Single-step: Theta, IRK, ERK

y_{n+1} is solely determined from y_n

Multi-step: AB, AM, ...

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

$$Y(t_{n+1}) = Y(t_n) + \int_{t_n}^{t_{n+1}} f(t', Y(t'))\,dt'$$

linear polynomial interpolating $g(t) = f(t, y(t))$ at $\{x_n, x_{n-1}\}$ is

$$P_1(t) = \frac{1}{h}\left[(t_n - t)\,g(t_{n-1}) + (t - t_{n-1})\,g(t_n)\right]$$

$$\int_{t_n}^{t_{n+1}} g(t')\,dt' \approx \int_{t_n}^{t_{n+1}} \frac{1}{h}\left[(t_n - t')\,g(t_{n-1}) + (t' - t_{n-1})\,g(t_n)\right] dt'$$

$$= \frac{1}{h}\left[t_n g_{n-1} - t_{n-1} g_n\right] + \frac{t^2}{2h}\Big|_{t_n}^{t_{n+1}} (g_n - g_{n-1})$$

using $t_{n-1} = t_n - h$

$t_{n+1} = t_n + h$

$$\int_{t_n}^{t_{n+1}} g(t')\,dt' \approx \frac{3h}{2} g_n - \frac{h}{2} g_{n-1}$$

$$\therefore \int_{t_n}^{t_{n+1}} g(t')\,dt' = \frac{h}{2}(3g_n - g_{n-1}) + \frac{5}{12} h^3 g''(\xi_n)$$

$$t_{n-1} \le \xi_n \le t_n$$

$$\therefore \boxed{y_{n+1} = y_n + \frac{h}{2}\left[3 \cdot f(t_n, y_n) - f(t_{n-1}, y_{n-1})\right]}$$

Note: need both y_0 & y_1

Note: y_1 can be computed using Euler's method with an accuracy of $O(h^2)$, AB will be of order 2 (global error)
the truncation error is bounded by $O(h^3)$

3rd order AB:

Interpolate $g(x)$ using a quadratic polynomial at t_n, t_{n-1}, t_{n-2}

$$P_2(t) = \frac{(t_n - t)(t_{n-1} - t)}{(t_n - t_{n-2})(t_{n-1} - t_{n-2})} g_{n-2} + \frac{(t_n - t)(t_{n-2} - t)}{(t_n - t_{n-1})(t_{n-2} - t_{n-1})} g_{n-1}$$

$$+ \frac{(t_{n-2} - t)(t_{n-1} - t)}{(t_{n-2} - t_n)(t_{n-1} - t_n)} g_n$$

$$= \frac{1}{2h^2}\Big[(t_n - t)(t_{n-1} - t)\, g_{n-2} - 2(t_n - t)(t_{n-2} - t)\, g_{n-1} + (t_{n-2} - t)(t_{n-1} - t)\, g_n \Big]$$

$$\int_{t_n}^{t_{n+1}} P_2(t')\,dt' = \frac{h}{12}\left[23 g_n - 16 g_{n-1} + 5 g_{n-2}\right]$$

$$\therefore \int_{t_n}^{t_{n+1}} g(t')\,dt' = \frac{h}{12}\left[23 g_n - 16 g_{n-1} + 5 g_{n-2}\right] + \frac{3}{8} h^4 g^{(3)}(\xi_n)$$

$$t_{n-2} \le \xi_n \le t_{n+1}$$

$$\therefore \boxed{y_{n+1} = y_n + \frac{h}{12}\left[23 f(t_n, y_n) - 16 f(t_{n-1}, y_{n-1}) + 5 f(t_{n-2}, y_{n-2})\right] + \frac{3}{8} h^4 Y^{4}(\xi_n)}$$

$q+1$ order AB method : interpolate $f(t, y(t))$ at the nodes :

$$\{t_n, t_{n-1}, \cdots, t_{n-q}\}$$

$q+1$ order AM method : interpolate $f(t, y(t))$ at the nodes

$$\{t_{n+1}, t_n, t_{n-1}, \cdots, t_{n-q+1}\}$$

2nd order AM method :

