who are removed from the affected population at a given time t by isolation, recovery and consequent immunity, or death. This quite naturally complicates the problem, but it can be shown (see [Ba2]) that an approximate solution can be given in the form

$$x(t) = x(0)e^{-(k_1/k_2)z(t)} \quad \text{and} \quad y(t) = m - x(t) - z(t),$$

where k_1 is the infective rate, k_2 is the removal rate, and $z(t)$ is determined from the differential equation

$$z'(t) = k_2\left(m - z(t) - x(0)e^{-(k_1/k_2)z(t)}\right).$$

The authors are not aware of any technique for solving this problem directly, so a numerical procedure must be applied. Find an approximation to $z(30)$, $y(30)$, and $x(30)$, assuming that $m = 100{,}000$, $x(0) = 99{,}000$, $k_1 = 2 \times 10^{-6}$, and $k_2 = 10^{-4}$.

5.6 Multistep Methods

The methods discussed to this point in the chapter are called **one-step methods** because the approximation for the mesh point t_{i+1} involves information from only one of the previous mesh points, t_i. Although these methods might use function evaluation information at points between t_i and t_{i+1}, they do not retain that information for direct use in future approximations. All the information used by these methods is obtained within the subinterval over which the solution is being approximated.

The approximate solution is available at each of the mesh points $t_0, t_1, \ldots, t_i$ before the approximation at t_{i+1} is obtained, and because the error $|w_j - y(t_j)|$ tends to increase with j, so it seems reasonable to develop methods that use these more accurate previous data when approximating the solution at t_{i+1}.

Methods using the approximation at more than one previous mesh point to determine the approximation at the next point are called *multistep* methods. The precise definition of these methods follows, together with the definition of the two types of multistep methods.

Definition 5.14 An ***m*-step multistep method** for solving the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha, \tag{5.23}$$

has a difference equation for finding the approximation w_{i+1} at the mesh point t_{i+1} represented by the following equation, where m is an integer greater than 1:

$$\begin{aligned} w_{i+1} = {} & a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ & + h[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) \\ & + \cdots + b_0 f(t_{i+1-m}, w_{i+1-m})], \end{aligned} \tag{5.24}$$

for $i = m - 1, m, \ldots, N - 1$, where $h = (b - a)/N$, the $a_0, a_1, \ldots, a_{m-1}$ and $b_0, b_1, \ldots, b_m$ are constants, and the starting values

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad \ldots, \quad w_{m-1} = \alpha_{m-1}$$

are specified. ■

When $b_m = 0$ the method is called **explicit**, or **open**, because Eq. (5.24) then gives w_{i+1} explicitly in terms of previously determined values. When $b_m \neq 0$ the method is called

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implicit, or **closed**, because w_{i+1} occurs on both sides of Eq. (5.243), so w_{i+1} is specified only implicitly.

For example, the equations

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3,$$

$$w_{i+1} = w_i + \frac{h}{24}[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})], \tag{5.25}$$

The Adams-Bashforth techniques are due to John Couch Adams (1819–1892), who did significant work in mathematics and astronomy. He developed these numerical techniques to approximate the solution of a fluid-flow problem posed by Bashforth.

for each $i = 3, 4, \ldots, N-1$, define an *explicit* four-step method known as the **fourth-order Adams-Bashforth technique**. The equations

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2,$$

$$w_{i+1} = w_i + \frac{h}{24}[9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})], \tag{5.26}$$

for each $i = 2, 3, \ldots, N-1$, define an *implicit* three-step method known as the **fourth-order Adams-Moulton technique**.

Forest Ray Moulton (1872–1952) was in charge of ballistics at the Aberdeen Proving Grounds in Maryland during World War I. He was a prolific author, writing numerous books in mathematics and astronomy, and developed improved multistep methods for solving ballistic equations.

The starting values in either (5.25) or (5.26) must be specified, generally by assuming $w_0 = \alpha$ and generating the remaining values by either a Runge-Kutta or Taylor method. We will see that the implicit methods are generally more accurate then the explicit methods, but to apply an implicit method such as (5.25) directly, we must solve the implicit equation for w_{i+1}. This is not always possible,and even when it can be done the solution for w_{i+1} may not be unique.

Example 1 In Example 3 of Section 5.4 (see Table 5.8 on page 289) we used the Runge-Kutta method of order four with $h = 0.2$ to approximate the solutions to the initial value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

The first four approximations were found to be $y(0) = w_0 = 0.5$, $y(0.2) \approx w_1 = 0.8292933$, $y(0.4) \approx w_2 = 1.2140762$, and $y(0.6) \approx w_3 = 1.6489220$. Use these as starting values for the fourth-order Adams-Bashforth method to compute new approximations for $y(0.8)$ and $y(1.0)$, and compare these new approximations to those produced by the Runge-Kutta method of order four.

Solution For the fourth-order Adams-Bashforth we have

$$\begin{aligned} y(0.8) \approx w_4 &= w_3 + \frac{0.2}{24}(55f(0.6, w_3) - 59f(0.4, w_2) + 37f(0.2, w_1) - 9f(0, w_0)) \\ &= 1.6489220 + \frac{0.2}{24}(55f(0.6, 1.6489220) - 59f(0.4, 1.2140762) \\ &\quad + 37f(0.2, 0.8292933) - 9f(0, 0.5)) \\ &= 1.6489220 + 0.0083333(55(2.2889220) - 59(2.0540762) \\ &\quad + 37(1.7892933) - 9(1.5)) \\ &= 2.1272892, \end{aligned}$$

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and

$$\begin{aligned} y(1.0) \approx w_5 &= w_4 + \frac{0.2}{24}\left(55f(0.8, w_4) - 59f(0.6, w_3) + 37f(0.4, w_2) - 9f(0.2, w_1)\right) \\ &= 2.1272892 + \frac{0.2}{24}(55f(0.8, 2.1272892) - 59f(0.6, 1.6489220) \\ &\quad + 37f(0.4, 1.2140762) - 9f(0.2, 0.8292933)) \\ &= 2.1272892 + 0.0083333(55(2.4872892) - 59(2.2889220) \\ &\quad + 37(2.0540762) - 9(1.7892933)) \\ &= 2.6410533, \end{aligned}$$

The error for these approximations at $t = 0.8$ and $t = 1.0$ are, respectively

$$|2.1272295 - 2.1272892| = 5.97 \times 10^{-5} \quad \text{and} \quad |2.6410533 - 2.6408591| = 1.94 \times 10^{-4}.$$

The corresponding Runge-Kutta approximations had errors

$$|2.1272027 - 2.1272892| = 2.69 \times 10^{-5} \quad \text{and} \quad |2.6408227 - 2.6408591| = 3.64 \times 10^{-5}.$$

■

Adams was particularly interested in the using his ability for accurate numerical calculations to investigate the orbits of the planets. He predicted the existence of Neptune by analyzing the irregularities in the planet Uranus, and developed various numerical integration techniques to assist in the approximation of the solution of differential equations.

To begin the derivation of a multistep method, note that the solution to the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha,$$

if integrated over the interval $[t_i, t_{i+1}]$, has the property that

$$y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} y'(t)\, dt = \int_{t_i}^{t_{i+1}} f(t, y(t))\, dt.$$

Consequently,

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t))\, dt. \tag{5.27}$$

However we cannot integrate $f(t, y(t))$ without knowing $y(t)$, the solution to the problem, so we instead integrate an interpolating polynomial $P(t)$ to $f(t, y(t))$, one that is determined by some of the previously obtained data points (t_0, w_0), (t_1, w_1), $\ldots$, (t_i, w_i). When we assume, in addition, that $y(t_i) \approx w_i$, Eq. (5.27) becomes

$$y(t_{i+1}) \approx w_i + \int_{t_i}^{t_{i+1}} P(t)\, dt. \tag{5.28}$$

Although any form of the interpolating polynomial can be used for the derivation, it is most convenient to use the Newton backward-difference formula, because this form more easily incorporates the most recently calculated data.

