Topics for today (Lecture 9) 23.5.2023

- Orthogonal polynomials ✓
- Gauss quadrature ✓
- Some discussion on error estimates of Gauss quadrature
- Weighted orthogonal polynomials ✓ → Homework

- Initial value problems
- Euler's method I

Orthogonal polynomials

"orthogonality" w.r.t. the inner product

given by $\langle p, q \rangle = \int_a^b p(x)\,q(x)\,dx$, p, q are

real-valued polynomials on $[a, b]$.

$\mathcal{P} := \{ p : p : [a,b] \to \mathbb{R}$ is polynomial$\}$

Then $(\mathcal{P}, \langle \cdot, \cdot \rangle)$ is a pre-Hilbert space,

just a (real) vector space with a positive-definite

inner product.

__Definition__

(Inner product space) A $\overset{\text{real}}{\text{vector}}$ space X is called $\overset{\text{an}}{\text{inner}}$ product space if there exists a map

$$X \times X \to \mathbb{R}$$

$$\langle \cdot , \cdot \rangle : X \times X \to \mathbb{R}$$

such that

$\langle p, q \rangle = \langle q, p \rangle \quad \forall\, p, q \in X$ (symmetry)

$\langle \alpha x + \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle \quad \forall\, \alpha, \beta \in \mathbb{R}$ $\forall\, x, y, z \in X$ (bilinearity)

$\langle x, x \rangle > 0$ iff $x \neq 0$. (positive definiteness)

Define

(norm), any real inner product space becomes a normed space by setting

$$\|x\| := \sqrt{\langle x, x\rangle}$$

Norm:
$$\begin{cases} \|x+y\| \le \|x\| + \|y\| & \Delta\text{-inequality} \quad \forall x, y \in X \\ \|\alpha x\| = |\alpha| \cdot \|x\| & \forall \alpha \in \mathbb{R} \ \forall x \in X \\ \|x\| = 0 \ \underbrace{\text{iff}}_{= \text{ if and only if}} \ x = 0 & \text{(definiteness)} \end{cases}$$

Orthogonality

p, q are called orthogonal if $\langle p, q \rangle = 0$, in symbols $p \perp q$

orthonormal

if $p \perp q$ and $\|p\| = \|q\| = 1$
$= \langle p, p \rangle = \langle q, q \rangle$,
"normalized"

Finding / constructing orthogonal sequences

inner product $\langle p, q \rangle = \int_a^b p(x)\, q(x)\, dx$

norm $\|q\| = \left(\int_a^b (q(x))^2 dx \right)^{\frac{1}{2}}$

Idea is to take a basis for $\mathcal{P}$

$\{1, x, x^2, \ldots, x^k, \ldots\}$

$\overline{\text{Gram-Schmidt}}$ procedure

$\{q_0, q_1, \ldots, q^k, \ldots\}$ is orthonormal basis of $\mathcal{P}$

$\{1, x, x^2, x^3, \dots, \dots\}$

$$q_0 = \frac{1}{\|1\|} = \frac{1}{\left[\left(\int_a^b 1^2 \, dx\right)^{\frac{1}{2}}\right]} = \frac{1}{\sqrt{b-a}}$$

Identify x with the function $x \mapsto x$

for $j = 1, 2, \dots$ (Induction!) assume that $\{q_0, q_1, \dots, q_{j-1}\}$ has been constructed.

$$\tilde{q}_j(x) = x\, q_{j-1}(x) - \sum_{i=0}^{j-1} \langle x q_{j-1}, q_i \rangle q_i(x)$$

$$\sum_{i=0}^{j-1} \left(\int_a^b z\, q_{j-1}(z)\, q_i(z) \, dz \right) q_i(x)$$

$$q_j(x) = \frac{\tilde{q}_j(x)}{\|\tilde{q}_j\|}$$

$$\left(\Longrightarrow \|q_j\| = 1 \right)$$

New basis is orthonormal!

$$\langle x\, q_{j-1}, q_i \rangle = \int_a^b x\, q_{j-1}(x)\, q_i(x)\, dx$$

$$\int_a^b q_{j-1}(x)\, x\, q_i(x)\, dx = \langle q_{j-1}, \underbrace{x\, q_i}_{\text{degree } i+1} \rangle$$

$$= 0 \quad \text{if}$$

$$i \le j-3$$

$q_{j-1} \perp$ "any polynomial of degree $\le j-2$"

$$i+1 \le j-2$$

$$\tilde{q}_j(x) = x\, q_{j-1}(x) - \sum_{i=0}^{j-1} \underbrace{\langle x q_{j-1}, q_i \rangle}_{=0 \text{ if } i \leq j-3} q_i(x)$$

$$= x\, q_{j-1}(x) - \langle x q_{j-1}, q_{j-1} \rangle q_{j-1}(x)$$

$$- \langle x q_{j-1}, q_{j-2} \rangle q_{j-2}(x)$$

Works only for polynomials!

(not in Hilbert spaces)

Q: Why $\tilde{q}_j \perp \operatorname{span}\{q_0, \dots, q_{j-1}\}$?

