rvert$	$\lvert e_3\rvert$
0.1	0.125	0.662	2.636
0.01	0.0134	0.0730	0.297
0.001	0.00135	0.00738	0.0301
0.0001	0.000136	0.000739	0.00301

error at times $t = 1, 2, 3$

- for fixed h: the further we proceed in time, the larger the error
- the smaller h, the smaller the error at a fixed time t

BUT: smaller step size $\Rightarrow$ more steps are needed to get to time t as h decreases

$\rightsquigarrow$ increase in computational effort

- Error is proportional to the step size

Decreasing h by a factor $\frac{1}{10}$

(roughly) $\Rightarrow$ error decreases by factor $\frac{1}{10}$

(and complexity increases by factor 10)

$\rightarrow$ linear dependence of error on step size

$$|e_{t_k}| = |y_k - y(t_k)| \leq \underbrace{C(t_k)}_{\text{function of time \& initial condition, but independent of } h} \cdot h^1$$

Methods with such a linear dependence:

First-order methods

(Explicit Euler: First-order method)

Implicit Euler Method

Recall form of explicit Euler:

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

This can interpreted as a forward difference approximation:

$$y'(t_k) \approx \frac{y(t_{k+1}) - y(t_k)}{t_{k+1} - t_k} \qquad (h = t_{k+1} - t_k)$$

Alternatively, one can use backward difference:

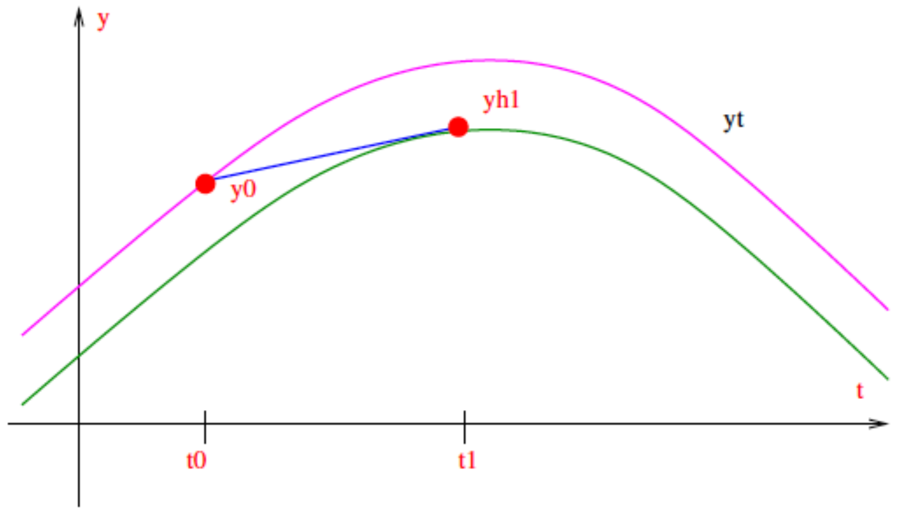
$$y'(t_{k+1}) \approx \frac{y(t_{k+1}) - y(t_k)}{t_{k+1} - t_k}$$

$$\left[\, y'(t_k) \approx \big(y(t_k) - y(t_{k-1})\big) \,/\, \big(t_k - t_{k-1}\big) \,\right]$$

$\Rightarrow$ $$\boxed{y_{k+1} = y_k + h f(y_{k+1})}$$

Implicit Euler Method

as a new scheme



Fundamental difference: RHS (for implicit Euler) depends on y_{k+1} which is not known at step k.

$\Rightarrow$ requires solution of a d-dimensional (possibly non-linear) system of equations! At each iteration step!

(Remark: solving non-linear systems will be discussed in Chapter 8 $\rightarrow$ e.g. Newton's method)

Benefits of such "implicit" methods? Better stability properties for stiff IVPs ($\rightsquigarrow$ will be discussed later)

Implicit midpoint method

Idea: central difference quotient as an approach

$$y'\left(\frac{1}{2}(t_k+t_{k+1})\right) \approx \frac{y(t_{k+1})-y(t_k)}{t_{k+1}-t_k}$$

$$\Rightarrow \; y(t_{k+1}) \approx y(t_k) + h \cdot \underline{f}\left(y\left(\frac{t_k+t_{k+1}}{2}\right)\right)$$