To derive an Adams-Bashforth explicit m-step technique, we form the backward-difference polynomial $P_{m-1}(t)$ through

$$(t_i, f(t_i, y(t_i))), \quad (t_{i-1}, f(t_{i-1}, y(t_{i-1}))), \ldots, \quad (t_{i+1-m}, f(t_{i+1-m}, y(t_{i+1-m}))).$$

Since $P_{m-1}(t)$ is an interpolatory polynomial of degree $m-1$, some number ξ_i in (t_{i+1-m}, t_i) exists with

$$f(t, y(t)) = P_{m-1}(t) + \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!}(t - t_i)(t - t_{i-1}) \cdots (t - t_{i+1-m}).$$

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Introducing the variable substitution $t = t_i + sh$, with $dt = h\,ds$, into $P_{m-1}(t)$ and the error term implies that

$$\begin{aligned}\int_{t_i}^{t_{i+1}} f(t, y(t))\,dt &= \int_{t_i}^{t_{i+1}} \sum_{k=0}^{m-1} (-1)^k \binom{-s}{k} \nabla^k f(t_i, y(t_i))\,dt \\ &\quad + \int_{t_i}^{t_{i+1}} \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!}(t - t_i)(t - t_{i-1}) \cdots (t - t_{i+1-m})\,dt \\ &= \sum_{k=0}^{m-1} \nabla^k f(t_i, y(t_i)) h (-1)^k \int_0^1 \binom{-s}{k} ds \\ &\quad + \frac{h^{m+1}}{m!} \int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_i, y(\xi_i))\,ds.\end{aligned}$$

The integrals $(-1)^k \int_0^1 \binom{-s}{k} ds$ for various values of k are easily evaluated and are listed in Table 5.12. For example, when $k = 3$,

$$\begin{aligned}(-1)^3 \int_0^1 \binom{-s}{3} ds &= -\int_0^1 \frac{(-s)(-s-1)(-s-2)}{1 \cdot 2 \cdot 3}\,ds \\ &= \frac{1}{6}\int_0^1 (s^3 + 3s^2 + 2s)\,ds \\ &= \frac{1}{6}\left[\frac{s^4}{4} + s^3 + s^2\right]_0^1 = \frac{1}{6}\left(\frac{9}{4}\right) = \frac{3}{8}.\end{aligned}$$

Table 5.12

k	$\int_0^1 \binom{-s}{k} ds$
0	1
1	$\frac{1}{2}$
2	$\frac{5}{12}$
3	$\frac{3}{8}$
4	$\frac{251}{720}$
5	$\frac{95}{288}$

As a consequence,

$$\begin{aligned}\int_{t_i}^{t_{i+1}} f(t, y(t))\,dt &= h\left[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) + \frac{5}{12}\nabla^2 f(t_i, y(t_i)) + \cdots\right] \\ &\quad + \frac{h^{m+1}}{m!}\int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_i, y(\xi_i))\,ds. \qquad (5.29)\end{aligned}$$

Because $s(s+1) \cdots (s+m-1)$ does not change sign on $[0, 1]$, the Weighted Mean Value Theorem for Integrals can be used to deduce that for some number μ_i, where $t_{i+1-m} < \mu_i < t_{i+1}$, the error term in Eq. (5.29) becomes

$$\begin{aligned}&\frac{h^{m+1}}{m!}\int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi_i, y(\xi_i))\,ds \\ &\qquad = \frac{h^{m+1} f^{(m)}(\mu_i, y(\mu_i))}{m!}\int_0^1 s(s+1) \cdots (s+m-1)\,ds.\end{aligned}$$

Hence the error in (5.29) simplifies to

$$h^{m+1} f^{(m)}(\mu_i, y(\mu_i))(-1)^m \int_0^1 \binom{-s}{m} ds. \qquad (5.30)$$

But $y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} f(t, y(t))\,dt$, so Eq. (5.27) can be written as

$$\begin{aligned}y(t_{i+1}) &= y(t_i) + h\left[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) + \frac{5}{12}\nabla^2 f(t_i, y(t_i)) + \cdots\right] \\ &\quad + h^{m+1} f^{(m)}(\mu_i, y(\mu_i))(-1)^m \int_0^1 \binom{-s}{m} ds. \qquad (5.31)\end{aligned}$$

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Example 2 Use Eq. (5.31) with $m = 3$ to derive the three-step Adams-Bashforth technique.

Solution We have

$$\begin{aligned} y(t_{i+1}) &\approx y(t_i) + h\left[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) + \frac{5}{12}\nabla^2 f(t_i, y(t_i))\right] \\ &= y(t_i) + h\left\{f(t_i, y(t_i)) + \frac{1}{2}[f(t_i, y(t_i)) - f(t_{i-1}, y(t_{i-1}))]\right. \\ &\quad \left. + \frac{5}{12}[f(t_i, y(t_i)) - 2f(t_{i-1}, y(t_{i-1})) + f(t_{i-2}, y(t_{i-2}))]\right\} \\ &= y(t_i) + \frac{h}{12}[23f(t_i, y(t_i)) - 16f(t_{i-1}, y(t_{i-1})) + 5f(t_{i-2}, y(t_{i-2}))]. \end{aligned}$$

The three-step Adams-Bashforth method is, consequently,

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2,$$

$$w_{i+1} = w_i + \frac{h}{12}[23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1})] + 5f(t_{i-2}, w_{i-2})],$$

for $i = 2, 3, \ldots, N-1$. ■

Multistep methods can also be derived using Taylor series. An example of the procedure involved is considered in Exercise 12. A derivation using a Lagrange interpolating polynomial is discussed in Exercise 11.

The local truncation error for multistep methods is defined analogously to that of one-step methods. As in the case of one-step methods, the local truncation error provides a measure of how the solution to the differential equation fails to solve the difference equation.

Definition 5.15 If $y(t)$ is the solution to the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha,$$

and

$$\begin{aligned} w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ &\quad + h[b_m f(t_{i+1}, w_{i+1}) + b_{m-1}f(t_i, w_i) + \cdots + b_0 f(t_{i+1-m}, w_{i+1-m})] \end{aligned}$$

is the $(i+1)$st step in a multistep method, the **local truncation error** at this step is

$$\begin{aligned} \tau_{i+1}(h) = \frac{y(t_{i+1}) - a_{m-1}y(t_i) - \cdots - a_0 y(t_{i+1-m})}{h} \\ - [b_m f(t_{i+1}, y(t_{i+1})) + \cdots + b_0 f(t_{i+1-m}, y(t_{i+1-m}))], \end{aligned} \tag{5.32}$$

for each $i = m-1, m, \ldots, N-1$. ■

Example 3 Determine the local truncation error for the three-step Adams-Bashforth method derived in Example 2.

Solution Considering the form of the error given in Eq. (5.30) and the appropriate entry in Table 5.12 gives

$$h^4 f^{(3)}(\mu_i, y(\mu_i))(-1)^3 \int_0^1 \binom{-s}{3} ds = \frac{3h^4}{8} f^{(3)}(\mu_i, y(\mu_i)).$$

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Using the fact that $f^{(3)}(\mu_i, y(\mu_i)) = y^{(4)}(\mu_i)$ and the difference equation derived in Example 2, we have

$$\tau_{i+1}(h) = \frac{y(t_{i+1}) - y(t_i)}{h} - \frac{1}{12}[23f(t_i, y(t_i)) - 16f(t_{i-1}, y(t_{i-1})) + 5f(t_{i-2}, y(t_{i-2}))]$$
$$= \frac{1}{h}\left[\frac{3h^4}{8}f^{(3)}(\mu_i, y(\mu_i))\right] = \frac{3h^3}{8}y^{(4)}(\mu_i), \quad \text{for some } \mu_i \in (t_{i-2}, t_{i+1}). \blacksquare$$

Adams-Bashforth Explicit Methods

Some of the explicit multistep methods together with their required starting values and local truncation errors are as follows. The derivation of these techniques is similar to the procedure in Examples 2 and 3.