Observe if $\tilde{q}_j \perp \operatorname{span}\{q_0, \dots, q_{j-1}\}$

$\Longrightarrow$ $q_j \perp \operatorname{span}\{q_0, \dots, q_{j-1}\}$

$\langle \tilde{q}_j, q_{j-1} \rangle$ (use bilinearity)

$= \langle x\, q_{j-1}, q_{j-1} \rangle$

$$- \sum_{j=0}^{j-1} \langle x\, q_{j-1}, q_i \rangle \cdot \underbrace{\langle q_i, q_{j-1} \rangle}_{=0 \text{ except for } i = j-1}$$

because $q_{j-1} \perp \operatorname{span}\{q_0, \dots, q_{j-2}\}$

$$= \langle x\, q_{j-1},\ q_{j-1} \rangle$$

$$- \sum_{i=0}^{j-1} \langle x\, q_{j-1},\ q_i \rangle \cdot \underbrace{\langle q_i,\ q_{j-1} \rangle}_{\substack{=0 \quad \text{except for} \\ i=j-1}}$$

$$= \langle x\, q_{j-1},\ q_{j-1} \rangle - \langle x\, q_{j-1},\ q_{j-1} \rangle \boxed{\cdot \langle q_{j-1},\ q_{j-1} \rangle}$$

$$\langle q_{j-1},\ q_{j-1} \rangle = \| q_{j-1} \|^2 = 1$$

$$= 0$$

THEOREM (Gauss quadrature)

Let $x_0, x_1, x_2, \dots, x_n$ roots of an orthogonal polynomial $q_{n+1}(x)$ on $[a,b]$

Then $\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$

where

$$A_i = \int_a^b \varphi_i(x)\,dx, \quad \varphi_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$$\int_a^b f(x)\,dx \approx \int_a^b \text{"interpolation polynomial of } f \text{ at } x_0, x_1, \dots, x_n\text{"}\,dx$$

is exact for all polynomials of degree $2n+1$ or less.

1. step: Compute orthonormal polynomials on [a,b]

2. step: Compute roots of q_{n+1}

3. step: Compute interpolation polynomial
w.r.t. the roots $x_0, x_1, x_2, \dots, x_n$

4. step: Integrate (Exact up to degree $2n+1$)

Error:

$$Q(f) = \sum_{i=0}^{n} f(x_i) \int_a^b \varphi_i(x)\,dx$$

$$\int_a^b f(x)\,dx - Q(f) = R(f)$$

Proof

Let f be a polynomial of degree $\leq 2n+1$

Division algorithm $\left(\frac{f}{q_{n+1}} = p_n + \frac{r_n}{q_{n+1}} \right)$

$$\underset{\deg = 2n+1}{f} = \boxed{\underset{\deg = n+1}{q_{n+1}} \; \underset{\deg = n}{p_n}} + \underset{\deg \leq n}{r_n}$$

$$\frac{5}{2} = 2 + \frac{1}{2}$$

$$5 = 2 \cdot 2 + 1$$

$$f(x_i) = \underbrace{q_{n+1}(x_i)}_{=0} p_n(x_i) + r_n(x_i)$$

Like integer division

$$= r_n(x_i)$$

Integrale

$$\int_a^b f(x)\,dx = \underbrace{\int_a^b \overset{\text{deg}=n+1}{\overline{q_{n+1}(x)}}\ \overset{\text{deg}=n}{\overline{p_n(x)}}\,dx}_{} + \int_a^b r_n(x)\,dx$$

$= \langle q_{n+1}, p_n \rangle$

$= 0$ because

$q_{n+1} \perp \operatorname{span}\{q_0, \dots, q_n\}$

$$= \int_a^b r_n(x)\,dx = \sum_{i=0}^{n} r_n(x_i) \underbrace{\int_a^b \varphi_i(x)\,dx}_{= A_i}$$

$$= \sum_{i=0}^{n} A_i\, r_n(x_i) = \sum_{i=0}^{n} A_i\, f(x_i)$$

$\square$

Def. Weighted orthogonal polynomials

$$\langle p, q \rangle_\omega = \int_a^b p(x)\, q(x)\, \omega(x)\, dx$$

$$\sqrt{\langle p, p \rangle_\omega} = \left(\int_a^b (p(x))^2\, \omega(x)\, dx \right)^{\frac{1}{2}}$$

$$\shortparallel$$

$$\|p\|_\omega$$

Typical weights e^{-x} $\rightsquigarrow$ Laguerre polynomials

$e^{-\frac{x^2}{2}}$ $\rightsquigarrow$ ~~Her~~ Hermite polynomials

Unweighted on $[-1, 1]$ $\rightsquigarrow$ Legendre polynomials
$(w = 1)$

Theorem (without proof)

The previous theorem holds for a w- orthonormal (orthogonal) polynomial q_{n+1}

$$A_i = \int_a^b \varphi_i(x)\, w(x)\, dx$$

Example (Gram-Schmidt) on $[-1,1]$

$$\tilde{q}_0 = 1$$

$$\tilde{q}_1 = x \cdot 1 - \frac{\langle x,1\rangle}{\langle 1,1\rangle} \cdot 1$$

$$= x - \left[\underbrace{\left(\int_{-1}^{1} x\,dx \right)}_{=0} \Big/ \left(\int_{-1}^{1} 1\,dx \right) \right] \cdot 1$$

odd function

$$f(x) = -f(-x)$$

$$\int_{-1}^{1} \text{"odd function"}\,dx = 0$$

$$= x$$

$$q_1 = \frac{\tilde{q}_1}{\|\tilde{q}_1\|} = \frac{x}{\left(\int_{-1}^{1} x^2 \, dx\right)^{\frac{1}{2}}} = \frac{x}{\sqrt{\frac{x^3}{3}\Big|_{-1}^{1}}}$$

$$\|q_1\|^2 = \frac{2}{3}$$

$$= \sqrt{\frac{3}{2}} \; x$$

$$\langle x, x\rangle = \frac{2}{3}$$

odd function

$$\tilde{q}_2 = x \cdot x - \frac{\overset{=0}{\langle x^2, 1\rangle}}{\underbrace{\langle 1, 1\rangle}_{=2}} \, \overset{q_0}{1} - \frac{\overset{=0}{\langle x^2, x\rangle}}{\underbrace{\langle x, x\rangle}_{=\frac{2}{3}}} \cdot \overset{q_1}{x}$$

$$= x^2 - \frac{\frac{2}{3}}{2} \cdot 1 = x^2 - \frac{1}{3}$$

$\tilde{q}_2 = x^2 - \frac{1}{3}$ Roots $x_0 = -\frac{1}{\sqrt{3}}, \; x_1 = \frac{1}{\sqrt{3}}$

