Linear Multistep Method

Note for RK method: it's one step. And to get higher order. We need to introduce several stages.

Rmk: But it's expensive if evaluate of f is expensive when apply several stages.

$\Rightarrow$ So we consider to reuse the value of f at previous steps.

pros: LMM:

i) Fewer compute of f

ii) Efficient for higher order.

RK:

i) Self-starting (one-step, only need y_0)

ii) better stability

iii) easier to do the adaptive time step.

(1) Derivation of LMMs:

Idea: To compute $t_{n-1} \to t_n$. We also use the info. from $t_{n-2}, t_{n-3} \dots$

① <u>Integration method</u>:

Note we can rewrite s.l. : For $\ell \in \mathbb{N}$.

$$y(t_n) = y(t_{n-\ell}) + \int_{t_{n-\ell}}^{t_n} f(s, y(s))\,ds \quad (*)$$

Evaluate RHS by quadrature by interpolating $f(t, y(t))$ by polynomial $p_m(t)$ of degree m in pts: $t_{k-m}, t_{k-(m-1)}, \cdots t_k$. $k \leq n$. S.t.

$p_m(t_{k-i}) = f(t_{k-i}, y(t_{k-i}))$. $0 \leq i \leq m$ holds.

i.e. $p_m(t) = \sum_0^m f(t_{k-i}, y(t_{k-i})) L_i^{(m)}(t)$ by Lagrange interpolation

<u>Rmk</u>: $f(t, y(t)) = p_m(t) + O(h^{m+1})$.

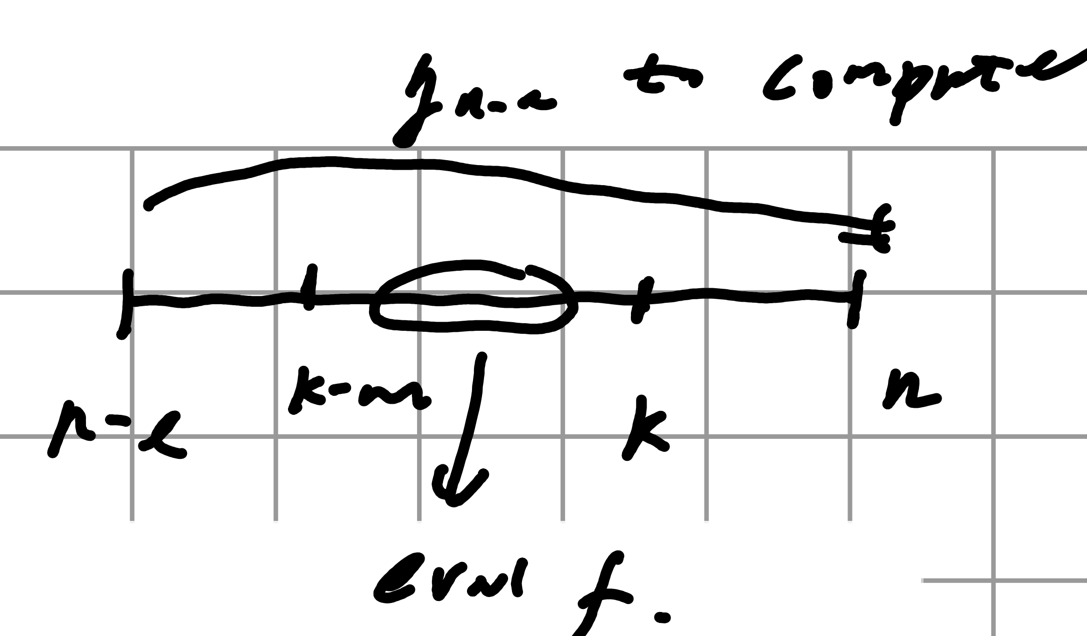
Plug into $(*)$, We have:

$$y(t_n) = y(t_{n-\ell}) + \sum_{i=0}^m f(t_{k-i}, y(t_{k-i})) \int_{t_{n-\ell}}^{t_n} L_i^{(m)}(s)\,ds + O(h^{m+2})$$

We need to chose: $\ell \in \mathbb{N}$. $k \in \{n-\ell, \cdots n\}$. and m. then we have form:

$y_n = y_{n-\ell} + h \sum_0^m \beta_i f_{k-i}$. $n \geq k$. where $f_j = f(t_j, y_j)$ and $\beta_i = \frac{1}{h} \int_{t_{n-\ell}}^{t_n} L_i^{(m)}(s)\,ds$