Adams-Bashforth Two-Step Explicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1,$$
$$w_{i+1} = w_i + \frac{h}{2}[3f(t_i, w_i) - f(t_{i-1}, w_{i-1})], \tag{5.33}$$

where $i = 1, 2, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = \frac{5}{12}y'''(\mu_i)h^2$, for some $\mu_i \in (t_{i-1}, t_{i+1})$.

Adams-Bashforth Three-Step Explicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2,$$
$$w_{i+1} = w_i + \frac{h}{12}[23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})], \tag{5.34}$$

where $i = 2, 3, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = \frac{3}{8}y^{(4)}(\mu_i)h^3$, for some $\mu_i \in (t_{i-2}, t_{i+1})$.

Adams-Bashforth Four-Step Explicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3, \tag{5.35}$$
$$w_{i+1} = w_i + \frac{h}{24}[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})],$$

where $i = 3, 4, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = \frac{251}{720}y^{(5)}(\mu_i)h^4$, for some $\mu_i \in (t_{i-3}, t_{i+1})$.

Adams-Bashforth Five-Step Explicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3, \quad w_4 = \alpha_4,$$
$$w_{i+1} = w_i + \frac{h}{720}[1901f(t_i, w_i) - 2774f(t_{i-1}, w_{i-1}) \tag{5.36}$$
$$+ 2616f(t_{i-2}, w_{i-2}) - 1274f(t_{i-3}, w_{i-3}) + 251f(t_{i-4}, w_{i-4})],$$

where $i = 4, 5, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = \frac{95}{288}y^{(6)}(\mu_i)h^5$, for some $\mu_i \in (t_{i-4}, t_{i+1})$.

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Adams-Moulton Implicit Methods

Implicit methods are derived by using $(t_{i+1}, f(t_{i+1}, y(t_{i+1})))$ as an additional interpolation node in the approximation of the integral

$$\int_{t_i}^{t_{i+1}} f(t, y(t))\, dt.$$

Some of the more common implicit methods are as follows.

Adams-Moulton Two-Step Implicit Method

$$\begin{aligned} w_0 &= \alpha, \quad w_1 = \alpha_1, \\ w_{i+1} &= w_i + \frac{h}{12}[5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})], \end{aligned} \tag{5.37}$$

where $i = 1, 2, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = -\frac{1}{24}y^{(4)}(\mu_i)h^3$, for some $\mu_i \in (t_{i-1}, t_{i+1})$.

Adams-Moulton Three-Step Implicit Method

$$\begin{aligned} &w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \\ &w_{i+1} = w_i + \frac{h}{24}[9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})], \end{aligned} \tag{5.38}$$

where $i = 2, 3, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = -\frac{19}{720}y^{(5)}(\mu_i)h^4$, for some $\mu_i \in (t_{i-2}, t_{i+1})$.

Adams-Moulton Four-Step Implicit Method

$$\begin{aligned} w_0 &= \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3, \\ w_{i+1} &= w_i + \frac{h}{720}[251f(t_{i+1}, w_{i+1}) + 646f(t_i, w_i) \\ &\quad - 264f(t_{i-1}, w_{i-1}) + 106f(t_{i-2}, w_{i-2}) - 19f(t_{i-3}, w_{i-3})], \end{aligned} \tag{5.39}$$

where $i = 3, 4, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = -\frac{3}{160}y^{(6)}(\mu_i)h^5$, for some $\mu_i \in (t_{i-3}, t_{i+1})$.

It is interesting to compare an m-step Adams-Bashforth explicit method with an $(m-1)$-step Adams-Moulton implicit method. Both involve m evaluations of f per step, and both have the terms $y^{(m+1)}(\mu_i)h^m$ in their local truncation errors. In general, the coefficients of the terms involving f in the local truncation error are smaller for the implicit methods than for the explicit methods. This leads to greater stability and smaller round-off errors for the implicit methods.

Example 4 Consider the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Use the exact values given from $y(t) = (t+1)^2 - 0.5e^t$ as starting values and $h = 0.2$ to compare the approximations from **(a)** by the explicit Adams-Bashforth four-step method and **(b)** the implicit Adams-Moulton three-step method.

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Solution **(a)** The Adams-Bashforth method has the difference equation

$$w_{i+1} = w_i + \frac{h}{24}[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})],$$

for $i = 3, 4, \ldots, 9$. When simplified using $f(t, y) = y - t^2 + 1$, $h = 0.2$, and $t_i = 0.2i$, it becomes

$$w_{i+1} = \frac{1}{24}[35w_i - 11.8w_{i-1} + 7.4w_{i-2} - 1.8w_{i-3} - 0.192i^2 - 0.192i + 4.736].$$

(b) The Adams-Moulton method has the difference equation

$$w_{i+1} = w_i + \frac{h}{24}[9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})],$$

for $i = 2, 3, \ldots, 9$. This reduces to

$$w_{i+1} = \frac{1}{24}[1.8w_{i+1} + 27.8w_i - w_{i-1} + 0.2w_{i-2} - 0.192i^2 - 0.192i + 4.736].$$

To use this method explicitly, we meed to solve the equation explicitly solve for w_{i+1}. This gives

$$w_{i+1} = \frac{1}{22.2}[27.8w_i - w_{i-1} + 0.2w_{i-2} - 0.192i^2 - 0.192i + 4.736],$$

for $i = 2, 3, \ldots, 9$.

The results in Table 5.13 were obtained using the exact values from $y(t) = (t + 1)^2 - 0.5e^t$ for α, α_1, α_2, and α_3 in the explicit Adams-Bashforth case and for α, α_1, and α_2 in the implicit Adams-Moulton case. Note that the implicit Adams-Moulton method gives consistently better results. ■

Table 5.13

t_i	Exact	Adams-Bashforth w_i	Error	Adams-Moulton w_i	Error
0.0	0.5000000				
0.2	0.8292986				
0.4	1.2140877				
0.6	1.6489406			1.6489341	0.0000065
0.8	2.1272295	2.1273124	0.0000828	2.1272136	0.0000160
1.0	2.6408591	2.6410810	0.0002219	2.6408298	0.0000293
1.2	3.1799415	3.1803480	0.0004065	3.1798937	0.0000478
1.4	3.7324000	3.7330601	0.0006601	3.7323270	0.0000731
1.6	4.2834838	4.2844931	0.0010093	4.2833767	0.0001071
1.8	4.8151763	4.8166575	0.0014812	4.8150236	0.0001527
2.0	5.3054720	5.3075838	0.0021119	5.3052587	0.0002132

Multistep methods are available as options of the *InitialValueProblem* command, in a manner similar to that of the one step methods. The command for the Adam Bashforth Four Step method applied to our usual example has the form

$C := InitialValueProblem(deq, y(0) = 0.5, t = 2, method = adamsbashforth,$
$submethod = step4, numsteps = 10, output = information, digits = 8)$

The output from this method is similar to the results in Table 5.13 except that the exact values were used in Table 5.13 and approximations were used as starting values for the Maple approximations.

To apply the Adams-Mouton Three Step method to this problem, the options would be changed to *method* = *adamsmoulton*, *submethod* = *step3*.

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Predictor-Corrector Methods

In Example 4 the implicit Adams-Moulton method gave better results than the explicit Adams-Bashforth method of the same order. Although this is generally the case, the implicit methods have the inherent weakness of first having to convert the method algebraically to an explicit representation for w_{i+1}. This procedure is not always possible, as can be seen by considering the elementary initial-value problem

$$y' = e^y, \quad 0 \le t \le 0.25, \quad y(0) = 1.$$

Because $f(t, y) = e^y$, the three-step Adams-Moulton method has

$$w_{i+1} = w_i + \frac{h}{24}[9e^{w_{i+1}} + 19e^{w_i} - 5e^{w_{i-1}} + e^{w_{i-2}}]$$

as its difference equation, and this equation cannot be algebraically solved for w_{i+1}.