(Legendre polynomials)

n = 1

2 roots

Quadrature

$$\int_{-1}^{1} f(x)\, dx = A_0 f\left(-\frac{1}{\sqrt{3}}\right) + A_1 f\left(\frac{1}{\sqrt{3}}\right)$$

by the way

$$\tilde{q}_3 = x^3 - \frac{3}{5} x$$

Now $\int_{-1}^{1} 1\,dx = 2 = A_0 + A_1$

$\int_{-1}^{1} x\,dx = 0 = -\frac{A_0}{\sqrt{3}} + \frac{A_1}{\sqrt{3}}$

$\Rightarrow A_0 = A_1 = 1$

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = 1 \cdot \left(-\frac{1}{\sqrt{3}}\right)^2 + 1\left(\frac{1}{\sqrt{3}}\right)^2$$

$$\int_{-1}^{1} x^3\,dx = 0 = 1\left(-\frac{1}{\sqrt{3}}\right)^3 + 1\left(\frac{1}{\sqrt{3}}\right)^3$$

$\rightarrow$ Gauss Quadrature is exact for degree $2n+1 = 3 = 2\cdot 1 + 1$

Error formula

for some $\xi(x) \in [a,b]$

$$\int_a^b f(x)\,dx - Q(f) = \underbrace{\frac{f^{(2n)}(\xi(x))}{(2n)!} \underbrace{\int_a^b p_n^2(x)\,dx}}_{R(f) =}$$

$$\underbrace{\int_a^b p_n^2(x)\,dx} = \langle p_n, p_n \rangle = \|p_n\|^2$$

$$M_4(f) = \max_{t \in [0,1]} |f^{(4)}(t)|$$

$$w = \frac{1}{\sqrt{x}}$$

$$R(f) \leq c_2 M_4(f)$$

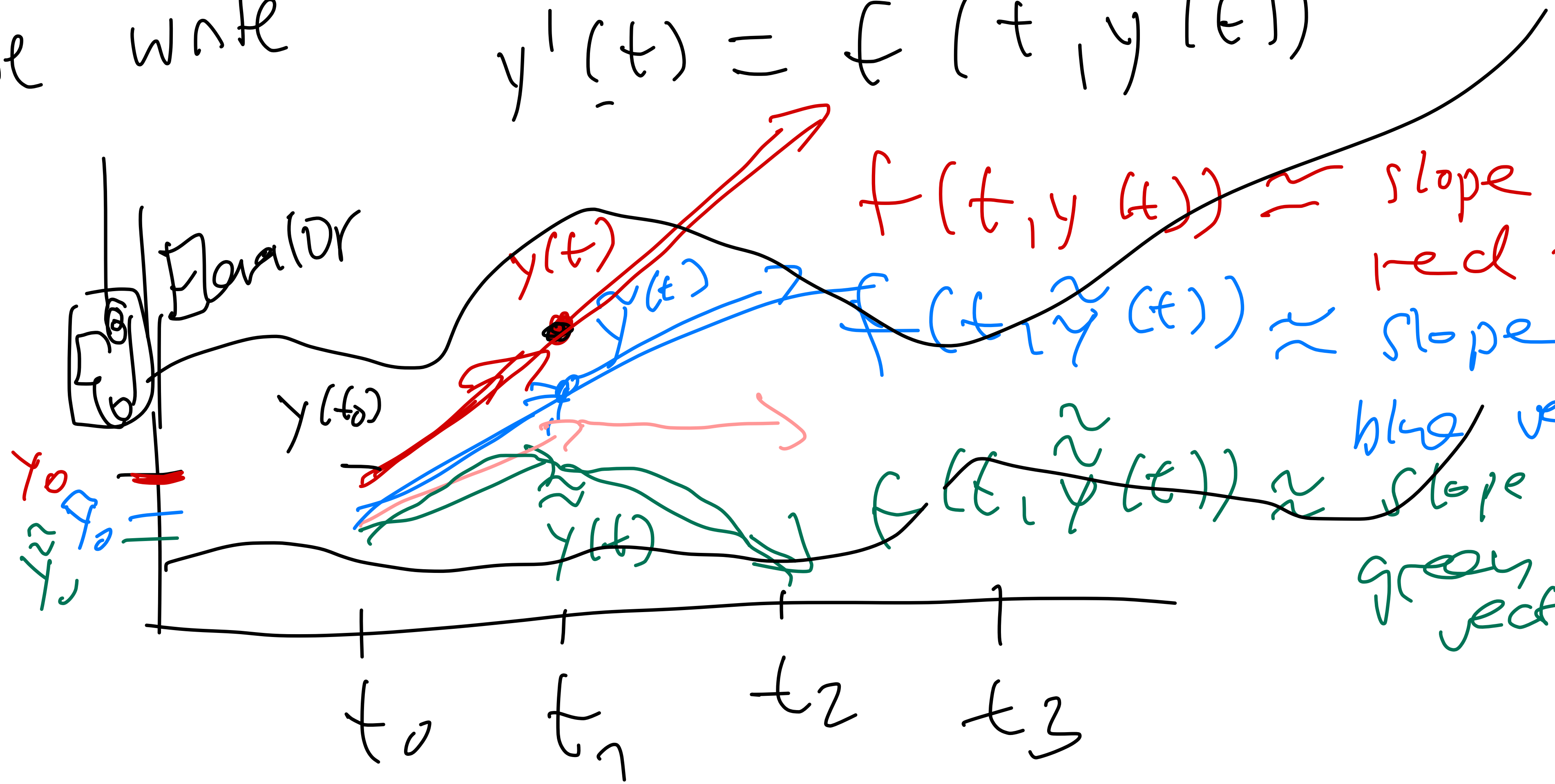
$$c_2 = \frac{\langle p_2, p_2 \rangle_w}{4!}$$

Initial value problems (IVP)

