Numerical methods for Ordinary Differential Equations

Problem: (Initial Value Problem)
Let $f(u,t)$ be a known function and $u_0 \in \mathbb{C}^N$.
Want to find a differentiable function $u(t)$ such that
(a) $u(0) = u_0$
(b) $u_t(t) = f(u(t),t)$, $\forall t \in [0,T]$.

Linear multistep formulas.

Def: An s-step linear multistep formula is a formula of the form

$$\sum_{j=0}^{s} a_j v^{n+j} = K \sum_{j=0}^{s} b_j f^{n+j}$$

with $a_s = 1$ and $a_0 \neq 0 \vee b_0 \neq 0$.
a) If $b_s = 0 \Leftrightarrow$ the LMF is explicit
b) If $b_s \neq 0 \Leftrightarrow$ the LMF is implicit

examples.
a) Euler formula: $v^{n+1} = v^n + kf^n$
b) Midpoint rule: $v^{n+1} = v^{n-1} + 2Kf^n$
c) Adams-Bashforth: $v^{n+1} = v^n + \frac{K}{24}(55f^n - 59f^{n-1} + 37f^{n-2} - 9f^{n-3})$

Remark: The purpose of LMFs is to approximate the solution of an ODE numerically. In particular, let

$$t_n = nk, \quad v^n = u(t_n), \quad f^n = f(v^n, t^n)$$

Then we want an LMF that will ~~appr~~ produce v^n that approximate the solution of

$$\dot{u} = f(u,t).$$

Convergence of LMFs.

Def: Let $\dot{u}=f(u,t)$, $u(0)=u_0$ be an initial value problem and $\sum_{j=0}^{s} a_j v^{n+j} = k\sum_{j=0}^{s} b_j f^{n+j}$ an LMF. with $v^0,\dots,v^{s-1}$ given.

a) Let $v^0(k), v^1(k),\dots, v^s(k)$ be functional representations of how we choose the LMF initialization as $k\to 0$. We say that they are consistent with the initial value problem iff

$$\lim_{k\to 0} v^n(k)=0 \quad , \forall n\in\{0,1,\dots,s-1\}.$$

b) We say that ~~an~~ the ODE is well-posed iff

i) $f(u,t)$ is continuous with respect to t.

ii) $\exists L>0 , \forall u,v\in\mathbb{C}^n , \forall t\in[0,T] : \|f(u,t)-f(v,t)\| \leq L\|u-v\|.$

c) An LMF is convergent $\Leftrightarrow$

$\forall$ well-posed ODEs , $\forall$ consistent $v^1(k), v^2(k),\dots, v^s(k)$:

$\exists \varphi(k) , \lim_{k\to 0}\varphi(k)=0 : \cancel{\forall t\in[0,T]}\ \|v^n(k)-u(nk)\| < \varphi(k). , \forall n\in\mathbb{N}^*.$

Remark: In order for an LMF to be useful, we must prove it is convergent. The following theory developed by Dahlquist explores this issue. Two fundamental concepts of this theory is consistency and stability.

Consistency of LMFs.

Def : Let $\sum_{j=0}^{s} a_j v^{n+j} = k\sum_{j=0}^{s} b_j f^{n+j}$ be an LMF. The polynomials:

$$\rho(z)=\sum_{j=0}^{s} a_j z^j \quad \text{and} \quad \sigma(z)=\sum_{j=0}^{s} b_j z^j$$

are called characteristic polynomials of the LMF.

Def : Let an LMF with characteristic polynomials $\rho(z)$ and $\sigma(z)$. and define

$$L(z) = \rho(e^{kz}) - kz\sigma(e^{kz}) = \sum_{n=0}^{+\infty} C_n (kz)^n$$

We say that

a) The LMF is consistent $\Leftrightarrow C_0 = C_1 = 0$.

b) The LMF is p-order accurate $\Leftrightarrow C_0 = C_1 = \cdots = C_p = 0 \wedge C_p \neq 0$.

Prop. : The coefficients C_n can be computed by:

$$\boxed{C_n = \sum_{j=0}^{s} \frac{a_j\, j^n}{n!} - \sum_{j=0}^{s} \frac{b_j \cdot j^{n-1}}{(n-1)!}}.$$

Thm : An LMF with characteristic polynomials $\rho(z), \sigma(z)$ is consistent $\Leftrightarrow$

$\Leftrightarrow \rho(1) = 0 \wedge \rho'(1) = \sigma(1)$.