We could use Newton's method or the secant method to approximate w_{i+1}, but this complicates the procedure considerably. In practice, implicit multistep methods are not used as described above. Rather, they are used to improve approximations obtained by explicit methods. The combination of an explicit method to predict and an implicit to improve the prediction is called a **predictor-corrector method**.

Consider the following fourth-order method for solving an initial-value problem. The first step is to calculate the starting values w_0, w_1, w_2, and w_3 for the four-step explicit Adams-Bashforth method. To do this, we use a fourth-order one-step method, the Runge-Kutta method of order four. The next step is to calculate an approximation, w_{4p}, to $y(t_4)$ using the explicit Adams-Bashforth method as predictor:

$$w_{4p} = w_3 + \frac{h}{24}[55f(t_3, w_3) - 59f(t_2, w_2) + 37f(t_1, w_1) - 9f(t_0, w_0)].$$

This approximation is improved by inserting w_{4p} in the right side of the three-step implicit Adams-Moulton method and using that method as a corrector. This gives

$$w_4 = w_3 + \frac{h}{24}[9f(t_4, w_{4p}) + 19f(t_3, w_3) - 5f(t_2, w_2) + f(t_1, w_1)].$$

The only new function evaluation required in this procedure is $f(t_4, w_{4p})$ in the corrector equation; all the other values of f have been calculated for earlier approximations.

The value w_4 is then used as the approximation to $y(t_4)$, and the technique of using the Adams-Bashforth method as a predictor and the Adams-Moulton method as a corrector is repeated to find w_{5p} and w_5, the initial and final approximations to $y(t_5)$. This process is continued until we obtain an approximation w_c to $y(t_N) = y(b)$.

Improved approximations to $y(t_{i+1})$ might be obtained by iterating the Adams-Moulton formula, but these converge to the approximation given by the implicit formula rather than to the solution $y(t_{i+1})$. Hence it is usually more efficient to use a reduction in the step size if improved accuracy is needed.

Algorithm 5.4 is based on the fourth-order Adams-Bashforth method as predictor and one iteration of the Adams-Moulton method as corrector, with the starting values obtained from the fourth-order Runge-Kutta method.

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ALGORITHM
5.4

Adams Fourth-Order Predictor-Corrector

To approximate the solution of the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha,$$

at $(N + 1)$ equally spaced numbers in the interval $[a, b]$:

INPUT endpoints a, b; integer N; initial condition α.

OUTPUT approximation w to y at the $(N + 1)$ values of t.

Step 1 Set $h = (b - a)/N$;
$t_0 = a$;
$w_0 = \alpha$;
OUTPUT (t_0, w_0).

Step 2 For $i = 1, 2, 3$, do Steps 3–5.
(*Compute starting values using Runge-Kutta method.*)

Step 3 Set $K_1 = hf(t_{i-1}, w_{i-1})$;
$K_2 = hf(t_{i-1} + h/2, w_{i-1} + K_1/2)$;
$K_3 = hf(t_{i-1} + h/2, w_{i-1} + K_2/2)$;
$K_4 = hf(t_{i-1} + h, w_{i-1} + K_3)$.

Step 4 Set $w_i = w_{i-1} + (K_1 + 2K_2 + 2K_3 + K_4)/6$;
$t_i = a + ih$.

Step 5 OUTPUT (t_i, w_i).

Step 6 For $i = 4, \ldots, N$ do Steps 7–10.

Step 7 Set $t = a + ih$;
$w = w_3 + h[55f(t_3, w_3) - 59f(t_2, w_2) + 37f(t_1, w_1) - 9f(t_0, w_0)]/24$; (*Predict* w_i.)
$w = w_3 + h[9f(t, w) + 19f(t_3, w_3) - 5f(t_2, w_2) + f(t_1, w_1)]/24$. (*Correct* w_i.)

Step 8 OUTPUT (t, w).

Step 9 For $j = 0, 1, 2$
set $t_j = t_{j+1}$; (*Prepare for next iteration.*)
$w_j = w_{j+1}$.

Step 10 Set $t_3 = t$;
$w_3 = w$.

Step 11 STOP. ■

Example 5 Apply the Adams fourth-order predictor-corrector method with $h = 0.2$ and starting values from the Runge-Kutta fourth order method to the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Solution This is continuation and modification of the problem considered in Example 1 at the beginning of the section. In that example we found that the starting approximations from Runge-Kutta are

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$$y(0) = w_0 = 0.5,\ y(0.2) \approx w_1 = 0.8292933,\ y(0.4) \approx w_2 = 1.2140762,\ \text{and}$$
$$y(0.6) \approx w_3 = 1.6489220.$$

and the fourth-order Adams-Bashforth method gave

$$\begin{aligned} y(0.8) \approx w_{4p} &= w_3 + \frac{0.2}{24}\left(55f(0.6, w_3) - 59f(0.4, w_2) + 37f(0.2, w_1) - 9f(0, w_0)\right) \\ &= 1.6489220 + \frac{0.2}{24}(55f(0.6, 1.6489220) - 59f(0.4, 1.2140762) \\ &\quad + 37f(0.2, 0.8292933) - 9f(0, 0.5)) \\ &= 1.6489220 + 0.0083333(55(2.2889220) - 59(2.0540762) \\ &\quad + 37(1.7892933) - 9(1.5)) \\ &= 2.1272892. \end{aligned}$$

We will now use w_{4p} as the predictor of the approximation to $y(0.8)$ and determine the corrected value w_4, from the implicit Adams-Moulton method. This gives

$$\begin{aligned} y(0.8) \approx w_4 &= w_3 + \frac{0.2}{24}\left(9f(0.8, w_{4p}) + 19f(0.6, w_3) - 5f(0.4, w_2) + f(0.2, w_1)\right) \\ &= 1.6489220 + \frac{0.2}{24}(9f(0.8, 2.1272892) + 19f(0.6, 1.6489220) \\ &\quad - 5f(0.4, 1.2140762) + f(0.2, 0.8292933)) \\ &= 1.6489220 + 0.0083333(9(2.4872892) + 19(2.2889220) - 5(2.0540762) \\ &\quad + (1.7892933)) \\ &= 2.1272056. \end{aligned}$$

Now we use this approximation to determine the predictor, w_{5p}, for $y(1.0)$ as

$$\begin{aligned} y(1.0) \approx w_{5p} &= w_4 + \frac{0.2}{24}\left(55f(0.8, w_4) - 59f(0.6, w_3) + 37f(0.4, w_2) - 9f(0.2, w_1)\right) \\ &= 2.1272056 + \frac{0.2}{24}(55f(0.8, 2.1272056) - 59f(0.6, 1.6489220) \\ &\quad + 37f(0.4, 1.2140762) - 9f(0.2, 0.8292933)) \\ &= 2.1272056 + 0.0083333(55(2.4872056) - 59(2.2889220) + 37(2.0540762) \\ &\quad - 9(1.7892933)) \\ &= 2.6409314, \end{aligned}$$

and correct this with

$$\begin{aligned} y(1.0) \approx w_5 &= w_4 + \frac{0.2}{24}\left(9f(1.0, w_{5p}) + 19f(0.8, w_4) - 5f(0.6, w_3) + f(0.4, w_2)\right) \\ &= 2.1272056 + \frac{0.2}{24}(9f(1.0, 2.6409314) + 19f(0.8, 2.1272892) \\ &\quad - 5f(0.6, 1.6489220) + f(0.4, 1.2140762)) \end{aligned}$$

