1) Definition: Initial value problem

Given an interval $J = [a,b] \subseteq \mathbb{R}$, initial time $t_0 \in (a,b)$,
and a function $f : J \times \Omega \to \mathbb{R}$ with $\Omega \subseteq \mathbb{R}^n$.
Find a function $y : J \to \Omega$ s.t

$$\frac{d}{dt} y(t) = y'(t) = \dot{y}(t) = f(t, y(t)) \quad \forall t \in J$$

satisfying the initial condition

$$y(t_0) = y_0 .$$

Sometimes to em

$$y(t; t_0, y_0)$$

2) Motivation / Examples

a) $\dot{y} = \lambda y$ for $\lambda \in \mathbb{R}$

$y(0) = y_0$ $y_0 \in \mathbb{R}$

Solution: $y(t) = y_0 e^{\lambda t}$

b) Chemical reaction kinetics.

Bimolecular reaction

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C + D$$

k_i reaction coefficients

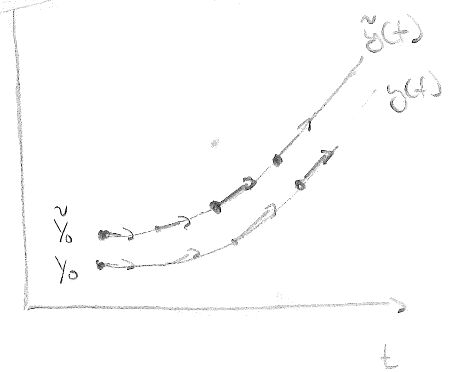
$$c_A' = c_B' = - k_1 c_A c_B + k_2 c_C c_D$$

$$c_C' = c_D' = k_1 c_A c_B - k_2 c_C c_D$$

- System
- nonlinear

Butcher

: First ideas



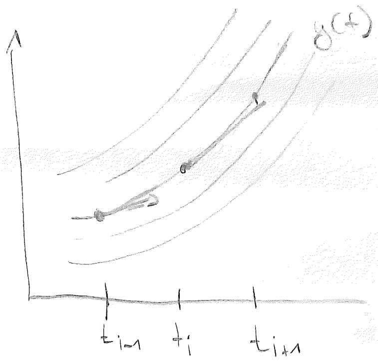
$t \mapsto (t, y(t)) = Y(t) \in \mathbb{R}^{n+1}$

Problem.

- For given start time t_0, stop time T, and initial value $y_0 = y(t_0)$, try to compute a numerical approximation $y_\Delta(t)$
- Introduce a subdivision $\{t_i\}_{i=0}^{n}$ of $[t_0, T]$ s.t. $t_i = t_0 + i\,\frac{T - t_0}{n}$.

  $\Delta t_i = \tau_i = t_{i+1} - t_i$ time-step size
- Equally space time-steps: Δt, τ.

a) Difference quotient approach:



$$y'(t_i) \approx \frac{y(t_{i+1}) - y(t_i)}{\tau}$$ Forward finite difference

So instead of $y'(t) = f(t, y(t))$ we solve

$$\frac{y(t_{i+1}) - y(t_i)}{\tau} \approx f(t_i, y(t_i))$$

$$\Rightarrow \quad y(t_{i+1}) \approx y(t_i) + \tau \cdot f(t_i, y(t_i)).$$

- Numerical method to compute approximation y_Δ defined at discrete time points

$$y_\Delta(t_{i+1}) := y_\Delta(t_i) + \tau_i\, f(t_i, y_\Delta(t_i))$$

$$y_{i+1} := y_i + \Delta t_i\, f(t_i, y_i) \qquad \text{for } i = 1, \dots n$$

$$y_0 := y(t_0) = y_0. \qquad \text{for } i = 0.$$

This is the

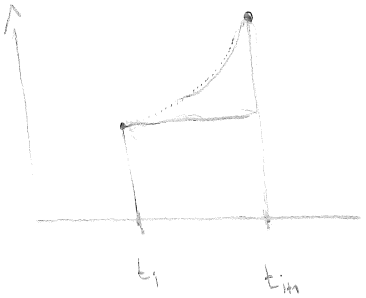
$\boxed{\text{Explicit Euler method}}$

Forward

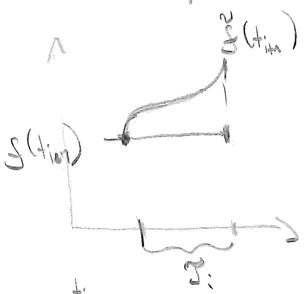
b) Integral approach

· $y'(t) = f(t, y(t))$ $\qquad \int_{t_i}^{t_{i+1}}$

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} \underbrace{f(t, y(t))}_{=: \tilde{f}(t)} \, dt$$



