2. Implicit Integration methods.

$$y_{n+1} = y_n + h\int_0^1 y'\, d\alpha$$

Trick: Shift the Newton backward diff formula by one pt

$$y = y_{n+1} + (\alpha-1)\nabla y_{n+1} + \frac{\alpha(\alpha-1)}{2}\nabla^2 y_{n+1} + \frac{(\alpha-1)\alpha(\alpha+1)}{6}\nabla^3 y_{n+1} + \cdots$$

$$y' = y'_{n+1} + (\alpha-1)\nabla y'_{n+1} + \frac{\alpha(\alpha-1)}{2}\nabla^2 y'_{n+1} + \frac{(\alpha-1)\alpha(\alpha+1)}{6}\nabla^3 y'_{n+1} + \cdots$$

$$y_{n+1} = y_n + h\int_0^1 y'\, d\alpha$$

$$= y_n + h\sum_{i=0}^{q} a_i \nabla^i y'_{n+1}$$

$$a_i = \int_0^1 \frac{(\alpha-1)\alpha(\alpha+1)\cdots(\alpha+i-2)}{i!}\, d\alpha$$

$$a_0 = 1$$

$$a_1 = \int_0^1 (\alpha-1)\, d\alpha = -\frac{1}{2}$$

$$a_2 = \int_0^1 \frac{(\alpha-1)\alpha}{2}\, d\alpha = -\frac{1}{12}$$

$\vdots$

General formula

$$y_{n+1} = y_n + h\left[1 - \frac{1}{2}\nabla - \frac{1}{12}\nabla^2 - \frac{1}{24}\nabla^3 + \cdots\right] y'_{n+1}$$

(1) Backward Euler, Implicit Euler.

$q = 0$

$$y_{n+1} = y_n + h\, y'_{n+1} + O(h^2)$$
$$= y_n + h\, f(y_{n+1}) + O(h^2)$$
$$\frac{y_{n+1} - y_n}{h} = f(y_{n+1}) + O(h).$$

* Implicit methods give non linear systems of algebraic equations at each time step.

initial guess.
iteration method
convergence.

(2) Crank-Nicolson method (Trapezoid rule, modified Euler, 2nd order Adams-Moulton)

$q = 1$

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

(3) Fourth order Adams-Moulton

$q=3$

$$y_{n+1} = y_n + \frac{h}{24}\left(9y'_{n+1} + 19y'_n - 5y'_{n-1} + y'_{n-2}\right) + O(h^5)$$

$*$ Problem for $\frac{dy}{dt} = f(y)$

Explicit Euler

$y_{n+1} = y_n + hf(y_n)$

1 func eval

Implicit Euler

$y_{n+1} = y_n + hf(y_{n+1})$

Solve

$R(y_{n+1}) = y_{n+1} - hf(y_{n+1}) - y_n = 0$

(4) Convergence

Think

- Solution is iterative
- Need initial guess $\{ y_{n+1}^{(0)} \}$
- Convergence ?

Each implicit method

$$y_{n+1} = h\, g(y_{n+1}) + w_n \qquad \text{subscript : time step}$$

Iterative solution at each time step

$$y_{n+1}^{(0)} \rightarrow \{ y_{n+1}^{(k)} \} \rightarrow \underset{\text{solution}}{y_{n+1}^{*}}$$

Imagine Fixed point iteration

$$y_{n+1}^{(k+1)} = h\, g(y_{n+1}^{(k)}) + w_n = F(y_{n+1}^{(k)})$$

$$L = \left| \frac{\partial F}{\partial y_{n+1}} \right| = \left| h \frac{\partial g}{\partial y_{n+1}} \right|$$

For convergence $L < 1$,

true for small enough h

h controls accuracy
Stability
convergence for NL eqn

(5) Stability of Implicit Method

$$\frac{dy}{dt} = -\lambda y$$

$$y = y_e + \epsilon(t)$$

$$\Downarrow$$

$$\frac{d\epsilon}{dt} = -\lambda \epsilon$$

i) Implicit Euler

$$\epsilon_{n+1} - \epsilon_n = -h\lambda \epsilon_{n+1}$$

$$\left|\frac{\epsilon_{n+1}}{\epsilon_n}\right| = \left|\frac{1}{1+h\lambda}\right| \quad \text{always stable}$$

ii) Trapezoid Rule

$$\epsilon_{n+1} - \epsilon_n = \frac{h}{2}\left[-\lambda \epsilon_{n+1} - \lambda \epsilon_n\right]$$

$$\epsilon_{n+1}\left(1 + \frac{h\lambda}{2}\right) = \epsilon_n\left(1 - \frac{h\lambda}{2}\right)$$

$$\left|\frac{\epsilon_{n+1}}{\epsilon_n}\right| = \left|\frac{1-\frac{h\lambda}{2}}{1+\frac{h\lambda}{2}}\right| < 1$$