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$$= 2.1272056 + 0.0083333(9(2.6409314) + 19(2.4872056) - 5(2.2889220) + (2.0540762))$$
$$= 2.6408286.$$

In Example 1 we found that using the explicit Adams-Bashforth method alone produced results that were inferior to those of Runge-Kutta. However, these approximations to $y(0.8)$ and $y(1.0)$ are accurate to within

$$|2.1272295 - 2.1272056| = 2.39 \times 10^{-5} \quad \text{and} \quad |2.6408286 - 2.6408591| = 3.05 \times 10^{-5},$$

respectively, compared to those of Runge-Kutta, which were accurate, respectively, to within

$$|2.1272027 - 2.1272892| = 2.69 \times 10^{-5} \quad \text{and} \quad |2.6408227 - 2.6408591| = 3.64 \times 10^{-5}.$$

The remaining predictor-corrector approximations were generated using Algorithm 5.4 and are shown in Table 5.14. ■

Table 5.14

t_i	$y_i = y(t_i)$	w_i	Error $\lvert y_i - w_i \rvert$
0.0	0.5000000	0.5000000	0
0.2	0.8292986	0.8292933	0.0000053
0.4	1.2140877	1.2140762	0.0000114
0.6	1.6489406	1.6489220	0.0000186
0.8	2.1272295	2.1272056	0.0000239
1.0	2.6408591	2.6408286	0.0000305
1.2	3.1799415	3.1799026	0.0000389
1.4	3.7324000	3.7323505	0.0000495
1.6	4.2834838	4.2834208	0.0000630
1.8	4.8151763	4.8150964	0.0000799
2.0	5.3054720	5.3053707	0.0001013

Adams Fourth Order Predictor-Corrector method is implemented in Maple for the example problem with

$C := InitialValueProblem(deq, y(0) = 0.5, t = 2, method = adamsbashforthmoulton, submethod = step4, numsteps = 10, output = information, digits = 8)$

and generates the same values as in Table 5.14.

Edward Arthur Milne (1896–1950) worked in ballistic research during World War I, and then for the Solar Physics Observatory at Cambridge. In 1929 he was appointed the W. W. Rouse Ball chair at Wadham College in Oxford.

Other multistep methods can be derived using integration of interpolating polynomials over intervals of the form $[t_j, t_{i+1}]$, for $j \le i-1$, to obtain an approximation to $y(t_{i+1})$. When an interpolating polynomial is integrated over $[t_{i-3}, t_{i+1}]$, the result is the explicit **Milne's method**:

$$w_{i+1} = w_{i-3} + \frac{4h}{3}[2f(t_i, w_i) - f(t_{i-1}, w_{i-1}) + 2f(t_{i-2}, w_{i-2})],$$

which has local truncation error $\frac{14}{45}h^4y^{(5)}(\xi_i)$, for some $\xi_i \in (t_{i-3}, t_{i+1})$.

Simpson's name is associated with this technique because it is based on Simpson's rule for integration.

Milne's method is occasionally used as a predictor for the implicit **Simpson's method**,

$$w_{i+1} = w_{i-1} + \frac{h}{3}[f(t_{i+1}, w_{i+1}) + 4f(t_i, w_i) + f(t_{i-1}, w_{i-1})],$$

which has local truncation error $-(h^4/90)y^{(5)}(\xi_i)$, for some $\xi_i \in (t_{i-1}, t_{i+1})$, and is obtained by integrating an interpolating polynomial over $[t_{i-1}, t_{i+1}]$.

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The local truncation error involved with a predictor-corrector method of the Milne-Simpson type is generally smaller than that of the Adams-Bashforth-Moulton method. But the technique has limited use because of round-off error problems, which do not occur with the Adams procedure. Elaboration on this difficulty is given in Section 5.10.

EXERCISE SET 5.6

1. Use all the Adams-Bashforth methods to approximate the solutions to the following initial-value problems. In each case use exact starting values, and compare the results to the actual values.

a. $y' = te^{3t} - 2y, \quad 0 \le t \le 1, \quad y(0) = 0,$ with $h = 0.2;$ actual solution $y(t) = \frac{1}{5}te^{3t} - \frac{1}{25}e^{3t} + \frac{1}{25}e^{-2t}.$

b. $y' = 1 + (t - y)^2, \quad 2 \le t \le 3, \quad y(2) = 1,$ with $h = 0.2;$ actual solution $y(t) = t + \frac{1}{1-t}.$

c. $y' = 1 + y/t, \quad 1 \le t \le 2, \quad y(1) = 2,$ with $h = 0.2;$ actual solution $y(t) = t \ln t + 2t.$

d. $y' = \cos 2t + \sin 3t, \quad 0 \le t \le 1, \quad y(0) = 1,$ with $h = 0.2;$ actual solution $y(t) = \frac{1}{2}\sin 2t - \frac{1}{3}\cos 3t + \frac{4}{3}.$

2. Use each of the Adams-Bashforth methods to approximate the solutions to the following initial-value problems. In each case use starting values obtained from the Runge-Kutta method of order four. Compare the results to the actual values.

a. $y' = \dfrac{2 - 2ty}{t^2 + 1}, \quad 0 \le t \le 1, \quad y(0) = 1,$ with $h = 0.1$ actual solution $y(t) = \dfrac{2t + 1}{t^2 + 2}.$

b. $y' = \dfrac{y^2}{1 + t}, \quad 1 \le t \le 2, \quad y(1) = -(\ln 2)^{-1},$ with $h = 0.1$ actual solution $y(t) = \dfrac{-1}{\ln(t + 1)}.$

c. $y' = (y^2 + y)/t, \quad 1 \le t \le 3, \quad y(1) = -2,$ with $h = 0.2$ actual solution $y(t) = \dfrac{2t}{1 - t}.$

d. $y' = -ty + 4t/y, \quad 0 \le t \le 1, \quad y(0) = 1,$ with $h = 0.1$ actual solution $y(t) = \sqrt{4 - 3e^{-t^2}}.$

3. Use each of the Adams-Bashforth methods to approximate the solutions to the following initial-value problems. In each case use starting values obtained from the Runge-Kutta method of order four. Compare the results to the actual values.

a. $y' = y/t - (y/t)^2, \quad 1 \le t \le 2, \quad y(1) = 1,$ with $h = 0.1;$ actual solution $y(t) = \dfrac{t}{1 + \ln t}.$

b. $y' = 1 + y/t + (y/t)^2, \quad 1 \le t \le 3, \quad y(1) = 0,$ with $h = 0.2;$ actual solution $y(t) = t\tan(\ln t).$

c. $y' = -(y + 1)(y + 3), \quad 0 \le t \le 2, \quad y(0) = -2,$ with $h = 0.1;$ actual solution $y(t) = -3 + 2/(1 + e^{-2t}).$

d. $y' = -5y + 5t^2 + 2t, \quad 0 \le t \le 1, \quad y(0) = 1/3,$ with $h = 0.1;$ actual solution $y(t) = t^2 + \frac{1}{3}e^{-5t}.$

4. Use all the Adams-Moulton methods to approximate the solutions to the Exercises 1(a), 1(c), and 1(d). In each case use exact starting values, and explicitly solve for w_{i+1}. Compare the results to the actual values.

5. Use Algorithm 5.4 to approximate the solutions to the initial-value problems in Exercise 1.

6. Use Algorithm 5.4 to approximate the solutions to the initial-value problems in Exercise 2.

7. Use Algorithm 5.4 to approximate the solutions to the initial-value problems in Exercise 3.

8. Change Algorithm 5.4 so that the corrector can be iterated for a given number p iterations. Repeat Exercise 7 with $p = 2, 3,$ and 4 iterations. Which choice of p gives the best answer for each initial-value problem?

