- 2nd-order Adams-Bashforth method (AB2) $y' = f(y,t)$

$$y_{n+1} = y_n + h\,\underbrace{y_n'}_{= f(y_n, t_n)} + \frac{1}{2}h^2 \underbrace{y_n''}_{= \frac{y_n' - y_{n-1}'}{h} + O(h)} + \frac{1}{6}h^3 y_n''' + \cdots$$

↑ widely used

$O(h^3)$

$$\rightarrow \quad y_{n+1} = y_n + h y_n' + \frac{1}{2}h\,(y_n' - y_{n-1}') + O(h^3)$$

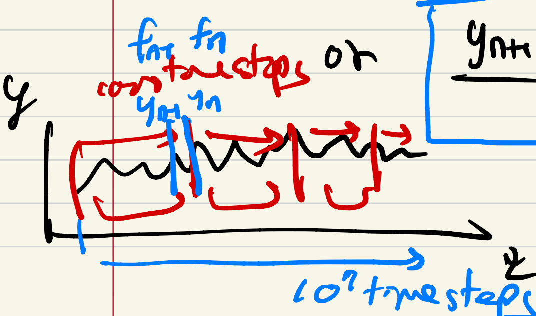
$$= y_n + h f(y_n, t_n) + \frac{1}{2}h\left(f(y_n, t_n) - f(y_{n-1}, t_{n-1})\right) + O(h^3)$$

$$\rightarrow \boxed{y_{n+1} = y_n + \frac{1}{2}h\left(3 f(y_n, t_n) - f(y_{n-1}, t_{n-1})\right)} + O(h^3)$$

AB2

or

$$\boxed{\frac{y_{n+1} - y_n}{h} = \frac{1}{2}\left(3 f_n - f_{n-1}\right)} + O(h^2)$$



globally second-order accurate

explicit

not self-starting ←

$y' = \lambda y$: $y_{n+1} = y_n + \frac{1}{2}h(3\lambda y_n - \lambda y_{n-1})$

$\rightarrow y_{n+1} - (1 + \frac{3}{2}\lambda h) y_n + \frac{1}{2}\lambda h y_{n-1} = 0$

Assume $y_n = \sigma^n y_0 \rightarrow \sigma^2 - (1 + \frac{3}{2}\lambda h)\sigma + \frac{1}{2}\lambda h = 0$

$\rightarrow \sigma = \frac{1}{2}\left[(1 + \frac{3}{2}\lambda h) \pm \sqrt{1 + \lambda h + \frac{9}{4}\lambda^2 h^2}\right]$

$(y_n = c_1 \sigma_1^n + c_2 \sigma_2^n)$ $\quad (\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{3}{68}x^3 + \cdots)$

$\rightarrow \sigma_1 = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \cdots$ $\quad \therefore$ 2nd-order accurate

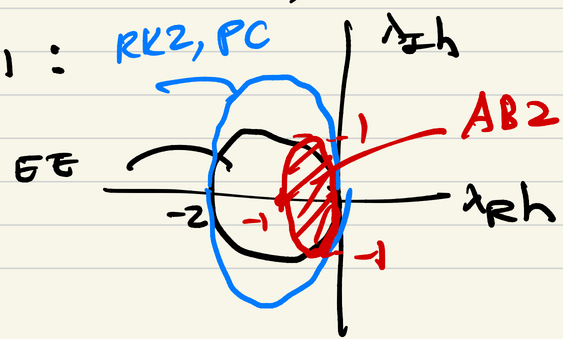
error

$\sigma_2 = \frac{1}{2}\lambda h - \frac{1}{2}\lambda^2 h^2 + \cdots$: spurious root

as $h \to 0$, $\sigma_2 \to 0$ $\therefore$ less dangerous

~~$\sigma_2 = -1 + \lambda h + \cdots$~~

$|\sigma| \le 1$:

