Classical Numerical Analysis, Chapter 20

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Chapter 20, Part 1 of 2
Linear Multistep Methods

What Are Multistep Methods?

The fundamental formula that defines mild solutions

$$\mathbf{u}(t_2) = \mathbf{u}(t_1) + \int_{t_1}^{t_2} \mathbf{f}(s, \mathbf{u}(s))\mathrm{d}s$$

was used in the previous chapter with $t_1 = t_k$ and $t_2 = t_{k+1}$. To approximate the integral, we used information about the slope function in the time interval $[t_k, t_{k+1}]$ only. However, we could use more information to build an approximation of the integral. For instance, for some $q \in \mathbb{N}_0$, we set $X_q = \{t_{k-q}, \dots, t_k, t_{k+1}\}$ and replace the slope function by its interpolant on X_q

$$\mathcal{I}_{X_q}[\mathbf{f}(\cdot, \mathbf{u}(\cdot))](t) \approx \mathbf{f}(t, \mathbf{u}(t)).$$

Then

$$\mathbf{u}(t_2) \approx \mathbf{u}(t_1) + \int_{t_1}^{t_2} \mathcal{I}_{X_q}[\mathbf{f}(\cdot, \mathbf{u}(\cdot))](s)\mathrm{d}s.$$

This is the basis of Adams-type methods and other multi-step methods, which we examine in this chapter.

Consistency of Linear Multi-step Methods

Definition (linear multi-step method)

Let $K, q \in \mathbb{N}$ with $q < K$. The finite sequence $\left\{\mathbf{w}^k\right\}_{k=0}^K \subset \mathbb{R}^d$ is called a **linear q-step approximation** *(or just a* **linear multi-step approximation***) to* $\mathbf{u}$*, solution of*

$$\mathbf{u}'(t) = \mathbf{f}(t, \mathbf{u}(t)), \quad 0 < t \leq T, \quad \mathbf{u}(0) = \mathbf{u}_0 \tag{1}$$

with starting values $\mathbf{w}^0, \mathbf{w}^1, \dots, \mathbf{w}^{q-1}$ if and only if, for $k = 0, \dots, K - q$,

$$\sum_{j=0}^{q} a_j \mathbf{w}^{k+j} = \tau \sum_{j=0}^{q} b_j \mathbf{f}(t_{k+j}, \mathbf{w}^{k+j}), \tag{2}$$

where $\{a_j\}_{j=0}^q, \{b_j\}_{j=0}^q \subseteq \mathbb{R}$. The multi-step approximation is called **explicit** *if $b_q = 0$; otherwise, it is called* **implicit***. As before, the* **global error** *of the multi-step approximation is the finite sequence $\left\{\mathbf{e}^k\right\}_{k=0}^K \subseteq \mathbb{R}^d$ defined via*

$$\mathbf{e}^k = \mathbf{u}(t_k) - \mathbf{w}^k.$$

Remark (convention)

Notice that, for the multi-step method (2) to make sense, we must have $a_q \neq 0$. In addition, observe that the coefficients $\{a_j\}_{j=0}^q, \{b_j\}_{j=0}^q$ are defined up to multiplication by a common constant. Because of these two considerations, here and in what follows we will assume that

$$a_q = 1.$$

Example

Consider the linear two-step ($q = 2$) method

$$\mathbf{w}^{k+2} - \mathbf{w}^{k} = \frac{\tau}{3}\left[\mathbf{f}(t_{k+2}, \mathbf{w}^{k+2}) + 4\mathbf{f}(t_{k+1}, \mathbf{w}^{k+1}) + \mathbf{f}(t_k, \mathbf{w}^{k})\right].$$

This method is implicit because $b_2 \neq 0$. The weights are

$$a_2 = 1,\ a_1 = 0,\ a_0 = -1,\ b_2 = \frac{1}{3},\ b_1 = \frac{4}{3},\ b_0 = \frac{1}{3}.$$

Definition (LTE and consistency)

