f. Use the answers generated in (e) and piecewise cubic Hermite interpolation to approximate y at the following values and compare them to the actual values of y.

i. $y(1.04)$ **ii.** $y(1.55)$ **iii.** $y(1.97)$

9. Given the initial-value problem

$$y' = \frac{1}{t^2} - \frac{y}{t} - y^2, \quad 1 \le t \le 2, \quad y(1) = -1$$

with the exact solution $y(t) = -1/t$.

a. Use Euler's method with $h = 0.05$ to approximate the solution and compare it with the actual values of y.

b. Use the answers generated in (a) and linear interpolation to approximate the following values of y and compare them to the actual values.

i. $y(1.052)$ **ii.** $y(1.555)$ **iii.** $y(1.978)$

c. Use Taylor's method of order 2 with $h = 0.05$ to approximate the solution and compare it with the actual values of y.

d. Use the answers generated in (c) and linear interpolation to approximate the following values of y and compare them to the actual values.

i. $y(1.052)$ **ii.** $y(1.555)$ **iii.** $y(1.978)$

e. Use Taylor's method of order 4 with $h = 0.05$ to approximate the solution and compare it with the actual values of y.

f. Use the answers generated in (e) and piecewise cubic Hermite interpolation to approximate the following values of y and compare them to the actual values.

i. $y(1.052)$ **ii.** $y(1.555)$ **iii.** $y(1.978)$

10. In an electrical circuit with impressed voltage $\mathcal{E}$, having resistance R, inductance L, and capacitance C in parallel, the current i satisfies the differential equation

$$\frac{di}{dt} = C\frac{d^2\mathcal{E}}{dt^2} + \frac{1}{R}\frac{d\mathcal{E}}{dt} + \frac{1}{L}\mathcal{E}.$$

Suppose $i(0) = 0$, $C = 0.3$ farads, $R = 1.4$ ohms, $L = 1.7$ henries, and the voltage is given by

$$\mathcal{E}(t) = e^{-0.06\pi t}\sin(2t - \pi).$$

Use Euler's method to find the current i for the values $t = 0.1j$, $j = 0, 1, \ldots, 100$.

11. A projectile of mass $m = 0.11$ kg shot vertically upward with initial velocity $v(0) = 8$ m/s is slowed due to the force of gravity $F_g = mg$ and due to air resistance $F_r = -kv|v|$, where $g = -9.8$ m/s^2 and $k = 0.002$ kg/m. The differential equation for the velocity v is given by

$$mv' = mg - kv|v|.$$

a. Find the velocity after $0.1, 0.2, \ldots, 1.0$ s.

b. To the nearest tenth of a second, determine when the projectile reaches its maximum height and begins falling.

5.3 Runge-Kutta Methods

In the last section we saw how Taylor methods of arbitrary high order can be generated. However, the application of these high-order methods to a specific problem is complicated by the need to determine and evaluate high-order derivatives with respect to t on the right side of the differential equation. The widespread use of computer algebra systems has simplified this process, but it still remains cumbersome.

In the later 1800s, Carl Runge (1856–1927) used methods similar to those in this section to derive numerous formulas for approximating the solution to initial-value problems.

In this section we consider Runge-Kutta methods, which modify the Taylor methods so that the high-order error bounds are preserved, but the need to determine and evaluate the high-order partial derivatives is eliminated. The strategy behind these techniques involves approximating a Taylor method with a method that is easier to evaluate. This approximation might increase the error, but the increase does not exceed the order of the truncation error that is already present in the Taylor method. As a consequence, the new error does not significantly influence the calculations.

In 1901, Martin Wilhelm Kutta (1867–1944) generalized the methods that Runge developed in 1895 to incorporate systems of first-order differential equations. These techniques differ slightly from those we currently call Runge-Kutta methods.

Runge-Kutta Methods of Order Two

The Runge-Kutta techniques make use of the Taylor expansion of f, the function on the right side of the differential equation. Since f is a function of two variables, t and y, we must first consider the generalization of Taylor's Theorem to functions of this type. This generalization appears more complicated than the single-variable form, but this is only because of all the partial derivatives of the function f.