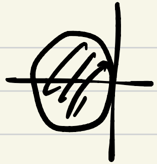


oval shape

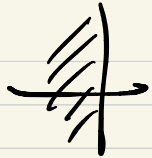
conditionally stable

unstable for $\lambda = i\omega$

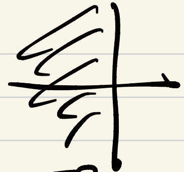
mild instability



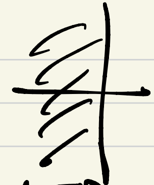
EE
$O(h)$
exp



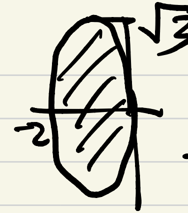
IE
$O(h)$
imp



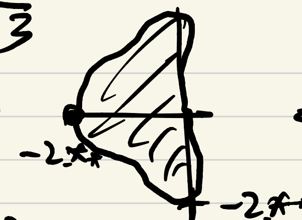
TR
$O(h^2)$
imp



LTR
$O(h^2)$
imp

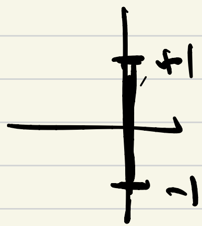


PC, RK2
$O(h^2)$
exp

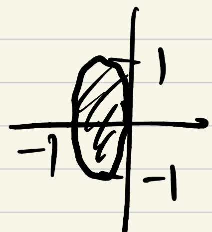


RK4
$O(h^4)$
exp

← Δt can be changed during simulation (in time)

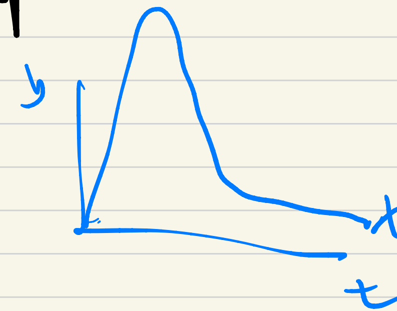


LF
$O(h^2)$
exp



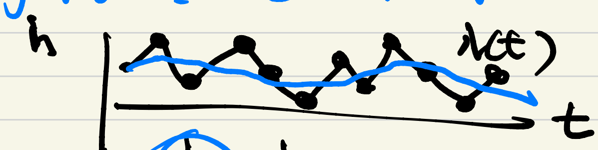
AB2
$O(h^2)$
exp

← Δt cannot be changed (fix Δt)



λ real & negative _ EE $|\lambda h| \le 2$ → For stability $h_{max} = \frac{2}{|\lambda|}$ $\lambda(t)$

$\lambda(t)$



$h = h_{max}$ $= 0.95 \times \frac{2}{|\lambda|}$

$h = h_{old} + (1-\alpha)\, h_{new} \quad (0 < \alpha \le 1)$

4.10 System of first-order ODEs

ex) chemical reaction

$$\begin{cases} \dfrac{dy_1}{dt} = \alpha_{11} y_1^2 + \alpha_{12} y_1 y_2 + \cdots \\ \dfrac{dy_2}{dt} = \alpha_{21} y_1 y_2 + \alpha_{22} y_2^2 + \cdots \\ \cdots\cdots \\ \cdots\cdots \end{cases}$$

a high-order ODE

$\downarrow$

system of 1st-order ODEs

ex) laminar boundary layer flow

(Blasius eq.)

$$f''' + ff'' = 0$$

$$y_1 = f$$

$$y_2 = y_1' = f'$$

$$y_3 = y_2' = f''$$

$$y_3' = f''' = -ff'' = -y_1 y_3$$

$$\Rightarrow \begin{cases} y_1' = y_2 \\ y_2' = y_3 \\ y_3' = -y_1 y_3 \end{cases}$$

From the conceptual point of view, there is only one fundamental difference between numerical sols. of one ODE and of a system of ODEs.

single ODE vs. System of ODEs

$\frac{dy}{dt} = f(y,t)$ $\qquad$ $\frac{dy_i}{dt} = f_i(t, y_1, y_2, \cdots, y_m)$

$i = 1, 2, \cdots, m$

model prob. $\quad \frac{dy}{dt} = \lambda y \qquad\qquad \frac{dy}{dt} = Ay$

Assume that A has a complete set of eigenvectors.