Let $\mathbf{u} \in C^1([0,T];\Omega)$ *be a classical solution on* $[0,T]$ *to* (1)*. Let the sequence* $\left\{\mathbf{w}^k\right\}_{k=0}^K$ *be obtained with the* q*-step method* (2) *with starting values* $\mathbf{w}^0, \mathbf{w}^1, \ldots, \mathbf{w}^{q-1}$*. The* **local truncation error** *(LTE) or* **consistency error** *of the multi-step approximation is defined as*

$$\begin{aligned}\boldsymbol{\mathcal{E}}[\mathbf{u}](t,\tau) \\ &= \frac{1}{\tau}\sum_{j=0}^{q}\left[a_j\mathbf{u}(t+(j-q)\tau) - \tau b_j \mathbf{f}(t+(j-q)\tau, \mathbf{u}(t+(j-q)\tau))\right] \quad (3)\end{aligned}$$

for any $t \in [t_q, T]$*. We make frequent use of the notation* $\boldsymbol{\mathcal{E}}^k[\mathbf{u}] = \boldsymbol{\mathcal{E}}[\mathbf{u}](t_k,\tau)$ *for* $k = q, \ldots, K$*.*

Definition (LTE and consistency Cont.)

We say that the linear multi-step approximation is **consistent to at least order** $p \in \mathbb{N}$ *if and only if, when*

$$\mathbf{u} \in C^{p+1}\Big([0, T]; \mathbb{R}^d\Big),$$

there is a constant $\tau_0 \in (0, T]$ *and a constant* $C > 0$ *such that, for all* $\tau \in (0, \tau_0]$ *and all* $t \in [t_q, T]$,

$$\|\mathcal{E}[\mathbf{u}](t, \tau)\|_2 \leq C\tau^p. \tag{4}$$

We say that the linear q-step approximation is **consistent to exactly order** p *if and only if p is the largest positive integer for which* (4) *holds.*

Definition (LTE and consistency Cont.)

We say that the multi-step approximation **converges globally**, *with at least order $p \in \mathbb{N}$, if and only if, when*

$$\mathbf{u} \in C^{p+1}\left([0, T]; \mathbb{R}^d\right),$$

there is some $\tau_1 \in (0, T]$ and a constant $C > 0$ such that

$$\left\|\mathbf{e}^k\right\|_2 \leq C\tau^p$$

for all $\tau \in (0, \tau_1]$ and any $k = 0, \ldots, K$.

Theorem (method of C's)

Let $\mathbf{f} \in \mathcal{F}^p(S)$ *and* $\mathbf{u} \in C^{p+1}([0,T];\mathbb{R}^d)$ *be a classical solution on* $[0,T]$ *to* (1). *Suppose that* $\mathbf{u}$ *is approximated by the linear q-step method* (2). *Define*

$$C_m = \begin{cases} \displaystyle\sum_{j=0}^{q} a_j, & m = 0, \\ \displaystyle\sum_{j=0}^{q} \left(\frac{j^m}{m!} a_j - \frac{j^{m-1}}{(m-1)!} b_j \right), & m \in \{1,2,3,\ldots\}, \end{cases} \tag{5}$$

with the convention that $0^0 = 1$. *The method is consistent to exactly order* p *if and only if* $C_0 = 0 = C_1 = \cdots = C_p$, *but* $C_{p+1} \neq 0$.

Proof.

For simplicity of notation, let us suppose that $d = 1$. Consider $t \in [t_q, T]$ and we extend, for any $k \in \mathbb{Z}$, the definition $t_k = k\tau$.

Proof Cont.

Using Taylor's Theorem, with the expansion point $t - t_q$, one finds, for each $j = 0, 1, \ldots, q$,

$$u(t + t_{j-q}) = \sum_{m=0}^{p} u^{(m)}(t - t_q)\frac{(j\tau)^m}{m!} + u^{(p+1)}(\zeta_j)\frac{(j\tau)^{p+1}}{(p+1)!}$$

and

$$\begin{aligned} u'(t + t_{j-q}) &= \sum_{m=0}^{p-1} u^{(m+1)}(t - t_q)\frac{(j\tau)^m}{m!} + u^{(p+1)}(\xi_j)\frac{(j\tau)^p}{p!} \\ &= \sum_{m=1}^{p} u^{(m)}(t - t_q)\frac{(j\tau)^{m-1}}{(m-1)!} + u^{(p+1)}(\xi_j)\frac{(j\tau)^p}{p!}. \end{aligned}$$

Proof Cont.

