8.3 (continued)

Recall : Heun's

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

- General 2-stage 2nd order RK

$$\begin{array}{c|cc} 0 & 0 & 0 \\ c_2 = a_{21} & a_{21} & 0 \\ \hline & b_1 & b_2 \end{array}$$

$$\begin{cases} x^{(2)} = x_i + h\, a_{21} f(t_i, x_i) \\ x_{i+1} = x_i + h\left(b_1 f(t_i, x_i) + b_2 f(t_i + \overset{a_{21}}{\cancel{c_2}} h, x^{(2)})\right) \end{cases}$$

$$x_{i+1} = x_i + h b_1 f(t_i, x_i) + h b_2 f(t_i + a_{21} h, x_i + h a_{21} f(t_i, x_i))$$

$$= x_i + h b_1 f(t_i, x_i) + h b_2 \big(f(t_i, x_i) + \partial_t f(t_i, x_i) \cdot a_{21} h$$

$$+ \partial_x f(t_i, x_i) \cdot h a_{21} f(t_i, x_i) + O(h^2) \big)$$

$$= x_i + h(b_1 + b_2) f(t_i, x_i)$$

$$+ h^2 b_2 a_{21} \left(\partial_t f(t_i, x_i) + \partial_x f(t_i, x_i) \cdot f(t_i, x_i)\right) + O(h^3)$$

$$\Rightarrow \begin{cases} b_1 + b_2 = 1 \\ b_2 a_{21} = \frac{1}{2} \end{cases}$$ "order conditions"

Example : $a_{21} = \frac{1}{2}$ $b_2 = 1$ $b_1 = 0$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$ "modified Euler method"

$$\begin{cases} x^* = x_i + \frac{1}{2} h f(t_i, x_i) \\ x_{i+1} = x_i + h f(t_i + \frac{1}{2} h, x^*) \end{cases}$$

Higher order accuracy analysis : Butcher series.

Classic 4th order RK

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

Adaptive RK w/ embedded table

$$\begin{array}{c|ccc} \underbrace{}_{c_j} & & a_{jk} & \\ \hline & b_1 & \cdots & b_s \\ & b_1^* & \cdots & b_s^* \end{array}$$

$b_1 \cdots b_s$ ↙ p-th order

$b_1^* \cdots b_s^*$ ↙ (p-1)-th order

$$x_{i+1} = x_i + h \sum_{k=1}^{s} b_k \, f(t_i + c_k h, x^{(k)})$$

$$x_{i+1}^* = x_i + h \sum_{k=1}^{s} b_k^* \, f(t_i + c_k h, x^{(k)})$$

x_{i+1} should be more accurate than x_{i+1}^*

⇝ error of $x_{i+1}^* \simeq |x_{i+1} - x_{i+1}^*|$

↳ an indicator of increasing/decreasing h.

$$\begin{cases} \text{If } |\cdot| \text{ is small, then } h \nearrow \\ \text{If } |\cdot| \text{ is large, then } h \searrow \end{cases}$$

Euler-Heun: $p=2$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \\ & 1 & 0 \end{array}$$

$\frac{1}{2} \ \frac{1}{2}$ ↙ Heun

$1 \ 0$ ↙ Euler

Runge-Kutta-Fehlberg: $p=5$ (w/ 6 stages)

8.4 Multistep methods

Idea: build formula for x_{i+1} using $x_i, x_{i-1}, \cdots, x_{i-k+1}$

For example: $x_{i+1} = x_i + a h f(t_i, x_i) + b h f(t_{i-1}, x_{i-1})$

To achieve second order accuracy,

$$x(t_{i+1}) = x(t_i) + a h \underbrace{f(t_i, x(t_i))}_{x'(t_i)} + b h \underbrace{f(t_{i-1}, x(t_{i-1}))}_{x'(t_{i-1})} + L.T.E.$$

$$x(t_{i+1}) = x(t_{i-1}) + 2h \cdot x'(t_{i-1}) + \frac{1}{2}(2h)^2 x''(t_{i-1}) + \cdots$$

$$x(t_i) = x(t_{i-1}) + h \cdot x'(t_{i-1}) + \frac{1}{2} h^2 x''(t_{i-1}) + \cdots$$

$$x'(t_i) = x'(t_{i-1}) + h \cdot x''(t_{i-1}) + \cdots$$

$$L.T.E. = h\, x'(t_{i-1}) \cdot \left(2 - 1 - a - b\right) + h^2 x''(t_{i-1}) \cdot \left(2 - \frac{1}{2} - a\right) + \cdots$$

$$\Rightarrow \begin{cases} a + b = 1 \\ a = \frac{3}{2} \end{cases} \qquad b = -\frac{1}{2}$$

$$x_{i+1} = x_i + \frac{3}{2} h f(t_i, x_i) - \frac{1}{2} h f(t_{i-1}, x_{i-1})$$

2nd order Adams-Bashforth method.

