(2) Linear Multi-step Methods (LMM)

<u>Def</u> An r-step LMM has the form of

$$\sum_{j=0}^{r} \alpha_j U^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(t^{n+j}, U^{n+j})$$

<u>Note</u> In this linear method, we note that at each $t = t^j$, $\exists$ only one fn evaluation of f.

Computationally, it's much more efficient to <u>store</u> $f(U^j)$ for each $t = t^j$, and reuse them in the rest of calculations.

<u>Rmk</u> $\begin{cases} \text{explicit if } \beta_r = 0 \\ \text{implicit if } \beta_r \neq 0. \end{cases}$

<u>Rmk</u> It is conventional to assume $\alpha_r = 1$.

<u>Ex.</u> <u>The Adams methods</u> have the form

$$U^{n+r} = U^{n+r-1} + \Delta t \sum_{j=0}^{r} \beta_j f(U^{n+j})$$

<u>Note</u>

(i) $\alpha_j = \begin{cases} 1, & j=r \\ -1, & j=r-1 \\ 0, & j<r-1 \end{cases}$

(ii) β_j are chosen to provide the order of accuracy to be r by examining Taylor series expansion as seen in E_{LT}^n calculation.

- Two types of the Adams methods

  (i) r-step Adams-Bashforth (explicit)
  (ii) r-step Adams-Moulton (implicit)

- The Adams methods are the most widely used multi-step methods.

- They are used to produce predictor-corrector algorithms in which one
  (i) first uses r-step explicit for prediction, &
  (ii) later uses r-step implicit for correction.

We'll discuss more on predictor-corrector algorithms later.

Derivations of LMM

- We can derive a given LMM using a couple of different approaches as we saw in one-step methods.

Ex. For example, we consider deriving the Adams methods using a quadrature rule:

→ We first write:

$$u(t^{n+r}) - u(t^{n+r-1}) = \int_{t^{n+r-1}}^{t^{n+r}} u'(t)\,dt$$

$$= \int_{t^{n+r-1}}^{t^{n+r}} f(u(t))\,dt \quad \text{--- (1)}$$

→ Applying a quadrature rule to (1):

$$\int_{t^{n+r-1}}^{t^{n+r}} f(u(t))\,dt \cong \Delta t \sum_{j=0}^{r} \beta_j f(u(t^{n+j})) \quad \text{--- (2)}$$

→ The final form becomes

$$U^{n+r} - U^{n+r-1} = \Delta t \sum_{j=0}^{r} \beta_j f(U^{n+j}).$$

→ Note that the Adams methods seek for a poly $p(t)$ that has properties of

(i) $r-1$ degree,

(ii) $p(t)$ interpolates $f(u(t))$ at $\underbrace{t^n, \cdots, t^{n+r-1}}_{r \text{ pts}}$

(i.e, $p(t^j) = f(u(t^j))$, $j = n, \cdots, n+r-1$)

(iii) integrate $p(t)$ to approximate (1)

→ obtain (2).

Ex. We now list few cases of the Adams-Bashforth (AB) methods (explicit)

$\boxed{\text{1 step AB}}$ $v^{n+1} = v^n + \Delta t f(v^n)$ (∴ 1 step AB = Forward Euler)

$\boxed{\text{2 step AB}}$ $v^{n+2} = v^{n+1} + \frac{\Delta t}{2}\left[-f(v^n) + 3f(v^{n+1})\right]$

$\boxed{\text{3 step AB}}$ $v^{n+3} = v^{n+2} + \frac{\Delta t}{12}\left[5f(v^n) - 16f(v^{n+1}) + 23f(v^{n+2})\right]$

$\boxed{\text{4 step AB}}$ $v^{n+4} = v^{n+3} + \frac{\Delta t}{24}\left[-9f(v^n) + 37f(v^{n+1}) - 59f(v^{n+2}) + 55f(v^{n+3})\right]$

Ex. few of the Adams-Moulton (AM) methods (Implicit)

$\boxed{\text{1 step AM}}$ $v^{n+1} = v^n + \frac{\Delta t}{2}\left[f(v^n) + f(v^{n+1})\right]$ (∴ 1 step AM = trapezoidal)

$\boxed{\text{2 step AM}}$ $v^{n+2} = v^{n+1} + \frac{\Delta t}{12}\left[-f(v^n) + 8f(v^{n+1}) + 5f(v^{n+2})\right]$

$\boxed{\text{3 step AM}}$ $v^{n+3} = v^{n+2} + \frac{\Delta t}{24}\left[f(v^n) - 5f(v^{n+1}) + 19f(v^{n+2}) + 9f(v^{n+3})\right]$

$\boxed{\text{4 step AM}}$ $v^{n+4} = v^{n+3} + \frac{\Delta t}{720}\left[-19f(v^n) + 106f(v^{n+1}) - 264f(v^{n+2}) + 646f(v^{n+3}) + 251f(v^{n+4})\right]$

Several more properties on LMM

(1). LMM is not self-starting

(i) one strategy is to use a one-step method to generate first few step solns at enough $t^0, t^1, \cdots,$ points to begin with a LMM.

(ii) Another option is to use a low-order method initially, and gradually increase the order as additional solns become available.

(2) Predictor-corrector method

— Implicit methods are, in general, usually more stable (and also more accurate) than explicit multi-step methods

— But implicit methods require an initial guess to begin nonlinear iterative processes.

