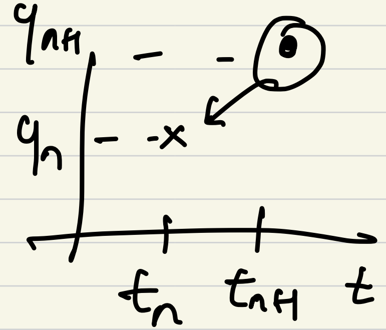
4.4 Implicit Euler or backward Euler method

$$y' = f(y, t) \xrightarrow{\text{IE}} \boxed{\begin{aligned} \frac{y_{n+1} - y_n}{h} &= f(y_{n+1}, t_{n+1}) \\ y_{n+1} &= y_n + h f(y_{n+1}, t_{n+1}) \end{aligned}}$$



cost/timestep is higher than explicit Euler

model prob. $y' = \lambda y$

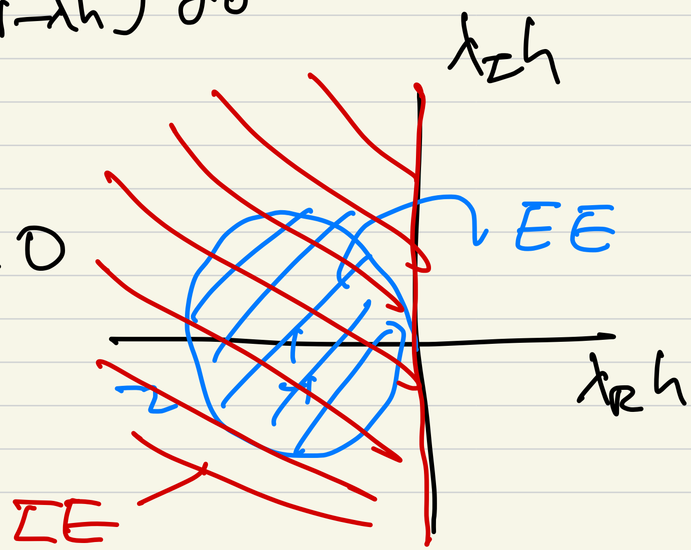
IE : $y_{n+1} = y_n + h\lambda y_{n+1} \rightarrow y_{n+1} = \frac{1}{1-\lambda h} y_n$

$\rightarrow y_n = \left(\frac{1}{1-\lambda h}\right)^n y_0$

$$\sigma = \frac{1}{1-\lambda h} = \frac{1}{1-\lambda_R h - i\lambda_I h}$$

$$|\sigma|^2 = \frac{1}{(1-\lambda_R h)^2 + (\lambda_I h)^2} \leq 1 \quad \text{for } \lambda_R \leq 0$$

$\therefore$ IE is unconditionally stable.
A - stable



4.5 Numerical accuracy

$$\text{IE}: \quad \sigma = \frac{1}{1-\lambda h} = 1 + \lambda h + (\lambda h)^2 + (\lambda h)^3 + \cdots$$

$$\text{exact sol.}: \quad e^{\lambda h} = 1 + \lambda h + \frac{1}{2}(\lambda h)^2 + \frac{1}{6}(\lambda h)^3 + \cdots$$

$$\text{IE}: \quad y_n = \sigma^n y_0 = (1 + \lambda h + (\lambda h)^2 + (\lambda h)^3 + \cdots)^n y_0$$

error

$$\lambda^2 h^2 \cdot n = \lambda^2 h^2 \cdot \frac{T}{h} = O(h)$$

$\therefore$ IE is 2nd-order accurate for one timestep.