Always stable but if $\frac{h\lambda}{2} > 1$
error oscillates with "n"

3. Predictor corrector method.

(1) Euler / Implicit Euler

Implicit Euler $y_{n+1} = y_n + hf(y_{n+1})$

Predictor

Euler to generate an initial guess

$$y_{n+1}^{p} = y_n + hf(y_n)$$

Corrector

$$y_{n+1} = y_n + hf(y_{n+1}^{p})$$

P-C algorithm become equivalent to fully implicit method if corrector step is iterated to convergence.

(2) Euler - Predictor / Crank-Nicolson Corrector

Predict $y_{n+1}^{p} = y_n + hf(y_n)$

Correct $y_{n+1} = y_n + \frac{h}{2}(f(y_{n+1}^{p}) + f(y_n))$

4. Runge – Kutta method

$$\frac{dy}{dt} = f(t, y(t))$$

weighting coeff

Formula (ν-th order)

$$\boxed{\begin{aligned} y_{n+1} &\equiv y(t_{n+1}) = y_n + \sum_{i=1}^{\nu} w_i k_i \\ k_i &= hf\Big(\underbrace{t_n + c_i h}_{\text{fraction step}},\ y_n + \sum_{j=1}^{i-1} a_{ij} k_j\Big), \quad c_1 \equiv 0 \end{aligned}}$$

$h \equiv t_{n+1} - t_n$

coeff $\{c_i\}$, $\{a_{ij}\}$ $\{w_i\}$

Taylor series expansion

$$y_{n+1} = y_n + y_n' h + \frac{h^2}{2} y_n'' + \frac{h^3}{6} y_n''' + \cdots$$

$$y_n' = f_n = f(t_n, y_n)$$

$$y_n'' = \left[\frac{d}{dt} f(t,y)\right]_{t_n} = \left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}\frac{dy}{dt}\right]_{t_n}$$

$$= (f_t + f f_y)_{t_n}$$

$$y_n''' = \big[f_{tt} + f_t f_y + f f_{ty} + f_{ty} f + f_y^2 f + f^2 f_{yy}\big]_{t_n}$$

$$y_{n+1} = y_n + h f_n + \frac{h^2}{2}(f_t + f f_y)_n + \frac{h^3}{6}(f_{tt} + f_t f_y + 2 f f_{ty} + f f_y^2 + f^2 f_{yy})_n \quad (A)$$

$$k_1 = h\, f(t_n + \overset{0}{\cancel{c_1}} h,\ y_n) = hf(t_n, y_n) = h f_n$$

$$k_2 = h f(t_n + c_2 h,\ y_n + a_{21} k_1)$$

$f(t+\alpha, y+\beta)$

$$= h f(t_n + c_2 h,\ y_n + a_{21} h f_n)$$

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

expansion in terms of h

$$\cong h f(t_n, y_n) + h^2 [f_t c_2 + f_y a_{21} f_n]_{t_n}$$

$$+ h^3 \left[\frac{c_2^2}{2} f_{tt} + f_{ty} c_2 \cdot a_{21} f_n + \frac{a_{21}^2}{2} f_n^2 f_{yy}\right]_{t_n}$$