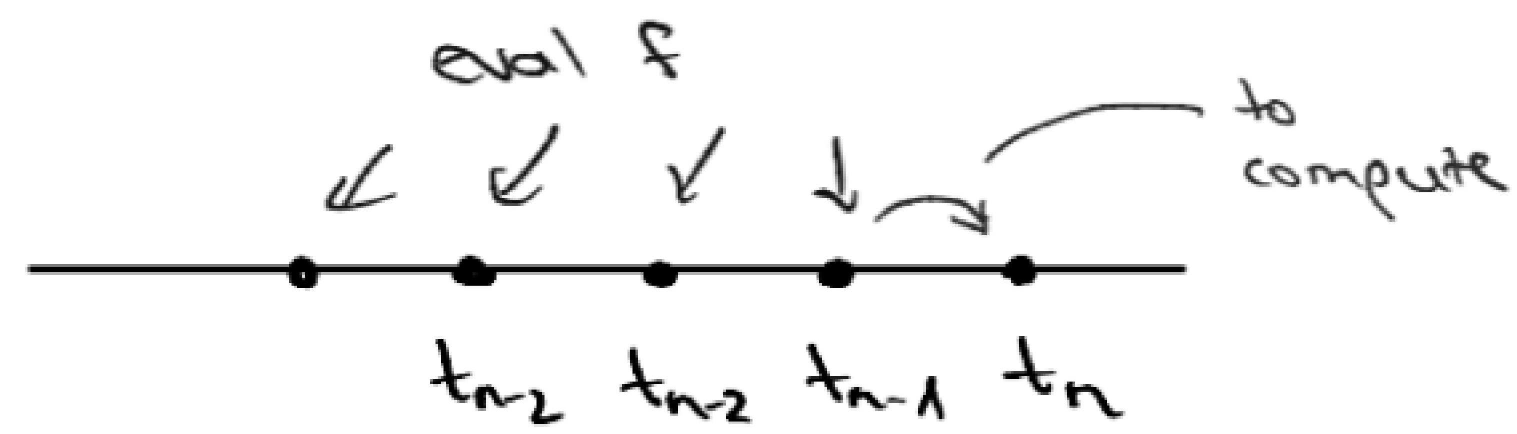
Examples:



(1) Adams-Bashforth methods:

$\ell = 1,\ k = n-1$

$\Rightarrow$ explicit



$$y_n = y_{n-1} + \sum_{\mu=0}^{m} f(t_{n-1-\mu}, y_{n-1-\mu}) \int_{t_{n-1}}^{t_n} L_\mu^{(m)}(s)\,ds, \quad n \geq m+1 \tag{4.7}$$

$m = 0$: $\quad y_n = y_{n-1} + h f_{n-1}$ (expl E) $\quad$ (4.8)

$m = 1$: $\quad y_n = y_{n-1} + \frac{1}{2} h (3 f_{n-1} - f_{n-2})$ $\quad$ (4.9)

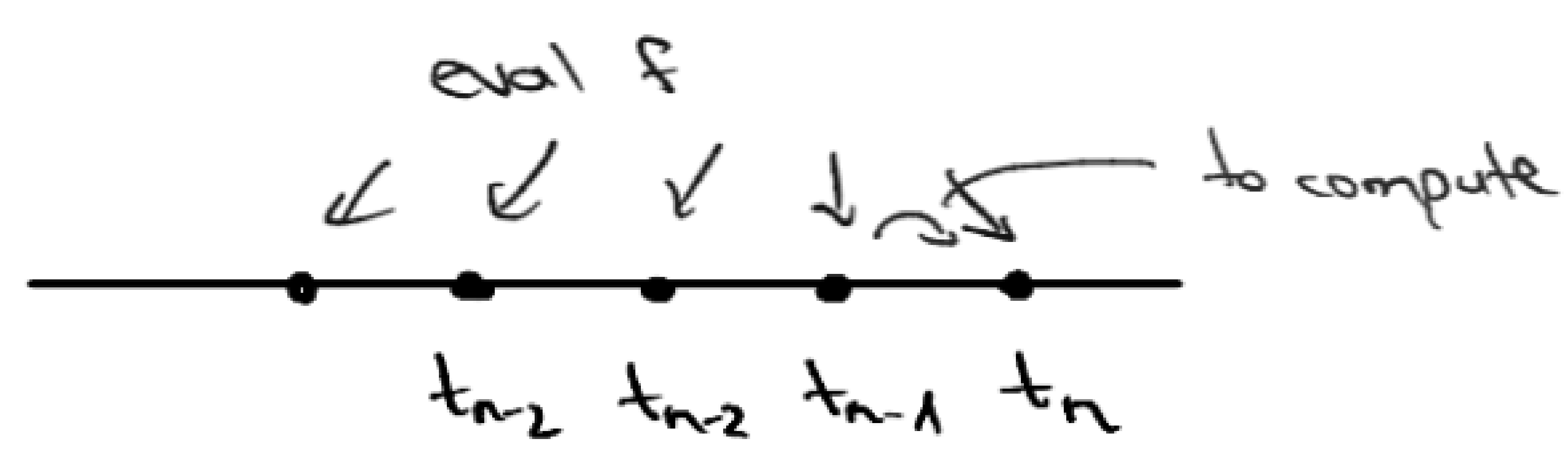
$m = 2$: $\quad y_n = y_{n-1} + \frac{1}{12} h (23 f_{n-1} - 16 f_{n-2} + 5 f_{n-3})$ $\quad$ (4.10)

$m = 3$: $\quad y_n = y_{n-1} + \frac{1}{24} h (55 f_{n-1} - 59 f_{n-2} + 37 f_{n-3} - 9 f_{n-4})$ $\quad$ (4.11)

(2) Adams-Moulton methods

$\ell = 1,\ k = n$

$\Rightarrow$ implicit



$$y_n = y_{n-1} + \sum_{\mu=0}^{m} f_{n-\mu} \int_{t_{n-1}}^{t_n} L_\mu^{(m)}(s)\,ds, \quad n \geq m. \tag{4.12}$$

$m = 0$: $\quad y_n = y_{n-1} + h f_n$ (impl E) $\quad$ (4.13)

$m = 1$: $\quad y_n = y_{n-1} + \frac{1}{2} h (f_n + f_{n-1})$ (Trapezoidal) $\quad$ (4.14)

$m = 2$: $\quad y_n = y_{n-1} + \frac{1}{12} h (5 f_n + 8 f_{n-1} - f_{n-2})$ $\quad$ (4.15)