9. The initial-value problem

$$y' = e^y, \quad 0 \le t \le 0.20, \quad y(0) = 1$$

has solution

$$y(t) = 1 - \ln(1 - et).$$

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Applying the three-step Adams-Moulton method to this problem is equivalent to finding the fixed point w_{i+1} of

$$g(w) = w_i + \frac{h}{24}\left(9e^{w} + 19e^{w_i} - 5e^{w_{i-1}} + e^{w_{i-2}}\right).$$

a. With $h = 0.01$, obtain w_{i+1} by functional iteration for $i = 2, \ldots, 19$ using exact starting values w_0, w_1, and w_2. At each step use w_i to initially approximate w_{i+1}.

b. Will Newton's method speed the convergence over functional iteration?

10. Use the Milne-Simpson Predictor-Corrector method to approximate the solutions to the initial-value problems in Exercise 3.

11. **a.** Derive the Adams-Bashforth Two-Step method by using the Lagrange form of the interpolating polynomial.

b. Derive the Adams-Bashforth Four-Step method by using Newton's backward-difference form of the interpolating polynomial.

12. Derive the Adams-Bashforth Three-Step method by the following method. Set

$$y(t_{i+1}) = y(t_i) + ahf(t_i, y(t_i)) + bhf(t_{i-1}, y(t_{i-1})) + chf(t_{i-2}, y(t_{i-2})).$$

Expand $y(t_{i+1})$, $f(t_{i-2}, y(t_{i-2}))$, and $f(t_{i-1}, y(t_{i-1}))$ in Taylor series about $(t_i, y(t_i))$, and equate the coefficients of h, h^2 and h^3 to obtain a, b, and c.

13. Derive the Adams-Moulton Two-Step method and its local truncation error by using an appropriate form of an interpolating polynomial.

14. Derive Simpson's method by applying Simpson's rule to the integral

$$y(t_{i+1}) - y(t_{i-1}) = \int_{t_{i-1}}^{t_{i+1}} f(t, y(t))\, dt.$$

15. Derive Milne's method by applying the open Newton-Cotes formula (4.29) to the integral

$$y(t_{i+1}) - y(t_{i-3}) = \int_{t_{i-3}}^{t_{i+1}} f(t, y(t))\, dt.$$

16. Verify the entries in Table 5.12 on page 305.

5.7 Variable Step-Size Multistep Methods

The Runge-Kutta-Fehlberg method is used for error control because at each step it provides, at little additional cost, *two* approximations that can be compared and related to the local truncation error. Predictor-corrector techniques always generate two approximations at each step, so they are natural candidates for error-control adaptation.

To demonstrate the error-control procedure, we construct a variable step-size predictor-corrector method using the four-step explicit Adams-Bashforth method as predictor and the three-step implicit Adams-Moulton method as corrector.

The Adams-Bashforth four-step method comes from the relation

$$y(t_{i+1}) = y(t_i) + \frac{h}{24}[55f(t_i, y(t_i)) - 59f(t_{i-1}, y(t_{i-1})) + 37f(t_{i-2}, y(t_{i-2})) - 9f(t_{i-3}, y(t_{i-3}))] + \frac{251}{720}y^{(5)}(\hat{\mu}_i)h^5,$$

for some $\hat{\mu}_i \in (t_{i-3}, t_{i+1})$. The assumption that the approximations $w_0, w_1, \ldots, w_i$ are all exact implies that the Adams-Bashforth local truncation error is

$$\frac{y(t_{i+1}) - w_{i+1,p}}{h} = \frac{251}{720}y^{(5)}(\hat{\mu}_i)h^4. \tag{5.40}$$

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A similar analysis of the Adams-Moulton three-step method, which comes from

$$y(t_{i+1}) = y(t_i) + \frac{h}{24}[9f(t_{i+1}, y(t_{i+1})) + 19f(t_i, y(t_i)) - 5f(t_{i-1}, y(t_{i-1})) + f(t_{i-2}, y(t_{i-2}))] - \frac{19}{720}y^{(5)}(\tilde{\mu}_i)h^5,$$

for some $\tilde{\mu}_i \in (t_{i-2}, t_{i+1})$, leads to the local truncation error

$$\frac{y(t_{i+1}) - w_{i+1}}{h} = -\frac{19}{720}y^{(5)}(\tilde{\mu}_i)h^4. \tag{5.41}$$

To proceed further, we must make the assumption that for small values of h, we have

$$y^{(5)}(\hat{\mu}_i) \approx y^{(5)}(\tilde{\mu}_i).$$

The effectiveness of the error-control technique depends directly on this assumption.

If we subtract Eq. (5.40) from Eq. (5.39), we have

$$\frac{w_{i+1} - w_{i+1,p}}{h} = \frac{h^4}{720}[251y^{(5)}(\hat{\mu}_i) + 19y^{(5)}(\tilde{\mu}_i)] \approx \frac{3}{8}h^4y^{(5)}(\tilde{\mu}_i),$$

so

$$y^{(5)}(\tilde{\mu}_i) \approx \frac{8}{3h^5}(w_{i+1} - w_{i+1,p}). \tag{5.42}$$

Using this result to eliminate the term involving $y^{(5)}(\tilde{\mu}_i)h^4$ from Eq. (5.41) gives the approximation to the Adams-Moulton local truncation error

$$|\tau_{i+1}(h)| = \frac{|y(t_{i+1}) - w_{i+1}|}{h} \approx \frac{19h^4}{720} \cdot \frac{8}{3h^5}|w_{i+1} - w_{i+1,p}| = \frac{19|w_{i+1} - w_{i+1,p}|}{270h}.$$

Suppose we now reconsider (Eq. 5.41) with a new step size qh generating new approximations $\hat{w}_{i+1,p}$ and $\hat{w}_{i+1}$. The object is to choose q so that the local truncation error given in Eq. (5.41) is bounded by a prescribed tolerance ε. If we assume that the value $y^{(5)}(\mu)$ in Eq. (5.41) associated with qh is also approximated using Eq. (5.42), then

$$\frac{|y(t_i + qh) - \hat{w}_{i+1}|}{qh} = \frac{19q^4h^4}{720}|y^{(5)}(\mu)| \approx \frac{19q^4h^4}{720}\left[\frac{8}{3h^5}|w_{i+1} - w_{i+1,p}|\right] = \frac{19q^4}{270}\frac{|w_{i+1} - w_{i+1,p}|}{h},$$

and we need to choose q so that

$$\frac{|y(t_i + qh) - \hat{w}_{i+1}|}{qh} \approx \frac{19q^4}{270}\frac{|w_{i+1} - w_{i+1,p}|}{h} < \varepsilon.$$

That is, choose q so that

$$q < \left(\frac{270}{19}\frac{h\varepsilon}{|w_{i+1} - w_{i+1,p}|}\right)^{1/4} \approx 2\left(\frac{h\varepsilon}{|w_{i+1} - w_{i+1,p}|}\right)^{1/4}.$$

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A number of approximation assumptions have been made in this development, so in practice q is chosen conservatively, often as

$$q = 1.5\left(\frac{h\varepsilon}{|w_{i+1} - w_{i+1,p}|}\right)^{1/4}.$$

A change in step size for a multistep method is more costly in terms of function evaluations than for a one-step method, because new equally-spaced starting values must be computed. As a consequence, it is common practice to ignore the step-size change whenever the local truncation error is between $\varepsilon/10$ and ε, that is, when

$$\frac{\varepsilon}{10} < |\tau_{i+1}(h)| = \frac{|y(t_{i+1}) - w_{i+1}|}{h} \approx \frac{19|w_{i+1} - w_{i+1,p}|}{270h} < \varepsilon.$$

In addition, q is given an upper bound to ensure that a single unusually accurate approximation does not result in too large a step size. Algorithm 5.5 incorporates this safeguard with an upper bound of 4.

Remember that the multistep methods require equal step sizes for the starting values. So any change in step size necessitates recalculating new starting values at that point. In Steps 3, 16, and 19 of Algorithm 5.5 this is done by calling a Runge-Kutta subalgorithm (Algorithm 5.2), which has been set up in Step 1.