$$k_3 = h f(t_n + c_3 h,\ y_n + a_{31} k_1 + a_{32} k_2)$$

$$= h f(t_n, y_n) + h [f_t \cdot c_3 h + f_y (a_{31} k_1 + a_{32} k_2)]_{t_n}$$

$$+ h \Big[\frac{c_3^2 h^2}{2} f_{tt} + f_{ty} c_3 h (a_{31} k_1 + a_{32} k_2)$$

$$+ f_{yy} \frac{(a_{31} k_1 + a_{32} k_2)^2}{2} \Big]$$

$$= hf(t_n, y_n) + h^2 (c_3 f_t + a_{31} f f_y + a_{32} f f_y)_{t_n}$$

$$+ h^3 (f_y a_{32} (f_t c_2 + f_y a_{21} f)$$

$$+ \frac{c_3^2}{2} f_{tt} + c_3 f_{ty} (a_{31} + a_{32}) f$$

$$+ \frac{1}{2} (a_{31} + a_{32})^2 f^2 f_{yy}]_{t_n}$$

$$y_{n+1} = y_n + w_1 k_1 + w_2 k_2 + w_3 k_3$$

$$= y_n + w_1 h f_n + w_2 h f_n + w_2 h^2 (f_t c_2 + a_{21} f f_y)$$
$$+ w_2 h^3 \left[\frac{c_2^2}{2} f_{tt} + f_{ty} c_2 a_{21} f + \frac{a_{21}^2}{2} f^2 f_{yy}\right]$$
$$+ w_3 h f_n + w_3 h^2 (c_3 f_t + a_{31} f f_y + a_{32} f f_y) + w_3 h^3 (\cdots) + \cdots$$
$$= y_n + h (w_1 + w_2 + w_3 + \cdots) f_n$$
$$+ h^2 f_t (c_2 w_2 + c_3 w_3 + \cdots)$$
$$+ h^2 f f_y (w_2 a_{21} + w_3 (a_{31} + a_{32}) + \cdots)$$
$$+ O(h^3) \qquad (B)$$

Compare (A) & (B)

$$w_1 + w_2 + \cdots w_v = 1.0$$
$$w_2 c_2 + w_3 c_3 + \cdots + w_v c_v = 0.5$$
$$w_2 a_{21} + w_3 (a_{31} + a_{32}) + \cdots + w_v \sum_{i=1}^{v-1} a_{vi} = 0.5$$

i) $V = 2$

$$w_1 + w_2 = 1.0$$
$$\left.\begin{aligned} w_2 c_2 &= 0.5 \\ w_2 a_{21} &= 0.5 \end{aligned}\right\} \rightarrow c_2 = a_{21}$$

3 eqns, 4 unknowns.

a) $c_2 = \frac{1}{2}$

$w_2 = 1$, $a_{21} = \frac{1}{2}$, $w_1 = 0$.

$k_1 = h f_n$

$k_2 = h f(t_n + 0.5h, y_n + 0.5 h f_n)$

$$\boxed{y_{n+1} = y_n + h f(t_n + 0.5h, y_n + 0.5 h f_n)}$$

Midpoint Scheme

predictor-corrector scheme that uses f evaluated at the Euler approximation to the midpoint between t_n & t_{n+1}

b) $c_2 = 1$

$a_{21} = 1, \quad w_2 = \frac{1}{2}, \quad w_1 = \frac{1}{2}$

$k_1 = h f_n$

$k_2 = h f(t_n + h, \; y_n + h f_n)$

$$\boxed{y_{n+1} = y_n + \frac{h}{2}\left(f_n + f(t_n + h, y_n + h f_n)\right)}$$

equivalent to Euler predictor / Trapezoid rule corrector.

II) $V = 3$.

1. $w_1 + w_2 + w_3 = 1$
2. $w_2 c_2 + w_3 c_3 = \frac{1}{2}$
3. $a_{21} w_2 + w_3 a_{31} + w_3 a_{32} = \frac{1}{2}$
4. $c_2 a_{21} w_2 + c_3 (a_{31} + a_{32}) w_3 = \frac{1}{3}$
5. $\frac{1}{2} c_2^2 w_2 + \frac{1}{2} c_3^2 w_3 = \frac{1}{6}$
6. $\frac{1}{2} a_{21}^2 w_2 + \frac{1}{2} (a_{31} + a_{32})^2 w_3 = \frac{1}{6}$
7. $a_{21} a_{31} w_3 = \frac{1}{6}$
8. $c_2 a_{31} w_3 = \frac{1}{6}$

8 equations $\rightarrow$ only 6 are independent

8 unknowns $\quad w_1, w_2, w_3.$
$\quad c_2, c_3$
$\quad a_{21}, a_{31}, a_{32}$

two constants at will. $\rightarrow$ Third-order Runge-Kutta method

iv) $\nu = 4$ Runge-Kutta-Gill method

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + k_4) + \frac{1}{3}(b k_2 + d k_3)$$

$$k_1 = h f_n$$

$$k_2 = h f\left(t_n + \tfrac{1}{2}h,\ y_n + \tfrac{1}{2}k_1\right)$$

$$k_3 = h f\left(t_n + \tfrac{1}{2}h,\ y_n + a k_1 + b k_2\right)$$

$$k_4 = h f\left(t_n + h,\ y_n + c k_2 + d k_3\right)$$

$$a = \frac{\sqrt{2}-1}{2}, \quad b = \frac{2-\sqrt{2}}{2}$$

$$c = -\frac{\sqrt{2}}{2} \qquad d = 1 + \frac{\sqrt{2}}{2}$$