Lecture Multistep methods 1. Introductory

- $[t_0, T]$, $\{t_i\}_{i=0}^{N}$ $t_i = t_0 + i \frac{T-t_0}{N}$
- One-step methods: progress from y_i to compute y_{i+1}, no "memory" of earlier time-steps
- **Example**: Assume y_i, y_{i+1} are given. We know that

$$y(t_{n+2}) - y(t_n) = \int_{t_n}^{t_{n+2}} y'(t)\,dt = \int_{t_n}^{t_{n+2}} f(t, y(t))\,dt \quad *)$$

- Applying the midpoint quadrature rule yields the two-step method

$$y_{n+2} - y_n = 2\tau f(t_{n+1}, y_{n+1}),$$

also known as leap-frog method.

Definition

A k-step linear multistep method (LMM) applied to the IVP

$$\begin{cases} y' = f(t,y) \\ y(t_0) = y_0 \end{cases}$$

is given by

$$\sum_{\ell=0}^{k} \alpha_\ell y_{n+\ell} = \underbrace{\tau \sum_{\ell=0}^{k} \beta_\ell f_{n+\ell}}_{=: \Phi(t_n, y_n, \dots, y_{n+k}, \tau)}$$

where $\{\alpha_\ell\}_{\ell=0}^{k}$, $\{\beta_\ell\}_{\ell=0}^{k}$ are the coefficients of the method, and $f_{n+\ell} := f(t_{n+\ell}, y_{n+\ell})$.

- **Remarks**

a) To get started, a k-step LMM needs k values $y_\ell \approx y(t_\ell)$ $\ell = 0, \dots, k-1$.
(Initial / startup phase). Needs to store $k-1$ values to get y_{i+k}.

b) Usually we require that $\alpha_k = 1$ and $|\alpha_0| + |\beta_0| \neq 0$

c) If $\beta_k = 0$ $\Rightarrow$ LMM is explicit, otherwise it is called implicit.

- **Question**: Convergence properties of a general LMM?

2) Consistency

Definition

A multistep method is said to be consistent of order p if the local discretization/truncation error

$$\boxed{\eta(t,\tau) = \sum_{l=0}^{k} \alpha_l y(t+l\tau) - \tau \Phi(t, y(t), y(t+\tau), \dots, y(t+k\tau), \tau)}$$

satisfies the condition

$$\eta(t,\tau) = \mathcal{O}(\tau^{p+1}), \quad \tau \to 0$$

- Very similar to definition for OSM.

THM: (Consistency of k-step LMM)

A k-step LMM has consistency order p $\Leftrightarrow$

$$C_0 := \sum_{l=0}^{k} \alpha_l = 0 \quad \text{and} \quad C_q := \frac{1}{q!} \sum_{l=0}^{k} (l^q \alpha_l - q l^{q-1} \beta_l) = 0$$

for $q = 1, \dots, p$.

Proof. (sketch) Do a Taylor-expansion of

$y(t_i + l\tau)$ and $y'(t_i + l\tau) = f(t+l\tau, y(t+l\tau))$

around t_i, insert this into:

$$\eta(t,\tau) = \sum_{l=0}^{k} \alpha_l y(t+l\tau) - \tau \sum_{l=0}^{k} \beta_l f($$

$$= \sum_{l=0}^{k} \alpha_l y(t+l\tau) - \tau \sum_{l=0}^{k} \beta_l y'(t+l\tau).$$

$$y(t+l\tau) = y(t) + \frac{(l\tau)}{1!} y'(t) + \frac{(l\tau)^2}{2!} y''(t) + \dots \frac{(l\tau)^q}{q!} y^{(q)}(t)$$

$$y'(t+l\tau) = y'(t) + \frac{(l\tau)}{1!} y''(t) + \dots \frac{(l\tau)^{q-1}}{(q-1)!} y^{(q)}(t).$$

Then the Taylor expansion of $\eta(t,\tau)$ around t is

$$\eta(t,\tau) = \sum_{l=0}^{k} \alpha_l y(t) + \frac{\tau}{1!} y'(t) \left(\sum_{l=0}^{k} \alpha_l l - \sum_{l=0}^{k} \beta_l \right)$$

$$+ \frac{\tau^2}{2!} y''(t) \left(\sum_{l=0}^{k} (\alpha_l l^2 - 2 l \beta_l) \right)$$

$$+ \dots \frac{\tau^q}{q!} y^{(q)}(t) \left(\sum_{l=0}^{k} \alpha_l l^q - q l^{q-1} \beta_l \right) + \mathcal{O}(\tau^{q+1}).$$

$\square$

Questions Is ensuring consistency already enough to design a convergent LMM?

Recall: For OSM, p-consistency + Lipschitz condition $\Rightarrow$ p-convergence.