ALGORITHM
5.5

Adams Variable Step-Size Predictor-Corrector

To approximate the solution of the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$$

with local truncation error within a given tolerance:

INPUT endpoints a, b; initial condition α; tolerance TOL; maximum step size $hmax$; minimum step size $hmin$.

OUTPUT i, t_i, w_i, h where at the ith step w_i approximates $y(t_i)$ and the step size h was used, or a message that the minimum step size was exceeded.

Step 1 Set up a subalgorithm for the Runge-Kutta fourth-order method to be called $RK4(h, v_0, x_0, v_1, x_1, v_2, x_2, v_3, x_3)$ that accepts as input a step size h and starting values $v_0 \approx y(x_0)$ and returns $\{(x_j, v_j) \mid j = 1, 2, 3\}$ defined by the following:

for $j = 1, 2, 3$
set $K_1 = hf(x_{j-1}, v_{j-1})$;
$K_2 = hf(x_{j-1} + h/2, v_{j-1} + K_1/2)$
$K_3 = hf(x_{j-1} + h/2, v_{j-1} + K_2/2)$
$K_4 = hf(x_{j-1} + h, v_{j-1} + K_3)$
$v_j = v_{j-1} + (K_1 + 2K_2 + 2K_3 + K_4)/6$;
$x_j = x_0 + jh$.

Step 2 Set $t_0 = a$;
$w_0 = \alpha$;
$h = hmax$;
$FLAG = 1$; (*FLAG will be used to exit the loop in Step 4.*)
$LAST = 0$; (*LAST will indicate when the last value is calculated.*)
OUTPUT (t_0, w_0).

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Step 3 Call $RK4(h, w_0, t_0, w_1, t_1, w_2, t_2, w_3, t_3)$;
Set $NFLAG = 1$; (*Indicates computation from RK4.*)
$i = 4$;
$t = t_3 + h$.

Step 4 While ($FLAG = 1$) do Steps 5–20.

Step 5 Set $WP = w_{i-1} + \frac{h}{24}[55f(t_{i-1}, w_{i-1}) - 59f(t_{i-2}, w_{i-2})$
$+ 37f(t_{i-3}, w_{i-3}) - 9f(t_{i-4}, w_{i-4})]$; (*Predict* w_i.)

$WC = w_{i-1} + \frac{h}{24}[9f(t, WP) + 19f(t_{i-1}, w_{i-1})$
$- 5f(t_{i-2}, w_{i-2}) + f(t_{i-3}, w_{i-3})]$; (*Correct* w_i.)

$\sigma = 19|WC - WP|/(270h)$.

Step 6 If $\sigma \le TOL$ then do Steps 7–16 (*Result accepted.*)
else do Steps 17–19. (*Result rejected.*)

Step 7 Set $w_i = WC$; (*Result accepted.*)
$t_i = t$.

Step 8 If $NFLAG = 1$ then for $j = i - 3, i - 2, i - 1, i$
OUTPUT (j, t_j, w_j, h);
(*Previous results also accepted.*)
else OUTPUT (i, t_i, w_i, h).
(*Previous results already accepted.*)

Step 9 If $LAST = 1$ then set $FLAG = 0$ (*Next step is* 20.)
else do Steps 10–16.

Step 10 Set $i = i + 1$;
$NFLAG = 0$.

Step 11 If $\sigma \le 0.1\,TOL$ or $t_{i-1} + h > b$ then do Steps 12–16.
(*Increase h if it is more accurate than required or decrease h to include b as a mesh point.*)

Step 12 Set $q = (TOL/(2\sigma))^{1/4}$.

Step 13 If $q > 4$ then set $h = 4h$
else set $h = qh$.

Step 14 If $h > hmax$ then set $h = hmax$.

Step 15 If $t_{i-1} + 4h > b$ then
set $h = (b - t_{i-1})/4$;
$LAST = 1$.

Step 16 Call $RK4(h, w_{i-1}, t_{i-1}, w_i, t_i, w_{i+1}, t_{i+1}, w_{i+2}, t_{i+2})$;
Set $NFLAG = 1$;
$i = i + 3$. (*True branch completed. Next step is 20.*)

Step 17 Set $q = (TOL/(2\sigma))^{1/4}$. (*False branch from Step 6: Result rejected.*)

Step 18 If $q < 0.1$ then set $h = 0.1h$
else set $h = qh$.

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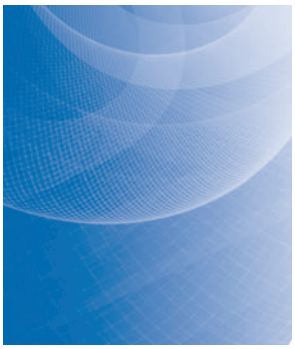

Step 19 If $h < hmin$ then set $FLAG = 0$;
OUTPUT ('$hmin$ exceeded')
else
if $NFLAG = 1$ then set $i = i - 3$;
(*Previous results also rejected.*)
Call $RK4(h, w_{i-1}, t_{i-1}, w_i, t_i, w_{i+1}, t_{i+1}, w_{i+2}, t_{i+2})$;
set $i = i + 3$;
$NFLAG = 1$.

Step 20 Set $t = t_{i-1} + h$.

Step 21 STOP. ■

Example 1 Use Adams variable step-size predictor-corrector method with maximum step size $hmax = 0.2$, minimum step size $hmin = 0.01$, and tolerance $TOL = 10^{-5}$ to approximate the solution of the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Solution We begin with $h = hmax = 0.2$, and obtain w_0, w_1, w_2 and w_3 using Runge-Kutta, then find wp_4 and wc_4 by applying the predictor-corrector method. These calculations were done in Example 5 of Section 5.6 where it was determined that the Runge-Kutta approximations are

$$y(0) = w_0 = 0.5,\ y(0.2) \approx w_1 = 0.8292933,\ y(0.4) \approx w_2 = 1.2140762,\ \text{and}$$
$$y(0.6) \approx w_3 = 1.6489220.$$

The predictor and corrector gave

$$y(0) = w_0 = 0.5,\ y(0.2) \approx w_1 = 0.8292933,\ y(0.4) \approx w_2 = 1.2140762,\ \text{and}$$
$$y(0.6) \approx w_3 = 1.6489220.$$

$$y(0.8) \approx w_{4p} = w_3 + \frac{0.2}{24}\left(55f(0.6, w_3) - 59f(0.4, w_2) + 37f(0.2, w_1) - 9f(0, w_0)\right)$$
$$= 2.1272892,$$

and

$$y(0.8) \approx w_4 = w_3 + \frac{0.2}{24}\left(9f(0.8, w_{4p}) + 19f(0.6, w_3) - 5f(0.42, w_2) + f(0.2, w_1)\right)$$
$$= 2.1272056.$$

We now need to determine if these approximations are sufficiently accurate or if there needs to be a change in the step size. First we find

$$\delta = \frac{19}{270h}|w_4 - w_{4p}| = \frac{19}{270(0.2)}|2.1272056 - 2.1272892| = 2.941 \times 10^{-5}.$$

Because this exceeds the tolerance of 10^{-5} a new step size is needed and the new step size is

$$qh = \left(\frac{10^{-5}}{2\delta}\right)^{1/4} = \left(\frac{10^{-5}}{2(2.941 \times 10^{-5})}\right)^{1/4}(0.2) = 0.642(0.2) \approx 0.128.$$

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As a consequence, we need to begin the procedure again computing the Runge-Kutta values with this step size, and then use the predictor-corrector method with this same step size to compute the new values of w_{4p} and w_4. We then need to run the accuracy check on these approximations to see that we have been successful. Table 5.15 shows that this second run is successful and lists the all results obtained using Algorithm 5.5. ■