General multistep method

$$a_k x_i + \cdots + a_0 x_{i-k} = h\,(b_k f_i + \cdots + b_0 f_{i-k})$$

$$f_j := f(t_j, x_j)$$

$b_k = 0 \longrightarrow$ explicit

$b_k \neq 0 \longrightarrow$ implicit

To analyze L.T.E., (take $i=k$, $t_0=0$)

$$a_k x(kh) + \cdots + a_0 x(t_0) = h(b_k x'(kh) + \cdots + b_0 x'(t_0)) + \text{L.T.E.}$$

$$\text{L.T.E.} = \sum_{j=0}^{k} \left(a_j x(jh) - h b_j x'(jh) \right)$$

$$x(jh) = \sum_{m=0}^{\infty} \frac{1}{m!} (jh)^m x^{(m)}(0)$$

$$x'(jh) = \sum_{m=0}^{\infty} \frac{1}{m!} (jh)^m x^{(m+1)}(0) = \sum_{m=1}^{\infty} \frac{1}{(m-1)!} (jh)^{m-1} x^{(m)}(0)$$

$$m \rightsquigarrow m-1$$

$$\text{L.T.E.} = \sum_{j=0}^{k} \left(a_j x(0) + \sum_{m=1}^{\infty} \left(a_j \frac{1}{m!} (jh)^m x^{(m)}(0) - h b_j \frac{1}{(m-1)!} (jh)^{m-1} x^{(m)}(0) \right) \right)$$

$$= \sum_{j=0}^{k} a_j x(0) + \sum_{j=0}^{k} \sum_{m=1}^{\infty} h^m x^{(m)}(0) \cdot \left(a_j \frac{1}{m!} j^m - b_j \frac{1}{(m-1)!} j^{m-1} \right)$$

$$= \sum_{j=0}^{k} a_j x(0) + \sum_{m=1}^{\infty} h^m x^{(m)}(0) \underbrace{\sum_{j=0}^{k} \left(a_j \frac{1}{m!} j^m - b_j \frac{1}{(m-1)!} j^{m-1} \right)}$$

order conditions:

$m=0$: $\displaystyle\sum_{j=0}^{k} a_j = 0$

$m \geq 1$: $\displaystyle\sum_{j=0}^{k} \left(a_j \frac{1}{m!} j^m - b_j \frac{1}{(m-1)!} j^{m-1} \right) = 0$

$$\begin{cases} m=1: & \displaystyle\sum_{j=0}^{k} (a_j \cdot j - b_j) = 0 \\ m=2: & \displaystyle\sum_{j=0}^{k} \left(a_j \cdot \frac{j^2}{2} - b_j \cdot j\right) = 0 \\ m=3: & \displaystyle\sum_{j=0}^{k} \left(a_j \cdot \frac{j^3}{6} - b_j \cdot \frac{j^2}{2}\right) = 0 \\ \quad \cdots & \end{cases}$$

To have p-th order accuracy, one needs to satisfy order conditions $m = 0, 1, \cdots, p$.

2nd order Adams-Bashforth:

$\vec{a} = (a_0, a_1, a_2) = (0, -1, 1)$ $\qquad$ $\vec{b} = (-\frac{1}{2}, \frac{3}{2}, 0)$

explicit.

$m=1: \quad \sum a_j \cdot j = 1 \qquad \sum b_j = 1$

$m=2: \quad \sum a_j \cdot \frac{j^2}{2} = \frac{3}{2} \qquad \sum b_j \cdot j = \frac{3}{2}$ $\qquad \Rightarrow$ 2nd order accuracy.

p-th order Adams-Bashforth

$\vec{a} = (\underset{0}{0}, \underset{1}{\cdots}, \underset{\cdots}{0}, \underset{p-1}{-1}, \underset{p}{1})$ $\qquad$ $\vec{b} = (b_0, \cdots, b_{p-1}, 0)$ $\qquad k = p$

explicit

$$\sum_{j=0}^{p} \left(a_j \frac{1}{m!} j^m - b_j \frac{1}{(m-1)!} j^{m-1} \right) = 0 \quad , m = 1, \cdots, p$$

$$\sum_{j=0}^{p-1} \frac{1}{(m-1)!} j^{m-1} b_j = \frac{1}{m!} p^m - \frac{1}{m!} (p-1)^m$$

$$\sum_{j=0}^{p-1} j^{m-1} b_j = \frac{1}{m} \left(p^m - (p-1)^m \right) , \quad m = 1, \cdots, p$$

$p \times p$ linear system for $b_0, \cdots, b_{p-1}$ w/ Vandermonde matrix as coeffs $\rightsquigarrow$ $\exists!$ sol'n.