$\rightarrow A = S^{-1}\Lambda S \qquad \Lambda$: eigenvalue matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_m \end{pmatrix}$$

$\frac{dy}{dt} = Ay = S^{-1}\Lambda S y$

$S\frac{dy}{dt} = \Lambda S y \rightarrow \frac{d}{dt}(Sy) = \Lambda(Sy) \qquad u \equiv Sy$

$\rightarrow \dfrac{du}{dt} = \Lambda u \rightarrow \boxed{\dfrac{du_i}{dt} = \lambda_i u_i}$ $\quad i = 1, 2, \cdots, m$

$$EE: \ u_i^n = (1 + \lambda_i h)^n u_i^0$$

for stability : $|1 + \lambda_i h| \le 1 \quad i = 1, 2, \cdots, m$

largest λ $\rightarrow$ smallest h

$\boxed{\dfrac{dy}{dt} = Ay}$ $\quad EE: \ y_{n+1} = y_n + hAy_n = (I + hA)y_n$

$$\rightarrow y_n = (I + hA)^n y_0 \equiv B^n y_0$$

α_i : eigenvalues of B : $|\alpha_i| \le 1$ for stability

λ_i : " of A : $\alpha_i = 1 + h\lambda_i$

$\Rightarrow |1 + h\lambda_i| \le 1$ for stability

for λ real & negative, $-1 \le 1 + h\lambda_i \le 1$

$$\Rightarrow h \le \frac{2}{|\lambda_{max}|}$$

$$\text{Stiffness} \equiv \frac{|\lambda_{max}|}{|\lambda_{min}|} \gg 1 \Rightarrow \text{System is stiff.}$$

Stiffness can arise in physical systems with several degrees of freedom, but with widely different response times.

ex) a system composed of two springs, one very stiff and the other very flexible.

ex) a mixture of chemical species with very different reaction times

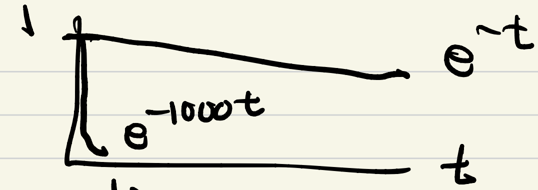
$$\begin{cases} u' = 998u - 1998v \\ v' = -999u - 1999v \end{cases} \qquad u(0) = v(0) = 1$$

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = \underbrace{\begin{pmatrix} 998 & -1998 \\ -999 & -1999 \end{pmatrix}}_{A} \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\det(A - \lambda I) = 0$$

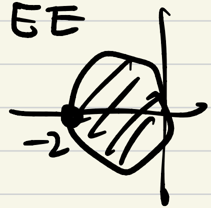
$$\rightarrow \left.\begin{aligned} \lambda_1 &= -1 \\ \lambda_2 &= -1000 \end{aligned}\right\} \text{stiff!}$$

exact sol. $\begin{cases} u = 4e^{-t} - 3e^{-1000t} \\ v = -2e^{-t} + 3e^{-1000t} \end{cases}$



$\lambda_1 = -1,\ \lambda_2 = -1000$: λ real & negative

EE



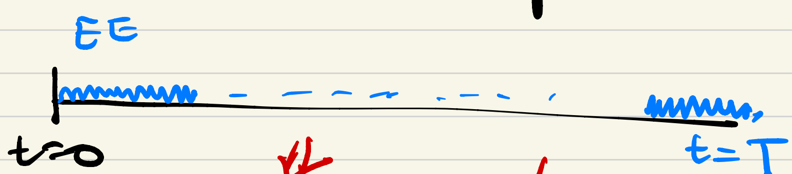
$|\lambda h| \le 2$ to be stable $\rightarrow h \le \dfrac{2}{|\lambda_1|}$ or $\dfrac{2}{|\lambda_2|}$

