If n_1 molecules of $K_2Cr_2O_7$, n_2 molecules of H_2O, and n_3 molecules of S are originally available, the following differential equation describes the amount $x(t)$ of KOH after time t:

$$\frac{dx}{dt} = k\left(n_1 - \frac{x}{2}\right)^2\left(n_2 - \frac{x}{2}\right)^2\left(n_3 - \frac{3x}{4}\right)^3,$$

where k is the velocity constant of the reaction. If $k = 6.22 \times 10^{-19}$, $n_1 = n_2 = 2 \times 10^3$, and $n_3 = 3 \times 10^3$, use the Runge-Kutta method of order 4 to determine how many units of potassium hydroxide will have been formed after 0.2 s.

20. Show that Heun's Method can be expressed in difference form, similar to that of the Runge-Kutta method of order 4, as

$$\begin{aligned}
w_0 &= \alpha,\\
k_1 &= hf(t_i, w_i),\\
k_2 &= hf\left(t_i + \frac{h}{3}, w_i + \frac{1}{3}k_1\right),\\
k_3 &= hf\left(t_i + \frac{2h}{3}, w_i + \frac{2}{3}k_2\right),\\
w_{i+1} &= w_i + \frac{1}{4}(k_1 + 3k_3),
\end{aligned}$$

for each $i = 0, 1, \ldots, N-1$.

5.4 Predictor-Corrector Methods

The Taylor and Runge-Kutta methods are examples of **one-step methods** for approximating the solution to initial-value problems. These methods use w_i in the approximation w_{i+1} to $y(t_{i+1})$ but do not involve any of the prior approximations $w_0, w_1, \ldots, w_{i-1}$. Generally some functional evaluations of f are required at intermediate points, but these are discarded as soon as w_{i+1} is obtained.

Since $|y(t_j) - w_j|$ decreases in accuracy as j increases, better approximation methods can be derived if, when approximating $y(t_{i+1})$, we include in the method some of the approximations prior to w_i. Methods developed using this philosophy are called **multistep methods**. In brief, one-step methods consider what occurred at only one previous step; multistep methods consider what happened at more than one previous step.

To derive a multistep method, suppose that the solution to the initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad \text{for } a \le t \le b, \quad \text{with } y(a) = \alpha,$$

is integrated over the interval $[t_i, t_{i+1}]$. Then

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

and

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

Since we cannot integrate $f(t, y(t))$ without knowing $y(t)$, which is the solution to the problem, we instead integrate an interpolating polynomial, $P(t)$, for $f(t, y(t))$ 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 $y(t_i) \approx w_i$, we have

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

If w_{m+1} is the first approximation generated by the multistep method, then we need to supply starting values $w_0, w_1, \ldots, w_m$ for the method. These starting values are generated using a one-step Runge-Kutta method with the same error characteristics as the multistep method.

There are two distinct classes of multistep methods. In an **explicit method,** w_{i+1} does not involve the function evaluation $f(t_{i+1}, w_{i+1})$. A method that does depend in part on $f(t_{i+1}, w_{i+1})$ is an **implicit** method.

Adams-Bashforth Explicit Methods

Some of the explicit multistep methods, together with their required starting values and local error terms, are given next.

Adams-Bashforth Two-Step Explicit Method

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

where $i = 1, 2, \ldots, N-1$, with local error $\frac{5}{12}y'''(\mu_i)h^3$ for some μ_i in (t_{i-1}, t_{i+1}).

Adams-Bashforth Three-Step Explicit Method

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

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

Adams-Bashforth Four-Step Explicit Method

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

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

Adams-Bashforth Five-Step Explicit Method

$$w_0 = \alpha,\ w_1 = \alpha_1,\ w_2 = \alpha_2,\ w_3 = \alpha_3,\ w_4 = \alpha_4$$

$$w_{i+1} = w_i + \frac{h}{720}[1901 f(t_i, w_i) - 2774 f(t_{i-1}, w_{i-1}) + 2616 f(t_{i-2}, w_{i-2}) - 1274 f(t_{i-3}, w_{i-3}) + 251 f(t_{i-4}, w_{i-4})]$$

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

Adams-Moulton Implicit Methods

Implicit methods use $(t_{i+1}, f(t_{i+1}, w_{i+1}))$ 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 listed next. Notice that the local error of an $(m-1)$-step implicit method is $O(h^{m+1})$, the same as that of an m-step explicit method. They both use m function evaluations, however, because the implicit methods use $f(t_{i+1}, w_{i+1})$, but the explicit methods do not.

