

Multistep methods

2.1 The Adams method

A typical numerical method for an initial-value ODE system computes the solution on a step-by-step basis. Thus, the Euler method advances the solution from t_0 to t_1 using \mathbf{y}_0 as an initial value. Next, to advance from t_1 to t_2 , we *discard* \mathbf{y}_0 and employ \mathbf{y}_1 as the new initial value.

Numerical analysts, however, are thrifty by nature. Why discard a potentially valuable vector \mathbf{y}_0 ? With greater generality, why not make the solution depend on several past values, provided that these values are available?

There is one perfectly good reason why not – the exact solution of

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \quad t \geq t_0, \quad \mathbf{y}(t_0) = \mathbf{y}_0 \quad (2.1)$$

is uniquely determined (\mathbf{f} being Lipschitz) by a single initial condition. Any attempt to pin the solution down at more than one point is mathematically nonsensical or, at best, redundant. This, however, is valid only with regard to the true solution of (2.1). When it comes to computation, this redundancy becomes our friend and past values of \mathbf{y} can be put to a very good use – provided, however, that we are very careful indeed.

Let us thus suppose again that \mathbf{y}_n is the numerical solution at $t_n = t_0 + nh$, where $h > 0$ is the step-size, and let us attempt to derive an algorithm that intelligently exploits past values. To that end, we assume that

$$\mathbf{y}_m = \mathbf{y}(t_m) + \mathcal{O}(h^{s+1}), \quad m = 0, 1, \dots, n+s-1, \quad (2.2)$$

where $s \geq 1$ is a given integer. Our wish being to advance the solution from t_{n-s+1} to t_{n+s} , we commence from the trivial identity

$$\mathbf{y}(t_{n+s}) = \mathbf{y}(t_{n+s-1}) + \int_{t_{n+s-1}}^{t_{n+s}} \mathbf{y}'(\tau) d\tau = \mathbf{y}(t_{n+s-1}) + \int_{t_{n+s-1}}^{t_{n+s}} \mathbf{f}(\tau, \mathbf{y}(\tau)) d\tau. \quad (2.3)$$

Wishing to exploit (2.3) for computational ends, we note that the integral on the right incorporates \mathbf{y} not just at the grid points – where approximants are available – but throughout the interval $[t_{n+s-1}, t_{n+s}]$. The main idea of an *Adams method* is to use past values of the solution to approximate \mathbf{y}' in the interval of integration. Thus, let \mathbf{p} be an interpolation polynomial (cf. A.2.2.1–A.2.2.5) that matches $\mathbf{f}(t_m, \mathbf{y}_m)$ for $m = n, n+1, \dots, n+s-1$. Explicitly,

$$\mathbf{p}(t) = \sum_{m=0}^{s-1} p_m(t) \mathbf{f}(t_{n+m}, \mathbf{y}_{n+m}),$$

where the functions

$$p_m(t) = \prod_{\substack{\ell=0 \\ \ell \neq m}}^{s-1} \frac{t - t_{n+\ell}}{t_{n+m} - t_{n+\ell}} = \frac{(-1)^{s-1-m}}{m!(s-1-m)!} \prod_{\substack{\ell=0 \\ \ell \neq m}}^{s-1} \left(\frac{t - t_n}{h} - \ell \right), \quad (2.4)$$

for every $m = 0, 1, \dots, s-1$, are *Lagrange interpolation polynomials*. It is an easy exercise to verify that indeed $p(t_m) = f(t_m, y_m)$ for all $m = n, n+1, \dots, n+s-1$. Hence, (2.2) implies that $p(t_m) = y'(t_m) + \mathcal{O}(h^s)$ for this range of m . We now use interpolation theory from A.2.2.2 to argue that, y being sufficiently smooth,

$$p(t) = y'(t) + \mathcal{O}(h^s), \quad t \in [t_{n+s-1}, t_{n+s}].$$

We next substitute p in the integrand of (2.3), replace $y(t_{n+s-1})$ by y_{n+s-1} there and, having integrated along an interval of length h , we incur an error of $\mathcal{O}(h^{s+1})$. In other words, the method

$$y_{n+s} = y_{n+s-1} + h \sum_{m=0}^{s-1} b_m f(t_{n+m}, y_{n+m}), \quad (2.5)$$

where

$$b_m = h^{-1} \int_{t_{n+s-1}}^{t_{n+s}} p_m(\tau) d\tau = h^{-1} \int_0^h p_m(t_{n+s-1} + \tau) d\tau, \quad m = 0, 1, \dots, s-1,$$

is of order $p = s$. Note from (2.4) that the coefficients b_0, b_1, \dots, b_{s-1} are independent of n and of h – thus we can subsequently use them to advance the iteration from t_{n+s} to t_{n+s+1} and so on.