Observe that the $j = 0$ case holds if we agree that $0^0 = 1$. Therefore,

$$\begin{aligned}
\tau\mathcal{E}[u](t,\tau) &= \sum_{j=0}^{q} a_j u(t + t_{j-q}) - \tau \sum_{j=0}^{q} b_j u'(t + t_{j-q}) \\
&= \sum_{j=0}^{q} a_j \sum_{m=0}^{p} u^{(m)}(t - t_q)\frac{(j\tau)^m}{m!} - \tau \sum_{j=0}^{q} b_j \sum_{m=1}^{p} u^{(m)}(t - t_q)\frac{(j\tau)^{m-1}}{(m-1)!} \\
&\quad + \tau^{p+1} \sum_{j=0}^{q} \left[a_j u^{(p+1)}(\zeta_j)\frac{j^{p+1}}{(p+1)!} - b_j u^{(p+1)}(\xi_j)\frac{j^p}{p!} \right].
\end{aligned}$$

Proof Cont.

Interchanging the summations, so that we sum by powers of τ, we have

$$\begin{aligned}\tau\mathcal{E}[u](t,\tau) &= u(t-t_q)\sum_{j=0}^{q} a_j + \sum_{m=1}^{p}\tau^m u^{(m)}(t-t_q)\sum_{j=0}^{q}\left[a_j\frac{j^m}{m!} - b_j\frac{j^{m-1}}{(m-1)!}\right] \\ &\quad + \tau^{p+1}\sum_{j=0}^{q}\left[a_j u^{(p+1)}(\zeta_j)\frac{j^{p+1}}{(p+1)!} - b_j u^{(p+1)}(\xi_j)\frac{j^p}{p!}\right] \\ &= C_0 u(t-t_q) + \sum_{m=1}^{p} C_m\tau^m u^{(m)}(t-t_q) \\ &\quad + \tau^{p+1}\sum_{j=0}^{q}\left[a_j u^{(p+1)}(\zeta_j)\frac{j^{p+1}}{(p+1)!} - b_j u^{(p+1)}(\xi_j)\frac{j^p}{p!}\right]\end{aligned} \tag{6}$$

for some constants $\zeta_j, \xi_j \in [t-t_q, t]$, $j = 0, \dots, q$.

Proof Cont.

($\Longrightarrow$) Suppose that the method is of exactly order p. Then, from (6), we must have $C_0 = C_1 = \cdots = C_p = 0$. If the true solution has higher regularity, say $u \in C^{p+2}([0,T])$, then we can extend the Taylor expansion by one term to obtain

$$\tau\mathcal{E}[u](t,\tau) = C_{p+1}\tau^{p+1}u^{(p+1)}(t-t_q) \\ + \tau^{p+2}\sum_{j=0}^{q}\left[a_j u^{(p+2)}(\tilde{\zeta}_j)\frac{j^{p+2}}{(p+2)!} - b_j u^{(p+2)}(\tilde{\xi}_j)\frac{j^{p+1}}{(p+1)!}\right].$$

Since the method does not exceed order p, it must be true that $C_{p+1} \neq 0$ generically, by the definition of the local truncation error.

Proof Cont.

($\Longleftarrow$) Suppose that $C_0 = C_1 = \cdots = C_p = 0$, but $C_{p+1} \neq 0$. Then

$$\mathcal{E}[u](t,\tau) = \tau^p \sum_{j=0}^{q} \left[a_j u^{(p+1)}(\zeta_j) \frac{j^{p+1}}{(p+1)!} - b_j u^{(p+1)}(\xi_j) \frac{j^p}{p!} \right]$$

and the method is consistent to at least order p. Since $C_{p+1} \neq 0$, the order of accuracy cannot exceed p, even if the true solution has higher regularity, say $u \in C^{p+2}([0, T])$. $\square$

Definition (characteristic polynomials)

For the linear q-step method (2), we define the **first** *and* **second characteristic polynomials**, *respectively, as*

$$\psi(z) = \sum_{j=0}^{q} a_j z^j \in \mathbb{P}_q, \qquad \chi(z) = \sum_{j=0}^{q} b_j z^j \in \mathbb{P}_q.$$

Corollary (first-order consistency)

Let $\mathbf{f} \in \mathcal{F}^1(S)$*. Assume that the function* $\mathbf{u} \in C^2([0,T];\mathbb{R}^d)$ *is a classical solution to the initial value problem (IVP)* (1)*. Suppose that* $\mathbf{u}$ *is approximated by the linear q-step method* (2)*. The method is consistent to at least first order if and only if*

$$\psi(1) = 0, \qquad \psi'(1) - \chi(1) = 0.$$

Proof.

