$$y' = f(x) \qquad x \geq x_0 \qquad y(x_0) = y_0$$

$$y(x) = y_0 + \int_{x_0}^{x} f(x')\,dx'$$

$\Rightarrow$ replacing the integral with a finite sum

$\Rightarrow$ quadrature procedure

First let ω be a non-negative function in the interval (a,b) s.t.

$$0 < \int_a^b \omega(x')\,dx' < \infty \qquad \left| \int_a^b \tau^j \omega(\tau)\,d\tau \right| < \infty \quad j = 1, 2, \cdots$$

(ω be the weight function)

$$\int_a^b f(x')\,\omega(x')\,dx' \approx \sum_{j=1}^{\nu} b_j f(c_j) \qquad \text{— } (*)$$

$b_1, b_2, \cdots b_\nu \rightarrow$ quadrature weights

$c_1, c_2, \cdots c_\nu \rightarrow$ quadrature nodes

for every f with p smooth derivatives

$$\left| \int_a^b f(x)\,\omega(x)\,dx - \sum_{j=1}^{\nu} b_j f(c_j) \right| \leq C \max_{a \leq x \leq b} \left| f^{(p)}(x) \right|$$

constant $C > 0$ is independent of f.

$\Rightarrow$ such a quadrature is said of order p.

NOTE: for every $f \in \mathbb{P}_{p-1}$ (real poly of degree $p-1$)

$(*)$ is of order p if it is exact for every $f \in \mathbb{P}_{p-1}$

Lemma: Given any distinct set of nodes $c_1, c_2, \cdots, c_\nu$, it is possible to find a unique set of weights $b_1, b_2, \cdots, b_\nu$ s.t. the quadrature formula is of order $p \geq \nu$

$\Rightarrow$ choose the simplest poly basis: $\{1, t, t^2, \cdots, t^{\nu-1}\}$

$$\Rightarrow \sum_{j=1}^{\nu} b_j c_j^m = \int_a^b \tau^m \omega(\tau) d\tau \quad , \quad m = 0, 1, \cdots, \nu-1$$

$\Rightarrow$ ν equations in the ν unknowns $b_1, b_2, \cdots, b_\nu$

$$[\, V \,] \cdot [\, b \,] = \left[\int_a^b \tau^m \omega(\tau) d\tau \right] \quad \text{—} \quad (**)$$

$\downarrow$

Vandermonde matrix $\Rightarrow$ non singular for distinct nodes

$\Rightarrow$ can always find the weight $[b]$ uniquely

$\Rightarrow$ a unique solution for a quadrature of order $p \geq \nu$ ※

$\boxed{\text{quadrature \& orthogonal polynomial family}}$

Thm:

Let $c_1, c_2, \cdots, c_\nu$ be the zeros of p_ν and let $b_1, b_2, \cdots b_\nu$ be the solution of the Vandermonde system $(**)$.

then the quadrature method $(*)$ is of order 2ν

proof: Let $\hat{p} \in \mathbb{P}_{2\nu-1}$, there exists $q, r \in \mathbb{P}_{\nu-1}$ s.t.

$$\hat{p} = p_\nu q + r$$

$$\int_a^b \hat{p}(\tau) \omega(\tau) d\tau = \langle p_\nu, q \rangle + \int_a^b r(\tau) \omega(\tau) d\tau = \int_a^b r(\tau) \omega(\tau) d\tau$$

moreover $$\sum_{j=1}^{\nu} b_j \hat{p}(c_j) = \cancel{\sum_{j=1}^{\nu} b_j p_\nu(c_j) q(c_j)} + \sum_{j=1}^{\nu} b_j r(c_j)$$

Since $r \in \mathbb{P}_{\nu-1}$, Lemma implies that

$$\int_a^b r(\tau)\,\omega(\tau)\,d\tau = \sum_{j=1}^{\nu} b_j\, r(c_j) = \int_a^b \hat{p}(\tau)\,\omega(\tau)\,d\tau, \quad \hat{p} \in \mathbb{P}_{2\nu-1}$$

thus the quadrature using $c_1, c_2 \ldots c_\nu$ as nodes
$b_1, b_2 \ldots b_\nu$ as weights

is of order $p \geq 2\nu$.