Adams-Moulton Two-Step Implicit Method

$$w_0 = \alpha,\ w_1 = \alpha_1$$

$$w_{i+1} = w_i + \frac{h}{12}[5 f(t_{i+1}, w_{i+1}) + 8 f(t_i, w_i) - f(t_{i-1}, w_{i-1})]$$

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

Adams-Moulton Three-Step Implicit Method

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

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

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

Adams-Moulton Four-Step Implicit Method

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

$$w_{i+1} = w_i + \frac{h}{720}[251 f(t_{i+1}, w_{i+1}) + 646 f(t_i, w_i) - 264 f(t_{i-1}, w_{i-1}) + 106 f(t_{i-2}, w_{i-2}) - 19 f(t_{i-3}, w_{i-3})]$$

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

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

Example 1 In Example 2 of Section 5.3 (see Table 5.8 on page 188) we used the Runge-Kutta method of order 4 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 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 4.

Solution For the fourth-order Adams-Bashforth we have

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

and

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

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

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

The corresponding Runge-Kutta approximations had errors

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

■

The implicit Adams-Moulton methods generally give considerably better results than the explicit Adams-Bashforth method of the same order. However, the implicit methods have the inherent weakness of first having to convert the method algebraically to an explicit representation for w_{i+1}. That this procedure can become difficult, if not impossible, can be seen by considering the elementary initial-value problem

$$y' = e^y, \quad \text{for } 0 \le t \le 0.25, \quad \text{with } y(0) = 1.$$

Since $f(t, y) = e^y$, the Adams-Moulton Three-Step 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 solved explicitly 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.

Predictor-Corrector Methods

In practice, implicit multistep methods are not used alone. Rather, they are used to improve approximations obtained by explicit methods. The combination of an explicit and implicit technique is called a **predictor-corrector method**. The explicit method predicts an approximation, and the implicit method corrects this prediction.

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 explicit Adams-Bashforth Four-Step method. To do this, we use a fourth-order one-step method, specifically, the Runge-Kutta method of order 4. The next step is to calculate an approximation, w_{4p}, to $y(t_4)$ using the explicit Adams-Bashforth Four-Step 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 use of the implicit Adams-Moulton Three-Step method as corrector:

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

The value w_4 is now used as the approximation to $y(t_4)$. Then 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 to $y(t_N) = y(b)$.

The program PRCORM53 implements the Adams Predictor-Corrector method.

Program PRCORM53 is based on the Adams-Bashforth Four-Step method as predictor and one iteration of the Adams-Moulton Three-Step method as corrector, with the starting values obtained from the Runge-Kutta method of order 4.

Example 2 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 a 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

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

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

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

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

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

and correct this with

$$\begin{aligned}
y(1.0) \approx w_5 &= w_4 + \frac{0.2}{24}[9f(1.0, w_{5p}) + 19f(0.8, w_4) - 5f(0.6, w_3) + f(0.4, w_2)]\\
&= 2.1272056 + \frac{0.2}{24}[9f(1.0, 2.6409314) + 19f(0.8, 2.1272892)\\
&\quad - 5f(0.6, 1.6489220) + f(0.4, 1.2140762)]\\
&= 2.1272056 + 0.0083333[9(2.6409314) + 19(2.4872056)\\
&\quad - 5(2.2889220) + (2.0540762)]\\
&= 2.6408286.
\end{aligned}$$

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

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

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

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

Other multistep methods can be derived using integration of interpolating polynomials over intervals of the form $[t_j, t_{i+1}]$ for $j \leq i-1$, where some of the data points are omitted. Milne's method is an explicit technique that results when a Newton Backward-Difference interpolating polynomial is integrated over $[t_{i-3}, t_{i+1}]$.

Milne's Method

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

where $i = 3, 4, \ldots, N-1$, with local error $\frac{14}{45}h^5 y^{(5)}(\mu_i)$ for some μ_i in (t_{i-3}, t_{i+1}).

This method is used as a predictor for an implicit method called Simpson's method. Its name comes from the fact that it can be derived using Simpson's rule for approximating integrals.