This follows from the method of C's and is an exercise. ☐

Theorem (the log-method)

Let $\mathbf{f} \in \mathcal{F}^p(S)$. *Assume that the function* $\mathbf{u} \in C^{p+1}([0, T]; \mathbb{R}^d)$ *is a classical solution to the IVP* (1). *Suppose that* $\mathbf{u}$ *is approximated by the linear q-step method* (2). *The method is consistent to exactly order p if and only if the function*

$$\phi(\mu) = \frac{\psi(\mu)}{\ln(\mu)} - \chi(\mu),$$

which is complex analytic in a neighborhood of $\mu = 1$, *has the property that* $\mu = 1$ *is a p-fold zero or, equivalently, that*

$$\tilde{\phi}(\mu) = \psi(\mu) - \chi(\mu) \ln(\mu),$$

which is also complex analytic in a neighborhood of $\mu = 1$, *has the property that* $\mu = 1$ *is a* $p + 1$*-fold zero.*

Example

Consider the linear two-step method

$$\mathbf{w}^{k+2} - \mathbf{w}^{k} = \frac{\tau}{3}\left[\mathbf{f}(t_{k+2}, \mathbf{w}^{k+2}) + 4\mathbf{f}(t_{k+1}, \mathbf{w}^{k+1}) + \mathbf{f}(t_k, \mathbf{w}^{k})\right].$$

This method is implicit and consistent to exactly order $p = 4$. Clearly, $C_0 = 0$. Now

$$C_1 = \sum_{j=0}^{2} (ja_j - b_j) = 2 \cdot 1 + 1 \cdot 0 + 0 \cdot (-1) - \left(\frac{1}{3} + \frac{4}{3} + \frac{1}{3}\right) = 2 - 2 = 0,$$

$$C_2 = \sum_{j=0}^{2} \left(\frac{j^2}{2!} a_j - jb_j\right) = \frac{2^2}{2} \cdot 1 - \left(2 \cdot \frac{1}{3} + 1 \cdot \frac{4}{3}\right) = 2 - 2 = 0,$$

$$C_3 = \sum_{j=0}^{2} \left(\frac{j^3}{6} a_j - \frac{j^2}{2} b_j\right) = \frac{2^3}{6} \cdot 1 - \left(\frac{2^2}{2} \cdot \frac{1}{3} + \frac{1^2}{2} \cdot \frac{4}{3}\right) = \frac{8}{6} - \frac{8}{6} = 0,$$

$$C_4 = \sum_{j=0}^{2} \left(\frac{j^4}{24} a_j - \frac{j^3}{6} b_j\right) = \frac{2^4}{24} \cdot 1 - \left(\frac{2^3}{6} \cdot \frac{1}{3} + \frac{1^3}{6} \cdot \frac{4}{3}\right) = \frac{2}{3} - \frac{2}{3} = 0.$$

Example (Cont.)

But

$$C_5 = \sum_{j=0}^{2} \left(\frac{j^5}{120} a_j - \frac{j^4}{24} b_j \right) = \frac{2^5}{120} \cdot 1 - \left(\frac{2^4}{24} \cdot \frac{1}{3} + \frac{1^4}{24} \cdot \frac{4}{3} \right) = \frac{4}{15} - \frac{5}{18} \neq 0.$$

Thus the method is exactly order $p = 4$, according to the method of C's.

Example

In this example, we use the log method to show that the two-step implicit method

$$\mathbf{w}^{k+2} - \mathbf{w}^{k+1} = \tau\left[\frac{5}{12}\mathbf{f}(t_{k+2}, \mathbf{w}^{k+2}) + \frac{8}{12}\mathbf{f}(t_{k+1}, \mathbf{w}^{k+1}) - \frac{1}{12}\mathbf{f}(t_k, \mathbf{w}^k)\right]$$

is consistent to exactly order $p = 3$. To do so, it is convenient to make the change of variables $z = \mu - 1$. Then

$$\begin{aligned}
\psi(\mu) &= \mu^2 - \mu \\
&= (z+1)^2 - (z+1) \\
&= z^2 + z, \\
\chi(\mu) &= \frac{5}{12}\mu^2 + \frac{8}{12}\mu - \frac{1}{12} \\
&= \frac{5}{12}(z+1)^2 + \frac{8}{12}(z+1) - \frac{1}{12} \\
&= \frac{5}{12}z^2 + \frac{3}{2}z + 1.
\end{aligned}$$

Example (Cont.)