$\Rightarrow$ Quadrature & Explicit RK schemes

$$y' = f(x, y)$$

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(\xi, y(\xi))\,d\xi \qquad x_{n+1} = x_n + h$$

$$= y(x_n) + \int_0^1 f(x_n + h\tau,\ y(x_n + h\tau))\,d\tau$$

$\Rightarrow$ replace the integral by a quadrature

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j\, f(x_n + c_j h,\ y(x_n + c_j h)) \quad n = 0, 1, \ldots$$

$\Rightarrow$ problems : we do not know values of y at nodes $x_n + c_i h$

Explicit RK : updating y_n with a linear combination of

$f(x_n, \tilde{y}_1)$
$f(x_n + hc_2, \tilde{y}_2)$
$\vdots$
$f(x_n + hc_\nu, \tilde{y}_\nu)$

$\xrightarrow{\text{specifically}}$

$$\tilde{y}_1 = y_n$$
$$\tilde{y}_2 = y_n + h a_{2,1} f(x_n, \tilde{y}_1)$$
$$\tilde{y}_3 = y_n + h a_{3,1} f(x_n, \tilde{y}_1) + h a_{3,2} f(x_n + c_2 h, \tilde{y}_2)$$
$$\vdots$$
$$\tilde{y}_\nu = y_n + h \sum_{i=1}^{\nu-1} a_{\nu,i}\, f(x_n + c_i h, \tilde{y}_i)$$

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j f(x_n + c_j h, \tilde{y}_j)$$

is the final update of y_n

RK Matrix : $A = (a_{j,i})_{j,i=1,2,\dots,\nu}$

RK weights : $b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_\nu \end{bmatrix}$

RK nodes $c = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_\nu \end{bmatrix}$

previously for RK2, we have found that

$$c = \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} \begin{array}{c|cc} & & \\ & \frac{1}{2} & \\ \hline & [0 & 1] = b^T \end{array} \qquad \begin{array}{c|cc} 0 & & \\ \frac{2}{3} & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \qquad \begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

in general the matrix A needs to be found specifically for $[b]$ & $[c]$

for RK − p, $p \le 3$, we can use Taylor expansion,
for example, for RK3

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad \begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{8} & \frac{3}{8} \end{array}$$

ERK4:

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

Implicit RK (IRK)

$$\tilde{y}_j = y_n + h \sum_{i=1}^{\nu} a_{j,i} \, f(x_n + c_i h, \tilde{y}_i) \qquad j = 1, 2, \dots, \nu$$

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j \, f(x_n + c_j h, \tilde{y}_j)$$

$\Rightarrow$ for every $\nu \geq 1$ a unique IRK method of order 2ν exists $\Rightarrow$ a natural extension of the Gaussian quadrature formulae of the previous theorem.

Consider

$$\tilde{y}_1 = y_n + \tfrac{1}{4} h \left[f(x_n, \tilde{y}_1) - f(x_n + \tfrac{2}{3} h, \tilde{y}_2) \right]$$

$$\tilde{y}_2 = y_n + \tfrac{1}{12} h \left[3 f(x_n, \tilde{y}_1) + 5 f(x_n + \tfrac{2}{3} h, \tilde{y}_2) \right]$$

$$y_{n+1} = y_n + \tfrac{1}{4} h \left[f(x_n, \tilde{y}_1) + 3 f(x_n + \tfrac{2}{3} h, \tilde{y}_2) \right]$$

$$
\begin{array}{c|cc}
[c] = \begin{bmatrix} 0 \\ \frac{2}{3} \end{bmatrix} & \begin{matrix} \frac{1}{4} \\ \frac{1}{4} \end{matrix} & \begin{matrix} -\frac{1}{4} \\ \frac{5}{12} \end{matrix} \\
\hline
 & \multicolumn{2}{c}{b^T = \begin{bmatrix} \frac{1}{4} & \frac{3}{4} \end{bmatrix}}
\end{array}
$$