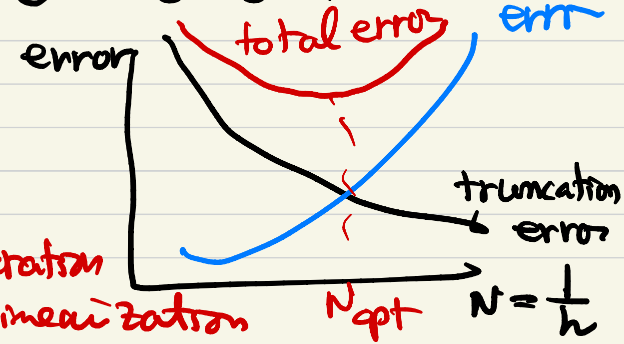
$\dfrac{2}{|\lambda_1|} = 2$, $\quad \dfrac{2}{|\lambda_2|} = 1/500 = h_{max}$

Advance 5 timesteps, $t = 5 \cdot \frac{1}{500} = 0.01$

$\rightarrow e^{-1000t} = 4.5 \times 10^{-5}$, $\quad e^{-t} = 0.99$

take 3500 timesteps to drive e^{-t} to 10^{-3}.





use implicit method!

↳ nonlinear algebraic eqs. → iteration or linearization

$$\frac{dy}{dt} = \underline{f}(y_1, y_2, \cdots, y_m) = \underline{f}(\underline{y})$$

$$\text{TR}: \quad \boxed{\underline{y}_{n+1} - \underline{y}_n = \frac{h}{2}\left[\underline{f}(\underline{y}_{n+1}) + \underline{f}(\underline{y}_n)\right]} + O(h^3)$$

① Linearization

② Iterative method

Midterm : November 8 (Wed) (~Ch. 4) (6pm – 9pm)

eTL.

HW3 : Nov. 15. upload before this saturday on

Nov. 1 : video lecture. uploaded on Oct. 31. watch this video before 11/6

- $\dfrac{d\underline{y}}{dt} = \underline{f}(y_1, y_2, \cdots, y_m) = \underline{f}(\underline{y})$

TR : $\boxed{\underline{y}_{n+1} - \underline{y}_n = \frac{h}{2}[\underline{f}(\underline{y}_{n+1}) + \underline{f}(\underline{y}_n)]} + O(h^3)$

$\approx O(h^3)$

① Linearization

$$f_i(\underline{y}_{n+1}) = f_i(\underline{y}_n) + (y_{1n+1} - y_{1n})\frac{\partial f_i}{\partial y_1}\Big|_n + (y_{2n+1} - y_{2n})\frac{\partial f_i}{\partial y_2}\Big|_n$$

$$+ \cdots + (y_{mn+1} - y_{mn})\frac{\partial f_i}{\partial y_m}\Big|_n + O(h^2), \quad i = 1, 2, \cdots, m$$

neglect

$$\rightarrow \underline{f}(\underline{y}_{n+1}) = \underline{f}(\underline{y}_n) + A(\underline{y}_{n+1} - \underline{y}_n) + O(h^2)$$

w/o losing accuracy

$$A = \begin{pmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_m} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & \cdots & \frac{\partial f_2}{\partial y_m} \\ \vdots & & & \\ \frac{\partial f_m}{\partial y_1} & \frac{\partial f_m}{\partial y_2} & \cdots & \frac{\partial f_m}{\partial y_m} \end{pmatrix}_{t_n}$$

Jacobian matrix

full matrix

$$\Rightarrow y_{n+1} - \underline{y}_n = \frac{h}{2}\left[\underline{f}(\underline{y}_n) + A(\underline{y}_{n+1} - \underline{y}_n) + \underline{f}(\underline{y}_n)\right] + O(h^3)$$

$$\Rightarrow \boxed{(I - \tfrac{h}{2}A)\,\underline{y}_{n+1} = (I - \tfrac{h}{2}A)\,\underline{y}_n + h\,\underline{f}(\underline{y}_n)}$$

linearized TR method

full matrix $\rightarrow$ direct inversion of $(I - \frac{h}{2}A)$ requires $O(m^3)$ operations. ✗

$\rightarrow$ may require iterative methods to solve the eq. at each timestep.