Recall the expansion for the log function:

$$\begin{aligned}\ln(\mu) &= (\mu-1) - \frac{1}{2}(\mu-1)^2 + \frac{1}{3}(\mu-1)^3 - \frac{1}{4}(\mu-1)^4 + \frac{1}{5}(\mu-1)^5 + \cdots \\ &= z - \frac{1}{2}z^2 + \frac{1}{3}z^3 - \frac{1}{4}z^4 + \frac{1}{5}z^5 + \cdots .\end{aligned}$$

We need to consider the difference

$$\frac{\psi(\mu)}{\ln(\mu)} - \chi(\mu).$$

To do so, we first find an expansion, in terms of z, for $\frac{\psi(\mu)}{\ln(\mu)}$:

$$\frac{\psi(\mu)}{\ln(\mu)} = c_0 + c_1 z + c_2 z^2 + c_3 z^3 + c_4 z^4 + \cdots .$$

Example (Cont.)

Then

$$\left(c_0 + c_1 z + c_2 z^2 + c_3 z^3 + \cdots\right)\left(z - \frac{1}{2}z^2 + \frac{1}{3}z^3 - \frac{1}{4}z^4 + \cdots\right) = z + z^2,$$

which implies that

$$\begin{aligned} c_0 &= 1, && \\ c_1 - \frac{1}{2}c_0 &= 1 && \implies c_1 = \frac{3}{2}, \\ c_2 - \frac{1}{2}c_1 + \frac{1}{3}c_0 &= 0 && \implies c_2 = \frac{5}{12}, \\ c_3 - \frac{1}{2}c_2 + \frac{1}{3}c_1 - \frac{1}{4}c_0 &= 0 && \implies c_3 = -\frac{1}{24}. \end{aligned}$$

Example (Cont.)

Finally,

$$\frac{\psi(\mu)}{\ln(\mu)} - \chi(\mu) = 1 + \frac{3}{2}z + \frac{5}{12}z^2 - \frac{1}{24}z^3 + c_4 z^4 + \cdots - \left(1 + \frac{3}{2}z + \frac{5}{12}z^2\right)$$
$$= -\frac{1}{24}z^3 + c_4 z^4 + \cdots ,$$

which proves that the method is of exactly third order.

Adams–Bashforth and Adams–Moulton Methods

AB and AM Methods

In this section, we derive some examples of the so-called Adams–Moulton and Adams–Bashforth multi-step methods. We make use of the Lagrange interpolation techniques of Chapter 9. Let $q < K$. Assume that we have computed $k + q - 1 < K$ approximations $\{\mathbf{w}^j\}_{j=0}^{k+q-1}$. Now, from the definition of mild solution, we have that

$$\mathbf{u}(t_{k+q}) - \mathbf{u}(t_{q+k-1}) = \int_{t_{k+q-1}}^{t_{k+q}} \mathbf{f}(s, \mathbf{u}(s)) \mathrm{d}s.$$

We could approximate this integral using the values $\mathbf{w}^k$ and $\mathbf{w}^{k+1}$, and this is the idea behind the single-step methods studied in Chapter 18. However, in doing so, we are not making use of all the information that we had computed before, i.e., $\{\mathbf{w}^j\}_{j=0}^{k+q-1}$.

AB and AM Methods

The idea of the *Adams methods* is to use a subset of $\{\mathbf{f}(t_j, \mathbf{w}^j)\}_{j=0}^{k+q-1}$ to construct an interpolating polynomial and use this polynomial to approximate the integral in the previous identity.

Two important classes of methods here are:

1. *Adams–Bashforth* methods, which use $\{\mathbf{f}(t_j, \mathbf{w}^j)\}_{j=k}^{k+q-1}$ and thus are *explicit* methods.
2. *Adams–Moulton* methods, which use $\{\mathbf{f}(t_j, \mathbf{w}^j)\}_{j=k}^{k+q}$ and thus are *implicit*.