Ordinary differential equations (ODEs)

instead of $y'(x) = F(x, y(x)) \longleftrightarrow y' = F(x,y)$

we write $y'(t) = f(t, y(t))$



$f(t, y(t)) \approx$ slope of red vector

$f(t, \tilde{y}(t)) \approx$ slope of blue vector

$f(t, \tilde{\tilde{y}}(t)) \approx$ slope of green vector problem

$$\begin{cases} y'(t) = f(t, y(t)) \\ y(t_0) = y_0 \in \mathbb{R} \end{cases}$$

initial datum

Assumptions: Existence and uniqueness are understood (e.g. Picard iteration)

"in the ideal world" = "world of idealized physics & mathematics"

I. f is continuous

$$f : [a,b] \times \mathbb{R} \to \mathbb{R}$$

$a \leq t_0$

II. f Lipschitz continuous in the 2nd variable, i.e., for all $t \in [a,b]$, $y_1, y_2 \in \mathbb{R}$

$$|f(t,y_1) - f(t,y_2)| \leq L\,|y_1 - y_2|$$

for some constant $L \geq 0$ which is independent of t, y_1, y_2.

(III. Later: Assume $|y''(t)| \leq M$)

Euler's method (Forward Euler / explicit)

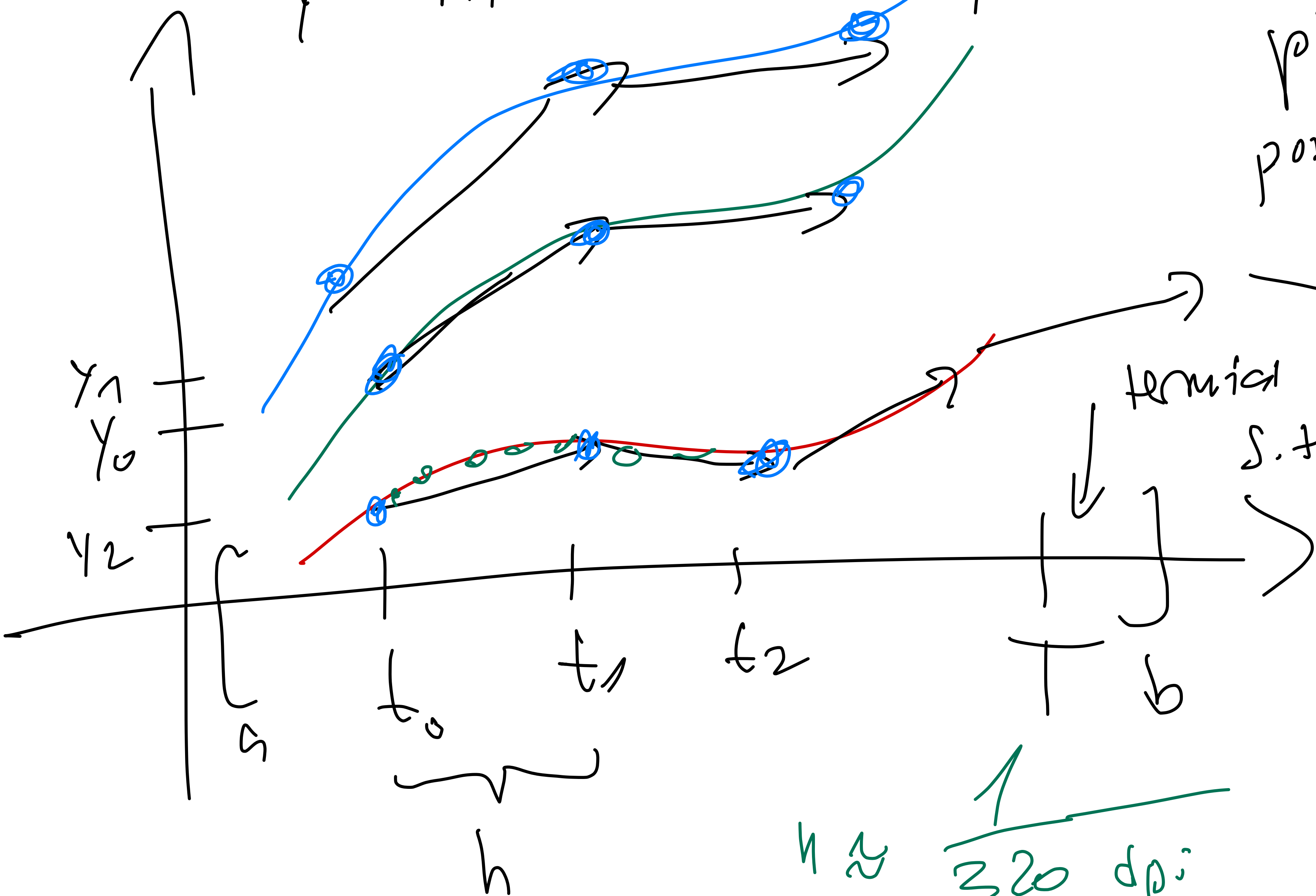
Step size h (constant), $0 < h \leq b-a$.

$$\begin{cases} y_0 = y(t_0) \\ y_{k+1} = y_k + h f(t_k, y_k) \\ \qquad\qquad k = 0, 1, 2, \dots \\ t_{k+1} = t_k + h \end{cases}$$