$m=3$: $y_n = y_{n-1} + \frac{1}{24} h \left(9f_n + 19 f_{n-1} - 5 f_{n-2} + f_{n-3}\right)$ (4.16)

(3) <u>Nyström methods</u>:

$\ell = 2$, $k = n-1$ $\Rightarrow$ <u>explicit</u>

$$y_n = y_{n-2} + \sum_{\mu=0}^{m} f_{n-1-\mu} \int_{t_{n-2}}^{t_n} L_\mu^{(m)}(s)\,ds, \quad n \geq m \qquad (4.17)$$

$m=0$: $y_n = y_{n-2} + 2h f_{n-1}$ (Midpoint rule) (4.18)
(leapfrog)

(4) <u>Milne-Simpson methods</u>:

$\ell = 2$, $k = n$ $\Rightarrow$ <u>implicit</u>

$$y_n = y_{n-2} + \sum_{\mu=0}^{m} f_{n-\mu} \int_{t_{n-2}}^{t_n} L_\mu^{(m)}(s)\,ds, \quad n \geq m \qquad (4.19)$$

$m=2$: $y_n = y_{n-2} + \frac{1}{3} h \left(f_n + 4 f_{n-1} + f_{n-2}\right)$ (4.20)

<u>Rmk</u>: i) Different to RK methods, even for higher order scheme. One only need to do one new evaluation of f in each time step. (Value of previous steps can be stored. But be careful: For implicit scheme, we still need to evaluate f_n additionally to solve it)

ii) $k = n \Rightarrow$ implicit method.

② Differentiation Method:

We consider form: $y'(t) = f(t, y(t))$. And next we try to interpolate y rather f.

s.t. $p_m(t_{k-i}) = y(t_{k-i})$. $0 \le i \le m$.

Then: $\sum_{i=0}^{m} L_i^{(m)'}(t_n) y(t_{k-i}) = f(t_n, y(t_n)) + O(h^{m+1})$

Rmk: $p_m(t)$ inteplote y. $\Rightarrow p_m'(t) = f(t, y(t))$

$\rightarrow p_m'(t_k) = ch^{-1}\ \forall k$

c can be solved by set $h = t_j - t_{j-1}$

Most famous methods:

Backward differentiation formula (BDF)

$t_k = t_n \Rightarrow \sum_{\mu=0}^{m} L_\mu^{(m)'}(t_n) y_{n-\mu} = f_n, \ n \ge m \quad (4.23)$

$m=1: \quad y_n - y_{n-1} = hf_n$ (impl E) $\quad (4.24)$

$m=2: \quad y_n - \frac{4}{3} y_{n-1} + \frac{1}{3} y_{n-2} = \frac{2}{3} hf_n \quad (4.25)$

$m=3: \quad y_n - \frac{18}{11} y_{n-1} + \frac{9}{11} y_{n-2} - \frac{2}{11} y_{n-3} = \frac{6}{11} hf_n \quad (4.26)$

And we can combine it with RK method by choosing $\{\alpha_k\}_0^k$, $\{\beta_k\}_0^k$ to get general k-step formula: $\sum_{r=1}^{k} \alpha_{k-r} y_{n-r} = h \sum_{0}^{k} \beta_{k-r} f_{n-r}$.

Where $\alpha_k = 1$ (normalization). $|\alpha_0| + |\beta_0| \neq 0$.

(So that $n-k$ is the oldest step)

Rmk: i) For $\beta_k = 0 \Rightarrow$ explicit

For $\beta_k \neq 0 \Rightarrow$ implicit

ii) Different from method ①. We store the value $\{y_k\}$ rather $\{f_k\}$ (But it need to eval. f_n for every n)

For $t_k - t_{k-1} \neq h$. We can extend the method:

$\sum_0^k \alpha_{n,k-r} y_{n-r} = h_n \sum_0^k \beta_{n,k-r} f_{n-r}$ where the coefficients $\{\alpha_{k,k-r}\}, \{\beta_{k,k-r}\}$ depend on the dist. of $\{t_k\}$.

Rmk: So it'll be significantly difficult to do the adaptive time stepping than RK-method.

(2) Consistency and Convergence:

Def: Truncated error is defined as $\tau_n :=$

$h^{-1} \sum_{r=0}^k \alpha_{k-r}\, y(t_{n-r}) - \sum_{r=0}^k \beta_{k-r} f(t_{n-r}, y(t_{n-r}))$

Rmk: As RK method, we insert exact solution into the one-step formula and divided by h

Lem. Under exact starting values condition: $y_{n-r} = y(t_{n-r})$. $r=1,\cdots k$. For explicit LMM i.e. $\beta_k = 0$. We have $y(t_n) - y_n = h z_n$. For general case: $y(t_n) - y_n = (1+O(hL|\beta_k|))h z_n$

L is Lip. const. of f

Pf: Note LMM scheme holds:

$$\sum_{r=0}^{k} \alpha_{k-r} y_{n-r} - h\sum_{r=0}^{k} \beta_{k-r} f_{n-r} = 0.$$

Subtract hz_n and use the cond.

$$\Rightarrow \alpha_k (y(t_n) - y_n) - h\beta_k (f(t_n, y(t_n)) - f(t_n, y_n)) = h z_n. \text{ (only "}r=0\text{" left)}$$

Let $\beta_k = 0$. We get first claim

Set $e_n = y(t_n) - y_n$.

$$\alpha_k e_n - h z_n = h\beta_k (f(t_n, y(t_n)) - f(t_n, y_n))$$

$$\overset{\alpha_k=1}{\Rightarrow} \|h z_n - e_n\| \overset{\text{Lip.}}{\leq} h|\beta_k| L \|e_n\|$$

So $e_n = h z_n + \delta_n$. $\|\delta_n\| \leq hL|\beta_k| \|e_n\|$

$$\Rightarrow e_n \approx h z_n + hL|\beta_k| e_n.$$

i.e. $e_n \approx (1 - hL|\beta_k|)^{-1} h z_n$

$\approx (1 + O(hL|\beta_k|)) h z_n$.