Example

The *Adams–Bashforth four-step method* (AB4) is defined as follows: for $k = 0, \ldots, K-4$,

$$\mathbf{w}^{k+4} - \mathbf{w}^{k+3} = \tau \left[\frac{55}{24}\mathbf{f}^{k+3} - \frac{59}{24}\mathbf{f}^{k+2} + \frac{37}{24}\mathbf{f}^{k+1} - \frac{9}{24}\mathbf{f}^{k} \right], \tag{7}$$

where $\mathbf{f}^j = \mathbf{f}(t_j, \mathbf{w}^j)$. This requires the starting values $\mathbf{w}^0$, $\mathbf{w}^1$, $\mathbf{w}^2$, $\mathbf{w}^3$. The coefficients (weights) are

$$a_4 = 1, \; a_3 = -1, \; a_2 = a_1 = a_0 = 0,$$

and

$$b_4 = 0, \; b_3 = \frac{55}{24}, \; b_2 = -\frac{59}{24}, \; b_1 = \frac{37}{24}, \; b_0 = -\frac{9}{24}.$$

Theorem (LTE of AB4)

Suppose that $\mathbf{f} \in \mathcal{F}^4(S)$ *and* $\mathbf{u} \in C^5([0,T];\mathbb{R}^d)$ *is the classical solution to* (1). *Then the local truncation error for the AB4 method* (7) *may be expressed as*

$$\boldsymbol{\mathcal{E}}^{k+4}[\mathbf{u}] \leq \frac{251 d^{1/2}}{720} \max_{\eta \in [t_k, t_{k+4}]} \|\mathbf{u}^{(5)}(\eta)\|_2 \tau^4$$

for every $k = 0, 1, \ldots, K-4$.

Proof.

Suppose that $0 \leq k \leq K-4$. Let $\mathbf{p}_k \in [\mathbb{P}_3]^d$ be the vector-valued Lagrange interpolating polynomial with respect to the four interpolation points

$$\left\{ (t_{k+j}, \mathbf{f}(t_{k+j}, \mathbf{u}(t_{k+j}))) \right\}_{j=0}^{3}.$$

Then, for all $t \in [t_k, t_{k+4}]$,

$$\mathbf{f}(t, \mathbf{u}(t)) = \mathbf{p}_k(t) + \mathbf{E}_k(t),$$

where $\mathbf{E}_k$ is an error function.

Proof (Cont.)

Thus,

$$\mathbf{u}(t_{k+4}) - \mathbf{u}(t_{k+3}) = \int_{t_{k+3}}^{t_{k+4}} \mathbf{f}(t, \mathbf{u}(t))\mathrm{d}t = \int_{t_{k+3}}^{t_{k+4}} \mathbf{p}_k(t)\mathrm{d}t + \int_{t_{k+3}}^{t_{k+4}} \mathbf{E}_k(t)\mathrm{d}t.$$

According to the error theory for Lagrange interpolation from Chapter 9, we have, for all $i = 1, \ldots, d$,

$$[\mathbf{E}_k]_i(t) = \frac{1}{4!}\frac{\mathrm{d}^4}{\mathrm{d}t^4}\left[\mathbf{f}(t, \mathbf{u}(t))\right]_{i|t=\xi_i} \prod_{j=0}^{3}(t - t_{k+j}) = \frac{1}{24}[\mathbf{u}^{(5)}]_i(\xi_i(t)) \prod_{j=0}^{3}(t - t_{k+j})$$

for all $t \in [t_k, t_{k+4}]$ and some $\xi_i = \xi_i(t) \in (t_k, t_{k+4})$. We find then that, after the change of variables $t = r\tau + t_{k+3}$,

$$\int_{t_{k+3}}^{t_{k+4}} [\mathbf{E}_k]_i(t)\mathrm{d}t = \frac{\tau^5}{24}\int_0^1 r(r+1)(r+2)(r+3)[\mathbf{u}^{(5)}]_i(\xi_i(t))\mathrm{d}r.$$

Proof (Cont.)

Evidently, $\mathbf{E}_k$ is a continuous function on $[0, T]$ since it is the difference of continuous functions. Now set

$$g(r) = r(r+1)(r+2)(r+3)$$

and observe that $g \geq 0$ on $[0,1]$. Then, taking norms,

$$\begin{aligned}
\left\| \int_{t_{k+3}}^{t_{k+4}} \mathbf{E}_k(t)\mathrm{d}t \right\|_2 &\leq \frac{\tau^5}{24} \int_0^1 g(r) \left(\sum_{i=1}^{d} \left| [\mathbf{u}^{(5)}]_i(\xi_i(t)) \right|^2 \right)^{1/2} \mathrm{d}r \\
&\leq d^{1/2} \max_{\xi \in [t_k, t_{k+4}]} \left\| \mathbf{u}^{(5)}(\xi) \right\|_2 \frac{\tau^5}{24} \int_0^1 g(r)\mathrm{d}r \\
&= \max_{\xi \in [t_k, t_{k+4}]} \left\| \mathbf{u}^{(5)}(\xi) \right\|_2 \frac{\tau^5}{24} \frac{251 d^{1/2}}{30} \\
&= \frac{251 d^{1/2}}{720} \tau^5 \max_{\xi \in [t_k, t_{k+4}]} \left\| \mathbf{u}^{(5)}(\xi) \right\|_2 .
\end{aligned}$$

Proof (Cont.)

