General multistep method

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

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

order conditions:

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

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

p-th order Adams-Moulton: $\qquad k = p-1$

$$\vec{a} = (0, \ldots 0, \underset{\substack{\uparrow \\ p-2}}{-1}, \underset{\substack{\uparrow \\ p-1}}{1}), \quad \vec{b} = (b_0, \cdots, \underset{\substack{\uparrow \\ \text{implicit}}}{b_{p-1}})$$

$$\frac{1}{(m-1)!} \sum_{j=0}^{p-1} b_j j^{m-1} = \frac{1}{m!} \sum_{j=0}^{p-1} a_j j^m = \frac{1}{m!} \left((p-1)^m - (p-2)^m \right)$$

$$\sum_{j=0}^{p-1} b_j j^{m-1} = \frac{1}{m} \left((p-1)^m - (p-2)^m \right) \qquad m = 1, \cdots, p$$

$p \times p$ linear system in $b_0, \cdots, b_{p-1}$ w/ Vandemonde coeff matrix

$\Rightarrow$ unique sol'n

Backward differentiation formula (BDF): $\quad$ (p-th order, $k = p$)

$$\vec{a} = (a_0, \cdots, a_p), \quad \vec{b} = (0, \cdots, 0, \underset{\substack{\uparrow \\ \text{implicit}}}{1})$$

$$m = 0: \quad \sum_{j=0}^{p} a_j = 0$$

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

$$\sum_{j=0}^{p} a_j j^m = m p^{m-1} \qquad \leftarrow \text{works for } m = 0, \cdots, p$$

$\Rightarrow$ unique sol'n.

Compare multistep methods vs. RK

Advantages:

- Cheaper in one step. (only one evaluation of f in each step for explicit multistep method)
- Easy to design high order method

Disadvantages:

- Need initialization (one needs $x_0, \cdots, x_{k-1}$ to get the method started, usually by another method)
- Harder to do adaptive step size
- less flexibility in parameters.

8.5 zero-stability of multistep methods

Suppose we solve $x' = f(t, x)$ by a multistep method

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

We aim to analyze the <u>convergence</u> of the method, i.e., when fix a final time T, taking $h = \frac{T - t_0}{n}$, is it true that

$$\lim_{h \to 0} (x_n - x(T)) = 0 \quad ? \qquad (\text{for reasonable } f)$$

- A necessary condition: the method is convergent for $f \equiv 0$ "zero-stability"

In this case, for given initial values $x_0, \cdots, x_{k-1}$. we have

$$x_i = -\frac{1}{a_k}(a_{k-1} x_{i-1} + \cdots + a_0 x_{i-k}) \qquad i \geq k$$

Denote $\vec{y}_i = \begin{pmatrix} x_{i-k+1} \\ \vdots \\ x_i \end{pmatrix}$ $\quad i \geq k-1$ Then

$\vec{y}_{k-1} = \begin{pmatrix} x_0 \\ \vdots \\ x_{k-1} \end{pmatrix}$, $\quad \vec{y}_i = A\,\vec{y}_{i-1}$

$$\begin{pmatrix} x_{i-k+1} \\ \vdots \\ x_i \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & & 1 \\ -\frac{a_0}{a_k} & \cdots & & & -\frac{a_{k-1}}{a_k} \end{pmatrix} \begin{pmatrix} x_{i-k} \\ \vdots \\ x_{i-1} \end{pmatrix}$$

The eigenvalues of A are zeros of the polynomial

$$p(z) = a_k z^k + a_{k-1} z^{k-1} + \cdots + a_0$$

- If some zero of $p(z)$ has $|\cdot| > 1$, then the component along its eigen-direction is magnified in the iteration $\rightsquigarrow$ unstable (no convergence)
- If all zeros of $p(z)$ have $|\cdot| \leq 1$ and any zero w/ $|\cdot| = 1$ is simple, then any error (initial / round-off) is not magnified $\longrightarrow$ stable

- Adams-Bashforth, Adams-Moulton $\quad p(z) = z^k - z^{k-1} = z^{k-1}(z-1)$ have zero-stability

BDF is zero-stable up to 6-th order

<u>Thm</u> A multistep method is convergent $\Leftrightarrow$ It is zero-stable and consistent

$\hookrightarrow \sum a_j = 0, \ \sum (j a_j - b_j) = 0$

8.6 Systems and high order ODEs

- System of ODEs

$$\begin{cases} x_1' = f_1(t, x_1, \cdots, x_n) \\ \cdots\cdots \\ x_n' = f_n(t, x_1, \cdots, x_n) \end{cases}$$

initial values

$$x_1(t_0) = x_{1,0}$$

$$\cdots$$

$$x_n(t_0) = x_{n,0}$$

Vector notation

$$\vec{x}(t) = \begin{pmatrix} x_1(t) \\ \vdots \\ x_n(t) \end{pmatrix}, \quad \vec{f}(t, \vec{x}) = \begin{pmatrix} f_1(t, x_1, \cdots, x_n) \\ \vdots \\ f_n(t, x_1, \cdots, x_n) \end{pmatrix}$$

$$\vec{x}_0 = \begin{pmatrix} x_{1,0} \\ \vdots \\ x_{n,0} \end{pmatrix}$$

$$\rightsquigarrow \quad \vec{x}'(t) = \vec{f}(t, \vec{x}(t)), \quad \vec{x}(t_0) = \vec{x}_0$$

RK, multistep can be directly applied.

2nd order Taylor method:

$$x_{i+1} = x_i + h f(t_i, x_i) + \frac{h^2}{2}\left(\partial_t f(t_i, x_i) + \partial_x f(t_i, x_i) f(t_i, x_i) \right)$$

$$\Downarrow$$

$$\vec{x}_{i+1} = \vec{x}_i + h \vec{f}(t_i, \vec{x}_i) + \frac{h^2}{2}\left(\partial_t \vec{f}(t_i, \vec{x}_i) + \nabla_{\vec{x}} \vec{f}(t_i, \vec{x}_i) \vec{f}(t_i, \vec{x}_i) \right)$$

- High order ODEs

$$y^{(n)} = f(t, y, y', \cdots, y^{(n-1)}), \quad y(t_0) = y_{0,0}, \; y'(t_0) = y_{1,0}, \; \cdots, \; y^{(n-1)}(t_0) = y_{n-1,0}$$

Define $x_1(t) = y(t)$, $x_2(t) = y'(t)$, $\cdots$, $x_n(t) = y^{(n-1)}(t)$. Then

$$\begin{cases} x_1'(t) = x_2(t) & x_1(t_0) = y_{0,0} \\ x_2'(t) = x_3(t) & x_2(t_0) = y_{1,0} \\ \quad \cdots & \quad \cdots \\ x_{n-1}'(t) = x_n(t) & x_n(t_0) = y_{n-1,0} \\ x_n'(t) = f(t, x_1, x_2, \cdots, x_n) & \end{cases}$$