$P_1(t)$ interpolates f at $\{t_{n+1}, t_n\}$

$$P_1(t) = \frac{1}{h}\left[(t_{n+1} - t) g_n + (t - t_n) g_{n+1}\right]$$

$$\int_{t_n}^{t_{n+1}} f(t', y(t'))\, dt' = \int_{t_n}^{t_{n+1}} g(t')\, dt' \approx \int_{t_n}^{t_{n+1}} P_1(t')\, dt'$$

$$= \frac{h}{2}(g_{n+1} + g_n)$$

$$\therefore \boxed{y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right]} - \frac{h^3}{12} Y'''(\xi_n)$$

2nd order AM $\longrightarrow$ Trapezoidal method

More generally, AB method can be derived using Newton backward difference formula:

$$P_p(t) = Y_n' + \frac{(t-t_n)}{h} \nabla Y_n' + \frac{(t-t_n)(t-t_{n-1})}{2!\, h^2} \nabla^2 Y_n' + \cdots$$

$$+ \frac{(t-t_n)(t-t_{n-1}) \cdots (t-t_{n-p+1})}{p!\, h^p} \nabla^p Y_n'$$

$$\nabla Y_n' \equiv Y'(t_n) - Y'(t_{n-1})$$

$$\int_{t_n}^{t_{n+1}} P_p(t')\, dt' = h Y_n' + \sum_{j=1}^{p} \frac{1}{j!\, h^j} \nabla^j Y_n' \int_{t_n}^{t_{n+1}} (t'-t_n)(t'-t_{n-1}) \cdots (t'-t_{n+1-j})\, dt'$$

$$= h \sum_{j=0}^{p} \gamma_j \nabla^j Y_n'$$

$$\gamma_0 = 1 \quad \gamma_1 = \frac{1}{2} \quad \gamma_2 = \frac{5}{12} \quad \gamma_3 = \frac{3}{8} \quad \cdots$$

Truncation error

$$Y'(t, y(t)) = P_p(t) + E_p(t)$$

$$E_p(t) = (t - X_{n-p}) \cdots (t - X_n)\, Y'[X_{n-p}, \cdots, X_n, t]$$

$$= \frac{(t - X_{n-p}) \cdots (t - X_n)}{(p+1)!} Y^{(p+2)}(\xi)$$

$$t_{n-p} \le \xi \le t_{n+1}$$

$$T_n(Y) = \int_{t_n}^{t_{n+1}} E_p(t')\,dt'$$

$$= \frac{Y^{(p+2)}(\xi)}{(p+1)!} \int_{t_n}^{t_{n+1}} (t'-t_{n-p})(t'-t_{n-p+1})\cdots(t'-t_n)\,dt'$$

$$= Y^{(p+2)}(\xi)\; h^{p+2}\; \gamma_{p+1} \qquad t_{n-p} \le \xi \le t_{n+1}$$

recall that $\quad |(t-t_{n-p})(t-t_{n-p+1})\cdots(t-t_n)| \le p!\,h^{p+1}$

for $t_{n-p} \le t \le t_n$ and equally spaced nodes.

$\therefore \quad p=0 \qquad y_{n+1} = y_n + hY_n' + \frac{1}{2}h^2 Y''(\xi_n)$

$p=1 \qquad y_{n+1} = y_n + \frac{h}{2}\left[3Y_n' - Y_{n-1}'\right] + \frac{5}{12}h^3 Y^{(3)}(\xi_n)$

$p=2 \qquad y_{n+1} = y_n + \frac{h}{12}\left[23Y_n' - 16Y_{n-1}' + 5Y_{n-2}'\right] + \frac{3}{8}h^4 Y^{(4)}(\xi_n)$

$\vdots$

$\Longrightarrow$

Definition: A numerical method

$$y_{n+1} = \sum_{j=0}^{p} a_j y_{n-j} + h\sum_{j=-1}^{p} b_j f(t_{n-j}, y_{n-j}) \qquad t_{p+1} \le t_{n+1} \le b$$

is consistent if

$$\frac{1}{h} \max_{t_p \le t_n \le b} |T_n(Y)| \to 0 \quad \text{as } h \to 0$$

for all functions Y continuously differentiable on $[a,b]$.

Note: Explicit methods $b_{-1} = 0$

Implicit methods: $b_{-1} \neq 0$

Truncation error
$$T_n(Y) \equiv Y(t_{n+1}) - \left[\sum_{j=0}^{p} a_j Y(t_{n-j}) + h \sum_{j=-1}^{p} b_j Y'(t_{n-j}) \right]$$

$n \geq p$.