Let us use the notation $\mathbf{f}_e^{k+j} = \mathbf{f}(t_{k+j}, \mathbf{u}(t_{k+j}))$, $j = 0, 1, 2, 3$. Then

$$\begin{aligned}\mathbf{p}_k(t) = \mathbf{f}_e^k & \frac{(t - t_{k+1})(t - t_{k+2})(t - t_{k+3})}{(t_k - t_{k+1})(t_k - t_{k+2})(t_k - t_{k+3})} \\ & + \mathbf{f}_e^{k+1} \frac{(t - t_k)(t - t_{k+2})(t - t_{k+3})}{(t_{k+1} - t_k)(t_{k+1} - t_{k+2})(t_{k+1} - t_{k+3})} \\ & + \mathbf{f}_e^{k+2} \frac{(t - t_k)(t - t_{k+1})(t - t_{k+3})}{(t_{k+2} - t_k)(t_{k+2} - t_{k+1})(t_{k+2} - t_{k+3})} \\ & + \mathbf{f}_e^{k+3} \frac{(t - t_k)(t - t_{k+1})(t - t_{k+2})}{(t_{k+3} - t_k)(t_{k+3} - t_{k+1})(t_{k+3} - t_{k+2})}.\end{aligned}$$

Observe that

$$\mathbf{p}_k(t_{k+j}) = \mathbf{f}_e^{k+j} = \mathbf{f}(t_{k+j}, \mathbf{u}(t_{k+j})), \quad j = 0, 1, 2, 3.$$

Proof (Cont.)

Integrating $\mathbf{p}_k$ on the interval $[t_{k+3}, t_{k+4}]$, the reader can confirm that

$$\int_{t_{k+3}}^{t_{k+4}} \mathbf{p}_k(t)\mathrm{d}t = \tau \left[\frac{55}{24}\mathbf{f}_e^{k+3} - \frac{59}{24}\mathbf{f}_e^{k+2} + \frac{37}{24}\mathbf{f}_e^{k+1} - \frac{9}{24} f_e^k \right].$$

Using the definition of the local truncation error (3), the result is proven. □

Consistency of AB4 by the Method of C's

Remark (consistency)

With the same hypotheses as in the previous theorem, we can use the method of C's to come to the same conclusion as above. In particular, for the AB4 method, we find

$$C_0 = C_1 = C_2 = C_3 = C_4 = 0, \qquad C_5 = \frac{251}{720}.$$

Does this mean that we should disregard the methodology used in the proof of the last theorem?

Example

The *Adams–Moulton four-step method* (AM4) is defined as follows: for $k = 0, \ldots, K-4$,

$$\mathbf{w}^{k+4} - \mathbf{w}^{k+3} = \tau \left[\frac{251}{720}\mathbf{f}^{k+4} + \frac{646}{720}\mathbf{f}^{k+3} - \frac{264}{720}\mathbf{f}^{k+2} + \frac{106}{720}\mathbf{f}^{k+1} - \frac{19}{720}\mathbf{f}^{k} \right], \quad (8)$$

where $\mathbf{f}^j = \mathbf{f}(t_j, \mathbf{w}^j)$. This requires the starting values $\mathbf{w}^0$, $\mathbf{w}^1$, $\mathbf{w}^2$, $\mathbf{w}^3$. The coefficients are

$$a_4 = 1, \ a_3 = -1, \ a_2 = a_1 = a_0 = 0,$$

and

$$b_4 = \frac{251}{720}, \ b_3 = \frac{646}{720}, \ b_2 = -\frac{264}{720}, \ b_1 = \frac{106}{720}, \ b_0 = -\frac{19}{720}.$$

Theorem (LTE for AM4)

Assume that $\mathbf{f} \in \mathcal{F}^5(S)$. *Let the function* $\mathbf{u} \in C^6([0, T]; \mathbb{R}^d)$ *be the classical solution to* (1). *Then the local truncation error for the AM4 method* (8) *may be expressed as*

$$\|\boldsymbol{\mathcal{E}}^{k+4}[\mathbf{u}]\|_2 \leq \frac{3d^{1/2}}{160} \max_{\eta \in [t_k, t_{k+4}]} \left\| \mathbf{u}^{(6)}(\eta) \right\|_2 \tau^5$$

for every $k = 0, 1, \dots, K-4$.