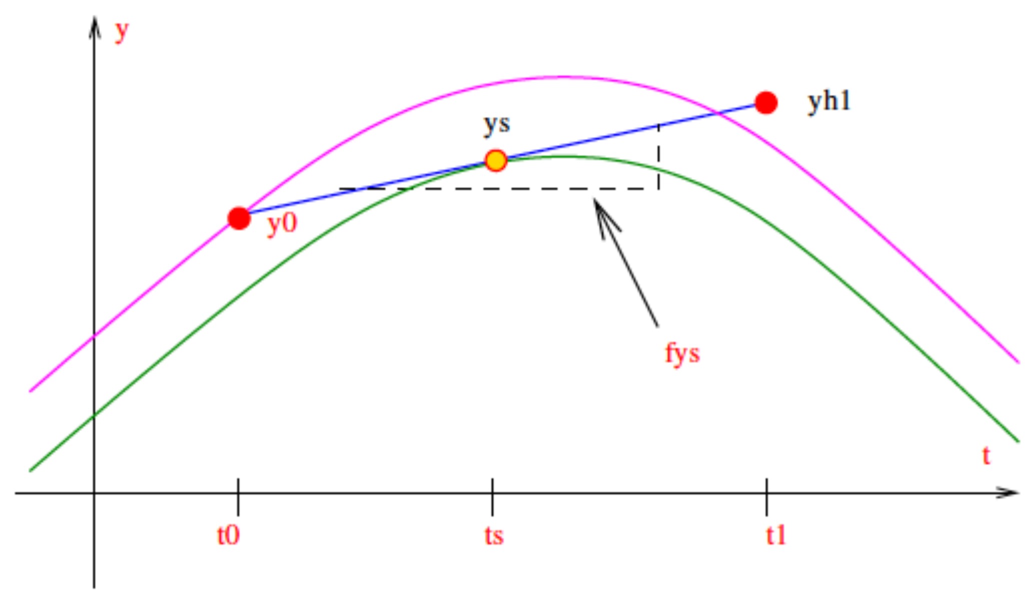
BUT: requires approximation of $y\left(\frac{t_k+t_{k+1}}{2}\right)$

$$\Rightarrow \; y\left(\frac{t_k+t_{k+1}}{2}\right) \approx \frac{1}{2}\left(y(t_k)+y(t_{k+1})\right)$$

$$\Rightarrow \; \boxed{y_{k+1} = y_k + h \cdot \underline{f}\left(\frac{1}{2}(y_k+y_{k+1})\right)}$$

Again: implicit method

Implicit midpoint method



Remark: Solutions of the non-linear systems in implicit Euler & implicit method exist, if h is sufficiently small.

Remark: expl. / impl. Euler & implicit midpoint method have in common that the new iterate y_{k+1} only involves the current state y_k.

such methods are called Single Step Methods

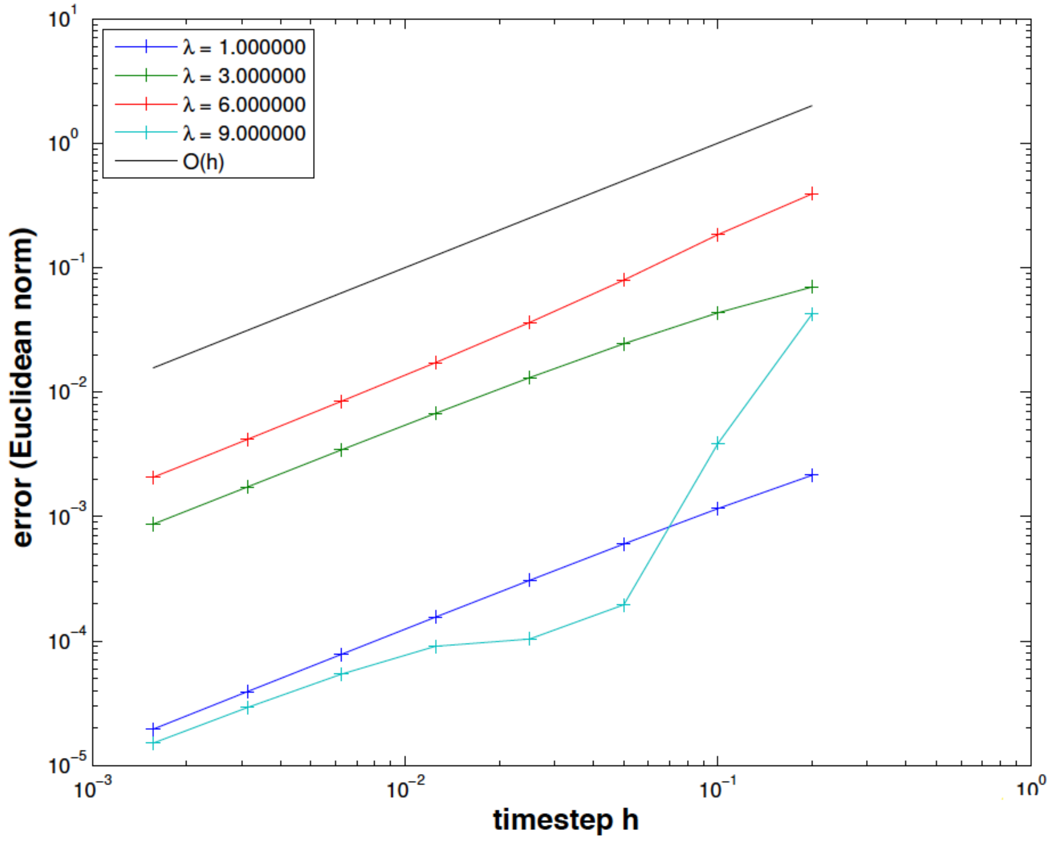
$[y_0, y_1, \dots, y_N]$ approximation of $[y(t_0), y(t_1), \dots, y(t_N)]$