The scheme (2.5) is called the *s-step Adams–Bashforth* method.

Having derived explicit expressions, it is easy to state Adams–Bashforth methods for moderate values of s . Thus, for $s = 1$ we encounter our old friend, the Euler method, whereas $s = 2$ gives

$$y_{n+2} = y_{n+1} + h \left[\frac{3}{2} f(t_{n+1}, y_{n+1}) - \frac{1}{2} f(t_n, y_n) \right] \quad (2.6)$$

and $s = 3$ gives

$$y_{n+3} = y_{n+2} + h \left[\frac{23}{12} f(t_{n+2}, y_{n+2}) - \frac{4}{3} f(t_{n+1}, y_{n+1}) + \frac{5}{12} f(t_n, y_n) \right]. \quad (2.7)$$

Figure 2.1 displays the logarithm of the error in the solution of $y' = -y^2$, $y(0) = 1$, by Euler's method and the schemes (2.6) and (2.7). The important information can be read off the y -scale: when h is halved, Euler's error decreases linearly, the error of (2.6) decays quadratically and (2.7) displays cubic decay. This is hardly surprising, since the order of the s -step Adams–Bashforth method is, after all, s and the global error decays as $\mathcal{O}(h^s)$.

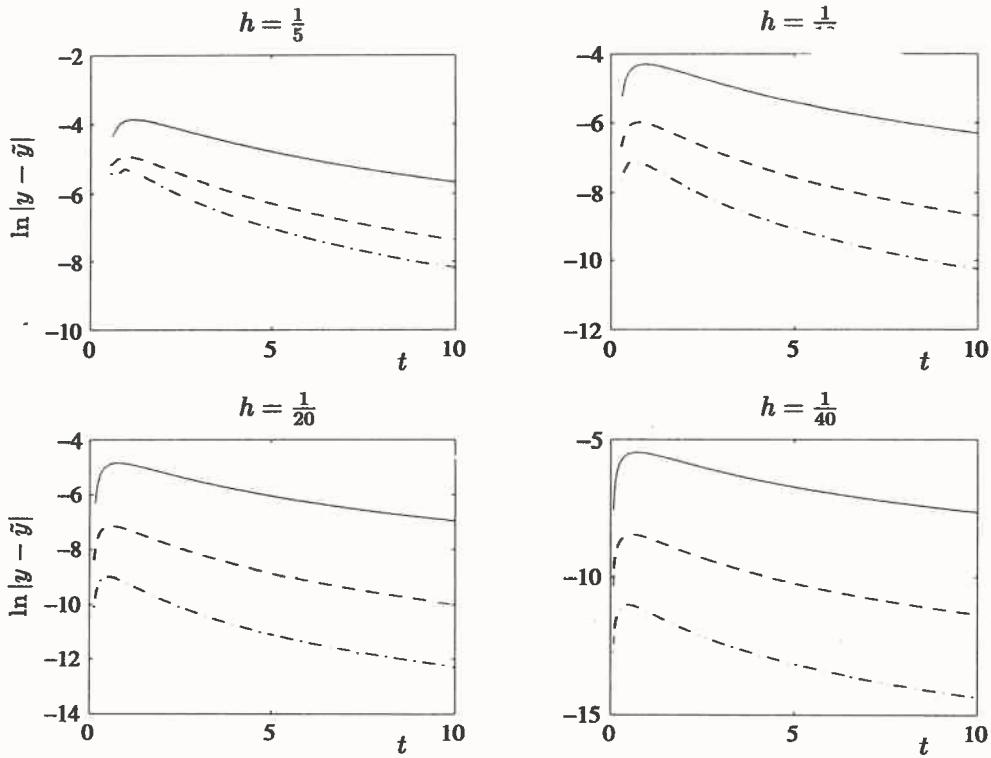


Figure 2.1 The first three Adams–Bashforth methods, as applied to the equation $y' = -y^2$, $y(0) = 1$. Euler's method, (2.6) and (2.7) correspond to the solid, broken and broken-and-dotted lines respectively.

Adams–Bashforth methods are just one instance of multistep methods. In the remainder of this chapter we will encounter several other families of such schemes. Later in this book we will learn that different multistep methods are suitable in different situations. First, however, we need to study the general theory of order and convergence.