3 Linear difference equations

Want to solve linear difference equation

$$\sum_{\ell=0}^{k} \alpha_\ell y_{n+\ell} = \varphi_n \qquad n = 0, 1, \ldots \qquad *_1)$$

yielding a solution sequence $\{y_n\}$ of numbers (or vectors)

- Now let $\{\tilde{y}_n\}$ be the general solution to the homogeneous problem

$$\sum_{\ell=0}^{k} \alpha_\ell y_{n+\ell} = 0 \qquad *_2)$$

- The general solution $\{y_n\}$ the inhomogeneous problem $*_1)$ can be represented as

$$y_n = \tilde{y}_n + \psi_n$$

where ψ_n is one particular solution of the inhomogeneous problem.

- Unique solution requires to set starting values $y_0, y_1, \ldots y_{k-1}$.

- Try $\tilde{y}_n = r^n$ for some $r \in \mathbb{R}$ as a solution
This is true if

$$0 = \sum_{\ell=0}^{k} \alpha_\ell r^{n+\ell} = r^n \underbrace{\sum_{\ell=0}^{k} \alpha_\ell r^\ell}_{\rho(r)}$$

<u>Definition</u>. $\rho(r)$ is called the (first) characteristic polynomial of a L.D.E.

- $\{r^n\}$ is a solution to $*_2)$ if r is a root of the characteristic polynomial.

- $\rho(r)$ - polynomial of order k
$\Rightarrow$ k roots $r_1, \ldots, r_k$.
If distinct simple $\{r_1^n\}, \ldots \{r_k^n\}$ are a linearly independent set of solutions to the homogeneous equation. $*)_2$

- For multiple roots say $r_1 = r_2 \ldots r_\mu$
$\{r_1^n\}, \{n r_1^n\}, \ldots \{n^{\mu-1} r_1^n\}$ linear ind. set of solutions. $\Rightarrow$ Found k- independent solutions $\{\tilde{y}_{n,\ell}\}$

$$y_n = \sum_{\ell=1}^{k} \gamma_\ell \tilde{y}_{n,\ell} + \psi_n \,. \qquad \text{sol}$$

Theorem

If $\varrho(r)$ has only k simple roots $r_1, \ldots, r_k$ then the solution sequence $\{\tilde{y}_n\}$ (to $*_2$) can be written as:

$$\tilde{y}_n = \sum_{\ell=1}^{k} \gamma_\ell \, r_\ell^n \qquad n = 0, 1, \ldots,$$

with $\gamma_\ell \in \mathbb{C}$.

$\boxed{\text{Proof}}$: Only sketched idea

Example

$$y'(t) = 0, \qquad y(0) = 0.1 \;\Rightarrow\; y(t) = 0.1$$

Consider the explicit LMM

$$y_{n+2} + 4\,y_{n+1} - 5\,y_n = \Delta t\left(4\, f(t_{n+1}, y_{n+1}) + 2 \cdot f(t_n, y_n)\right)$$

- Exercise: Determine coefficients $\{\alpha_\ell\}_{\ell=0}^{2}$ $\{\beta_\ell\}$ and show that this method has consistency order 3.
(see Example 8.3 for solution).

- Homogeneous difference equations:

$$y_{n+2} + 4\,y_{n+1} - 5\,y_n = 0$$

$$y_n = \gamma_1 r_1^n + \gamma_2 r_2^n \qquad r_1, r_2 \text{ root of the charact polynom}$$

$$\varrho(r) = r^2 + 4r - 5 = (r-1)(r+5).$$

$$\Rightarrow \; r_1 = 1, \quad r_2 = -5$$

- Take initial values $y_0 = 0.1$, $y_1 = 0.1 + \varepsilon$ with a small perturbation ε.

$$0.1 = \gamma_1 + \gamma_2$$

$$0.1 + \varepsilon = \gamma_1 - 5\gamma_2$$

$$\Rightarrow \boxed{\begin{array}{l} \gamma_1 = 0.1 + \frac{\varepsilon}{6} \\ \gamma_2 = -\frac{\varepsilon}{6} \end{array}}$$

$$\Rightarrow \tilde{y}_n = \left(0.1 + \frac{\varepsilon}{6}\right) \cdot 1^n - \frac{\varepsilon}{6}(-5)^n$$

$\tau = \frac{T}{n}$ for some $n \in \mathbb{N}$ then

$$\lim_{n \to \infty} |y(T) - y_n| = \lim \left| \left(\frac{\varepsilon}{6} - \frac{\varepsilon}{6}(-5)^n \right) \right| = \infty$$

No convergence :

Observation : Problem is the root $r_2 = -5$ leading to the divergence of the scheme

Definition

A k-step LMM is called zero-stable if the characteristic polynomial $\rho(r) = \sum_{l=0}^{k} \alpha_l r^l$ satisfies the Dahlquist root condition:

i) $|r_i| \leq 1$ for $i = 1, 2, \dots k$

ii) $|r_i| < 1$ for multiple roots

4) Convergence

Definition : A LMM with initial values

$$y_i = y(t_i) + \mathcal{O}(\tau^p) \quad \tau \to 0 \quad , \; i = 0, \dots k-1$$

is called convergent of order p if the global discretization error

$$e(t_i, \tau) := y(t_i) - y_n \qquad i = k, \dots n$$

satisfies $e(t_i, \tau) = \mathcal{O}(\tau^p) \quad \tau \to 0$

Theorem (Dahlquist) : A LMM is convergent of order p if and only if it is consistent of order p and zero-stable

In short

$$p\text{-Convergence} \Leftrightarrow p\text{-Consistency} + \text{zero-stability}.$$

5 Examples of LMM ..

- General construction either via difference quotients or numerical quadrature ..