Table 5.15

t_i	$y(t_i)$	w_i	h_i	σ_i	$\lvert y(t_i) - w_i \rvert$
0	0.5	0.5			
0.1257017	0.7002323	0.7002318	0.1257017	4.051×10^{-6}	0.0000005
0.2514033	0.9230960	0.9230949	0.1257017	4.051×10^{-6}	0.0000011
0.3771050	1.1673894	1.1673877	0.1257017	4.051×10^{-6}	0.0000017
0.5028066	1.4317502	1.4317480	0.1257017	4.051×10^{-6}	0.0000022
0.6285083	1.7146334	1.7146306	0.1257017	4.610×10^{-6}	0.0000028
0.7542100	2.0142869	2.0142834	0.1257017	5.210×10^{-6}	0.0000035
0.8799116	2.3287244	2.3287200	0.1257017	5.913×10^{-6}	0.0000043
1.0056133	2.6556930	2.6556877	0.1257017	6.706×10^{-6}	0.0000054
1.1313149	2.9926385	2.9926319	0.1257017	7.604×10^{-6}	0.0000066
1.2570166	3.3366642	3.3366562	0.1257017	8.622×10^{-6}	0.0000080
1.3827183	3.6844857	3.6844761	0.1257017	9.777×10^{-6}	0.0000097
1.4857283	3.9697541	3.9697433	0.1030100	7.029×10^{-6}	0.0000108
1.5887383	4.2527830	4.2527711	0.1030100	7.029×10^{-6}	0.0000120
1.6917483	4.5310269	4.5310137	0.1030100	7.029×10^{-6}	0.0000133
1.7947583	4.8016639	4.8016488	0.1030100	7.029×10^{-6}	0.0000151
1.8977683	5.0615660	5.0615488	0.1030100	7.760×10^{-6}	0.0000172
1.9233262	5.1239941	5.1239764	0.0255579	3.918×10^{-8}	0.0000177
1.9488841	5.1854932	5.1854751	0.0255579	3.918×10^{-8}	0.0000181
1.9744421	5.2460056	5.2459870	0.0255579	3.918×10^{-8}	0.0000186
2.0000000	5.3054720	5.3054529	0.0255579	3.918×10^{-8}	0.0000191

EXERCISE SET 5.7

1. Use the Adams Variable Step-Size Predictor-Corrector Algorithm with tolerance $TOL = 10^{-4}$, $hmax = 0.25$, and $hmin = 0.025$ to approximate the solutions to the given initial-value problems. Compare the results to the actual values.

a. $y' = te^{3t} - 2y, \quad 0 \le t \le 1, \quad y(0) = 0;$ actual solution $y(t) = \frac{1}{5}te^{3t} - \frac{1}{25}e^{3t} + \frac{1}{25}e^{-2t}$.

b. $y' = 1 + (t - y)^2, \quad 2 \le t \le 3, \quad y(2) = 1;$ actual solution $y(t) = t + 1/(1 - t)$.

c. $y' = 1 + y/t, \quad 1 \le t \le 2, \quad y(1) = 2;$ actual solution $y(t) = t \ln t + 2t$.

d. $y' = \cos 2t + \sin 3t, \quad 0 \le t \le 1, \quad y(0) = 1;$ actual solution $y(t) = \frac{1}{2}\sin 2t - \frac{1}{3}\cos 3t + \frac{4}{3}$.

2. Use the Adams Variable Step-Size Predictor-Corrector Algorithm with $TOL = 10^{-4}$ to approximate the solutions to the following initial-value problems:

a. $y' = (y/t)^2 + y/t, \quad 1 \le t \le 1.2, \quad y(1) = 1,$ with $hmax = 0.05$ and $hmin = 0.01$.

b. $y' = \sin t + e^{-t}, \quad 0 \le t \le 1, \quad y(0) = 0,$ with $hmax = 0.2$ and $hmin = 0.01$.

c. $y' = (y^2 + y)/t, \quad 1 \le t \le 3, \quad y(1) = -2,$ with $hmax = 0.4$ and $hmin = 0.01$.

d. $y' = -ty + 4t/y, \quad 0 \le t \le 1, \quad y(0) = 1,$ with $hmax = 0.2$ and $hmin = 0.01$.

3. Use the Adams Variable Step-Size Predictor-Corrector Algorithm with tolerance $TOL = 10^{-6}$, $hmax = 0.5$, and $hmin = 0.02$ to approximate the solutions to the given initial-value problems. Compare the results to the actual values.

a. $y' = y/t - (y/t)^2, \quad 1 \le t \le 4, \quad y(1) = 1;$ actual solution $y(t) = t/(1 + \ln t)$.

b. $y' = 1 + y/t + (y/t)^2, \quad 1 \le t \le 3, \quad y(1) = 0;$ actual solution $y(t) = t \tan(\ln t)$.

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c. $y' = -(y+1)(y+3), \quad 0 \le t \le 3, \quad y(0) = -2;$ actual solution $y(t) = -3 + 2(1 + e^{-2t})^{-1}$.

d. $y' = (t + 2t^3)y^3 - ty, \quad 0 \le t \le 2, \quad y(0) = \frac{1}{3};$ actual solution $y(t) = (3 + 2t^2 + 6e^{t^2})^{-1/2}$.

4. Construct an Adams Variable Step-Size Predictor-Corrector Algorithm based on the Adams-Bashforth five-step method and the Adams-Moulton four-step method. Repeat Exercise 3 using this new method.

5. An electrical circuit consists of a capacitor of constant capacitance $C = 1.1$ farads in series with a resistor of constant resistance $R_0 = 2.1$ ohms. A voltage $\mathcal{E}(t) = 110 \sin t$ is applied at time $t = 0$. When the resistor heats up, the resistance becomes a function of the current i,

$$R(t) = R_0 + ki, \quad \text{where } k = 0.9,$$

and the differential equation for $i(t)$ becomes

$$\left(1 + \frac{2k}{R_0} i\right) \frac{di}{dt} + \frac{1}{R_0 C} i = \frac{1}{R_0 C} \frac{d\mathcal{E}}{dt}.$$

Find $i(2)$, assuming that $i(0) = 0$.

5.8 Extrapolation Methods

Extrapolation was used in Section 4.5 for the approximation of definite integrals, where we found that by correctly averaging relatively inaccurate trapezoidal approximations exceedingly accurate new approximations were produced. In this section we will apply extrapolation to increase the accuracy of approximations to the solution of initial-value problems. As we have previously seen, the original approximations must have an error expansion of a specific form for the procedure to be successful.

To apply extrapolation to solve initial-value problems, we use a technique based on the Midpoint method:

$$w_{i+1} = w_{i-1} + 2h f(t_i, w_i), \quad \text{for } i \ge 1. \tag{5.43}$$

This technique requires two starting values since both w_0 and w_1 are needed before the first midpoint approximation, w_2, can be determined. One starting value is the initial condition for $w_0 = y(a) = \alpha$. To determine the second starting value, w_1, we apply Euler's method. Subsequent approximations are obtained from (5.43). After a series of approximations of this type are generated ending at a value t, an endpoint correction is performed that involves the final two midpoint approximations. This produces an approximation $w(t, h)$ to $y(t)$ that has the form

$$y(t) = w(t, h) + \sum_{k=1}^{\infty} \delta_k h^{2k}, \tag{5.44}$$

where the δ_k are constants related to the derivatives of the solution $y(t)$. The important point is that the δ_k do not depend on the step size h. The details of this procedure can be found in the paper by Gragg [Gr].

To illustrate the extrapolation technique for solving

$$y'(t) = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha,$$

assume that we have a fixed step size h. We wish to approximate $y(t_1) = y(a + h)$.

For the first extrapolation step we let $h_0 = h/2$ and use Euler's method with $w_0 = \alpha$ to approximate $y(a + h_0) = y(a + h/2)$ as

$$w_1 = w_0 + h_0 f(a, w_0).$$

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