2.2 Order and convergence of multistep methods

We write a general s -step method in the form

$$\sum_{m=0}^s a_m y_{n+m} = h \sum_{m=0}^s b_m f(t_{n+m}, y_{n+m}), \quad n = 0, 1, \dots, \quad (2.8)$$

where a_m, b_m , $m = 0, 1, \dots, s$, are given constants, independent of h , n and the underlying differential equation. It is conventional to normalize (2.8) by letting $a_s = 1$. When $b_s = 0$ (as is the case with the Adams–Bashforth method) the method is said to be *explicit*; otherwise it is *implicit*.

Since we are about to encounter several criteria that play an important role in choosing the coefficients a_m and b_m , a central consideration is to obtain a reasonable

value of the order. Recasting the definition from Chapter 1, we note that the method (2.8) is of *order* $p \geq 1$ if and only if

$$\psi(t, \mathbf{y}) := \sum_{m=0}^s a_m \mathbf{y}(t + mh) - h \sum_{m=0}^s b_m \mathbf{y}'(t + mh) = \mathcal{O}(h^{p+1}), \quad h \rightarrow 0, \quad (2.9)$$

for all sufficiently smooth functions \mathbf{y} and there exists at least one such function for which we cannot improve upon the decay rate $\mathcal{O}(h^{p+1})$.

The method (2.8) can be characterized in terms of the polynomials

$$\rho(w) := \sum_{m=0}^s a_m w^m \quad \text{and} \quad \sigma(w) := \sum_{m=0}^s b_m w^m.$$

Theorem 2.1 *The multistep method (2.8) is of order $p \geq 1$ if and only if there exists $c \neq 0$ such that*

$$\rho(w) - \sigma(w) \ln w = c(w - 1)^{p+1} + \mathcal{O}(|w - 1|^{p+2}), \quad w \rightarrow 1. \quad (2.10)$$

Proof We assume that \mathbf{y} is analytic and that its radius of convergence exceeds sh . Expanding in Taylor series and changing the order of summation,

$$\begin{aligned} \psi(t, \mathbf{y}) &= \sum_{m=0}^s a_m \sum_{k=0}^{\infty} \frac{1}{k!} \mathbf{y}^{(k)}(t) m^k h^k - h \sum_{m=0}^s b_m \sum_{k=0}^{\infty} \frac{1}{k!} \mathbf{y}^{(k+1)}(t) m^k h^k \\ &= \left(\sum_{m=0}^s a_m \right) \mathbf{y}(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^s m^k a_m - k \sum_{m=0}^s m^{k-1} b_m \right) h^k \mathbf{y}^{(k)}(t). \end{aligned}$$

Thus, to obtain order p it is necessary and sufficient that

$$\begin{aligned} \sum_{m=0}^s a_m &= 0, & \sum_{m=0}^s m^k a_m &= k \sum_{m=0}^s m^{k-1} b_m, & k &= 1, 2, \dots, p. \\ \sum_{m=0}^s m^{p+1} a_m &\neq (p+1) \sum_{m=0}^s m^p b_m. \end{aligned} \quad (2.11)$$

Let $w = e^z$; therefore $w \rightarrow 1$ corresponds to $z \rightarrow 0$. Expanding again in a Taylor series,

$$\begin{aligned} \rho(e^z) - z\sigma(e^z) &= \sum_{m=0}^s a_m e^{mz} - z \sum_{m=0}^s b_m e^{mz} \\ &= \sum_{m=0}^s a_m \left(\sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k \right) - z \sum_{m=0}^s b_m \left(\sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k \right) \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^s m^k a_m \right) z^k - \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \left(\sum_{m=0}^s m^{k-1} b_m \right) z^k. \end{aligned}$$

Therefore

$$\rho(e^z) - z\sigma(e^z) = cz^{p+1} + \mathcal{O}(z^{p+2})$$

for some $c \neq 0$ if and only if (2.11) is true. The theorem follows by restoring $w = e^z$. ■

An alternative derivation of the order conditions (2.11) assists in our understanding of them. The map $\mathbf{y} \mapsto \psi(t, \mathbf{y})$ is linear, consequently $\psi(t, \mathbf{y}) = \mathcal{O}(h^{p+1})$ if and only if $\psi(t, q) = 0$ for every polynomial q of degree p . Because of linearity, this is equivalent to

$$\psi(t, q_k) = 0, \quad k = 0, 1, \dots, p,$$

where $\{q_0, q_1, \dots, q_p\}$ is a basis of the $(p+1)$ -dimensional space of p -degree polynomials (cf. A.2.1.2–A.2.1.3). Setting $q_k(t) = t^k$ for $k = 0, 1, \dots, p$ we immediately obtain (2.11).