Def: A LMM is consistent with IVP if $\max_{0 \le n \le N} \|z_n\| \to 0$ $(h \to 0)$. It's of order p if for suff. smooth solution $y(t)$. s.t. $\max_{0 \le n \le N} \|z_n\| = O(h^p)$.

Lem. (Truncation error)

The truncation error of a LMM for an analytic sol. $y(t)$ can be written:

$z(t) = h^{-1} \sum_{i \ge 0} c_i h^i y^{(i)}(t)$ with $c_0 = \sum_0^k \alpha_{k-r}$

and $c_i = (-1)^i \left(\frac{1}{i!} \sum_{r=0}^{k} r^i \alpha_{k-r} + \frac{1}{(i-1)!} \sum_{r=0}^{k} r^{i-1} \beta_{k-r} \right)$

Pf: Taylor expand on $y(t_{n-r}) = y(t_n - rh)$

and $f_{n-r} = f(t_n - rh, y(t_n - rh))$ at t_n

Then plug it into z. $\square$.

Rmk: It's consistent if $c_0 = c_1 = 0$. i.e.

$\sum_0^k \alpha_{k-r} = 0$. $\sum_0^k r\alpha_{k-r} + \beta_{k-r} = 0$.

It's of order p if $c_0 = c_1 = \dots = c_p = 0$.

and $C_{p+1} \neq 0$. (also called error const.)

e.g. For 2-step method of consistency order 3 has form: ($\alpha \neq -1$ for $C_4 = -\frac{1}{4!}(1+\alpha) \neq 0$)

$y_n - (1+\alpha) y_{n-1} + \alpha y_{n-2} = \frac{1}{12} h [(5+\alpha) f_n + 8(1-\alpha) f_{n-1} - (1+5\alpha) f_{n-2}]$.

Rmk: For $\alpha = -1 \Rightarrow C_4 = 0$ but $C_5 \neq 0$.

it's Simpson method of order $p=4$.

For $\alpha = 0$: it's 2-step Adam-Moulton

For $\alpha = -5$: it's explicit but not a convergent method.

Def: A LMM is convergent for IVP if starting values $\max_{0 \le j \le k-1} \|y_j - y(t_j)\| \to 0$ ($h \to 0$) holds $\Rightarrow$ $\max_{1 \le n \le N} \|y_n - y(t_n)\| \to 0$ ($h \to 0$)

Rmk: Different to RK schemes which inherit stab. of Lip func f for LMM case: Consistency $\not\Rightarrow$ Convergence

e.g. $\alpha = -5$ in Rmk above.

Def: For a LMM. We set:

i) 1st characteristic polynomial is def by $\rho(\lambda) := \sum_{r=0}^{k} \alpha_r \lambda^r$.

ii) 2nd characteristic polynomial is def by $\sigma(\lambda) := \sum_{r=0}^{k} \beta_r \lambda^r$.

Rmk: To be consistent, it's equi. with:

$\rho(1) = 0$ and $\rho'(1) = -\sigma(1)$.

Def: A LMM is zero-stable if roots $\lambda_i \in \mathbb{C}$ of $\rho(\lambda)$ satisfy:

a) $|\lambda_i| \le 1 \ \forall i$. b) $|\lambda_i| = 1 \Rightarrow \lambda_i$ is simple.

Lem. If a LMM is convergent. Then: for roots $\lambda_i \in \mathbb{C}$ of $\rho(\lambda)$ should satisfy $|\lambda_i| \le 1$ if λ_i is simple; $|\lambda_i| < 1$ if λ_i is multiple root. (i.e. zero stable)

Pf: $\max_{0 \le n \le N} \| y_n - y(t_n) \| \to 0$ for $\forall$ IVP with converging starting value cond. $\Rightarrow$

In particular it holds for $\begin{cases} y'(t) = 0 \\ y(0) = 0. \end{cases}$

which has unique sol. $y(t) \equiv 0$.

So: LMM reduces to $\sum_{0}^{k} \alpha_{k-r} y_{k-r} \overset{f=0}{=} 0$.

Assume $y_n = \lambda^n$. Next we find λ s.t.

$\sum_0^k \alpha_{k-r} \lambda^{n-r} = \lambda^{n-k} \rho(\lambda) = 0$ holds

So: roots (λ_i) of $\rho(\lambda)$ generates sol. of LMM scheme through $y_n = \lambda_i^n$.

Besides, if λ_i is multiple root of $\rho(\lambda)$

$\Rightarrow y_n = n\lambda_i^n$ is also sol. of LMM scheme by using $\rho(\lambda_i) = \rho'(\lambda_i) = 0$.

Set $y_n = h(\lambda_1^n + n\lambda_2^n)$. where λ_1 is some simple root and λ_2 is some multiple.

$\Rightarrow$ a) $y_n \to 0 \ (h \to 0)$. $\forall n \leq k-1$. (Converging start value)

b) y_n solve LMM scheme.