- Basic idea: Integration of differential equation some time-interval $[t_{i+m-r}, t_{i+m}]$

$$y(t_{i+m}) - y(t_{i+m-r}) = \int_{t_{i+m-r}}^{t_{i+m}} y'(t)\,dt$$

$$= \int_{t_{i+m-r}}^{t_{i+m}} f(t, y(t))\,dt$$

- Replace $f(t, y(t))$ by some interpolation polynomial q, we obtain the general numerical method

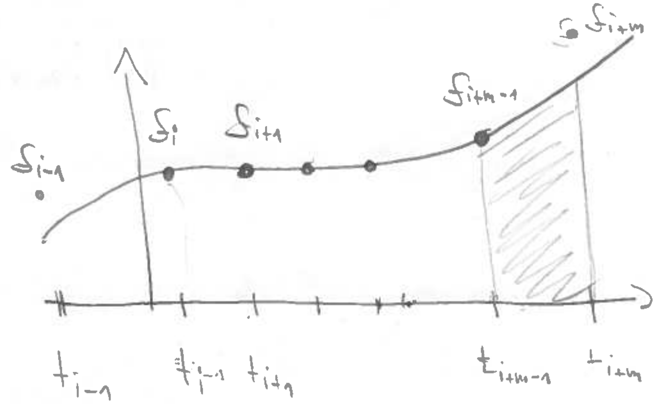
$$y_{i+m} - y_{i+m-r} = \int_{t_{i+m-r}}^{t_{i+m}} q(t)\,dt$$

- The trick is now to choose the interpolation nodes based on previously time-steps which may also lie outside of the time integration interval $[t_{i+m-r}, t_{i+m}]$

Adams-Bashforth methods:

- $r = 1$ and $q \in \mathbb{P}_{m-1}$ with

$$q(t_{i+j}) = f(t_{i+j}, y_{i+j}) \quad j = 0, \dots, m-1$$



$\boxed{\text{A-B methods are explicit, zero-stable and have consistency order } m.}$

$m = 1: \quad y_{i+1} = y_i + \tau f_i \quad (= \text{explicit Euler})$

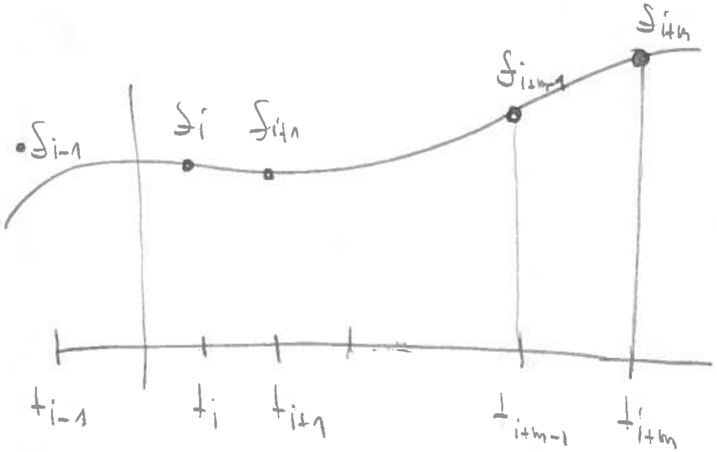
$m = 2: \quad y_{i+2} = y_{i+1} + \frac{\tau}{2}(3 f_{i+1} - f_i)$

$m = 3: \quad y_{i+3} = y_{i+2} + \frac{\tau}{12}(23 f_{i+2} - 16 f_{i+1} + 5 f_i)$

Adams-Moulton

- $r = 1$, $q \in \mathbb{P}_m$ with

$$q(t_{i+j}) = f(t_{i+j}, y_{i+j}) \quad j = 0, \dots, m.$$



- A-M methods are implicit, zero-stable and have consistency order $p = m + 1$

$m = 1$ $\quad y_{i+1} = y_i + \frac{\tau}{2}(f_{i+1} + f_i)$ ($\hat{=}$ trapezoidal rule)

$m = 2$ $\quad y_{i+2} = y_{i+1} + \frac{\tau}{12}(5 f_{i+2} + 8 f_{i+1} - f_i)$

$m = 3$ $\quad y_{i+3} = y_{i+2} + \frac{\tau}{24}(9 f_{i+3} + 19 f_{i+2} - 5 f_{i+1} + f_i)$

- Similar construction to obtain
  - Nyström methods
  - Milne-Simpson