Proof.

The proof is in the textbook. □

Backward Differentiation Formula Methods

Definition (BDF)

A linear q-step method (2) is called a **BDF method** *(or a* **BDFq method***) if and only if it is of order q, exactly, and*

$$b_q \neq 0, \quad b_{q-1} = b_{q-2} = \cdots = b_1 = b_0 = 0.$$

Theorem (construction of BDF)

Let $q \in \mathbb{N}$ and set $\beta = \left[\sum_{j=1}^{q} \frac{1}{j}\right]^{-1}$. Suppose that the linear q-step method (2) is a BDF method. Then $b_q = \beta$ and

$$\psi(z) = \sum_{j=0}^{q} a_j z^j = \beta \sum_{j=1}^{q} \frac{1}{j} z^{q-j}(z-1)^j$$

or, equivalently,

$$a_q = 1, \qquad a_{q-m} = \beta \sum_{j=m}^{q} \frac{(-1)^m}{j} \binom{j}{m}, \quad m = 1, \ldots, q.$$

Proof.

For the interested reader, the proof is in the book. □

Example

BDF1: For $q = 1$, we find

$$b_1 = 1, \quad a_1 = 1, \quad a_0 = -1.$$

Of course, this corresponds to the single-step backward Euler method.

Example

BDF2: For $q = 2$, we find

$$b_2 = \frac{2}{3}, \quad a_2 = 1, \quad a_1 = -\frac{4}{3}, \quad a_0 = \frac{1}{3}.$$

Example

BDF3: For $q = 3$, we find

$$b_3 = \frac{6}{11}, \quad a_3 = 1, \quad a_2 = -\frac{18}{11}, \quad a_1 = \frac{9}{11}, \quad a_0 = -\frac{2}{11}.$$

Example

Let us review the traditional way to derive the BDF methods, in particular, the BDF2 method. Let $d = 1$ and $u \in C^1([0, T])$ be a classical solution to (1). For $0 \le k \le K - 2$, and any $t \in [t_k, t_{k+2}]$,

$$
\begin{aligned}
u(t) = u(t_k)\frac{(t - t_{k+1})(t - t_{k+2})}{(t_k - t_{k+1})(t_k - t_{k+2})} + u(t_{k+1})\frac{(t - t_k)(t - t_{k+2})}{(t_{k+1} - t_k)(t_{k+1} - t_{k+2})} \\
+ u(t_{k+2})\frac{(t - t_k)(t - t_{k+1})}{(t_{k+2} - t_k)(t_{k+2} - t_{k+1})} + \mathcal{E}(t),
\end{aligned}
$$

where $\mathcal{E}$ is an error term.

Example (Cont.)

Differentiating and evaluating at $t = t_{k+2}$, we get

$$
\begin{aligned}
u'(t_{k+2}) &= u(t_k)\frac{(t_{k+2}-t_{k+1})+(t_{k+2}-t_{k+2})}{(t_k-t_{k+1})(t_k-t_{k+2})} \\
&\quad + u(t_{k+1})\frac{(t_{k+2}-t_k)+(t_{k+2}-t_{k+2})}{(t_{k+1}-t_k)(t_{k+1}-t_{k+2})} \\
&\quad + u(t_{k+2})\frac{(t_{k+2}-t_k)+(t_{k+2}-t_{k+1})}{(t_{k+2}-t_k)(t_{k+2}-t_{k+1})} + \mathcal{E}'(t_{k+2}) \\
&= \frac{1}{2\tau}u(t_k) - \frac{2}{\tau}u(t_{k+1}) + \frac{3}{2\tau}u(t_{k+2}) + \mathcal{E}'(t_{k+2}) \\
&= f(t_{k+2}, u(t_{k+2})).
\end{aligned}
$$

Equivalently,

$$u(t_{k+2}) - \frac{4}{3}u(t_{k+1}) + \frac{1}{3}u(t_k) + \frac{2\tau}{3}\mathcal{E}'(t_{k+2}) = \frac{2\tau}{3}f(t_{k+2}, u(t_{k+2})).$$

This yields the BDF2 method.