Convergence rates of these 3 methods:

- all algebraic
- the two Euler methods are first-order
- the implicit midpoint method is second-order

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

consider error $|e_1|$ at final time $t = 1$

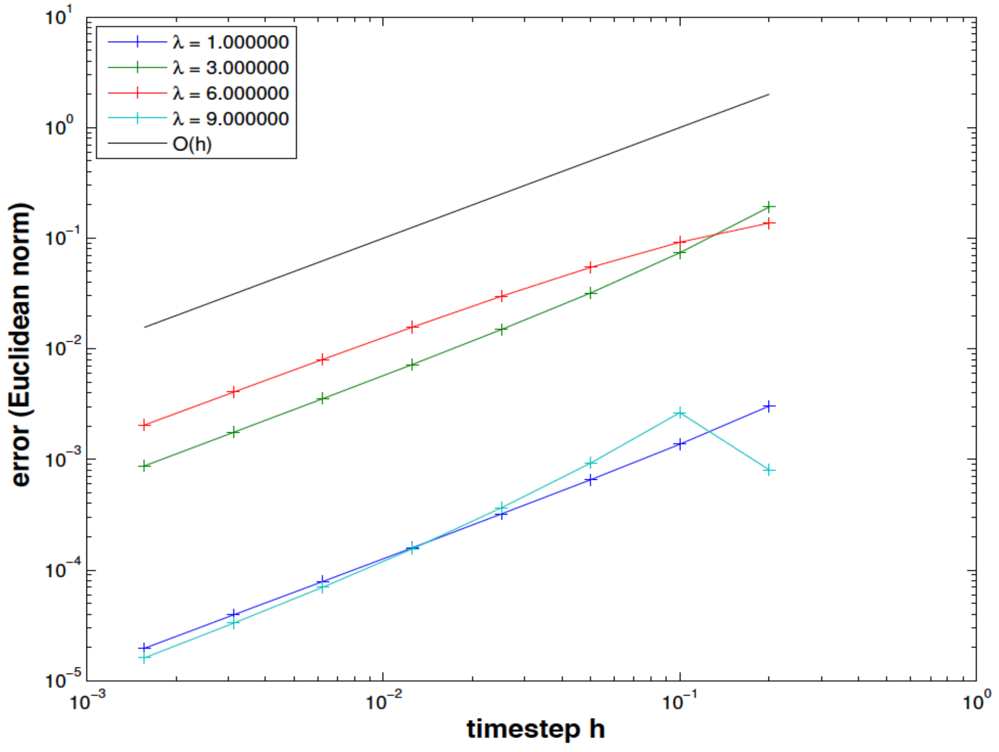


explicit Euler method

log-log-plot

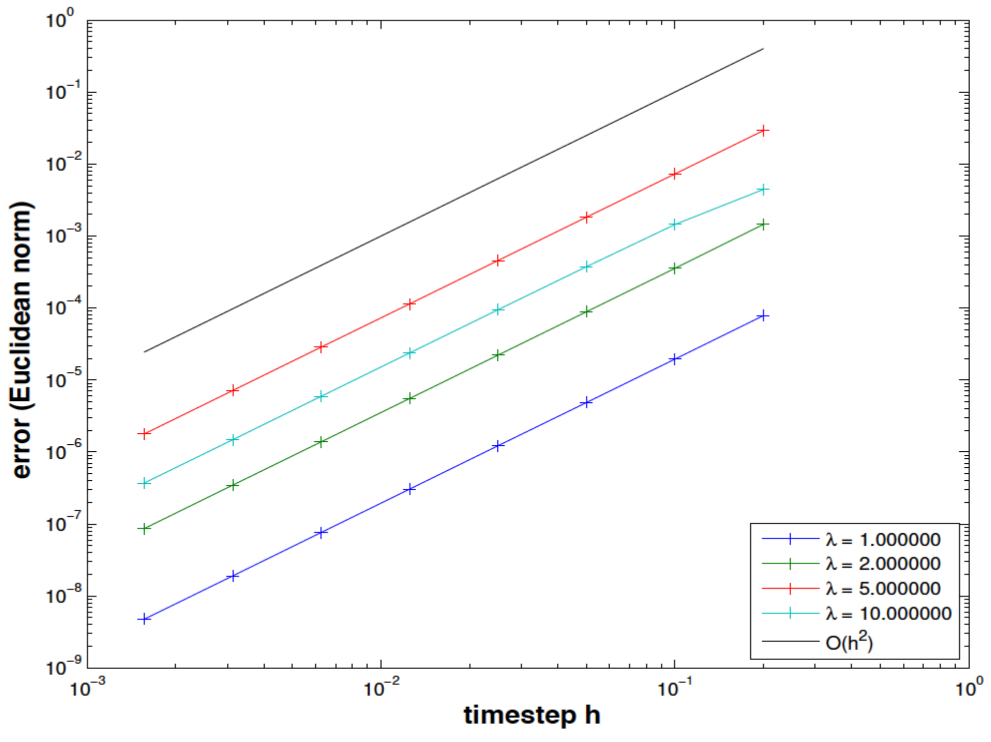
algebraic

$\mathcal{O}(h)$



implicit Euler method

$\mathcal{O}(h)$



implicit midpoint method

$|e_1| = \mathcal{O}(h^2)$

$\Rightarrow$ implicit midpoint method is a second order method

$$|e_{t_k}| \leq C(t_k)\, h^2$$

General Single Step Methods

So far:

$$y_{k+1} = \underbrace{y_k + h_k f(y_k)}_{\Psi(h_k, y_k)} \qquad \text{[Explicit Euler]}$$

$$y_{k+1} = y_k + h_k f(y_{k+1}) \qquad \text{[Implicit Euler]}$$

$$y_{k+1} = y_k + h_k f\left(\tfrac{1}{2}(y_k + y_{k+1})\right) \qquad \text{[Implicit midpoint]}$$

General SSM:

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

$\uparrow$ discrete evolution operator (approximates the true evolution operator Φ)

Single step: Ψ only takes in state y_k

Analytical setting:

$$y(t_1) = \Phi^{h_1} y_0$$

$$y(t_{k+1}) = \Phi^{t_{k+1}} y_0 = \Phi^{h_k}[y(t_k)]$$

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

$D \subset \mathbb{R}^d$

$\overset{?}{\approx}$

Numerical setting

$$y_1 = \Psi^{h_0} y_0$$

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

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

Explicit Euler: $y_{k+1} = \Psi^{h_k} y_k = y_k + h_k f(y_k)$

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

Recall: $\frac{\partial \Phi}{\partial t}(t, y) = f(y)$