$y' = \sqrt{|y|}$

$y \to \sqrt{|y|}$ is not Lipschitz

phase portrait



terminal time s.th. $kh \le T - t_0$

$dpi = \frac{dots}{in}$

$h \approx \frac{1}{320\ dpi} = \frac{1\ in}{320\ dots}$

$$y_0 = y(t_0)$$

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

$$k = 0, 1, 2, \dots$$

$$t_{k+1} = t_k + h \implies t_{k+1} - t_k = h$$

$$y_k \approx y(t_k)$$

$$y_{k+1} \approx y(t_{k+1})$$

$$y'(t_k) \approx \frac{y_{k+1} - y_k}{\underbrace{t_{k+1} - t_k}_{=h}} = f(t_k, y_k)$$

$$y' = \frac{1}{t}$$

$$y' = \frac{1}{y}$$

$$y\,dy = 1\,dt$$

$$\frac{y^2}{2} = t + c$$

$$\frac{d}{dt} y = \frac{d\cancel{t}}{t}$$

$$\int dy = \int \frac{1}{t}\, dt$$

$$y = \sqrt{2t+c}$$

$$y = \sqrt{2t+c}$$

$$y = \ln(t) + C$$

$$y = \sqrt{2t + 2c}$$

Error estimates : Taylor $\quad (h = t_{k+1} - t_k)$

$$y(t_{k+1}) = y(t_k) + h\, y'(t_k) + \frac{h^2}{2} y''(\xi_k)$$

$$= y(t_k) + h\, f(t_k, y(t_k)) + \frac{h^2}{2} y''(\xi_k)$$

$\xi_k \in [a, b]$

2 Types of errors

(A) truncation error (local)

(B) global error

$$\boxed{L = \max_{\substack{y \in \mathbb{R} \\ t \in [a,b]}} |\partial_y f|}$$

Notation

$y(t_k)$ exact at $t = t_k$

y_k approximate (outcome of Euler)

local error $O(h)$

Euler $\dfrac{y_{k+1} - y_k}{h} = f(t_k, y_k) + \dfrac{h}{2} y''(\xi_k)$

If f does not depend on time, then

$$y'' = \frac{d}{dt} f = \partial_t f + \underbrace{\partial_y f}_{\leq L} \cdot y'$$

$|y''| \leq L|y'|$

$|y'| \leq |f|$

Global error at fixed $t = t_k$

$$| y(t_k) - y_k | \leq ?$$

uniformly independent of t

local $\lim_{h \to 0} \frac{y_{k+1} - y_k}{h} = y'(t_k) = f(t_k, y(t_k))$

(t_k fixed)

We are going to prove: uniform convergence

global Consider $\lim_{h \to 0} \max_k | y(t_k) - y_k | = 0$?

Theorem

I. f is continuous and Lipschitz in the 2nd variable

II. $|y''| \le M$

III. $y_0 \to y(t_0)$ as $h \to 0$

Euler's method is uniformly convergent, that is $\lim_{h \to 0} \max_k |y(t_k) - y_k| = 0$

Note: for each h we get another set of k's.

k depends on h.

<u>Proof</u> Let $d_j = y(t_j) - y_j$

Taylor & Euler

$$d_{k+1} = d_k + h\Big[\underbrace{\big|f(t_k, y(t_k)) - f(t_k, y_k)\big|}_{\leq L\,|y(t_k) - y_k|}\Big] + \frac{h^2}{2}\underbrace{\boxed{y''(\xi_k)}}_{\leq M}$$

$$|d_{k+1}| \leq |d_k| + hL|d_k| + \frac{h^2}{2}M$$

$$|d_{k+1}| \leq |d_k| + hL|d_k| + \frac{h^2}{2}M$$
$$= (1+hL)|d_k| + \frac{h^2}{2}M.$$

"a priori" estimate

(contrast to "a posteriori")

Lemma Assume that for some $\alpha, \beta > 0$

$$\gamma_{k+1} \leq (1+\alpha)\gamma_k + \beta \quad \forall k$$

then

$$\gamma_n \leq e^{n\alpha}\gamma_0 + \frac{e^{n\alpha}-1}{\alpha}\beta .$$

Later: $\gamma_n = |d_n|$

$\alpha = hL \quad , \quad \beta = \frac{h^2}{2}M$

Proof

$$(1+\alpha) \le 1 + \alpha + \frac{\alpha^2}{2} e^{\xi} \overset{\text{Taylor}}{=} e^{\alpha}$$

$$\left(\text{Taylor}: \quad e^{\alpha} = e^{0} + e^{0} \cdot \alpha + \frac{\alpha^2}{2} e^{\xi} \right)$$

$$\Rightarrow \quad (1+\alpha) \le e^{\alpha}$$

$$\gamma_{k+1} \le (1+\alpha)\gamma_k + \beta$$

$$\begin{aligned} \gamma_n &\le (1+\alpha)\gamma_{n-1} + \beta \\ &\le (1+\alpha)^2 \gamma_{n-2} + \left[(1+\alpha) + 1 \right] \beta \\ &\le (1+\alpha)^n \gamma_0 + \left[\sum_{j=0}^{n-1} (1+\alpha)^j \right] \beta \end{aligned}$$

$$\gamma_n \leq (1+\alpha)^n \gamma_0 + \left[\sum_{j=0}^{n-1} (1+\alpha)^j \right] \beta$$

$$\leq e^{\alpha n} \gamma_0 + \frac{1-(1+\alpha)^n}{1-(1+\alpha)} \beta$$

$$\leq e^{\alpha n} \gamma_0 + \frac{e^{\alpha n} - 1}{\alpha} \beta$$

$$\sum_{i=0}^{n-1} q^i = \frac{1-q^n}{1-q}$$

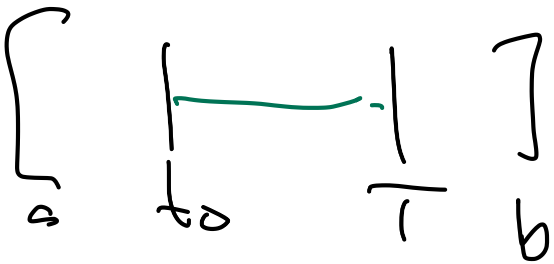
$$|d_{k+1}| \leq |d_k| + hL|d_k| + \frac{h^2}{2}M$$

$$= (1+hL)|d_k| + \frac{h^2}{2}M$$

$$|d_n| \leq e^{nhL}|d_0|$$

$$+ \frac{e^{nhL}-1}{L}\frac{h}{2}M$$

$$|d_k| \le e^{khL}\,|d_0| + \frac{e^{khL}-1}{L}\,\frac{h}{2}\,M$$



$$|y(t_k) - y_k| \le e^{khL}\,\cancel{|y(t_0) - y_0|} + \frac{e^{khL}-1}{L}\,\frac{h}{2}\,M$$

$\to 0$ by Ass.