Note:
$$T_n(\alpha Y + \beta W) = \alpha T_n(Y) + \beta T_n(W)$$

Assuming $Y(x)$ is $m+1$ times continuously differentiable

$$Y(x) = \sum_{i=0}^{m} \frac{1}{i!} (t-t_n)^i Y^{(i)}(t_n) + R_{m+1}(t)$$

$$\therefore T_n(Y) = \sum_{i=0}^{m} \frac{1}{i!} Y^{(i)}(t_n) \cdot T_n((t-t_n)^i) + T_n(R_{m+1}(t))$$

$i=0$ $\quad T_n(1) = 1 - \sum_{j=0}^{p} a_j \equiv C_0$

$i \geq 1$, $\quad T_n((t-t_n)^i)$

$$\equiv (t_{n+1}-t_n)^i - \left[\sum_{j=0}^{p} a_j (t_{n-j}-t_n)^i + h \sum_{j=-1}^{p} b_j\, i\, (t_{n-j}-t_n)^{i-1} \right]$$

$$= h^i - h^i \sum_{j=0}^{p} a_j (-j)^i - h^i \sum_{j=-1}^{p} b_j\, i\, (-j)^{i-1}$$

$$= h^i \cdot \left[1 - \sum_{j=0}^{p} a_j (-j)^i - \sum_{j=-1}^{p} i\, b_j (-j)^{i-1} \right] \equiv h^i C_i$$

To satisfy the condition that the truncation error

$$\frac{1}{h} \max_{t_a \le t_n \le t_b} |T_n(Y)| \to 0 \quad \text{as} \quad h \to 0$$

$T_n(Y)$ must be at least $O(h^2)$

since

$$T_n(Y) = \sum_{i=0}^{m} \frac{C_i}{i!} h^i Y^{(i)}(t_n) + T_n(R_{m+1})$$

$$C_0 = 0 \implies 1 - \sum_{j=0}^{p} a_j = 0$$

$$C_1 = 0 \implies 1 - \left[\sum_{j=0}^{p} (-j)^i a_j + i \sum_{j=-1}^{p} (-j)^{i-1} b_j \right] = 0$$

$\implies$ consistency condition for multi-step methods

if $Y(t)$ is $m+1$ times continuously differentiable
convergence condition requires $\frac{1}{h} T_n(Y) \to O(h^m)$

$\implies C_i = 0, \quad i = 2, 3, \ldots, m$

$\therefore$ the largest value of m s.t. $\frac{1}{h} T_n(Y) = O(h^m)$ holds is called the 'order' or 'order of convergence' of the method. For example, $\frac{1}{h} T_n(Y) \sim O(h^2)$ for 2nd order AB method.

Determine the order of the following two-step method:

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

Sol:

$$y_{n+2} = y_n + y_n' \cdot 2h + y_n'' \frac{(2h)^2}{2!} + y_n^{(3)} \frac{(2h)^3}{3!} + \cdots$$

$$y_{n+2}' = y_n' + y_n^{(2)} \cdot 2h + y_n^{(3)} \frac{(2h)^2}{2!} + y_n^{(4)} \frac{(2h)^3}{3!} + \cdots$$

$$y_{n+1}' = \cancel{y_{n+1}}\, y_n' + y_n^{(2)} \cdot h + y_n^{(3)} \frac{h^2}{2!} + y_n^{(4)} \frac{h^3}{3!}$$

$$+)\ y_n' = y_n'$$

$$y_n' + y_{n+1}' + y_{n+2}' = 3y_n' + 3h\, y_n^{(2)} + \frac{5h^2}{2} y_n^{(3)} + \frac{9h^3}{6!} y_n^{(4)} + \cdots$$

$$y_{n+2} - y_n - \frac{2}{3}h\left[y_{n+2}' + y_{n+1}' + y_n' \right]$$

$$= y_n' \cdot 2h + y_n^{(2)} \frac{(2h)^2}{2!} + y_n^{(3)} \frac{(2h)^3}{3!} + \cdots$$

$$- \frac{2h}{3}\left[3y_n' + 3h y_n^{(2)} + \frac{5h^2}{2} y_n^{(3)} + \frac{9h^3}{6!} y_n^{(4)} \right]$$

$$= \left(\frac{8h^3}{3!} - \frac{10h^3}{6} \right) y_n^3 + O(h^4)$$

$$= -\frac{h^3}{3} y_n^3 + O(h^4) \longrightarrow \text{the two-step method is 2 order}$$