Basic requirement on Ψ:

At $h=0$: $\frac{d}{dh}\Psi^h = f(y)$?

Consistent discrete evolution

The discrete evolution $\mathbf{\Psi}$ defining a single step method according to definition 8.3.1 and (8.33) for the autonomous ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ invariably is of the form

$$\boxed{\mathbf{\Psi}^h\mathbf{y} = \mathbf{y} + h\boldsymbol{\psi}(h,\mathbf{y})} \quad \text{with} \quad \begin{array}{l} \boldsymbol{\psi} : I \times D \to \mathbb{R}^d \text{ continuous,} \\ \boldsymbol{\psi}(0,\mathbf{y}) = \mathbf{f}(\mathbf{y}) . \end{array} \tag{8.34}$$

$f(y) =$

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

$$= \psi(0, y)$$

Note: Explicit Euler: $\psi(h, y) = f(y)$

General SSM: $\psi(0, y) = f(y)$

Example: Consistency of implicit Euler:

$$\Psi^h y = y + h \underbrace{f(\Psi^h y)}_{=\psi(h,y)}$$

$$\psi(0, y) = f(\underbrace{\Psi^0 y}_{=y}) = f(y) \quad \checkmark$$

Order of accuracy for SSMs

All SSMs converge algebraically

there is a $p \in \mathbb{N}$ such that the sequence $(\mathbf{y}_k)_k$ generated by the single step method for $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$ on a mesh $\mathcal{M} := \{t_0 < t_1 < \cdots < t_N = T\}$ satisfies

$$\boxed{\max_k \|\mathbf{y}_k - \mathbf{y}(t_k)\| \leq Ch^p} \quad \text{for} \quad h := \max_{k=1,\dots,N} |t_k - t_{k-1}| \to 0\,, \tag{8.37}$$

with $C > 0$ independent of $\mathcal{M}$

Definition 8.3.3 (Order of a single step method). The minimal integer $p \in \mathbb{N}$ for which (8.37) holds for a single step method when applied to an ODE with (sufficiently) smooth right hand side, is called the *order* of the method.