Remark. : The prop and thm provide means to prove that an LMF is consistent and to obtain the order of accuracy. The significance of order of accuracy is given by the following theorem:

Thm : Let $\dot{u} = f(u,t)$, $u(0) = u_0$ be a well-posed initial value problem and $u^n(k)$ a discretized solution obtained by a convergent LMF with order of accuracy p and ~~initial~~ consistent ~~not~~ initialization $v^0(k), v^1(k), \ldots, v^s(k)$.

~~Then $\lim_{k\to 0} \|$~~

Then : $\exists \varphi(k) > 0$, $\lim_{k \to 0} \varphi(k) = 0$: $\dfrac{\|v^n(k) - u(nk)\|}{k^p} < \varphi(k)$, $\forall k > 0$, $\forall n \in \mathbb{N}^*$

Stability of LMFs

<u>Def</u>: An LMF with characteristic polynomials $\rho(z), \sigma(z)$ is <u>stable</u> iff all roots $\rho_1, \rho_2, \dots, \rho_m$ of $\rho(z)$ satisfy:

a) $|\rho_n| \leq 1$, $\forall n \in \{1, 2, \dots, m\}$

b) $|\rho_n| = 1 \Rightarrow \rho_n$ is a simple root of $\rho(z)$.

Dahlquist theory of convergence

<u>Thm</u> (Dahlquist equivalence theorem)
An LMF is convergent $\Leftrightarrow$ the LMF is consistent and stable

<u>Thm</u>: (1st Dahlquist stability barrier)
For a <u>stable</u> LMF with order of accuracy p and s steps:

a) If the LMF is explicit $\Rightarrow p \leq s$

b) If $s = 2n+1 \Rightarrow p \leq s+1$

c) If $s = 2n \Rightarrow p \leq s+2$

<u>Remark</u>. For a consistent LMF, $p \leq 2s$, therefore the above bounds are also bounds for convergent LMFs.

Remarkable LMFs

Adams–Bashforth formulas.

<u>Def</u> : Let v^n be an arbitrary sequence. Then:

$$\nabla v^n = v^n - v^{n-1}$$
$$\nabla^k v^n = \nabla^{k-1} v^n - \nabla^{k-1} v^{n-1}.$$

<u>Prop.</u> : $\boxed{\nabla^k v^n = \sum_{j=0}^{k} (-1)^j \binom{k}{j} v^{n-j}}$

<u>Def</u> : The s-step Adams-Bashforth formula is the LMF given by:

$$\boxed{v^{n+s} = v^{n+s-1} + k \sum_{j=0}^{s-1} \gamma_j \nabla^j f^{n+s-1}}$$

where

$$\boxed{\gamma_j = (-1)^j \int_0^1 \binom{-\tau}{j} d\tau}$$

<u>Thm</u> : The coefficients γ_j can be computed by the following reccurence:

$$\boxed{\begin{aligned} &\gamma_1 = 1 \\ &\gamma_j + \frac{1}{2}\gamma_{j-1} + \frac{1}{3}\gamma_{j-2} + \dots + \frac{1}{j+1}\gamma_0 = 1 \end{aligned}}$$

<u>Thm</u> : The s-step Adams-Bashforth LMFs are convergent, $\forall s \geq 1$.

<u>Prop.</u> : The low-order AB LMFs are given by:

a) $v^n = v^{n-1} + k\left(\frac{3}{2} f^{n-1} - \frac{1}{2} f^{n-2}\right)$ $\rightsquigarrow$ order $p=2$

b) $v^n = v^{n-1} + k\left(\frac{23}{12} f^{n-1} - \frac{16}{12} f^{n-2} + \frac{5}{12} f^{n-3}\right)$. $\rightsquigarrow$ order $p=3$

c) $v^n = v^{n-1} + k\left(\frac{55}{24} f^{n-1} - \frac{59}{24} f^{n-2} + \frac{37}{24} f^{n-3} - \frac{9}{24} f^{n-4}\right)$. $\rightsquigarrow$ order $p=4$.

Adams-Moulton formulas.

Def : The s-step Adams-Moulton LMF is defined as:

$$\boxed{v^{n+s} = v^{n+s-1} + k\sum_{j=0}^{s} \gamma_j^* \nabla^j f^{n+s}}$$

with $$\boxed{\gamma_j^* = (-1)^j \int_{-1}^{0} \binom{-\tau}{j} d\tau}$$

Prop. : The coefficients γ_j^* satisfy the following recurrence:

$$\boxed{\begin{array}{l} \gamma_1 = 1. \\ \gamma_j^* + \frac{1}{2}\gamma_{j-1}^* + \frac{1}{3}\gamma_{j-2}^* + \cdots + \frac{1}{j+1}\gamma_0^* = 0. \end{array}}$$

Thm : The Adams-Moulton LMFs are convergent, $\forall s \geq 1$. with order of accuracy $p = s+1$.