So with LMM converge. We have:

$y_N = h(\lambda_1^N + N\lambda_2^N) \to 0. \ (h \to 0)$

Since $h = T/N$. T fixed. So:

$\frac{T}{N}(\lambda_1^N + N\lambda_2^N) \to 0 \ (N \to \infty$, i.e. $h \to 0)$

$\Rightarrow |\lambda_1| \leq 1$ & $|\lambda_2| < 1$

Next, we want to figure out whether

the zero-stability is sufficient condition:

Consider perturbed LMM scheme: $\tilde{y}_n = y_n + e_n$.

$n = 0, \cdots k-1$; $\sum_{r=0}^{k} \alpha_{n-r} \tilde{y}_{n-r} = h \sum_{r=0}^{k} \beta_{k-r} f(t_{n-r}, \tilde{y}_{n-r}) + \xi_n$

Rmk. If L is global Lip. const. of f. Apply Banach fixed pt Thm: $\beta_k \neq 0$, $h < 1/L|\beta_k|$ $\Rightarrow$ $(\tilde{y}_n)$. $n \geq 0$ are uniquely determined. (Note $\beta_k \neq 0 \Rightarrow$ implicit method)

Thm. (Discrete stability)

If f is globally Lip. conti. on $I \times \mathbb{R}^k$ and let LMM be zero-stable. Then: $h < 1/L|\beta_k|$. $\beta_k \neq 0$ $\Rightarrow$ $\exists$ 2 sol's y_n. $\tilde{y}_n$ of LMM scheme & perturbed LMM scheme respectively. st. $\exists$ const. K. $\Gamma > 0$

$$\|\tilde{y}_n - y_n\| \leq K e^{\Gamma(t_n - t_0)} \left(\max_{0 \leq i \leq k-1} \|e_i\| + \sum_{k}^{n} \|\xi_j\| \right)$$

for $n \geq k$. where K. Γ depend on L and α_r. β_r. $r = 0 \cdots k$. St. K. $\Gamma \to \infty$ for $h|\beta_k|L \to 1$.

Pf: For $\lambda = 1$: Set $e_n \stackrel{\Delta}{=} \tilde{y}_n - y_n = e_n$

Subtract LMM schemes of $y_n, \tilde{y}_n$:

$$e_n = -\sum_{r=1}^{k} \alpha_{k-r} e_{n-r} + h\beta_k (f(t_n, \tilde{y}_n) - f(t_n, y_n))$$

$$+ h \sum_{r=1}^{k} \beta_{k-r} (f(t_{n-r}, \tilde{y}_{n-r}) - f(t_{n-r}, y_{n-r})) + \rho_n$$

(To use Lip. of f)

Set $b_n = h \sum_{r=1}^{k} \beta_{k-r} (f(t_{n-r}, \tilde{y}_{n-r}) - f(t_{n-r}, y_{n-r})) + \rho_n$.

and $\sigma_n = (f(t_n, \tilde{y}_n) - f(t_n, y_n)) / e_n \cdot I_{\{e_n \neq 0\}}$.

So: $|\sigma_n| \stackrel{Lip}{\leq} L \, I_{\{e_n \neq 0\}}$.

Now $e_n = -\sum_{r=1}^{k} \alpha_{k-r} e_{n-r} + h\beta_k \sigma_n e_n + b_n$

i.e. $(1 - h\beta_k \sigma_n) e_n = -\sum_{r=0}^{k} \alpha_{k-r} e_{k-r} + b_n$.

It can be written: $D_n E_n = C_n A E_{n-1} + B_n$

Where $E_n = (e_{n-k}, \cdots e_{n-1}, e_n)^T \in \mathbb{R}^{k+1}$. $B_n = (0, \cdots 0, b_n)^T \in \mathbb{R}^{k+1}$. $D_n = \text{diag}\{1 - h\beta_k \sigma_{n-k}, \cdots 1 - h\beta_k \sigma_n\}$. $C_n = \text{diag}\{1 - h\beta_k \sigma_{n-k}, \cdots, 1 - h\beta_k \sigma_{n-1}, 1\}$. $A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & & 1 & & \\ & \ddots & & \ddots & \\ & & \ddots & 0 & 1 \\ 0 & -\alpha_0 & \cdots & \cdots & -\alpha_{k-1} \end{pmatrix} \in \mathbb{R}^{k+1}$

(Only n^{th} component is nontrivial relation)

So if $h < 1/L|\beta_k|$, then D_n is invertible.

$\Rightarrow E_n = D_n^{-1}(C_n A E_{n-1} + B_n)$. $n \geq 1$

Note A is Frobenius matrix has eigenfunc.:

$f_A(\lambda) = \sum_{i=0}^{k} \lambda^{k+1-i} \alpha_{k-i} = \lambda g(\lambda)$. g is 1^{st} ch. poly.

<u>Lem.</u> $\forall A \in \mathbb{C}^{m\times m}$. $\forall \varepsilon > 0$. $\exists$ induced matrix norm $\|\cdot\|_{A,\varepsilon}^{(A)}$

s.t. for spectral radius $r(A) = \max\{|\lambda_i| : \lambda_i$ is eigenvalues of $A\}$. We have:

$$r(A) \leq \|A\|_{A,\varepsilon} \leq r(A) + \varepsilon.$$

Besides, if $\forall$ eigenvalue λ, s.t. $|\lambda| = r(A)$ is simple. $\Rightarrow \exists$ induced norm $\|\cdot\|_0$, s.t. $r(A) = \|A\|_0$.

<u>Ref</u>: (A) is norm on matrix induced from vector norm $\|\cdot\|$ by $\|A\| = \max_{x\neq 0} \|Ax\|/\|x\|$.