Stiff ODE:

$$y' = \Lambda y \qquad y(0) = y_0 \qquad \Lambda = \begin{bmatrix} -100 & 1 \\ 0 & -\frac{1}{10} \end{bmatrix}$$

using Euler's method

$$y_1 = y_0 + h\Lambda y_0 = (I + h\Lambda) y_0$$

$$y_2 = y_1 + h\Lambda y_1 = (I + h\Lambda)^2 y_0$$

$$\vdots$$

$$y_n = (I + h\Lambda)^n y_0 \qquad n = 0, 1, 2, \dots$$

$$\boxed{\begin{aligned} &(VV^{-1} + hVDV^{-1})^n \\ &= V(I + hD)^n V^{-1} = Ve^{Dt}V^{-1} \end{aligned}}$$

$$\Lambda = VDV^{-1} \quad \text{where} \quad V = \begin{bmatrix} 1 & 1 \\ 0 & \frac{999}{10} \end{bmatrix} \qquad D = \begin{bmatrix} -100 & 0 \\ 0 & -\frac{1}{10} \end{bmatrix}$$

$$y(t) = e^{t\Lambda} = Ve^{tD}V^{-1}y_0 \quad \text{for } t \geq 0$$

$$e^{tD} = \begin{bmatrix} e^{-100t} & 0 \\ 0 & e^{-t/10} \end{bmatrix}$$

$$y(t) = e^{-100t} \cdot \underbrace{X_1}_{\text{first eigenvector}} + e^{-t/10} \underbrace{X_2}_{\text{second eigenvector}}$$

for $t \gg 0$ $\quad y(t) \sim e^{-t/10} X_2$

Euler solution :

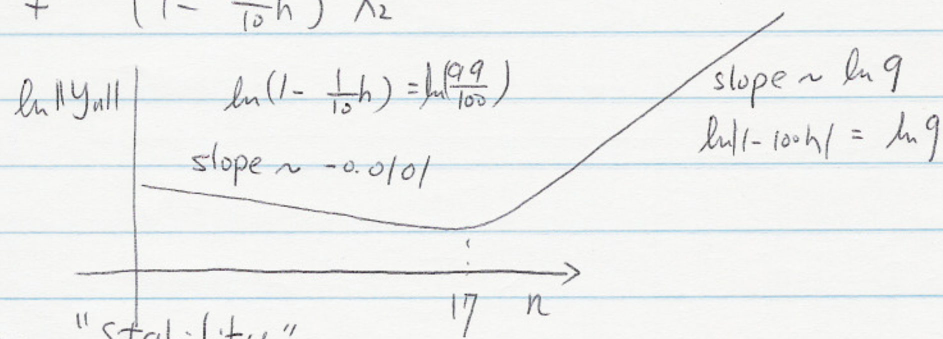
$$y_n = (I + h\Lambda)^n y_0$$

$$= V(I + hD)^n V^{-1} y_0$$

$$(I+hD)^n = \begin{bmatrix} (1-100h)^n & 0 \\ 0 & (1-\frac{1}{10}h)^n \end{bmatrix}$$

$$\therefore \; y_n = (1-100h)^n X_1 + (1-\tfrac{1}{10}h)^n X_2$$

if $y_0 = \begin{bmatrix} 1 \\ \frac{999}{10} \end{bmatrix}$



need to decrease h for "Stability"
not for "accuracy".

What if we use Trapezoidal rule ?

$$y_n = \left(\frac{I + \frac{1}{2}h\Lambda}{I - \frac{1}{2}h\Lambda} \right)^n y_0 \qquad n = 0, 1, \ldots$$

$$y_n = \left(\frac{1-50h}{1+50h}\right)^n X_1 + \left(\frac{1-\frac{1}{20}h}{1+\frac{1}{20}h}\right)^n X_2$$

$$\left|\frac{1-50h}{1+50h}\right| < 1 \qquad \left|\frac{1-\frac{1}{20}h}{1+\frac{1}{20}h}\right| < 1 \qquad \text{for all } h$$

$\Rightarrow$ need to choose h small enough so that error does not lead to numerical instability

Suppose we are considering a given numerical method.
Apply it with a constant step size $h > 0$ to the scalar linear equation

$$y' = \lambda y, \quad t \geq 0, \quad y(0) = 1 \quad \lambda \in \mathbb{C} \quad \text{— } (*)$$

The solution $y(t) = e^{\lambda t}$, $\lim_{t \to \infty} y(t) = 0$ iff $Re(\lambda) < 0$

Definition: linear stability domain D of the underlying numerical method is the set of all numbers $h\lambda \in \mathbb{C}$ s.t. $\lim_{n \to \infty} y_n = 0$.