$$\boxed{\therefore \text{ IE is 1st-order accurate}}$$

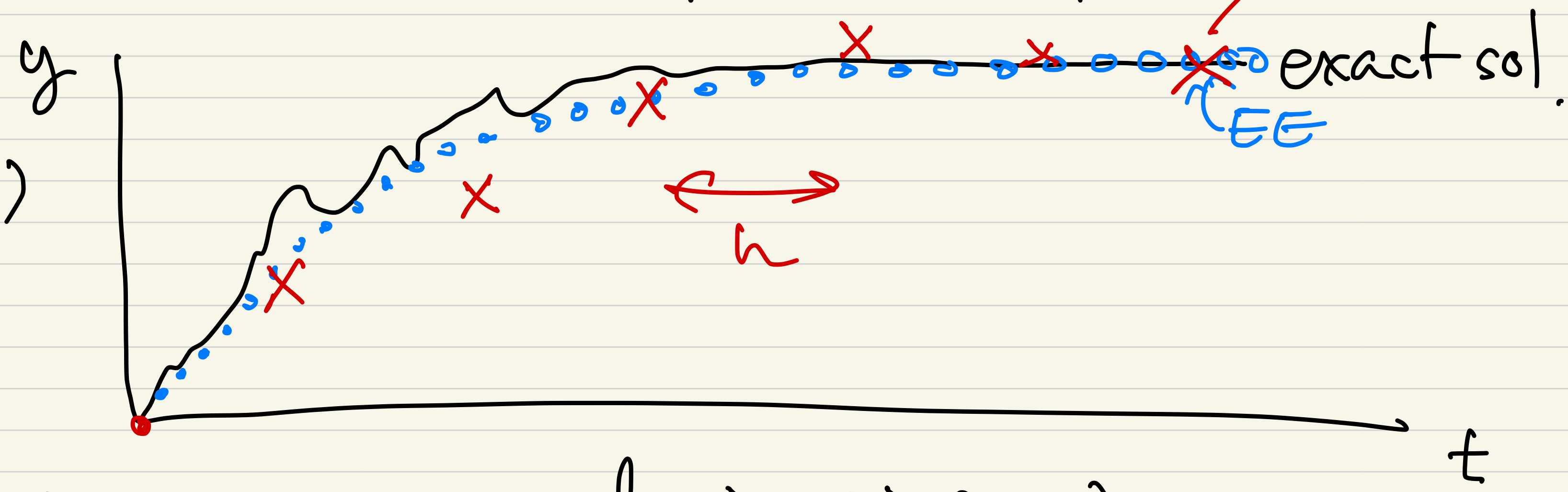
$$\text{IE}: \quad e^{\lambda h} - \sigma = e^{\lambda h} - \frac{1}{1-\lambda h} = -\frac{1}{2}\lambda^2 h^2 + \cdots$$

$$\text{EE}: \quad e^{\lambda h} - \sigma = e^{\lambda h} - (1 + \lambda h) = \frac{1}{2}\lambda^2 h^2 + \cdots$$

$\Rightarrow$ stability is nothing to do with accuracy.

From stability point of view,
our objective is to take largest time step h.

$y' = f(y,t)$



- Accuracy for $\lambda = i\omega$ (purely imaginary)

$y' = \lambda y = i\omega y$

exact sol. $y = y_0 e^{i\omega t} = y_0 (\cos\omega t + i \sin\omega t)$

EE : $y_{n+1} = y_n + \lambda h y_n = (1+\lambda h) y_n$

$\rightarrow y_n = (1+i\omega h)^n y_0 = \sigma^n y_0$, $\sigma = 1 + i\omega h$

exact sol. : amplitude $|e^{i\omega t}| = 1$

EE : amplitude $|\sigma| = \sqrt{1+\omega^2 h^2} > 1$ unstable !

$$\sigma = |\sigma| e^{i\theta}$$

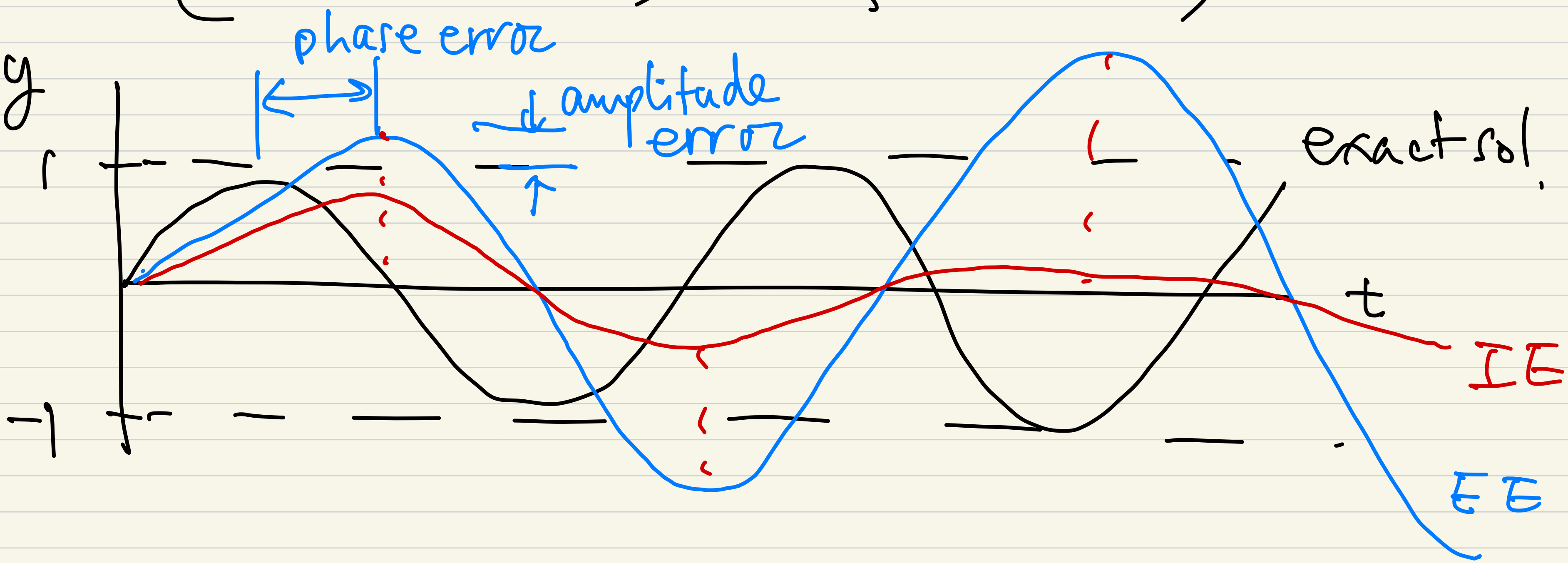
phase $\theta = \tan^{-1}\dfrac{Im(\sigma)}{Re(\sigma)} = \tan^{-1}\dfrac{\omega h}{1} = \tan^{-1}\omega h$