- ◊ Adams–Bashforth revisited... Theorem 2.1 obviates the need for ‘special tricks’ such as used in our derivation of the Adams–Bashforth methods in Section 2.1. Given any multistep scheme (2.8), we can verify its order by a fairly painless expansion into series. It is convenient to express everything in the currency $\xi := w - 1$. For example, (2.6) results in

$$\rho(w) - \sigma(w) \ln w = (\xi + \xi^2) - (1 + \frac{3}{2}\xi)(\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 + \dots) = \frac{5}{12}\xi^3 + \mathcal{O}(\xi^4);$$

thus order two is validated. Likewise, we can check that (2.7) is indeed of order three from the expansion

$$\begin{aligned} \rho(w) - \sigma(w) \ln w &= \xi + 2\xi^2 + \xi^3 \\ &\quad - (1 + \frac{5}{2}\xi + \frac{23}{12}\xi^2)(\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 - \frac{1}{4}\xi^4 + \dots) \\ &= \frac{3}{8}\xi^4 + \mathcal{O}(\xi^5). \end{aligned}$$

◊

Nothing, unfortunately, could be further from good numerical practice than to assess a multistep method solely – or primarily – in terms of its order. Thus, let us consider the two-step implicit scheme

$$y_{n+2} - 3y_{n+1} + 2y_n = h \left[\frac{13}{12}f(t_{n+2}, y_{n+2}) - \frac{5}{3}f(t_{n+1}, y_{n+1}) - \frac{5}{12}f(t_n, y_n) \right]. \quad (2.12)$$

It is easy to ascertain that the order of (2.12) is two. Encouraged by this – and not being very ambitious – we attempt to use this method to solve numerically the exceedingly simple equation $y' \equiv 0, y(0) = 1$. A single step reads $y_{n+2} - 3y_{n+1} + 2y_n = 0$, a recurrence relation whose general solution is $y_n = c_1 + c_2 2^n$, $n = 0, 1, \dots$, where $c_1, c_2 \in \mathbb{R}$ are arbitrary. Suppose that $c_2 \neq 0$; we need both y_0 and y_1 to launch time-stepping and it is trivial to verify that $c_2 \neq 0$ is equivalent to $y_1 \neq y_0$. It is easy to prove that the method fails to converge. Thus, choose $t > 0$ and let $h \rightarrow 0$ so that $nh \rightarrow t$: Obviously, $n \rightarrow \infty$, and this implies that $|y_n| \rightarrow \infty$, which is far from the exact value $y(t) \equiv 1$.

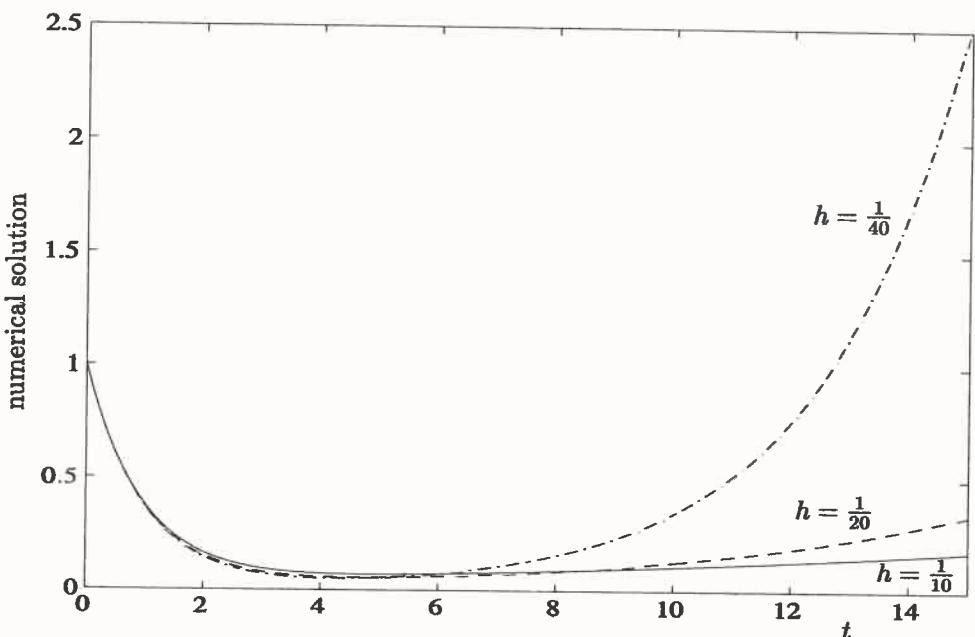


Figure 2.2 The breakdown in the numerical solution of $y' = -y$, $y(0) = 1$, by a nonconvergent numerical scheme, showing how the situation worsens with decreasing step-size.