Prop : The low-order Adams-Moulton LMFs are:

a) $v^{n+1} = v^n + k\left(\frac{1}{2} f^n + \frac{1}{2} f^{n-1}\right)$.

b) $v^{n+1} = v^n + k\left(\frac{5}{12} f^n + \frac{8}{12} f^{n-1} - \frac{1}{12} f^{n-2}\right)$.

c) $v^{n+1} = v^n + k\left(\frac{9}{24} f^n + \frac{19}{24} f^{n-1} - \frac{5}{24} f^{n-2} + \frac{1}{24} f^{n-3}\right)$.

Backwards differentiation formulas.

~~Thm~~

Def : The s-step backwards differentiation formula is given by

$$\boxed{\sum_{j=1}^{s} \frac{1}{j} \nabla^j v^{n+s} = k f^{n+s}.}$$

Thm : The s-step backwards differentiation formula is:

a) Consistent, $\forall s \geq 0$,

b) Has order of accuracy $s = p$.

c) Is stable $\Leftrightarrow 1 \leq s \leq 6$!!!

d) Is convergent $\Leftrightarrow 1 \leq s \leq 6$.

Prop. : The following are low order backwards differentiation formulas:

a) $v^n - v^{n-1} = kf^n$

b) $v^n - \frac{4}{3} v^{n-1} + \frac{1}{3} v^{n-2} = \cancel{kf^n}\ \frac{2}{3} kf^n$

c) $v^n - \frac{18}{11} v^{n-1} + \frac{9}{11} v^{n-2} - \frac{2}{11} v^{n-3} = \frac{6}{11} kf^n.$

d) $v^n - \frac{48}{25} v^{n-1} + \frac{36}{25} v^{n-2} - \frac{16}{25} v^{n-3} + \frac{3}{25} v^{n-4} = \frac{12}{25} kf^n.$

▼ More about stability.

In order for an LMF to be practically useful, it needs to be convergent. Another property that is required is "absolute stability".

Def: Suppose that we have an LMF with characteristic polynomials $\rho(z)$ and $\sigma(z)$. The stability polynomial $\pi_\lambda(z)$ is then defined as:

$$\boxed{\pi_\lambda(z) = \rho(z) - \lambda\sigma(z).}$$

Def: An LMF with characteristic polynomials $\rho(z), \sigma(z)$ is absolutely stable at $\lambda \in \mathbb{C}$ iff the roots $\rho_1, \rho_2, \dots, \rho_n$ of $\pi_\lambda(z)$ have the following properties:

a) $|\rho_j| \leq 1, \ \forall j \in \{1, 2, \dots, n\}$

b) $|\rho_j| = 1 \Rightarrow \rho_j$ is a simple root.

Def: The stability region $S \subseteq \mathbb{C}$ of an LMF is a subset of the complex plane such that

$$S = \{\lambda \in \mathbb{C} : \text{the LMF is absolutely stable at } \lambda \in \mathbb{C}\}.$$

The interpretation of absolute stability is given by the following theorem:

Thm: If an LMF is absolutely stable at $ak \in \mathbb{C}$, then all solutions to the recurrence relation

$$\sum_{j=0}^{s} a_j v^{n+j} = ak \sum_{j=0}^{s} b_j v^{n+j}$$

are bounded as $n \to +\infty$.

Remark : The LMF in the theorem approximates the ODE

$$\frac{du}{dt} = au.$$

Absolute stability guarantees that the LMF approximation does not blow up. According to the ODE, if $Re(a) < 0$, then this is true. Therefore it is desirable that as much of the $Re(\lambda) < 0$ plane lies in the stability region as possible.
Establishing results for other model ODEs is difficult.
OTOH absolute stability is a good rule for measuring which LMFs are "better".

~~**Def** : A(α)L~~
~~a) An LMF is A-stable $\Rightarrow$~~

▼ Von-Neumann polynomials.

The theory of von-Neumann polynomials allows us to establish stability results.

Def : Let $\varphi(z)$ be a polynomial with roots $\rho_1, \rho_2, \ldots, \rho_n$.

a) φ is a Schur polynomial $\Leftrightarrow \forall j \in [n] : |\rho_j| < 1$.

b) φ is a Von Neumann polynomial $\Leftrightarrow \forall j \in [n] : |\rho_j| \leq 1$.

c) φ is a simple Von Neumann polynomial $\Leftrightarrow$

$$\Leftrightarrow \begin{cases} \varphi \text{ is a Von Neumann polynomial} \\ \forall j \in [n] : (|\rho_j| = 1 \Rightarrow \rho_j \text{ is a simple root}). \end{cases}$$

d) φ is a conservative polynomial $\Leftrightarrow \forall j \in [n] : |\rho_j| = 1$.