exact sol. : $y = y_0 e^{i\omega t} = y_0 e^{i\omega h n} = y_0 \cdot 1 \cdot e^{i\omega h n}$

EE : $y_n = \sigma^n y_0 = y_0 |\sigma|^n e^{i\theta n}$

phase error $= \omega h - \theta = \omega h - \tan^{-1}\omega h = \frac{1}{3}(\omega h)^3 + \cdots$

$$\left(\tan^{-1}\omega h = \omega h - \frac{1}{3}(\omega h)^3 + \frac{1}{5}(\omega h)^5 + \cdots\right)$$



IE : $y_{n+1} = \frac{1}{1-\lambda h} y_n = \frac{1}{1-i\omega h} y_n \rightarrow y_n = \left(\frac{1}{1-i\omega h}\right)^n y_0$

$\frac{1+i\omega h}{1+\omega^2 h^2}$

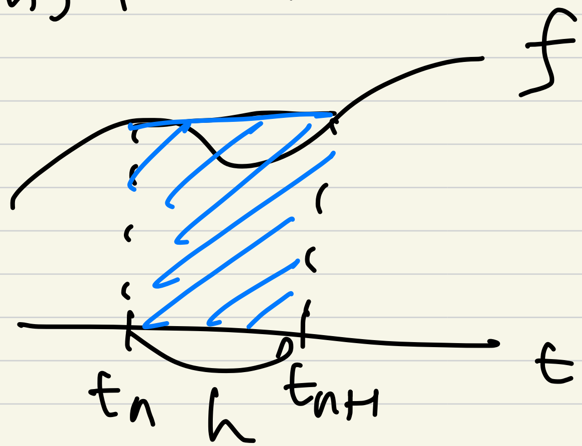
$\sigma = \frac{1}{1-i\omega h} = |\sigma| e^{i\theta}$

$|\sigma|^2 = \frac{1}{1+\omega^2 h^2} < 1$ stable. $\rightarrow$ but decaying sol.

$\theta = \tan^{-1} \frac{\omega h}{1} = \tan^{-1} \omega h$; same as that of EE.

phase error $= \omega h - \theta = \frac{1}{3}(\omega h)^3 + \cdots$

4.6 Trapezoidal method (TR)



$y' = f(y,t)$

$\rightarrow y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f(y,t)\,dt$

$\rightarrow \boxed{y_{n+1} = y_n + \frac{h}{2}\left[f(y_{n+1}, t_{n+1}) + f(y_n, t_n)\right]}$ TR

implicit method

$$y' = f \Rightarrow \frac{y_{n+1} - y_n}{h} = \frac{1}{2}(f_{n+1} + f_n) \quad : \text{TR implicit}$$

$$= f_n \quad : \text{EE explicit}$$

$$= f_{n+1} \quad : \text{IE implicit}$$

When TR is applied to PDE, it is called 'Crank-Nicolson' method.

Model prob. $y' = \lambda y$

TR : $y_{n+1} = y_n + \frac{h}{2}(\lambda y_{n+1} + \lambda y_n)$

$$\rightarrow \quad y_{n+1} = \frac{1 + \lambda h/2}{1 - \lambda h/2} y_n = \sigma y_n$$

$$\frac{1}{1-\varepsilon} = 1 + \varepsilon + \varepsilon^2 + \cdots$$

$$\sigma = \frac{1 + \lambda h/2}{1 - \lambda h/2} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{4}\lambda^3 h^3 + \cdots$$

error

exact sol. $e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \cdots$

$\therefore$ TR is 3rd-order accurate for one timestep
globally $\boxed{\text{2nd-order}}$ accurate.