$\boxed{\text{A-stable?}}$

$$\sum_{m=0}^{s} a_m y_{n+m} = h\lambda \sum_{m=0}^{s} b_m y_{n+m} \qquad n=0,1,\cdots$$

$$\sum_{m=0}^{s} (a_m - h\lambda b_m) y_{n+m} = 0$$

$$\sum_{m=0}^{s} (a_m - h\lambda b_m) \frac{y_{n+m}}{y_n} = 0$$

$$y_{n+m}/y_n = \omega^m$$

$$\sum_{m=0}^{s} (a_m - h\lambda b_m)\, \omega^m = 0 \quad \text{——} (*) \text{ characteristic equation}$$

A-stability for multi-step method

all roots of equation —— (*)

$|\omega_i(h\lambda)| < 1 \quad i=1,2,\cdots,q(z) \quad$ for $z \in \mathbb{C}^- \rightarrow$ root condition

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multistep method

$$\sum_{m=0}^{s} a_m y_{n+m} = h \sum_{m=0}^{s} b_m f(t_{n+m}, y_{n+m}) \quad n=0,1,\cdots$$

is a convergent numerical method if the solution

$\{y_n\}$ ~~is~~ converges to $Y(t)$ as

$$\max_{t_0 \le t_n \le b} |Y(t_n) - y_n| \to 0 \quad \text{as } h \to 0$$

convergence $\Longleftrightarrow$ Root condition $\Longleftrightarrow$ stability

Example: 2nd order A-B method

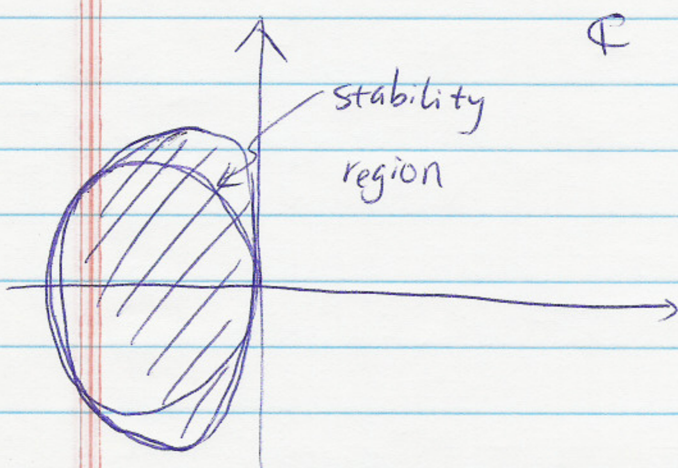
$$y_{n+1} = y_n + \frac{h}{2}\left[3y_n' - y_{n-1}' \right]$$

characteristic equation is applying AB 2nd order to the linear equation. $y' = \lambda y$

$\therefore$ get $r^2 - \left(1 + \frac{3h\lambda}{2}\right) y_n + \frac{1}{2}h\lambda = 0$

$$r_0 = \frac{1}{2}\left\{ 1 + \frac{3}{2}h\lambda + \sqrt{1 + h\lambda + \frac{9}{4}h^2\lambda^2} \right\}$$

$$r_1 = \frac{1}{2}\left\{ 1 + \frac{3}{2}h\lambda - \sqrt{1 + h\lambda + \frac{9}{4}h^2\lambda^2} \right\}$$



$\Longrightarrow$ Dahlquist second barrier

The highest order of an A-stable multistep method is two.

Backward-differentiation formula (BDF)

A-stability of RK

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

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

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

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

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

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

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

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

$$z = h\lambda$$

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

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

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

$\therefore\ r(z) \equiv 1 + z b^T (\mathbb{I} - zA)^{-1} \mathbb{1}$ 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 $\det(I - zA) = 1$
$\Downarrow$
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

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

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

$|r(z)| < 1$ $\quad z = \rho \cdot e^{i\theta}$ 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.

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