$\Rightarrow \exists \|\cdot\|_0$ s.t. $\|A\|_0 = r(A) \leq 1$ by zero-stability.

So: $\|E_n\|_0 \leq \|D_n^{-1}\|_0 (\|C_n\|_0 \|E_{n-1}\|_0 + \|B_n\|_0)$

Then: $\|E_n\|_0 \leq \Gamma \sum_0^{n-1} h \|E_i\|_0 + \|E_0\|_0 + \Lambda \sum_1^{n} |\delta_i|$

where $\Gamma = \gamma^2 |\beta_k| L (1 + h\gamma^2 |\beta_k| L) / 1 - h|\beta_k| L + \gamma^2 L (|\beta_k| + \beta)$

$\Lambda = \gamma(1 + h\gamma^2 |\beta_k| L / 1 - h|\beta_k| L)$. $\gamma = \mathrm{const}(k)$

Apply discrete Grownwall's Lem.:

$\|E_n\|_0 \le e^{\Gamma(t_n - t_0)} (\|E_0\|_0 + \Lambda \sum^{n} |\zeta_i|)$

Use equiv. of norm.: $K = C\Lambda \to \infty$ $(h|\beta_k|L \to 1)$

Rmk: For explicit method, we also have such estimate (But const. are different) without cond.: $h < 1/|\beta_k|L$.

Thm. (Convergence)

f is globally Lip. and LMM is zero-stable $h < 1/|\beta_k|L$ $(\beta_k \neq 0)$. $\delta_h = \max_{0 \le k \le k-1} \|\eta_k - y(t_k)\| \xrightarrow{h \to 0} 0$.

Then: Consistency is sufficient for convergence. i.e. $\max_{0 \le n \le N} \|\eta_n - y(t_n)\| \to 0$ $(h \to 0)$ and

$\|\eta_n - y(t_n)\| \le K e^{\Gamma(t_n - t_0)} (\delta_h + (t_n - t_0) \max_{k \le k \le n} \|z_k\|)$

where z_i is truncated error and K, Γ are const. on Thm above.

Rmk: $\delta_h \to 0$ is converging starting value cond. we defined before. which means $\{\eta_k\}_{k \le k-1}$ are already closed to exact solution for k^{th}-step.

Pf: Note that exact sol. $y(t)$ satisfies perturbed LMM scheme:

$y(t_n) = y_n + (y(t_n) - y_n) \triangleq y_n + e_n$

and $\sum_0^k \alpha_{k-r}\, y(t_{n-r}) = h \sum_0^k \beta_{k-r} f(t_{n-r}, y(t_{n-r})) + h Z_n$. (def of Z_n)

$\Rightarrow g_n = h Z_n$. Apply Thm above.

So: f Lip. + zero-stable + consistent of order p.

$\Rightarrow$ Convergence of order p

Thm. LMM of type:

i) Adams - Bashforth ii) Adam - Moulton

iii) Nystrim iv) Milne - Simpson

are all convergent.

Pf: 1) Consistency: Note they all use poly. $P_m(t)$ of degree m to fit the LMM.

$\Rightarrow$ It has at least order $m+2-1 = m+1$ by (1) ①.

2) Zero - Stab.: They all have forms: $\alpha_k = 1$ and $\alpha_{k-1} = 1$. or $\alpha_{k-2} = -1$.

$\Rightarrow \rho(\lambda) = \lambda^k - \lambda^{k-1}$ or $\lambda^k - \lambda^{k-2}$.

which satisfies zero - stability.

Rmk: For BDF method:

a) $k \leq 6 \Rightarrow$ zero stable

b) $k \geq 7 \Rightarrow$ not zero stable!

Note for k-step LMM:

i) Implicit method has $2(k+1)-1$ free parameters

($\alpha_k = 1$ fixed)

ii) Explicit method has $2(k+1)-1-1$ free parameters

($\alpha_k = 1$ and $\beta_k = 0$ fixed)

$\Rightarrow$ Ideally, let $C_i = 0$ for as many i as possible.

We can achieve order $2k$ & $2k-1$.

But it's not true:

Thm. (First Dahlquist Barrier)

Zero stable k-step method can't attain the order $m > k+2$ if k even.

$m > k+1$ if k odd.

For explicit k-step method: the max order is $m = k$

Rmk: Zero-stable k-step method with order $k+2$ is called optimal. (e.g. Simpson's)

(3) <u>Numerical Stab.:</u>

Apply LMM on model problem: $y'(t) = \lambda y(t)$.

We have: $\sum_{r=0}^{k} \alpha_{k-r} y_{n-r} = h \sum_{r=0}^{k} \beta_{k-r} \lambda y_{n-r}$. $(*)$

$\Rightarrow \sum_{r=0}^{k} (\alpha_{k-r} - h\lambda\beta_{k-r}) y_{n-r} = 0$. Let $z = h\lambda$.

<u>Def</u>: Stab. region of an LMM $:= \{ z \in \mathbb{C} \mid \forall$

$\{y_n\}$ sol. of $(*)$ for $Re\,\lambda < 0$ stay bdd

when $n \to \infty \}$.

The LMM is A-stable if its stab.

region $\supseteq \{ x+iy \in \mathbb{C} \mid x \leq 0 \}$.

<u>Def</u>: Stab. polynomial of LMM is $\pi(\lambda, z) :=$

$\sum_{r=0}^{k} (\alpha_r - z\beta_r) \lambda^r = \rho(\lambda) - z\sigma(\lambda)$.