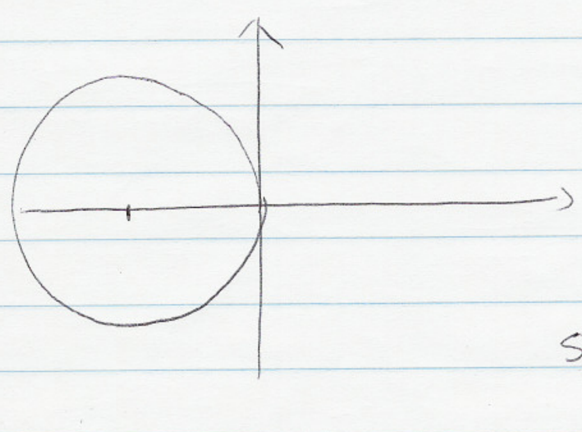
Equivalently: D is the set of all $h\lambda$ for which the correct asymptotic behavior of equation $(*)$ is recovered.

previously we have looked at Euler's method applied to $y' = \lambda y$

$\Rightarrow \quad y_n = (1 + h\lambda)^n, \quad n = 0, 1, \ldots$

$\lim_{n \to \infty} y_n = 0$ iff $|1 + h\lambda| < 1$

$\Rightarrow \quad D_{Euler} = \{ z \in \mathbb{C} : |1 + z| < 1 \}$
is the interior of a complex disc of unit radius centered at $z = -1$



what happens if

$$y' = \Lambda y$$

where Λ is an arbitrary $d \times d$ matrix?

Spectral factorization $\Lambda = VDV^{-1}$

where V is a nonsingular eigenvector matrix &

$D = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_d)$

$$y_n = \sum_{k=1}^{d} (1 + h\lambda_k)^n x_k$$

where x_k is the decomposition of the initial condition in the kth eigenvector

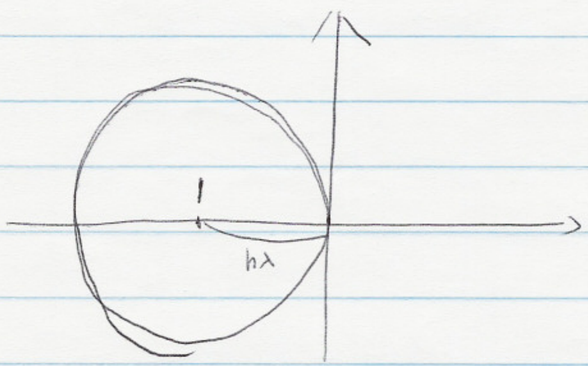
Assuming the exact solution of the linear system is asymptotically stable

$\Rightarrow$ iff $Re(\lambda_k) < 0$ for $k = 1, 2, \cdots, d$.

$$\therefore \quad |1 + h\lambda_k| < 1 \quad \text{for} \quad k = 1, 2, \cdots, d$$

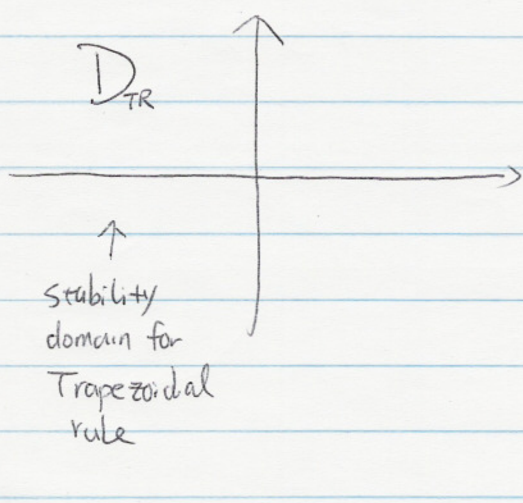
$\Rightarrow$ all the terms $h\lambda_k$ must lie in $\mathcal{D}$

$\Rightarrow$ step-size is determined by the stiffest component of the system



$$\text{maximum step size} = \frac{1}{\max(Re(\lambda_k))}$$

for trapezoidal rule : $\mathcal{D}_{TR} = \left\{ z \in \mathbb{C} \;\middle|\; \left| \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z} \right| < 1 \right\}$



$\Rightarrow$ A method is A-stable if the half-plane : $\{ z \in \mathbb{C} : Re\, z < 0 \}$ belongs to the stability domains.