Remark : An LMF is stable iff $\rho(z)$ is a simple Von Neumann polynomial. An LMF is absolutely stable at $\lambda \in \mathbb{C}$ iff $\pi_\lambda(z)$ is a simple von-Neumann polynomial

The Von-Neumann theory is based on the following result.

<u>Thm</u> : Let $\varphi(z) = \sum_{l=0}^{d} a_l z^l$ and $\varphi^*(z) = \sum_{l=0}^{d} \bar{a}_{d-l} z^l$

and $\psi(z) = \frac{1}{z}\left[\varphi^*(0)\varphi(z) - \varphi(0)\varphi^*(z)\right]$

a) φ simple Von Neumann $\Leftrightarrow \begin{cases} |\varphi(0)| < |\varphi^*(0)| \\ \psi \text{ simple Von Neumann} \end{cases} \vee \begin{cases} \psi(x) = 0 \\ \varphi' \text{ Schur} \end{cases}$

b) φ Schur $\Leftrightarrow \begin{cases} |\varphi(0)| < |\varphi^*(0)| \\ \psi \text{ Schur.} \end{cases}$

c) φ von Neumann $\Leftrightarrow \begin{cases} |\varphi(0)| < |\varphi^*(0)| \\ \psi \text{ Von Neumann} \end{cases} \vee \begin{cases} \varphi' \text{ von Neumann.} \\ \psi(x) = 0 \end{cases}$

d) φ conservative $\Leftrightarrow \psi = 0 \wedge \varphi'$ von Neumann.

<u>Remark.</u> : With the ~~follows~~ theorem above $\deg \psi < \deg \varphi$, so we can reduce the degree of the polynomial and compute stability regions explicitly.

▼ Stiff ODEs.

Stiffness is a non-well defined pathology that carries the following symptoms:

1) The problem contains widely varying time scales.
2) Stability is more of a constraint on k than accuracy.
3) Explicit methods don't work.

Stiffness maybe a local phenomenon: an ODE may be stiff at some timesteps and non-stiff at other timesteps.

To detect whether

$$\frac{du}{dt} = f(u,t)$$

is stiff we do the following:

- 1 Linearize the equation: $\dfrac{du}{dt} = J(t)u$.
- 2 Freeze coefficients at time of interest: $A = J(t)$.
- 3 Find the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of A.
- 4 Apply the following rule of thumb.

Rule of thumb

The timestep k must be small enough so that $\forall \lambda_j \in \lambda(A) : k\lambda \in S$ where S is the stability region of the LFM.

Note that this statement although useful in practice, is not a theorem. It may fail for one of the following reasons:

1) It may not be possible to linearize the ODE
2) Rounding errors may cause instability.
3) The timescale in which $J(t)$ varies may not be larger compared to the timestep. Then freezing time is not correct.
4) If the matrix A is very far from being normal, then instabilities due to that may ~~arize~~ arise.

To solve stiff problems effectively, one needs LMFs with large stability regions.

Def: An LMF with stability region S is:

a) A-stable $\Leftrightarrow \{\lambda \in \mathbb{C} : \text{Re}\,\lambda < 0\} \subseteq S$
b) $A(a)$-stable, $a \in (0, \pi/2) \Leftrightarrow \{\lambda \in \mathbb{C} : \cancel{\text{Re}}\ |\arg\lambda - \pi| < a\} \subseteq S$.
c) $A(0)$-stable $\Leftrightarrow \exists a \in (0, \pi/2)$: the LMF is $A(a)$ stable.

Unfortunately a result by Dahlquist shows that the price for A-stability is very high.

Def: An LMF with stability polynomial $\pi_\lambda(z)$ that has roots $\rho_1(\lambda), \rho_2(\lambda), \dots, \rho_n(\lambda)$ is L-stable iff

a) The LMF is A-stable

b) $\forall j \in [n]: \lim\limits_{\lambda \to +\infty} \rho_j(\lambda) = 0$.

Prop.:

a) Backwards Euler method: $v^{n+1} = v^n + k f^{n+1}$ is L-stable.

b) Trapezoid rule: $v^{n+1} = v^n + \frac{k}{2}(f^n + f^{n+1})$ is A-stable but not L-stable.

Remark:

A-stability guarantees reasonable stability.

L-stability guarantees robustness for extremely stiff problems.