Idea: Apply quadrature rules to compute integrals



· one node QR using left end point

$$\int_{t_i}^{t_{i+1}} \tilde{f}(t) \approx \tilde{f}(t_i) \cdot \tau_i$$

So we define

$$Y_{i+1} := Y_i + \tau_i f(t_i, Y_i)$$

Explicit Euler again !

· One point QR using right end point

Define:

$$Y_{i+1} = Y_i + \tau_i \tilde{f}(t_{i+1})$$

$$\Longleftrightarrow \quad Y_{i+1} = Y_i + \tau_i f(t_{i+1}, Y_{i+1}) \qquad *)$$

· Y_{i+1} only implicitly defined as solutions to $*)$

Implicit / Backward Euler:

Set $\quad Y_0 = y(t_0)$

For $i = 1, \dots N$ compute Y_i by solving

$$Y_{i+1} = Y_i + \tau_i f(t_{i+1}, Y_{i+1})$$

· How complicate this is to solve, depends on f.

For instance $\quad y' = \lambda y \quad f(t, y(t)) = \lambda y(t)$.

Then

$$Y_{i+1} = Y_i + \tau \lambda Y_{i+1}$$

$$\Rightarrow \quad Y_{i+1} = \frac{1}{(1 - \tau\lambda)} \cdot Y_i \quad \dots$$

· Exercise: Can you derive the implicit using a difference quotient?

Definition

A one-step method with the startvalue

$$y_0 = y(t_0) + \mathcal{O}(\tau^p) \qquad \tau \longrightarrow 0$$

is called convergent of order $p \in \mathbb{N}$, if the

$$e(t_i, \tau) = \mathcal{O}(\tau^p) \qquad \tau \longrightarrow 0.$$

Note the different powers in the consistency and convergence definition ! ..

Example

The explicit Euler method is consistent of order 1.
for smooth enough f.

Taylor-expansion

$$\begin{aligned} \eta(t, \tau) &= y(t) + \tau f(t, y(t)) - y(t+\tau) \\ &= y(t) + \tau f(t, y(t)) - y(t) - \tau \underbrace{y'(t)}_{f(t, y(t))} + \mathcal{O}(\tau^2) \\ &= \mathcal{O}(\tau^2). \end{aligned}$$

4) One-step methods

Definition:

A one-step method defines an approximation to the IVP (*) in the form of a discrete function $y_\Delta : \{t_0, \dots, t_N\} \longrightarrow \mathbb{R}^n$ given by

$$y_{i+1} = y_i + \tau_i \, \Phi(t_i, y_i, y_{i+1}, \Delta t)$$

for some increment function

$$\Phi : [a,b] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^+ \longrightarrow \mathbb{R}^n.$$

- A one-step method is called explicit if Φ does not depend on y_i

Exercise

Write up the increment function for

- Explicit Euler
- Implicit Euler
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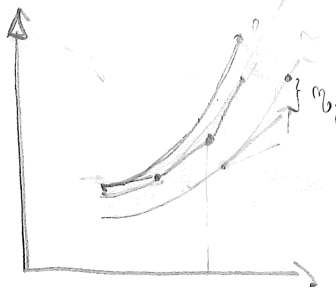
Questions

- Can we quantify the global discretization error $e(t_i, \tau) := y_\Delta(t_i) - y(t_i)$?



- Error sources
  - $y_0 - y(t_0)$? (floating point number!)
  - local truncation error
  - Accumulation? For time steps more errors ... (but probably smaller)

Definitions

a) The local discretization truncation error $\eta(t, \tau)$ is defined by

$$\eta(t,\tau) = \underbrace{y(t) + \tau \, \Phi(t, y(t), y(t+\tau), \tau)}_{\text{Approximation for } y(t+\tau) \text{ starting exact value of } y \text{ at } t} - y(t+\tau).$$

b) One-step method is called consistent if $\eta(t,\tau) \longrightarrow 0$ $\tau \longrightarrow 0$

c) consistent of order p if $\eta(t,\tau) = \mathcal{O}(\tau^{p+1})$