Taylor's Theorem for Two Variables

If f and all its partial derivatives of order less than or equal to $n+1$ are continuous on $D = \{(t, y) | a \le t \le b,\ c \le y \le d\}$ and (t, y) and $(t+\alpha, y+\beta)$ both belong to D, then

$$
\begin{aligned}
f(t+\alpha, y+\beta) \approx f(t, y) &+ \left[\alpha \frac{\partial f}{\partial t}(t, y) + \beta \frac{\partial f}{\partial y}(t, y)\right] \\
&+ \left[\frac{\alpha^2}{2}\frac{\partial^2 f}{\partial t^2}(t, y) + \alpha\beta \frac{\partial^2 f}{\partial t\, \partial y}(t, y) + \frac{\beta^2}{2}\frac{\partial^2 f}{\partial y^2}(t, y)\right] + \cdots \\
&+ \frac{1}{n!}\sum_{j=0}^{n} \binom{n}{j} \alpha^{n-j}\beta^{j} \frac{\partial^n f}{\partial t^{n-j}\partial y^{j}}(t, y).
\end{aligned}
$$

The error term in this approximation is similar to that given in Taylor's Theorem, with the added complications that arise because of the incorporation of all the partial derivatives of order $n+1$.

To illustrate the use of this formula in developing the Runge-Kutta methods, let us consider a Runge-Kutta method of order 2. We saw in the previous section that the Taylor method of order 2 comes from

$$
\begin{aligned}
y(t_{i+1}) &= y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \frac{h^3}{3!}y'''(\xi) \\
&= y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2}f'(t_i, y(t_i)) + \frac{h^3}{3!}y'''(\xi),
\end{aligned}
$$

or, since

$$
f'(t_i, y(t_i)) = \frac{\partial f}{\partial t}(t_i, y(t_i)) + \frac{\partial f}{\partial y}(t_i, y(t_i)) \cdot y'(t_i)
$$

and $y'(t_i) = f(t_i, y(t_i))$, we have

$$
\begin{aligned}
y(t_{i+1}) = y(t_i) + h&\left[f(t_i, y(t_i)) + \frac{h}{2}\frac{\partial f}{\partial t}(t_i, y(t_i)) + \frac{h}{2}\frac{\partial f}{\partial y}(t_i, y(t_i)) \cdot f(t_i, y(t_i))\right] \\
&+ \frac{h^3}{3!}y'''(\xi).
\end{aligned}
$$

Taylor's Theorem of two variables permits us to replace the term in the braces with a multiple of a function evaluation of f of the form $a_1 f(t_i + \alpha, y(t_i) + \beta)$. If we expand this term using Taylor's Theorem with $n = 1$, we have

$$\begin{aligned} a_1 f(t_i + \alpha, y(t_i) + \beta) &\approx a_1 \left[f(t_i, y(t_i)) + \alpha \frac{\partial f}{\partial t}(t_i, y(t_i)) + \beta \frac{\partial f}{\partial y}(t_i, y(t_i)) \right] \\ &= a_1 f(t_i, y(t_i)) + a_1 \alpha \frac{\partial f}{\partial t}(t_i, y(t_i)) + a_1 \beta \frac{\partial f}{\partial y}(t_i, y(t_i)). \end{aligned}$$

Equating this expression with the terms enclosed in the braces in the preceding equation implies that a_1, α, and β should be chosen so that

$$1 = a_1, \quad \frac{h}{2} = a_1 \alpha, \quad \text{and} \quad \frac{h}{2} f(t_i, y(t_i)) = a_1 \beta;$$

that is,

$$a_1 = 1, \quad \alpha = \frac{h}{2}, \quad \text{and} \quad \beta = \frac{h}{2} f(t_i, y(t_i)).$$

The error introduced by replacing the term in the Taylor method with its approximation has the same order as the error term for the method, so the Runge-Kutta method produced in this way, called the **Midpoint method**, is also a second-order method. As a consequence, the local error of the method is proportional to h^3, and the global error is proportional to h^2.