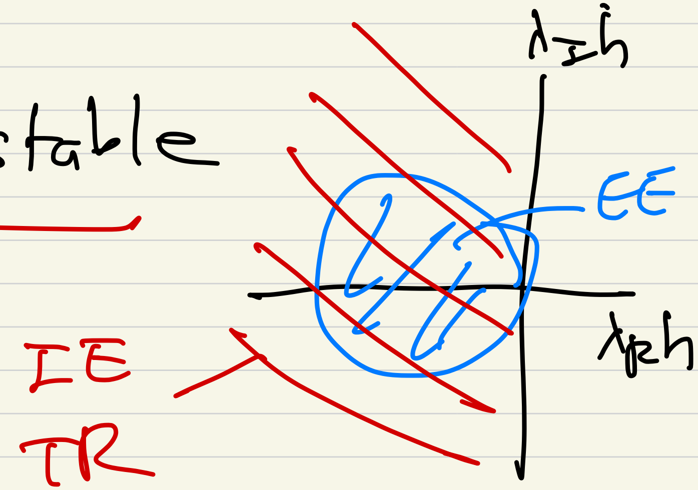
stability : $\lambda = \lambda_R + i\lambda_I$

$$\sigma = \frac{1+\lambda h/2}{1-\lambda h/2} = \frac{1+\lambda_R h/2 + i\lambda_I h/2}{1-\lambda_R h/2 - i\lambda_I h/2} = \frac{A e^{i\theta}}{B e^{i\alpha}} = \frac{A}{B} e^{i(\theta-\alpha)}$$

$$\theta = \tan^{-1} \frac{\frac{1}{2}\lambda_I h}{1+\frac{1}{2}\lambda_R h}, \quad \alpha = \tan^{-1} \frac{-\frac{1}{2}\lambda_I h}{1-\frac{1}{2}\lambda_R h}$$

$$|\sigma| = \frac{A}{B} = \frac{\sqrt{(1+\frac{1}{2}\lambda_R h)^2 + (\frac{1}{2}\lambda_I h)^2}}{\sqrt{(1-\frac{1}{2}\lambda_R h)^2 + (\frac{1}{2}\lambda_I h)^2}} \le 1 \quad \text{for } \lambda_R \le 0$$

$\therefore$ TR is unconditionally stable



For $\lambda_R = 0$, $y' = i\omega y$ $(\lambda = i\omega)$

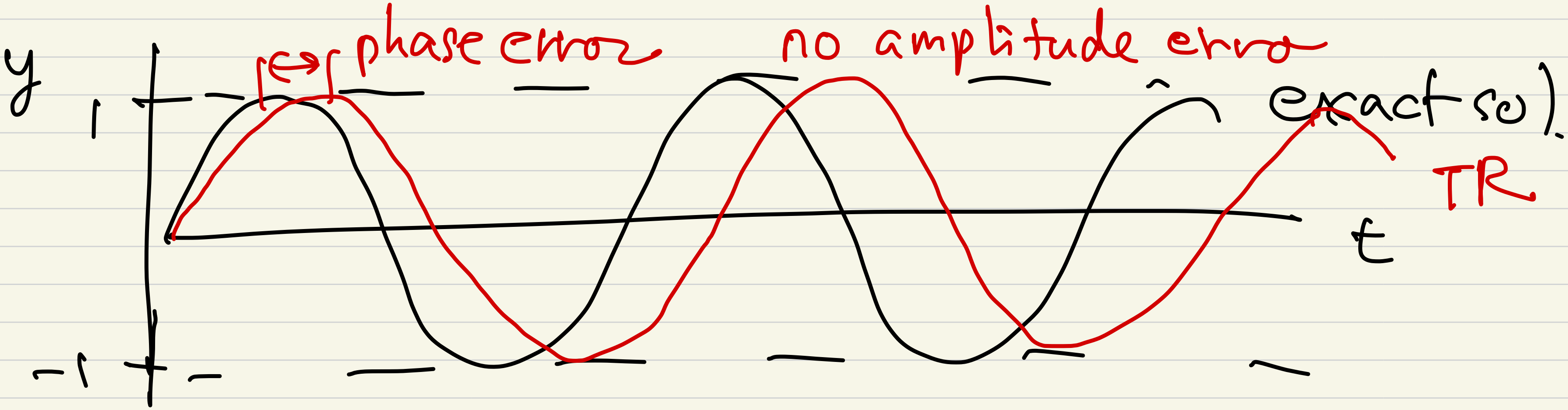
TR : $|\sigma| = 1$ $\therefore$ no amplitude error

phase : $\sigma = \dfrac{1 + i\frac{1}{2}\omega h}{1 - i\frac{1}{2}\omega h} = e^{i\cdot 2\theta}$ $\quad \theta = \tan^{-1}\dfrac{\omega h}{2}$

phase error $= \omega h - 2\tan^{-1}\dfrac{\omega h}{2}$

$$= \omega h - 2\left[\frac{\omega h}{2} - \frac{1}{24}(\omega h)^3 + \cdots\right] = \boxed{\frac{1}{12}}(\omega h)^3 + \cdots$$

four times better than that of EE & IE.