Note $\forall$ sol. $\{y_n\}$ of $(*)$ stay bdd require:

$|\lambda_i| \leq 1$ $\forall i$. and $|\lambda_i| < 1$ for λ_i is multiple

where (λ_i) is root of $\pi(\lambda, z)$.

So we call LMM is absolutely stable for

$z \neq 0$ if there holds.

<u>Rmk</u>: It motivates from: $y_n = \lambda_i^n$ or $n\lambda_i^n$

satisfies $\sum_{0}^{k} \alpha_{k-r} y_{n-r} = 0$. where λ_i is simple or multiple root of $g(\lambda)$. We can also replace y_{n-r} by λ^{n-r} in (*)

e.g. For $\pi(\lambda, z) = \rho(\lambda) - z\sigma(\lambda)$. First solve $\{\lambda_i(z)\}$. Let $|\lambda_i(z)| < 1$ or ≤ 1.

$\Rightarrow$ Restrict SR inside this domain.

We prefer A-stable methods for stiff problem. But we have following restriction:

Thm. i) An explicit LMM can't be A-stable.

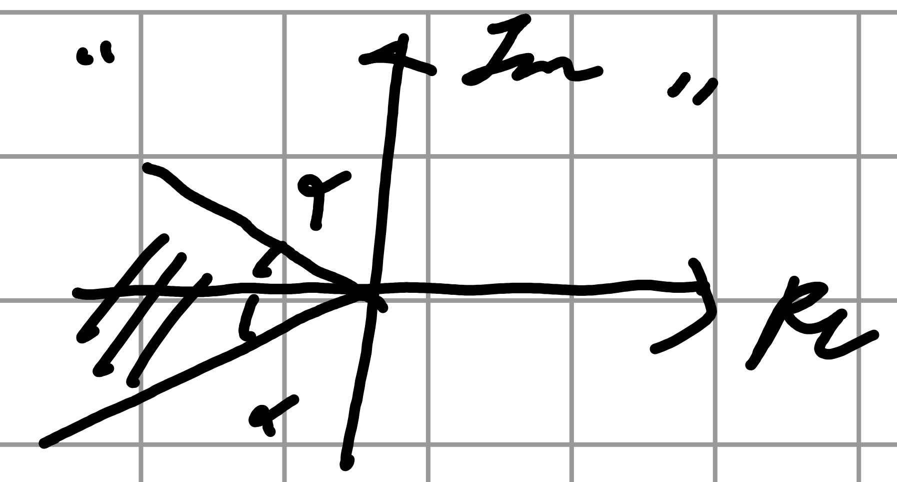
ii) Order of A-stable implicit LMM can not be higher than $p=2$.

iii) The A-stable implicit LMM with order $p=2$ with smallest error const. is the trapezoidal rule.

Rmk: In RK method. Radau method is implicit L-stable with order $2s-1 > 2$

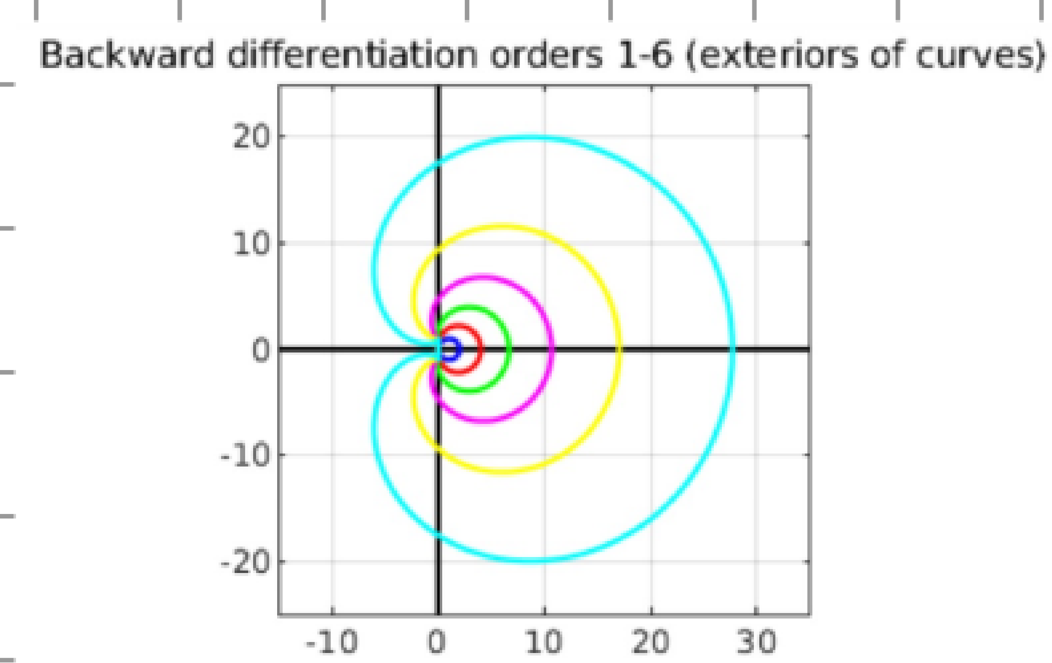
It's too demanding to require A-stable. So:

Def: A method is called $A(\alpha)$-stable for $\alpha \in (0, \frac{\pi}{2})$ if it stab. region contains



(So it's $A(0)$-stable if it contains negative x-axis)

<u>Rmk</u>: i) It motivates from SR of BDF:



When order ↑ after order > 2. ⇒ Its angle of SR will ↓.

ii) $A(0)$-stable method is well-suited to solve stiff IVPs with only real negative eigenvalue of $f_x(t, y(t))$

<u>e.g.</u> Heat equation $u_t = u_{xx}$.