Midpoint Method

$$\begin{aligned} w_0 &= \alpha \\ w_{i+1} &= w_i + h \left[f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2} f(t_i, w_i) \right) \right], \end{aligned}$$

where $i = 0, 1, \ldots, N - 1$, with local error $O(h^3)$ and global error $O(h^2)$.

Using $a_1 f(t + \alpha, y + \beta)$ to replace the term in the Taylor method is the easiest choice, but it is not the only one. If we instead use a term of the form

$$a_1 f(t, y) + a_2 f(t + \alpha, y + \beta f(t, y)),$$

the extra parameter in this formula provides an infinite number of second-order Runge-Kutta formulas. When $a_1 = a_2 = \frac{1}{2}$ and $\alpha = \beta = h$, we have the **Modified Euler method.**

Modified Euler Method

$$\begin{aligned} w_0 &= \alpha \\ w_{i+1} &= w_i + \frac{h}{2}[f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))] \end{aligned}$$

where $i = 0, 1, \ldots, N - 1$, with local error $O(h^3)$ and global error $O(h^2)$.

Example 1 Use the Midpoint method and the Modified Euler method with $N = 10$, $h = 0.2$, $t_i = 0.2i$, and $w_0 = 0.5$ to approximate the solution to our usual example,

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

Solution The difference equations produced from the various formulas are

$$\text{Midpoint method:} \quad w_{i+1} = 1.22w_i - 0.0088i^2 - 0.008i + 0.218;$$

$$\text{Modified Euler method:} \quad w_{i+1} = 1.22w_i - 0.0088i^2 - 0.008i + 0.216,$$

for each $i = 0, 1, \ldots, 9$. The first two steps of these methods give

$$\text{Midpoint method:} \quad w_1 = 1.22(0.5) - 0.0088(0)^2 - 0.008(0) + 0.218 = 0.828;$$

$$\text{Modified Euler method:} \quad w_1 = 1.22(0.5) - 0.0088(0)^2 - 0.008(0) + 0.216 = 0.826,$$

and

$$\text{Midpoint method:} \quad w_2 = 1.22(0.828) - 0.0088(0.2)^2 - 0.008(0.2) + 0.218 = 1.21136;$$

$$\text{Modified Euler method:} \quad w_2 = 1.22(0.826) - 0.0088(0.2)^2 - 0.008(0.2) + 0.216 = 1.20692,$$

Table 5.6 lists all the results of the calculations. For this problem, the Midpoint method is superior to the Modified Euler method.

Table 5.6

t_i	$y(t_i)$	Midpoint Method	Error	Modified Euler Method	Error
0.0	0.5000000	0.5000000	0	0.5000000	0
0.2	0.8292986	0.8280000	0.0012986	0.8260000	0.0032986
0.4	1.2140877	1.2113600	0.0027277	1.2069200	0.0071677
0.6	1.6489406	1.6446592	0.0042814	1.6372424	0.0116982
0.8	2.1272295	2.1212842	0.0059453	2.1102357	0.0169938
1.0	2.6408591	2.6331668	0.0076923	2.6176876	0.0231715
1.2	3.1799415	3.1704634	0.0094781	3.1495789	0.0303627
1.4	3.7324000	3.7211654	0.0112346	3.6936862	0.0387138
1.6	4.2834838	4.2706218	0.0128620	4.2350972	0.0483866
1.8	4.8151763	4.8009586	0.0142177	4.7556185	0.0595577
2.0	5.3054720	5.2903695	0.0151025	5.2330546	0.0724173

Higher-Order Runge-Kutta Methods

Karl Heun (1859–1929) was a professor at the Technical University of Karlsruhe. He introduced this technique in a paper published in 1900 [Heu].

The term $T^{(3)}(t, y)$ can be approximated with global error $O(h^3)$ by an expression of the form

$$f(t + \alpha_1, y + \delta_1 f(t + \alpha_2, y + \delta_2 f(t, y))),$$

involving four parameters, but the algebra involved in the determination of α_1, δ_1, α_2, and δ_2 is quite involved. The most common $O(h^3)$ is Heun's method.