→ linearization may have errors for strongly nonlinear eqs.

② Iterative method w/o linearization

TR : $\underline{y}_{n+1} - \underline{y}_n = \frac{h}{2}[\underline{f}(\underline{y}_{n+1}) + \underline{f}(\underline{y}_n)] + O(h^3)$

Newton iterative method $F(x) = 0$

$$\frac{dF}{dx} = \frac{F^{k+1} - F^k}{x^{k+1} - x^k} \qquad k: \text{iteration index}$$

$$\rightarrow \frac{dF}{dx}^k (x^{k+1} - x^k) = \underbrace{F^{k+1}}_{0} - F^k$$

$$\underline{F} \equiv \underline{y}_{n+1} - \underline{y}_n - \frac{h}{2}[\underline{f}(\underline{y}_{n+1}) + \underline{f}(\underline{y}_n)] = 0$$

$$\rightarrow \left.\frac{\partial F_i}{\partial y_j}\right|^k (y_j^{k+1} - y_j^k) = -F_i^k \qquad i = 1, 2, \cdots, m \qquad k: \text{iteration index}$$

$$= \left.\frac{\partial y_i}{\partial y_j}\right|^k - 0 - \frac{h}{2}\left[\left.\frac{\partial f_i}{\partial y_j}\right|^k + 0\right] = \delta_{ij} - \frac{h}{2}\left.\frac{\partial f_i}{\partial y_j}\right|^k$$

full matrix

$k=0 : \underline{y}^0 = \underline{y}_n \rightarrow [I - \frac{h}{2}A^k](\underline{y}^{k+1} - \underline{y}^k) = -\underline{F}^k = -\underline{y}^k + \underline{y}_n + \frac{h}{2}[\underline{f}(\underline{y}^k) + \underline{f}(\underline{y}_n)]$

Solve this system of eqs. iteratively at each time step.

→ 3 ~ 4 iterations / time step if initial guess y^0 is good. (actually it is good)

* <u>inherent instability</u>

consider $y'' - k^2 y = 0$, $y(0) = 0$, $y'(0) = -k y_0$ $(k > 0)$

→ exact sol. $y = y_0 e^{-kx}$

numerical sol. $y = c_1 e^{-kx} + c_2 e^{+kx}$

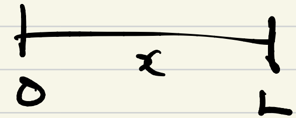
truncation & round-off errors will be exponentially amplified → sol. diverges.

⇒ Inherently unstable.

None of the standard numerical methods will provide the correct sol.!

4.1) Boundary value problems

$$\begin{cases} y'' = f(y, y', x) \\ y(0) = y_0, \quad y(L) = y_L \end{cases}$$



① shooting method
② direct "

① shooting method : boundary value prob
→ initial " "

$y'' = f$ → convert to two 1st-order ODEs

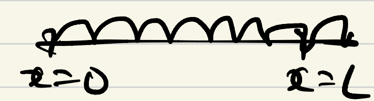
$u = y$

$v = u' = y'$ → $v' = y'' = f$ $\Rightarrow \begin{cases} u' = v \\ v' = f(u, v, x) \end{cases}$ $v(0)$ X

$u(0) = u_0$
$u(L) = u_L$

Guess for $v(0)$ → $v(0) = E$.

→ $u(0)$ & $v(0)$ → integrate up to $x \geq L$.



→ check if $u(L) = y_L$

→ If not, try a different $v(0)$

iteration

Consider a linear eq.

$$y''(x) + A(x)\,y'(x) + B(x)\,y(x) = f(x), \quad y(0) = y_0, \quad y(L) = y_L.$$

two guesses for $y'(0)$ $(= v(0))$ $\xrightarrow[\text{in } x]{\text{integrate}}$ $y_1(x)$ & $y_2(x)$

numerical sols.

Since the gov. eq. is linear, a linear combination of y_1 and y_2 is also a sol.