Fix $T \in [a,b]$ terminal time $T > t_0$ s. th. $kh \le T - t_0$

$$\max_k |d_k| \leq e^{L(T-t_0)} |d_0| + \frac{e^{L(T-t_0)} - 1}{L} \frac{h}{2} M$$

$h \to 0$ method is uniformly convergent global error is $O(h)$

- Heun's methods y_{k+1} y_k
- Adams-Moulton
- Backward Euler
- Linear multistep methods

$$\tilde{y}_{k+1} = y_k + h f(t_k, y_k)$$ Euler / prediction

$$y_{k+1} = y_k + \frac{h}{2}\left[f(t_k, y_k) + f(t_{k+1}, \tilde{y}_{k+1})\right]$$

correction

$$\tilde{y}_{k+1} = y_k + h f(t_k, y_k)$$

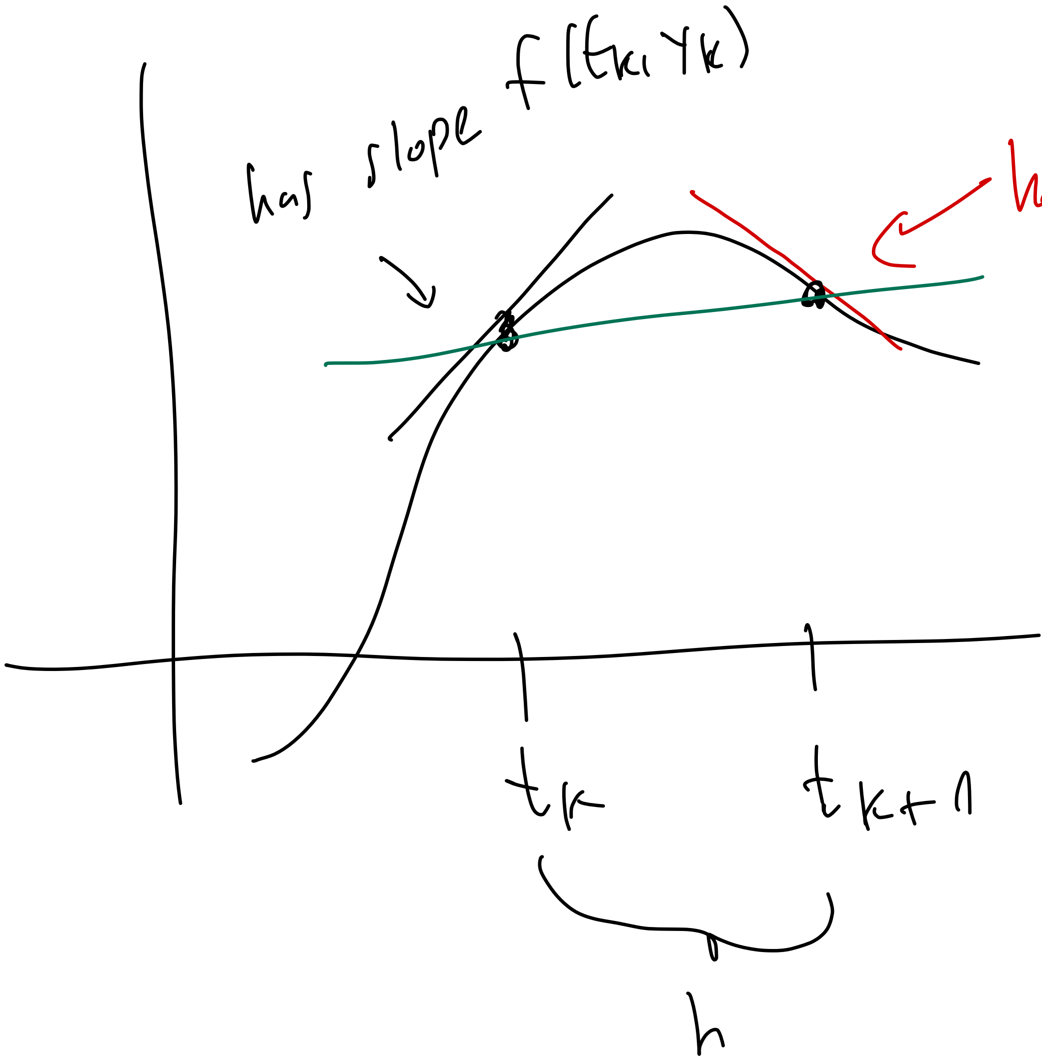
Euler / prediction

$$y_{k+1} = y_k + \frac{h}{2}\left[f(t_k, y_k) + f(t_{k+1}, \tilde{y}_{k+1}) \right]$$

correction

Do not know y_{k+1}

predict as $\tilde{y}_{k+1}$



has slope $f(t_{k+1}, y_{k+1})$

$$\frac{h}{2}\left(f(t_k, y_k) + f(t_{k+1}, \tilde{y}_{k+1}) \right)$$

trapezoid rule

Heun's method is called trapezoid method

$$y_{k+1} = y_k + \frac{h}{2}\left[f(t_k, y_k) + f(t_{k+1}, \boxed{\tilde{y}_{k+1}}) \right]$$

$$\Updownarrow$$

$$y_{k+1}$$

$$y'(t) = f(t, y(t))$$

can be expressed as integral equation

$$\boxed{y(t+h)} = \boxed{y(t)} + \underbrace{\int_t^{t+h} f(s, \boxed{y(s)})\, ds}$$

$$= \frac{h}{2}\left[f(t, y(t)) + f(t+h, \boxed{y(t+h)}) \right] + O(h^3)$$

Quadrature: (Trapezoid)