Simpson's Method

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

where $i = 1, 2, \ldots, N-1$, with local error $-\frac{1}{90}h^5 y^{(5)}(\mu_i)$ for some μ_i in (t_{i-1}, t_{i+1}).

Although the local error involved with a predictor-corrector method of the Milne-Simpson type is generally smaller than that of the Adams-Bashforth-Moulton method, the technique has limited use because of round-off error problems, which do not occur with the Adams procedure.

MATLAB uses methods that are more sophisticated than the standard Adams-Bashforth-Moulton techniques to approximate the solutions to ordinary differential equations. An introduction to methods of this type is considered in Section 5.6.

EXERCISE SET 5.4

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. $y' = te^{3t} - 2y$, for $0 \le t \le 1$, with $y(0) = 0$ and $h = 0.2$; actual solution $y(t) = \frac{1}{5}te^{3t} - \frac{1}{25}e^{3t} + \frac{1}{25}e^{-2t}$.
   b. $y' = 1 + (t-y)^2$, for $2 \le t \le 3$, with $y(2) = 1$ and $h = 0.2$; actual solution $y(t) = t + 1/(1-t)$.
   c. $y' = 1 + \frac{y}{t}$, for $1 \le t \le 2$, with $y(1) = 2$ and $h = 0.2$; actual solution $y(t) = t\ln t + 2t$.
   d. $y' = \cos 2t + \sin 3t$, for $0 \le t \le 1$ with $y(0) = 1$ and $h = 0.2$; actual solution $y(t) = \frac{1}{2}\sin 2t - \frac{1}{3}\cos 3t + \frac{4}{3}$.
2. Use all the Adams-Moulton methods to approximate the solutions to 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.
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 4. Compare the results to the actual values.
   a. $y' = \frac{y}{t} - \left(\frac{y}{t}\right)^2$, for $1 \le t \le 2$, with $y(1) = 1$ and $h = 0.1$; actual solution $y(t) = t/(1 + \ln t)$.
   b. $y' = 1 + \frac{y}{t} + \left(\frac{y}{t}\right)^2$, for $1 \le t \le 3$, with $y(1) = 0$ and $h = 0.2$; actual solution $y(t) = t\tan(\ln t)$.
   c. $y' = -(y+1)(y+3)$, for $0 \le t \le 2$, with $y(0) = -2$ and $h = 0.1$; actual solution $y(t) = -3 + 2/(1 + e^{-2t})$.
   d. $y' = -5y + 5t^2 + 2t$, for $0 \le t \le 1$, with $y(0) = 1/3$ and $h = 0.1$; actual solution $y(t) = t^2 + \frac{1}{3}e^{-5t}$.
4. Use the predictor-corrector method based on the Adams-Bashforth Four-Step method and the Adams-Moulton Three-Step method to approximate the solutions to the initial-value problems in Exercise 1.
5. Use the predictor-corrector method based on the Adams-Bashforth Four-Step method and the Adams-Moulton Three-Step method to approximate the solutions to the initial-value problem in Exercise 3.
6. The initial-value problem

   $$y' = e^y, \quad \text{for } 0 \le t \le 0.20, \quad \text{with } y(0) = 1$$

   has the exact solution

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

   Applying the Adams-Moulton Three-Step method to the problem requires solving for w_{i+1} in the equation

   $$g(w_{i+1}) = w_{i+1} - \left(w_i + \frac{h}{24}\left(9e^{w_{i+1}} + 19e^{w_i} - 5e^{w_{i-1}} + e^{w_{i-2}}\right)\right) = 0.$$

   Suppose that $h = 0.01$ and we use the exact starting values for w_0, w_1, and w_2.
   a. Apply Newton's method to this equation with the starting value w_2 to approximate w_3 to within 10^{-6}.
   b. Repeat the calculations in (a) using the starting value w_i to determine approximations accurate to within 10^{-6} for each w_{i+1} for $i = 2, \dots, 19$.
7. Use the Milne-Simpson Predictor-Corrector method to approximate the solutions to the initial-value problems in Exercise 3.

5.5 Extrapolation Methods

Extrapolation was used in Romberg integration for the approximation of definite integrals, where we found that, by correctly averaging relatively inaccurate trapezoidal approximations, we could produce new approximations that are exceedingly accurate. In this section