The failure in convergence does not require, realistically, that $c_2 \neq 0$ be induced by y_1 . Any calculation on a real computer introduces roundoff error which, sooner or later, is bound to render $c_2 \neq 0$ and bring about a geometric growth in the error.

Needless to say, a method that cannot integrate the simplest possible ODE with any measure of reliability should not be used for more substantial computational ends. Nontrivial order is not sufficient to ensure convergence! The need thus arises for a criterion that allows us to discard bad methods and narrow the field down to convergent multistep schemes.

◊ **Failure to converge** Suppose that the linear equation $y' = -y$, $y(0) = 1$, is solved by a two-step method with $\rho(w) = w^2 - 2.01w + 1.01$, $\sigma(w) = 0.995w - 1.005$. As will be soon evident, this method also fails the convergence criterion, although not by a wide margin! Figure 2.2 displays three solution trajectories, for progressively decreasing step-sizes $h = \frac{1}{10}, \frac{1}{20}, \frac{1}{40}$. In all instances, in its early stages the solution perfectly resembles the decaying exponential, but after a while small perturbations grow at an increasing pace and render the computation meaningless. It is a characteristic of nonconvergent methods that decreasing the step-size actually makes matters worse! ◇

We say that a polynomial obeys the *root condition* if all its zeros reside in the closed complex unit disc and all its zeros of unit modulus are simple.

Theorem 2.2 (The Dahlquist equivalence theorem) *Suppose that the error in the starting values y_1, y_2, \dots, y_{s-1} tends to zero as $h \rightarrow 0+$. The multistep method*

(2.8) is convergent if and only if it is of order $p \geq 1$ and the polynomial ρ obeys the root condition.

It is important to make crystal clear that convergence is not simply another attribute of a numerical method, to be weighed alongside its other features. If a method is not convergent – and regardless of how attractive it may look – do not use it!

Theorem 2.2 allows us to discard method (2.12) without further ado, since $\rho(w) = (w - 1)(w - 2)$ violates the root condition. Of course, this method is contrived and, even were it convergent, it is doubtful whether it would have been of much interest. However, more ‘respectable’ methods fail the convergence test. For example, the method

$$\begin{aligned} & y_{n+3} + \frac{27}{11}y_{n+2} - \frac{27}{11}y_{n+1} - y_n \\ &= h \left[\frac{3}{11}f(t_{n+3}, y_{n+3}) + \frac{27}{11}f(t_{n+2}, y_{n+2}) + \frac{27}{11}f(t_{n+1}, y_{n+1}) + \frac{3}{11}f(t_n, y_n) \right] \end{aligned}$$

is of order six; it is the *only* three-step method that attains this order! Unfortunately,

$$\rho(w) = (w - 1) \left(w + \frac{19 + 4\sqrt{15}}{11} \right) \left(w + \frac{19 - 4\sqrt{15}}{11} \right)$$

and the root condition fails. On the other hand, note that Adams–Bashforth methods are safe for all $s \geq 1$, since $\rho(w) = w^{s-1}(w - 1)$.

◊ **Analysis and algebraic conditions** Theorem 2.2 demonstrates a state of affairs that prevails throughout mathematical analysis. Thus, we desire to investigate an *analytic* condition, e.g. whether a differential equation has a solution, whether a continuous dynamical system is asymptotically stable, whether a numerical method converges. By their very nature, analytic concepts involve infinite processes and continua, hence one can expect analytic conditions to be difficult to verify, to the point of unmanageability. For all we know, the human brain (exactly like a digital computer) might be essentially an algebraic machine. It is thus an important goal in mathematical analysis to search for equivalent *algebraic* conditions. The Dahlquist equivalence theorem is a remarkable example of this: everything essentially reduces to the determination whether zeros of a polynomial reside in a unit disc, and this can be determined in a finite number of algebraic operations! In the course of this book we will encounter numerous other examples of this state of affairs. Cast your mind back to basic infinitesimal calculus and you are bound to recall further instances of analytic problems being rendered into an algebraic language. ◇

The multistep method (2.8) has $2s + 1$ parameters. Had order been the sole consideration, we could have utilized all the available degrees of freedom to maximize it. The outcome, an (implicit) s -step method of order $2s$, is unfortunately not convergent for $s \geq 3$ (we have already seen the case $s = 3$). In general, it is possible to prove that the maximal order of a convergent s -step method (2.8) is at most $2\lfloor(s+2)/2\rfloor$ for implicit schemes and just s for explicit ones; this is known as *the Dahlquist first barrier*.