1. Idea. Heun's method

predict $\tilde{y}_{k+1}$ via Euler (explicit)

2. Idea.

just use

$$\boxed{\Phi(y_{k+1}) = y_{k+1}}$$

Newton's method

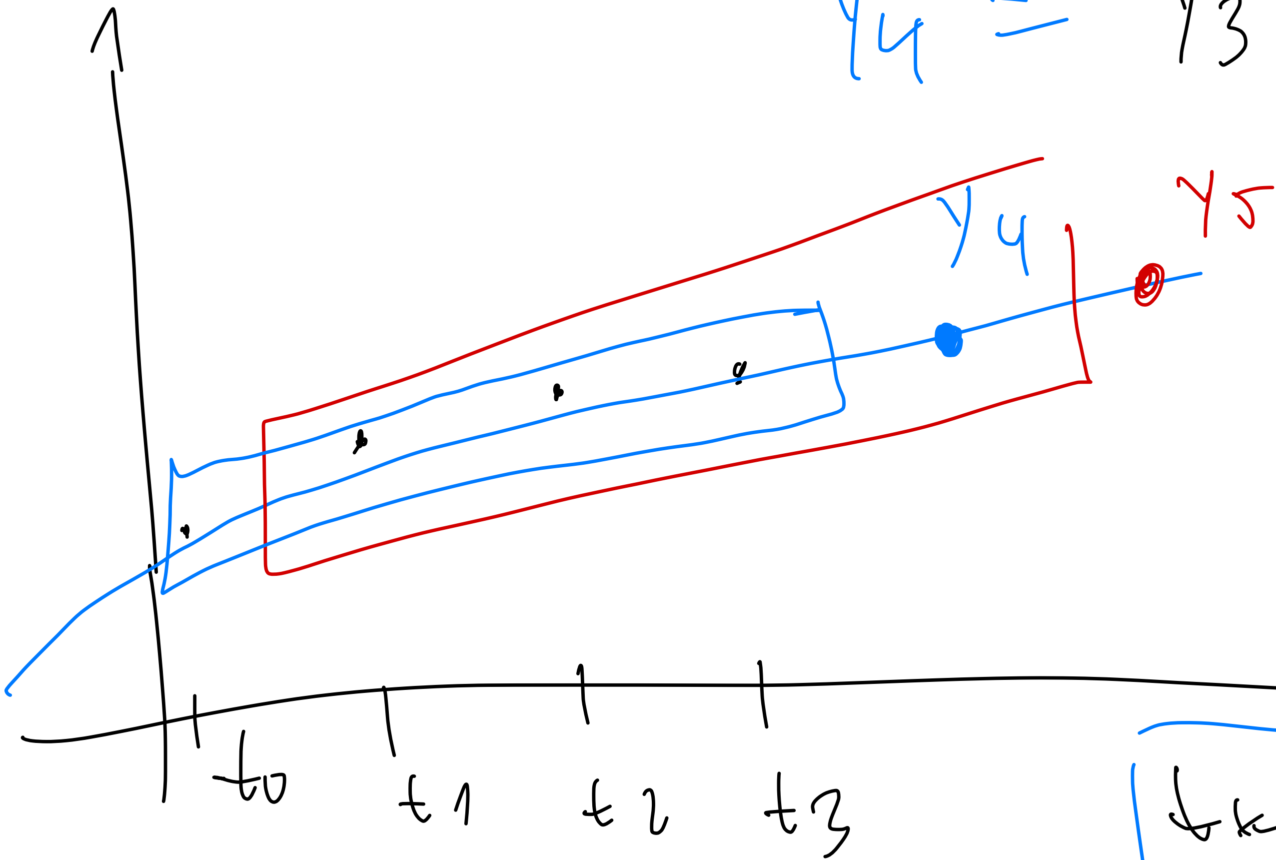
$$y_{k+1} = \underbrace{y_k + \frac{h}{2}\left[f(t_k, y_k) + f(t_{k+1}, y_{k+1})\right]}_{= \Phi(y_{k+1})}$$

(implicit)

Each step requires to solve a linear equation

Multistep methods

$$y_4 = y_3 + h\Big(b_2 f(t_2, y_2) + b_1 f(t_1, y_1) + b_0 f(t_0, y_0)\Big)$$



$$y(t_{k+1}) = y(t_k) + \boxed{\int_{t_k}^{t_{k+1}} f(s, y(s))\, ds}$$

Idea: Quadrature

General definition

$$y' = f(t, y)$$
$$y(t_0) = y_0$$

Linear multi step method

$$h = t_i - t_{i-1}$$

Idea is linear combination of several

y_i and $f(t_i, y_i)$

$$\sum_{j=0}^{s} a_j y_{n+j} = h \sum_{j=0}^{s} b_j f(t_{n+j}, y_{n+j}),$$

where $a_s = 1$.

$$\sum_{j=0}^{s} a_j y_{n+j} = h \sum_{j=0}^{s} b_j f(t_{n+j}, y_{n+j}),$$

where $a_s = 1$.

Coefficients $a_0, \dots, a_{s-1}, b_0, \dots, b_s$,

determine the method.