— A good initial guess is supplied by an explicit method

⇒ This approach of combining a pair of

(i) explicit as a predictor, &

(ii) implicit as a corrector

is called "predictor-corrector" method.

→ In this predictor – corrector pair, we use

(i) an explicit method :

$U^n \longrightarrow \hat{U}^{n+1}$, $\hat{U}^{n+1}$ is a temporary prediction value which is to be corrected

(ii) an implicit method ;

$\hat{U}^{n+1} \longrightarrow U^{n+1}$, U^{n+1} is a correction from $\hat{U}^{n+1}$ by applying any necessary extra correction step with implicit schems that reduces the local errors in a controled way.

Ex, 1step AB (or forward Euler) + 1step AM (or trapezoidal)

$$\begin{cases} \hat{U}^{n+1} = U^n + \Delta t\, f(U^n) & \Leftarrow \text{AB} \\ U^{n+1} = U^n + \frac{\Delta t}{2}\left[f(U^n) + f(\hat{U}^{n+1})\right] & \Leftarrow \text{AM} \end{cases}$$

→ 2nd order accurate, like the trapezoidal method.

Rmk One may use the corrector repeatedly until some convergence tolerance is met, but it is not worth the expense.

In practice, a fixed number of corrector steps, often only once, may be used instead.

Def Characteristic polynomials ρ & σ of LMM:

① $$\rho(\zeta) \equiv \sum_{j=0}^{r} \alpha_j \zeta^j$$

② $$\sigma(\zeta) \equiv \sum_{j=0}^{r} \beta_j \zeta^j$$

are characteristic polynomials of of an r-step LMM:

$$\sum_{j=0}^{r} \alpha U^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(t^{n+j}, U^{n+j})$$

Ex. The two-step AM method:

$$U^{n+2} = U^{n+1} + \frac{\Delta t}{12}\left[-f(U^n) + 8f(U^{n+1}) + 5f(U^{n+2})\right]$$

$$\Rightarrow \begin{cases} \rho(\zeta) = \zeta^2 - \zeta \\ \sigma(\zeta) = \frac{1}{12}(5\zeta^2 + 8\zeta - 1) \end{cases}$$

$\leftarrow$ (set $n=0$)

Ex. The 3-step AB method:

$$U^{n+3} = U^{n+2} + \frac{\Delta t}{12}\left[5f(U^n) - 16f(U^{n+1}) + 23f(U^{n+2})\right]$$

$$\Rightarrow \begin{cases} \rho(\zeta) = \zeta^3 - \zeta^2 \\ \sigma(\zeta) = \frac{1}{12}(23\zeta^2 - 16\zeta + 5) \end{cases}$$

Thm The LMM method is consistent if

$$\begin{cases} \rho(1) = 0 \\ \rho'(1) = \sigma(1) \end{cases}$$

proof.

We need to show $E_{LT}^{n+1} \to 0$ as $\Delta t \to 0$.

To see this, we notice that

$u^{n+j} = u(t^{n+j}) = u(t^n + j\Delta t)$

$$E_{LT}^{n+1} = \frac{1}{\Delta t}\left[\sum_{j=0}^{r} \alpha_j u^{n+j} - \Delta t \sum_{j=0}^{r} \beta_j \overbrace{f(u^{n+j})}^{u'(t^{n+j})}\right]$$

$$= \frac{1}{\Delta t}\sum_{j=0}^{r} \alpha_j \left\{ u(t^n) + (j\Delta t)\, u'(t^n) + \frac{(j\Delta t)^2}{2} u''(t^n) + O(\Delta t^3) \right\}$$

$$- \sum_{j=0}^{r} \beta_j \left\{ u'(t^n) + (j\Delta t)\, u''(t^n) + \frac{(j\Delta t)^2}{2} u'''(t^n) + O(\Delta t^3) \right\}$$

$$= \frac{1}{\Delta t}\left[\sum_{j=0}^{r} \alpha_j\right] u(t^n) \quad \text{--- } (*)$$

$$+ \left[\sum_{j=0}^{r} (j\alpha_j - \beta_j)\right] u'(t^n) \quad \text{--- } (**)$$

$$+ \Delta t \left[\sum_{j=0}^{r} \left(\frac{j^2}{2}\alpha_j - \beta_j\right)\right] u''(t^n)$$

$$+ \cdots$$

$$+ \Delta t^{q-1}\left[\sum_{j=0}^{r} \left(\frac{1}{q!} j^q \alpha_j - \frac{1}{(q-1)!} j^{q-1} \beta_j\right)\right] u^{(q)}(t^n)$$

$$+ O(\Delta t^q)$$

In order to get $E_{LT}^{n+1} \to 0$ as $\Delta t \to 0$, $(*)$ & $(**)$ should vanish.

$\Rightarrow$ ① $\sum_{j=0}^{r} \alpha_j = 0 \quad (\Leftrightarrow \rho(1) = 0)$

② $\sum_{j=0}^{r} (j\alpha_j - \beta_j) = 0 \quad \Big(\Leftrightarrow \underbrace{\sum_{j=0}^{r} j\alpha_j}_{=\rho'(1)} = \underbrace{\sum_{j=0}^{r} \beta_j}_{=\sigma(1)}\Big)$

$\Rightarrow$

If $\begin{cases} \rho(1) = 0 \\ \rho'(1) = \sigma(1), \end{cases}$

then the r-step LMM method is <u>consistent</u>.