The usual practice is to employ orders $s + 1$ and s for s -step implicit and explicit methods respectively. An easy procedure for constructing such schemes is as follows. Choose an arbitrary s -degree polynomial ρ that obeys the root condition and such that $\rho(1) = 0$ (according to (2.11), $\rho(1) = \sum a_m = 0$ is necessary for order $p \geq 1$). Dividing the order condition (2.10) by $\ln w$ we obtain

$$\sigma(w) = \frac{\rho(w)}{\ln w} + \mathcal{O}(|w - 1|^p). \quad (2.13)$$

(Note that division by $\ln w$ shaves off a power of $|w - 1|$ and that the singularity at $w = 1$ in the numerator and the denominator is removable.) Suppose first that $p = s + 1$ and no restrictions are placed on σ . We expand the fraction in (2.13) into a Taylor series about $w = 1$ and let σ be the s -degree polynomial that matches the series up to $\mathcal{O}(|w - 1|^{s+1})$. The outcome is a convergent, s -step method of order $s + 1$. Likewise, to obtain an explicit method of order s , we let σ be an $(s - 1)$ -degree polynomial (to force $b_m = 0$) that matches the series up to $\mathcal{O}(|w - 1|^s)$.

Let us, for example, choose $s = 2$ and $\rho(w) = w^2 - w$. Letting, as before, $\xi = w - 1$, we have

$$\begin{aligned} \frac{\rho(w)}{\ln w} &= \frac{\xi + \xi^2}{\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 + \mathcal{O}(\xi^4)} = \frac{1 + \xi}{1 - \frac{1}{2}\xi + \frac{1}{3}\xi^2} + \mathcal{O}(\xi^3) \\ &= (1 + \xi)(1 + \frac{1}{2}\xi - \frac{1}{12}\xi^2) + \mathcal{O}(\xi^3) = 1 + \frac{3}{2}\xi + \frac{5}{12}\xi^2 + \mathcal{O}(\xi^3). \end{aligned}$$

Thus, for quadratic σ and order 3 we truncate, obtaining

$$\sigma(w) = 1 + \frac{3}{2}(w - 1) + \frac{5}{12}(w - 1)^2 = -\frac{1}{12} + \frac{2}{3}w + \frac{5}{12}w^2,$$

whereas in the explicit case σ is linear, $p = 2$, and we recover, unsurprisingly, the Adams–Bashforth scheme (2.6).

The choice $\rho(w) = w^{s-1}(w - 1)$ is associated with *Adams* methods. We have already seen the explicit Adams–Bashforth schemes, whilst their implicit counterparts bear the name of Adams–Moulton methods. However, provided that we wish to maximize the order subject to convergence, without placing any extra constraints on the multistep method, Adams schemes are the most reasonable choice. After all, if – as implied in the statement of Theorem 2.2 – large zeros of ρ are bad, it makes perfect sense to drive as many zeros as we can to the origin!

2.3 Backward differentiation formulae

Classical texts in numerical analysis present several distinct families of multistep methods. For example, letting $\rho(w) = w^{s-2}(w^2 - 1)$ leads to s -order explicit *Nystrom* methods and to implicit *Milne* methods of order $s + 1$ (cf. Exercise 2.3). However, in a well-defined yet important situation, certain multistep methods are significantly better than other schemes of the type (2.8). These are the *backward differentiation formulae* (BDFs).

An s -order, s -step method is said to be a BDF if $\sigma(w) = \beta w^s$ for some $\beta \in \mathbb{R} \setminus \{0\}$.

Lemma 2.3 *For a BDF we have*

$$\beta = \left(\sum_{m=1}^s \frac{1}{m} \right)^{-1} \quad \text{and} \quad \rho(w) = \beta \sum_{m=1}^s \frac{1}{m} w^{s-m} (w-1)^m. \quad (2.14)$$

Proof The order being $p = s$, (2.10) implies that

$$\rho(w) - \beta w^s \ln w = \mathcal{O}(|w-1|^{s+1}), \quad w \rightarrow 1.$$

We substitute $v = w^{-1}$, hence

$$v^s \rho(v^{-1}) = -\beta \ln v + \mathcal{O}(|v-1|^{s+1}), \quad v \rightarrow 1.$$