Note for $\pi(\lambda, z) = \rho(\lambda) - z\sigma(\lambda)$. when $z = \lambda h \to -\infty$ ⇒ $\sigma(\lambda)$ is dominant. ⇒ roots of $\sigma(\lambda)$ will be dominant for stability.

So we need to choose $\{\lambda_i\}$ roots of $\sigma(\lambda)$ well inside unit ball $\{|z|<1\}$. <u>e.g.</u> BDF method has $\sigma(\lambda) = \beta_k \lambda^k$. Whose root falls on center.

(4) <u>Practical Aspects</u>:

① <u>Computation of start. value</u>:

Note LMM with k steps to compute y_n requires values $y_{n-1}, \cdots y_{n-k}$ which're not provided by IVP. So, we split LMM into:

i) Starting phase: compute starting pt $\{y_k\}_{n-k}^{n-1}$

ii) Run phase: execute LMM.

e.g. To apply BDF-2: $y_n - \frac{4}{3} y_{n-1} + \frac{1}{3} y_{n-2} = \frac{2}{3} h f_n$.

with y_0 given. We want to get y_1 to start BDF-2. The idea:

We use BDF-1 to get y_1 from y_0 at 1^{st} step. Then apply remaining $N-1$ steps with BDF-2. $\Rightarrow$ Order of error is:

$y_0 \to y_1$: $O(h^2)$.

$N-1$ step: $O(h^3) \cdot \underbrace{(N-1)}_{\sim h^{-1}} = O(h^2)$.

i.e. It's still method of order 2.

More generally to start a LMM of order p we need to use method of order $\geq p-1$ to retain the order of consistency:

We can use one-step method (e.g. RK schemes

Rmk: Since we only need $R-1$ steps of RK

Extra effort barely affects computation cost. $\Rightarrow$ One'd like to use the higher order method to keep initial error $\downarrow$

Alternatively people use Self-starting procedure: Use methods from same class of LMM with increasing R. e.g. BDF-1. BDF-2. BDF-3 ...

Rmk: The 1^{st}-step will negatively affect the desired order 3 since its local error is just $O(h^2)$. But we can use very small initial time step to avoid it.

③ Solution of implicit system:

Consider implicit LMM: $y_n - h\beta_R f(t_n, y_n) - g_n = 0$

where $g_n = h\sum_{r=1}^{R} \beta_{R-r} f_{n-r} - \sum_{r=1}^{R} a_{R-r} y_{n-r}$.

Recall for $h < 1/L|\beta_R|$. y_n is uniquely solved where L is Lip. const. of f:

method 1: Fixed point iteration

With start value $y_n^{(0)}$: $y_n^{(k+1)} = h\beta_R f(t_n, y_n^{(k)}) + g_n$

$\Rightarrow \|y_n^{(k)} - y_n\| \le q^k \|y_n^{(0)} - y_n\|$. $q = hL|\beta_k| < 1$ holds.

Rmk: For $L \sim 1$. Note accuracy of approxi. $\{y_n^{(k)}\}_k$ to y_n $\uparrow$. But for a LMM of order p. We want its local error to be order $p+1$ $\Rightarrow$ We can stop after $p+1$ iteration.

But for $L \gg 1$ (e.g. Stiff problem). We'd better to use:

method 2: Newton's method

Set $F(x) = x - h\beta_k f(t_n, x) - g_n$. So we have:

$$F'(x) = \mathbb{1} - h\beta_k f_x(t_n, x)$$

$$\Delta y_n^{(k)} = F(y_n^{(k)}) \cdot F'(y_n^{(k)})^{-1} \Rightarrow y_n^{(k+1)} = y_n^{(k)} + \Delta y_n^{(k)}.$$

③ Predictor - Corrector method:

It's a variant of using fixed pt. iteration for implicit LMM.

Idea: Try to find a good estimate for $y_n^{(0)}$ by other explicit LMM once.

e.g.: Predictor is from Adams-Bashforth of order 4 : $y_n^{(0)} = P(y_{n-1}, \cdots y_{n-4})$

Corrector is from Adam-Moulton of

order 4 : $f_n^{(k-1)} = E(y_n^{(k-1)})$

$$y_n^{(k)} = C(y_{n-1}, \cdots y_{n-3}, f_n^{(k-1)})$$

We run many iterations of "$E \to C$" in

specific number M. i.e.

$P(EC)^M : P \to E \to C \to E \to C \to \cdots\cdots$

Milne device:

Predictor-corrector method can be used for local error estimate and then for step length control:

e.g. Assume we have exact starting value

And given predictor, by expansion:

$$y_n^p = y_n^{(0)} = y(t_n) - C_5^{(p)} h^5 y^{(5)}(t_n) + O(h^6)$$

And after k iterations in corrector:

$$y_n^{(k)} = y(t_n) - C_5^{(c)} h^5 y^{(5)}(t_n) + O(h^6).$$ value

Compare these two equations, we can solve $y^{(5)}(t_n)$

$= (y_n^{(k)} - y_n^{(0)}) / h^5 (C_5^{(P)} - C_5^{(C)}) + O(h)$

So: we have: $z_n = |y_n^{(k)} - y(t_n)|$

$= |-C_5^{(C)} h^5 y^{(5)}(t_n) + O(h^6)|$

i.e. $z_n = \dfrac{C_5^{(C)}}{C_5^{(P)} - C_5^{(C)}} \cdot (y_n^{(k)} - y_n^{(0)}) / h + O(h^5)$

which's estimate for this step.