For $\lambda_I = 0$, λ is real & negative ($\lambda_R \leq 0$)

TR: $\sigma = \dfrac{1+\frac{1}{2}\lambda_R h}{1-\frac{1}{2}\lambda_R h} \longrightarrow y_n = \sigma^n y_0$

for large h, $\sigma \rightarrow -1$

σ^n oscillates between -1 and 1, but never blows up.

non-physical

should be careful!

try different numerical method.

$$* \quad y'' + \omega^2 y = 0 \qquad y(0) = y_0, \; y'(0) = 0$$

$$y_1 = y$$

$$y_2 = y_1' \longrightarrow y_2' = y_1'' = -\omega^2 y_1$$

$$\Rightarrow \begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}}_{A} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = S^{-1} \Lambda S \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

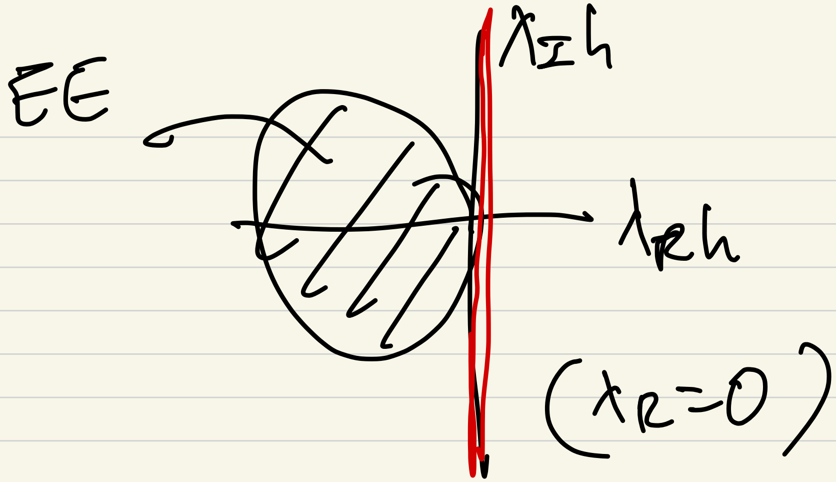
$$\det(A - \lambda I) = \begin{vmatrix} -\lambda & 1 \\ -\omega^2 & -\lambda \end{vmatrix} = 0 \longrightarrow \lambda^2 = -\omega^2$$

$$\lambda = \pm i\omega$$

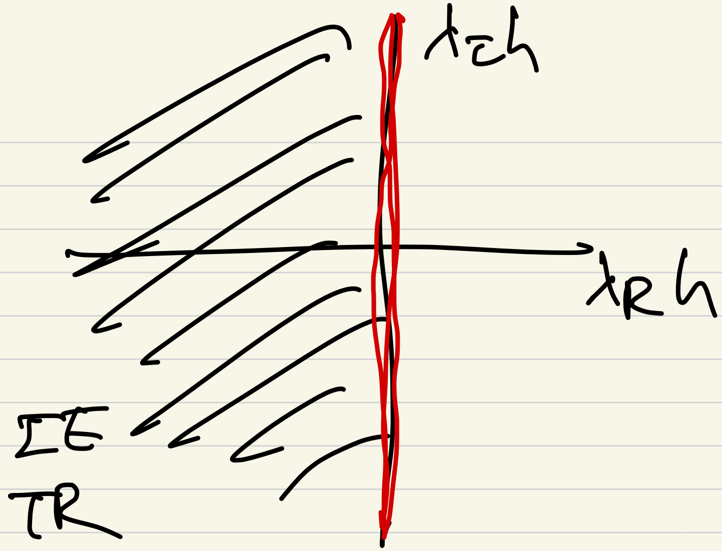
purely imaginary eigenvalues.

$$\underbrace{S \begin{pmatrix} y_1' \\ y_2' \end{pmatrix}} = \Lambda \underbrace{S \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}} \Rightarrow \begin{pmatrix} z_1' \\ z_2' \end{pmatrix} = \Lambda \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \rightarrow \begin{array}{l} z_1' = \lambda_1 z_1 \\ z_2' = \lambda_2 z_2 \end{array}$$

model prob.



EE is unstable



IE & TR are stable

4.7 Linearization for implicit methods

TR: $y' = f(y,t) \longrightarrow y_{n+1} = y_n + \frac{h}{2}\left[\boxed{f(y_{n+1}, t_{n+1})} + f(y_n, t_n)\right] + O(h^3)$

$\Rightarrow$ solve nonlinear algebraic eq.

$\rightarrow$ require iterative solution procedure

$\Rightarrow$ can be avoided by linearization technique.

$$f(y_{n+1}, t_{n+1}) = f(y_n, t_{n+1}) + (y_{n+1} - y_n)\left.\frac{\partial f}{\partial y}\right|_{y_n, t_{n+1}} + \boxed{\frac{1}{2}(y_{n+1} - y_n)^2 \left.\frac{\partial^2 f}{\partial y^2}\right|_{y_n, t_{n+1}} + \cdots}$$

$O(h^3)$ $\quad O(h^2)$

$$h\left.\frac{\partial y}{\partial t}\right|_n + \frac{1}{2}h^2 \left.\frac{\partial^2 y}{\partial t^2}\right|_n + \cdots$$

neglect this term w/o losing any accuracy

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

$$\rightarrow \boxed{y_{n+1} = y_n + \frac{h}{2}\,\frac{f(y_n, t_{n+1}) + f(y_n, t_n)}{1 - \frac{h}{2}\frac{\partial f}{\partial y}\Big|_{y_n, t_{n+1}}}} + O(h^3)$$

linearized TR (LTR)

this formula does not require iteration, while retaining global second-order accuracy.