Since

$$\ln v = \ln[1 + (v-1)] = \sum_{m=1}^s \frac{(-1)^{m-1}}{m} (v-1)^m + \mathcal{O}(|v-1|^{s+1}),$$

we deduce that

$$v^s \rho(v^{-1}) = \beta \sum_{m=1}^s \frac{(-1)^m}{m} (v-1)^m.$$

Therefore

$$\begin{aligned} \rho(w) &= \beta v^{-s} \sum_{m=1}^s \frac{(-1)^m}{m} (v-1)^m = \beta \sum_{m=1}^s \frac{(-1)^m}{m} w^s (w^{-1}-1)^m \\ &= \beta \sum_{m=1}^s \frac{1}{m} w^{s-m} (w-1)^m. \end{aligned}$$

To complete the proof of (2.14), we need only to derive the explicit form of β . It follows at once by imposing the normalization condition $a_s = 1$ on the polynomial ρ . ■

The simplest BDF has been already encountered in Chapter 1: when $s = 1$ we recover the backward Euler method (1.15). The next two BDFs are

$$s = 2 : \quad \mathbf{y}_{n+2} - \frac{4}{3}\mathbf{y}_{n+1} + \frac{1}{3}\mathbf{y}_n = \frac{2}{3}hf(t_{n+2}, \mathbf{y}_{n+2}), \quad (2.15)$$

$$s = 3 : \quad \mathbf{y}_{n+3} - \frac{18}{11}\mathbf{y}_{n+2} + \frac{9}{11}\mathbf{y}_{n+1} - \frac{2}{11}\mathbf{y}_n = \frac{6}{11}hf(t_{n+3}, \mathbf{y}_{n+3}). \quad (2.16)$$

Their derivation is trivial; for example, (2.16) follows by letting $s = 3$ in (2.14). Therefore

$$\beta = \frac{1}{1 + \frac{1}{2} + \frac{1}{3}} = \frac{6}{11}$$

and

$$\rho(w) = \frac{6}{11} [w^2(w-1) + \frac{1}{2}w(w-1)^2 + \frac{1}{3}(w-1)^3] = w^3 - \frac{18}{11}w^2 + \frac{9}{11}w - \frac{2}{11}.$$

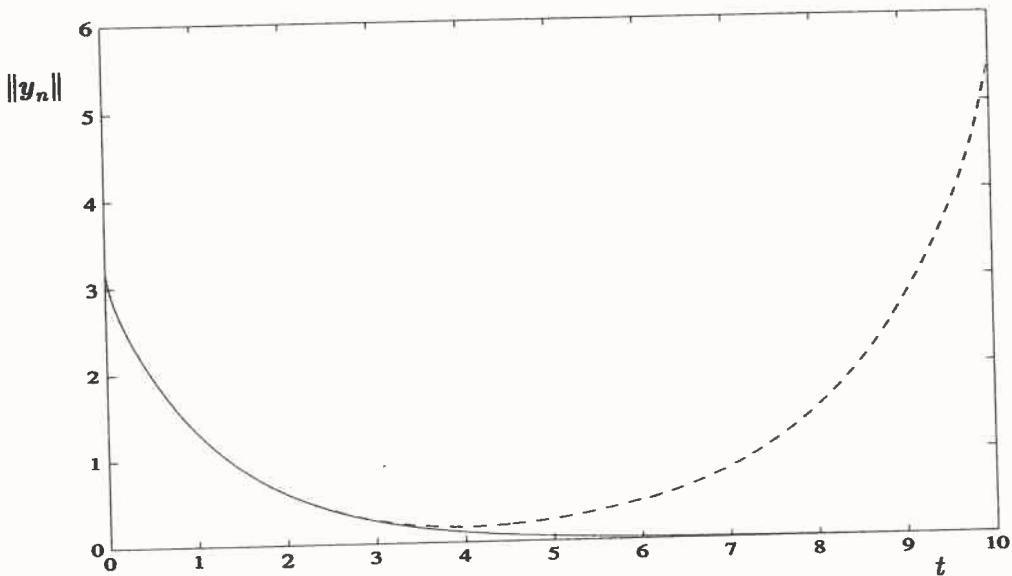


Figure 2.3 The norm of the numerical solution of (2.17) by the Adams–Bashforth method (2.6) for $h = 0.027$ (solid line) and $h = 0.0275$ (broken line).

Since BDFs are derived by specifying σ , we cannot be assured that the polynomial ρ of (2.14) obeys the root condition. In fact, the root condition fails for all but a few such methods.

Theorem 2.4 *The polynomial (2.14) obeys the root condition and the underlying BDF method is convergent if and only if $1 \leq s \leq 6$.*

Fortunately, the ‘good’ range of s is sufficient for all practical considerations.

Underscoring the importance of BDFs, we present a simple example that demonstrates the limitations of Adams schemes; we hasten to emphasize that this is by way of a trailer for our discussion of stiff ODEs in Chapter 4.