$\rightarrow$ $y(x) = c_1 y_1(x) + c_2 y_2(x)$

@ $x=0$, $y(0) = c_1 y_1(0) + c_2 y_2(0) = (c_1 + c_2)\,y_0 \rightarrow c_1 + c_2 = 1$

@ $x=L$, $\underset{\overset{\shortparallel}{y_L}}{y(L)} = c_1 \underbrace{y_1(L) + c_2\, y_2(L)}_{\text{num. sols.}}$

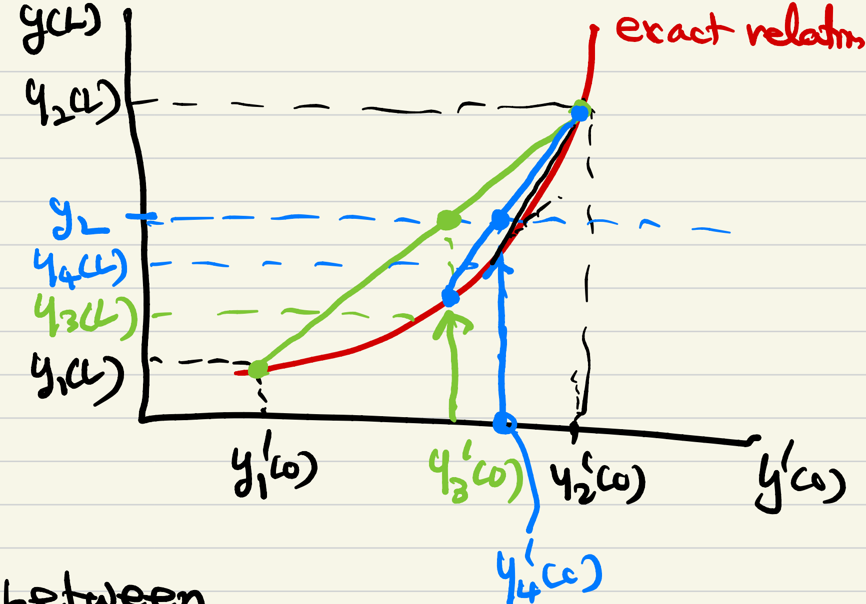
$$\Rightarrow \begin{cases} c_1 = \dfrac{y_L - y_2(L)}{y_1(L) - y_2(L)} \\ c_2 = 1 - c_1 \end{cases}$$

$\rightarrow$ $y(x) = c_1 y_1 + c_2 y_2$: num. sol satisfying $y(0) = y_0$ & $y(L) = y_L$

Consider a nonlinear eq.

$$\begin{cases} y'' = f(y, y', x) \\ y(0) = y_0 \;\&\; \underline{y(L) = y_L} \end{cases}$$

$y'(0) = \bigstar$



Secant method

$y_1'(0) \longrightarrow y_1(L) \neq y_L$

$y_2'(0) \longrightarrow y_2(L) \neq y_L$

$\rightarrow$ form a straight line between

$(y_1'(0), y_1(L))$ & $(y_2'(0), y_2(L))$.

find slope $m = \dfrac{y_1(L) - y_2(L)}{y_1'(0) - y_2'(0)} = \dfrac{y - y_2(L)}{y' - y_2'(0)}$

$$\rightarrow y' = y_2'(0) + \frac{1}{m}\left(y - y_2(L)\right)$$

next guess : $y_3'(0) = y_2'(0) + \frac{1}{m}\left(y_L - y_2(L)\right)$

$\vdots$

$$y'_{k+1}(0) = y'_k(0) + \frac{y'_k(0) - y'_{k-1}(0)}{y_k(L) - y_{k-1}(L)} (y_L - y_k(L))$$

k: iteration index

until finding correct $y'(0)$ that satisfies $y(L) = y_L$.

ex) Blasius eq. $f''' + ff'' = 0$ $f(0), f(L), f'(L)$ given

→ convert to 3 1st-order ODEs

require $f(0)$, $\underset{E_1}{\underset{\shortparallel}{f'(0)}}$, $\underset{E_2}{\underset{\shortparallel}{f''(0)}}$ → $f(L)$, $f'(L)$

HW3

② Direct method