Linear stability analysis $f = \lambda y$

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

$$= \frac{1 + \frac{1}{2}\lambda h}{1 - \frac{1}{2}\lambda h}\, y_n = \sigma y_n$$

unconditionally stable

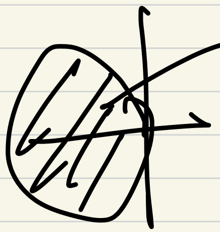
Linearization may lead to some loss of total stability for nonlinear f.

4.8 Runge-Kutta methods (RK)

① Predictor-corrector method (PC)

explicit method

EE

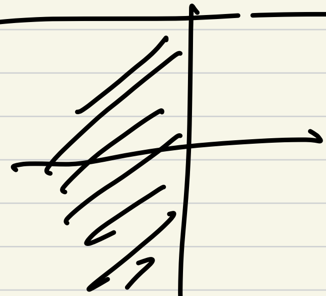


timestep limit

implicit method

IE

TR



iterative sol. → LTR

predictor-corrector method

↑ explicit method

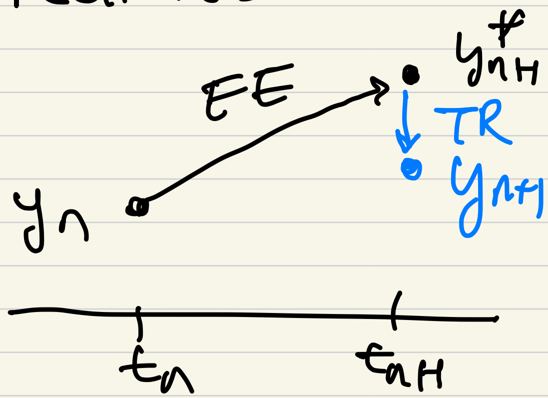
PC & RK methods provide better stability than explicit method like EE but less work/timestep than implicit method.

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

① $y^*_{n+1} = y_n + h f(y_n, t_n)$: EE as predictor

② $y_{n+1} = y_n + \frac{h}{2}\left[f(y^*_{n+1}, t_{n+1}) + f(y_n, t_n) \right]$

TR as corrector



model prob. : $y' = \lambda y$

① $y^*_{n+1} = y_n + h\lambda y_n = (1+\lambda h) y_n$

② $y_{n+1} = y_n + \frac{h}{2}\left[\lambda(1+\lambda h) y_n + \lambda y_n \right]$

$= y_n \left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2 \right) = \sigma y_n$ $O(h^3)$

exact sol. $e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \cdots$

$\therefore$ PC is 2nd-order accurate.

stability : $y_n = \sigma^n y_0$, $\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2$

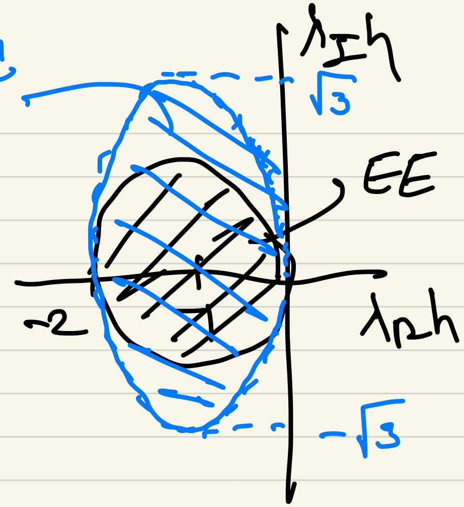
$\Rightarrow |\sigma| \le 1$ to be stable

$$|1+\lambda h+\tfrac{1}{2}\lambda^2h^2| \le 1$$

$$1+\lambda h+\tfrac{1}{2}\lambda^2h^2 = e^{i\theta}$$

find λh for different trials for θ

$\therefore$ PC is conditionally stable



For $\lambda = i\omega$, $\sigma = 1+\lambda h+\tfrac{1}{2}\lambda^2h^2 = 1+i\omega h-\tfrac{1}{2}\omega^2h^2$

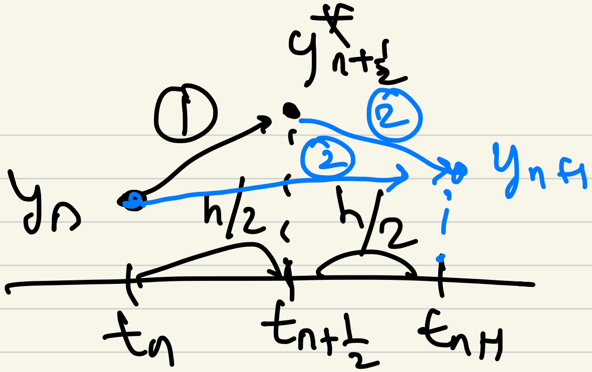
$$|\sigma|^2 = (1-\tfrac{1}{2}\omega^2h^2)^2+(\omega h)^2 = 1+\tfrac{1}{4}\omega^4h^4 > 1$$

unstable for purely imaginary λ.