Let us consider the linear ODE system

$$\mathbf{y}' = \begin{bmatrix} -20 & 10 & 0 & \cdots & 0 \\ 10 & -20 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & -20 & 10 \\ 0 & \cdots & 0 & 10 & -20 \end{bmatrix} \mathbf{y}, \quad \mathbf{y}(0) = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}. \quad (2.17)$$

We will encounter in this book numerous instances of similar systems; (2.17) is a handy paradigm for many linear ODEs that occur in the context of discretization of the partial differential equations of evolution.

Figure 2.3 displays the Euclidean norm of the solution of (2.17) by the second-order Adams–Bashforth method (2.6), with two (slightly) different step-sizes, $h = 0.027$ (the solid line) and $h = 0.0275$ (the broken line). The solid line is indistinguishable in the

figure from the norm of the true solution, which approaches zero as $t \rightarrow \infty$. Not so the norm for $h = 0.0275$: initially, it shadows pretty well the correct value but, after a while, it runs away. The whole qualitative picture is utterly false! And, by the way, things rapidly get considerably worse when h is increased: for $h = 0.028$ the norm reaches 2.5×10^4 , while for $h = 0.029$ it shoots to 1.3×10^{11} .

What is the mechanism that degrades the numerical solution and renders it so sensitive to small changes in h ? At the moment it suffices to state that the quality of local approximation (which we have quantified in the concept of ‘order’) is not to blame; taking the third-order scheme (2.7) in place of the current method would have only made matters worse. On the other hand, were we to attempt the solution of this ODE with (2.15), say, and with any $h > 0$, the norm would have tended to zero in tandem with the exact solution. In other words, methods such as BDFs are singled out by a favourable property that makes them the methods of choice for important classes of ODEs. Much more will be said about this in Chapter 4.

Comments and bibliography

There are several ways of introducing the theory of multistep methods. Traditional texts have emphasized the derivation of schemes by various interpolation formulae. The approach of Section 2.1 harks back to this approach, as does the name ‘backward differentiation formula’. Other books derive order conditions by sheer brute force, requiring that the multistep formula (2.8) be exact for all polynomials of degree p , since this is equivalent to order p . This can be expressed as a linear system of $p + 1$ equations in the $2s + 1$ unknowns $a_0, a_1, \dots, a_{s-1}, b_0, b_1, \dots, b_s$. A solution of this system yields a multistep method of requisite order (of course, we must check it for convergence!), although this procedure does not add much to our understanding of such methods.¹ Linking order with an approximation of the logarithm, *pace* Theorem 2.1, elucidates matters on a considerably more profound level. This can be shown by the following hand-waving argument.

Given an analytic function g , say, and a number $h > 0$, we denote $g_n^{(k)} = g^{(k)}(t_0 + hn)$, $k, n = 0, 1, \dots$, and define two operators that map such ‘grid functions’ into themselves, the shift operator $\mathcal{E}g_n^{(k)} := g_{n+1}^{(k)}$ and the differential operator $Dg_n^{(k)} := g_n^{(k+1)}$, $k, n = 0, 1, \dots$ (cf. Section 7.1). Expanding in a Taylor series about $t_0 + nh$,

$$\mathcal{E}g_n^{(k)} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} g_n^{(k+\ell)} h^\ell = \left(\sum_{\ell=0}^{\infty} \frac{1}{\ell!} (hD)^\ell \right) g_n^{(k)}, \quad k, n = 0, 1, \dots$$

Since this is true for every analytic g with a radius of convergence exceeding h , it follows that, at least formally, $\mathcal{E} = \exp(hD)$. The exponential of the operator, exactly like the more familiar matrix exponential, is defined by a Taylor series.

The above argument can be tightened at the price of some mathematical sophistication. The main problem with naively defining \mathcal{E} as the exponential of hD is that, in the standard spaces beloved by mathematicians, D is not a *bounded* linear operator. To recover boundedness we need to resort to a more exotic space.

Let $U \subseteq \mathbb{C}$ be an open connected set and denote by $\mathcal{A}(U)$ the vector space of analytic functions defined in U . The sequence $\{f_n\}_{n=0}^{\infty}$, where $f_n \in \mathcal{A}(U)$, $n = 0, 1, \dots$, is said to converge to f *locally uniformly* in $\mathcal{A}(U)$ if $f_n \rightarrow f$ uniformly in every compact (i.e., closed and

¹Though low on insight and beauty, brute force techniques are occasionally useful in mathematics just as in more pedestrian walks of life.