A-stability of RK

$$\xi_j = y_n + h\lambda \sum_{i=1}^{\nu} a_{j,i}\,\xi_i \qquad j = 1, 2, \ldots, \nu$$

$$\xi \equiv \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_\nu \end{bmatrix} \qquad \mathbb{1} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \in \mathbb{R}^\nu$$

$$\xi = \mathbb{1} \cdot y_n + h\lambda A \xi$$

$$(I - h\lambda A)\xi = \mathbb{1} \cdot y_n$$

$$\xi = \frac{\mathbb{1}}{I - h\lambda A} y_n ,$$

assuming $I - h\lambda A$ is non-singular

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j \xi_j$$

$$= y_n + h \sum_{j=1}^{\nu} b_j \left(\frac{\mathbb{1}}{I - h\lambda A} y_n \right)_j$$

$$= \left[1 + h\lambda\, b^T (I - h\lambda A)^{-1} \mathbb{1} \right] y_n$$

$$z = h\lambda$$

$$(I - zA)^{-1} = \frac{\operatorname{adj}(I - zA)}{\det(I - zA)}$$

$\operatorname{adj}(I - zA) \rightarrow$ determinant of $(\nu-1)\times(\nu-1)$ matrix $\in \mathbb{P}_{\nu-1}$

$\det(I - zA) \rightarrow \in \mathbb{P}_\nu$

$\therefore \; r(z) \equiv 1 + z b^T (I - zA)^{-1} \mathbb{1}$ is a ratio of $\mathbb{P}_\nu / \mathbb{P}_\nu$

stability domains:

$$\mathbb{D} = \{ z \in \mathbb{C} : |r(z)| < 1 \}$$

for the ERK methods, ① $r(z)$ is a polynomial

because $\det(\mathbb{I} - zA) = 1$
$\Downarrow$
lower ~~triangular~~
with unity diagonal
entries.

② $r(0) = 1$ for ERK
and because $r(z)$ is a polynomial,
$r(z)$ must be a constant to
be bound uniformally by value
unity in $\mathbb{C}^-$ (the left plane)
$r(z) = c \in [-1, 1)$
$\Rightarrow$ no A-stability for ERK.

For specific IRK schemes

$$c = \begin{bmatrix} 0 \\ \frac{2}{3} \end{bmatrix} \left| \begin{array}{cc} \frac{1}{4} & -\frac{1}{4} \\ \frac{1}{4} & \frac{5}{12} \\ \hline \multicolumn{2}{c}{b^T = \begin{bmatrix} \frac{1}{4} & \frac{3}{4} \end{bmatrix}} \end{array} \right.$$

$$r(z) = \frac{1 + \frac{1}{3}z}{1 - \frac{2}{3}z + \frac{1}{6}z^2}$$

$|r(z)| < 1$ $\quad z = \rho \cdot e^{i\theta}$
with $\rho > 0$
$|\theta + \pi| < \frac{1}{2}\pi$

$$\left| 1 + \frac{1}{3}\rho e^{i\theta} \right|^2 < \left| 1 - \frac{2}{3}\rho e^{i\theta} + \frac{1}{6}\rho^2 e^{2i\theta} \right|^2$$

$$1 + \frac{2}{3}\rho\cos\theta + \frac{1}{9}\rho^2 < 1 - \frac{4}{3}\rho\cos\theta + \rho^2\left(\frac{1}{3}\cos 2\theta + \frac{4}{9}\right)$$
$$- \frac{2}{3}\rho^3\cos\theta + \frac{1}{36}\rho^4$$

$$\underbrace{2\rho\left(1+\frac{1}{9}\rho^2\right)\cos\theta}_{\text{always less than zero on the left plane}} < \underbrace{\frac{2}{3}\rho^2\cos^2\theta + \frac{1}{36}\rho^4}_{\text{positive definite}}$$

$\Rightarrow$ this IRK is A-stable.

$$r(z) = \frac{1+\frac{1}{3}z}{1-\frac{2}{3}z+\frac{1}{6}z^2}$$

D