- Runge-Kutta methods — explicit methods

advantages:
1. good stability properties
2. timestep size can be changed during computation.
3. self starting

- 2nd-order Runge-Kutta method (RK2)



① $y^*_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(y_n, t_n)$: EE

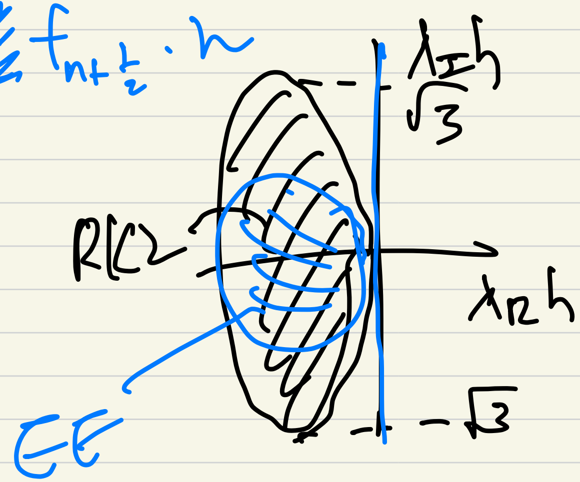
② $y_{n+1} = y_n + h f\left(y^*_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}\right)$: Midpoint rule

$\int_{n}^{n+1} f\,dt = f_{n+\frac{1}{2}} \cdot h$

model prob. $y' = \lambda y$

$\xrightarrow{①②}$ $y_{n+1} = y_n\left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2\right)$

2nd-order accurate



For $\lambda = i\omega$, unstable

$\sigma = 1 + i\omega h - \frac{1}{2}\omega^2 h^2$

$= |\sigma| e^{i\theta}$, $\quad \theta = \tan^{-1} \dfrac{\omega h}{1 - \frac{1}{2}\omega^2 h^2}$

$|\sigma| > 1$

phase error: $\omega h - \theta = -\frac{1}{6}\omega^3 h^3 + \cdots$

- RK4 (most popular scheme) - explicit

$y' = f(y, t)$

① $y^{*}_{n+\frac{1}{2}} = y_n + \frac{h}{2} \underline{f(y_n, t_n)}$

② $y^{**}_{n+\frac{1}{2}} = y_n + \frac{h}{2} \underline{f(y^{*}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}})}$

③ $y^{***}_{n+1} = y_n + h \underline{f(y^{**}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}})}$

④ $y_{n+1} = y_n + h\left[\frac{1}{6} f(y_n, t_n) + \frac{1}{3} f(y^{*}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}) + \frac{1}{3} f(y^{**}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}) + \frac{1}{6} \underline{f(y^{***}_{n+1}, t_{n+1})}\right]$

$\Rightarrow$ requires 4 function evaluations / time step

$\rightarrow$ expensive

$y' = \lambda y$: $y_{n+1} = \sigma y_n$

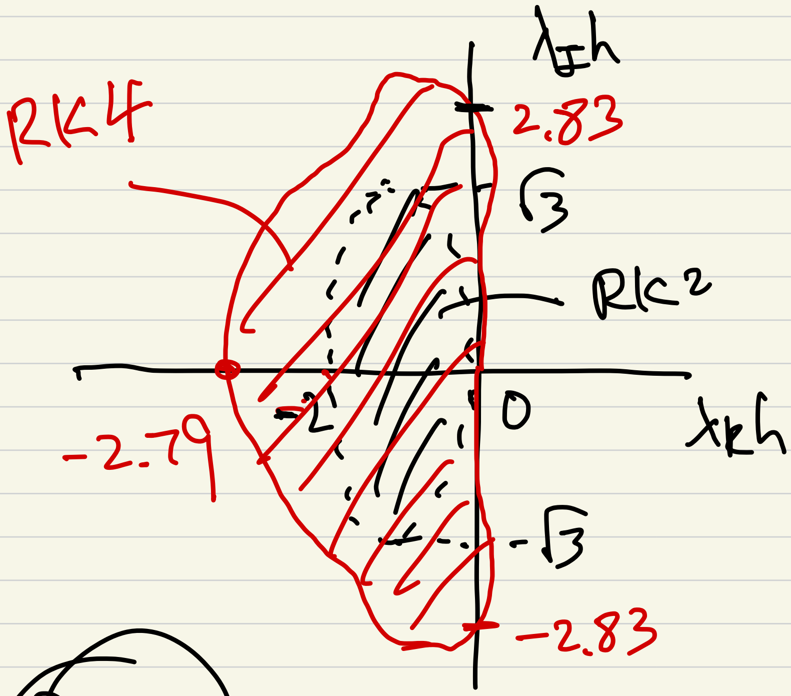
$\rightarrow \sigma = \underline{1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \frac{1}{24}\lambda^4 h^4}$

exact sol. : $e^{\lambda h} = \underline{1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \frac{1}{24}\lambda^4 h^4} + \cdots$