Euler: $s=1$, $a_1 = 1$, $a_0 = -1$, $b_1 = 0$, $b_0 = 1$

Implicit trapezoid rule

$s = 1$, $a_1 = 1$, $a_0 = -1$, $b_1 = b_0 = \frac{1}{2}$

The method is called explicit if $b_s = 0$, otherwise it is called implicit.
(Need to solve (nonlinear) equations / fixed point problem via Newton's method)

Resume 15:00

Bad example

$y' = -15y, \quad y(0) = 1, \quad t \geq 0$

$y(t) = e^{-15t}$ exact solution

However Euler's method $h = \frac{1}{4}$

oscillates about zero

Implicit trapezoidal rule does not oscillate.

$$y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} f(s, y(s))\, ds$$

Adams - Bashforth (Explicit)

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interpolation nodes $t_k, t_{k-1}, \dots, t_{k-m+1}$

Interpolation polynomial $p_{m-1}(s)$

Quadrature $$y_{k+1} = y_k + \int_{t_k}^{t_{k+1}} p_{m-1}(s)\, ds$$

$$y_{k+1} = y_k + \int_{t_k}^{t_{k+1}} p_{m-1}(s)\,ds$$

$$= y_k + h \sum_{\ell=0}^{m-1} b_\ell \, f(t_{k-\ell}, y_{k-\ell})$$

where $$b_\ell = \frac{1}{h} \int_{t_k}^{t_{k+1}} \left(\prod_{\substack{j=0 \\ j\neq \ell}}^{m-1} \frac{s - t_{k-j}}{t_{k-\ell} - t_{k-j}} \right) ds$$

Quadrature

$m = 1$, $\ell = 0$, $b_0 = 1$

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

Euler

Adams – Bashforth has truncation error of

$$O(h^m).$$

Adams – Moulton (Implicit)

$$y_{k+1} = y_k + h \sum_{\ell=0}^{m} c_\ell \, f(t_{k+1-\ell}, y_{k+1-\ell})$$

where

$$c_\ell = \frac{1}{h} \int_{t_k}^{t_{k+1}} \left(\prod_{\substack{j=0 \\ j \neq \ell}}^{m} \frac{s - t_{k+1-\ell}}{t_{k+1-\ell} - t_{k+1-j}} \right) ds$$

Truncation error $O(h^{m+1})$

$m=0 \quad , \quad \ell=0 \quad , \quad c_0 = 1$

we get

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

Implicit

Backward Euler

$$\sum_{j=0}^{s} a_j y_{n+j} \overset{(*)}{=} h \sum_{j=0}^{s} b_j f(t_{n+j}, y_{n+j}),$$

where $a_s = 1$.

Multistep method is called consistent if the truncation error is $O(h)$ or better.

$\boxed{\text{THM}}$ | Method $(*)$ is consistent iff

$$\sum_{k=0}^{s-1} a_k = -1 \quad \text{and} \quad \sum_{k=0}^{s} b_k = s + \sum_{k=0}^{s-1} k a_k$$

Euler: $b_0 = 1, b_1 = 0$, Backward Euler $b_0 = 0, b_1 = 1$

$s=1$

trapezoidal rule $b_0 = b_1 = \frac{1}{2}$

If, moreover,

$$q \sum_{k=0}^{s} k^{q-1} b_k = s^q + \sum_{k=0}^{s-1} k^q a_k$$

for every $q = 1, \dots, p$.

then the truncation error is $O(h^{p+1})$

Convention: $k^0 = 0$ for $k = 0$

$k^0 = 1$ otherwise

[Hairer, Nørsett, Wanner, Solving ODEs I: Nonstiff problems (2nd ed.), Springer, Berlin (1993)] (theory)

Stability (global error) of multistep methods depends on the convergence of the initial values $y_1, \dots, y_{s-1}$ to y_0 as $h \to 0$

Global error $O(h^p)$ under certain algebraic conditions on a_k and b_k

Example (Good bad example)

$$y_{k+2} - 3y_{k+1} + 2y_k =$$

$$h\left[\frac{13}{12} f(t_{k+2}, y_{k+2}) - \frac{5}{3} f(t_{k+1}, y_{k+1}) - \frac{5}{12} f(t_k, y_k)\right]$$

$\Rightarrow$ method is consistent

$s = 2$, $a_2 = 1$, $a_1 + a_2 = -1$

$$\sum_{k=0}^{s} b_k = s + \sum_{k=0}^{s-1} k a_k \qquad -1 = \frac{13}{12} - \frac{5}{3} - \frac{5}{12} = 2 - 3 = -1$$

Solve $y' = 0$, $y(0) = 1$, exact solution

$f \equiv 0$ ← constantly equal to

$y(t) = 1$, $t \geq 0$

$y \equiv 1$

Let us introduce an error to the initial value, $y_0 = 1$,

$y_1 = 1 + \delta$ $\left(\lim_{\delta \to 0} y_1 = y_0 \right)$

$y_2 = 3y_1 - 2y_0 = 1 + 3\delta$

$y_k = 3y_{k-1} - 2y_{k-2} = 1 + (2^k - 1)\delta$

$\delta \sim 2^{-53} \Rightarrow k = 100 \Rightarrow$ error $\sim 2^{47}$

Example (Effect of rounding error)

Euler (see proof) $|d_k| = |y_k - y(t_k)|$

$$|d_{k+1}| \leq (1+hL)|d_k| + \delta \qquad \delta \approx \frac{h^2}{2}M$$

$M = \max|y''|$

$$\Rightarrow \quad |d_{k+1}| \leq e^{L(T-t_0)}|d_0| + \underbrace{\frac{e^{L(T-t_0)}-1}{hL}\delta}_{\text{dominant term, if } h \text{ is very small.}}$$

initial error / uncertainty

Stability

$$q \sum_{k=0}^{s} k^{q-1} b_k = s^q + \sum_{k=0}^{s-1} k^q a_k$$

$$y_{k+2} - 3y_{k+1} + 2y_k = h\left[\frac{13}{12} f(t_{k+2}, y_{k+2}) - \frac{5}{3} f(t_{k+1}, y_{k+1}) - \frac{5}{12} f(t_k, y_k)\right]$$

Good bad example is not stable though it is consistent.

$q = 1$

$$b_1 + b_2 \overset{!}{=} s + a_1$$

$$-\frac{7}{12} = -\frac{5}{3} + \frac{13}{12} \neq 2 + (-3) = -1$$