$\therefore$ RK4 is fourth-order accurate.

stability $|\sigma| \leq 1$ to be stable

$$1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \frac{1}{24}\lambda^4 h^4 = e^{i\theta}$$



conditionally stable

for $\lambda = i\omega$, $|\lambda_I h| \leq 2.83$,
conditionally stable

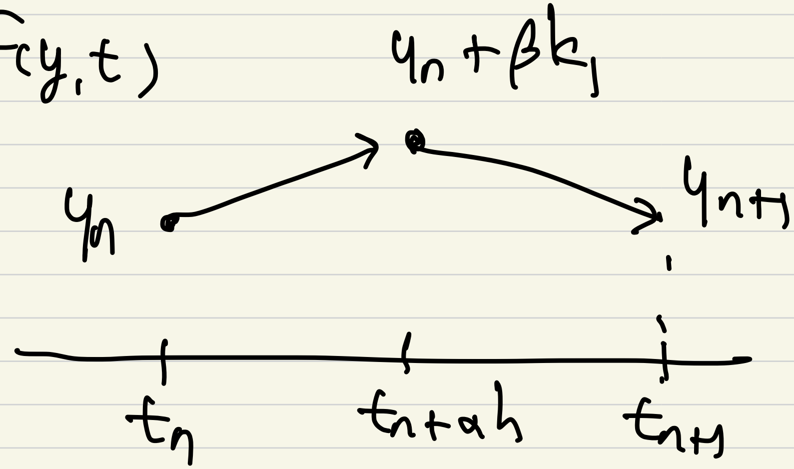
for $\lambda_i = 0$, $|\lambda_R h| \leq 2.79$

RK3

- How to construct RK2?

$y' = f(y, t)$

$$\begin{cases} k_1 = h f(y_n, t_n) \\ k_2 = h f(y_n + \beta k_1, t_n + \alpha h) \\ y_{n+1} = y_n + \gamma_1 k_1 + \gamma_2 k_2 \end{cases}$$



Find $\alpha, \beta, \gamma_1, \gamma_2$ to ensure the highest order of accuracy for the method.

Taylor series for k_2

$$k_2 = h\left[f(y_n, t_n) + \beta k_1 \frac{\partial f}{\partial y}\Big|_n + \alpha h \frac{\partial f}{\partial t}\Big|_n + \cdots \right]$$

$$\rightarrow \quad y_{n+1} = y_n + \gamma_1 h f_n + \gamma_2 h\left(f_n + \beta h f_n f_{y_n} + \alpha h f_{t_n} + \cdots\right)$$

$$= y_n + (\gamma_1+\gamma_2) h f_n + \gamma_2 \beta h^2 f_n f_{y_n} + \gamma_2 \alpha h^2 f_{t_n} + \cdots$$

$$\left(\begin{aligned} y(t_{n+1}) &= y(t_n) + h y'(t_n) + \tfrac{1}{2} h^2 y''(t_n) + \cdots \\ &= y_n + h f_n + \tfrac{1}{2} h^2 \left(f_{t_n} + f_{y_n} f_n\right) + \cdots \end{aligned} \right)$$

match the coeffs.

$$\begin{cases} \gamma_1 + \gamma_2 = 1 \\ \gamma_2 \beta = \frac{1}{2} \\ \gamma_2 \alpha = \frac{1}{2} \end{cases}$$

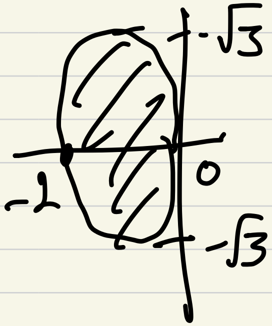
4 unknowns and 3 eqs.

$\downarrow$

α as a free parameter

$$\Rightarrow \gamma_2 = \frac{1}{2\alpha}, \quad \beta = \alpha, \quad \gamma_1 = 1 - \frac{1}{2\alpha}$$

RK2 : $\begin{cases} k_1 = hf(y_n, t_n) \\ k_2 = hf(y_n + \alpha k_1, t_n + \alpha h) \\ y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) k_1 + \frac{1}{2\alpha} k_2 \end{cases}$ $\quad 0 < \alpha < 1$



model prob. $y' = \lambda y \longrightarrow y_{n+1} = y_n \left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2\right)$

2nd-order accurate.

$y' = f(y, t)$: EE, IE, TR, LTR, PC, RK2, RK4