Heun's Method

$$w_0 = \alpha$$

$$w_{i+1} = w_i + \tfrac{h}{4}\left(f(t_i, w_i) + 3\left(f\left(t_i + \tfrac{2h}{3}, w_i + \tfrac{2h}{3} f\left(t_i + \tfrac{h}{3}, w_i + \tfrac{h}{3} f(t_i, w_i)\right)\right)\right)\right),$$

for $i = 0, 1, \ldots, N-1$, with local error $O(h^4)$ and global error $O(h^3)$.

Illustration Applying Heun's method with $N = 10$, $h = 0.2$, $t_i = 0.2i$, and $w_0 = 0.5$ to approximate the solution to our usual example,

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

gives the values in Table 5.7. Note the decreased error throughout the range over the Midpoint and Modified Euler approximations. □

Table 5.7

t_i	$y(t_i)$	Heun's Method	Error
0.0	0.5000000	0.5000000	0
0.2	0.8292986	0.8292444	0.0000542
0.4	1.2140877	1.2139750	0.0001127
0.6	1.6489406	1.6487659	0.0001747
0.8	2.1272295	2.1269905	0.0002390
1.0	2.6408591	2.6405555	0.0003035
1.2	3.1799415	3.1795763	0.0003653
1.4	3.7324000	3.7319803	0.0004197
1.6	4.2834838	4.2830230	0.0004608
1.8	4.8151763	4.8146966	0.0004797
2.0	5.3054720	5.3050072	0.0004648

The program RKO4M52 implements the Runge-Kutta Order 4 method.

Runge-Kutta Order Four

Runge-Kutta methods of order 3 are not generally used. The most common Runge-Kutta method in use is of order 4. It is given by the following.

Runge-Kutta Method of Order 4

$$\begin{aligned}
w_0 &= \alpha,\\
k_1 &= hf(t_i, w_i),\\
k_2 &= hf\left(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_1\right),\\
k_3 &= hf\left(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_2\right),\\
k_4 &= hf(t_{i+1}, w_i + k_3),\\
w_{i+1} &= w_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),
\end{aligned}$$

where $i = 0, 1, \ldots, N-1$, with local error $O(h^5)$ and global error $O(h^4)$.

Example 2 Use the Runge-Kutta method of order 4 with $h = 0.2$, $N = 10$, and $t_i = 0.2i$ to obtain approximations to the solution of the initial-value problem

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

Solution The approximation to $y(0.2)$ is obtained by

$$w_0 = 0.5$$
$$k_1 = 0.2f(0, 0.5) = 0.2(1.5) = 0.3$$
$$k_2 = 0.2f(0.1, 0.65) = 0.328$$
$$k_3 = 0.2f(0.1, 0.664) = 0.3308$$
$$k_4 = 0.2f(0.2, 0.8308) = 0.35816$$
$$w_1 = 0.5 + \frac{1}{6}(0.3 + 2(0.328) + 2(0.3308) + 0.35816) = 0.8292933.$$

The remaining results and their errors are listed in Table 5.8. ■

Table 5.8

t_i	Exact $y_i = y(t_i)$	Runge-Kutta Order 4 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	2.1272027	0.0000269
1.0	2.6408591	2.6408227	0.0000364
1.2	3.1799415	3.1798942	0.0000474
1.4	3.7324000	3.7323401	0.0000599
1.6	4.2834838	4.2834095	0.0000743
1.8	4.8151763	4.8150857	0.0000906
2.0	5.3054720	5.3053630	0.0001089

Computational Comparisons

The main computational effort in applying the Runge-Kutta methods involves the function evaluations of f. In the second-order methods, the local error is $O(h^3)$ and the cost is two functional evaluations per step. The Runge-Kutta method of order 4 requires four evaluations per step and the local error is $O(h^5)$. The relationship between the number of evaluations per step and the order of the global error is shown in Table 5.9. Because of the relative decrease in the order for n greater than 4, the methods of order less than 5 with smaller step size are used in preference to the higher-order methods using a larger step size.

Table 5.9

Evaluations per step:	2	3	4	$5 \le n \le 7$	$8 \le n \le 9$	$10 \le n$
Best possible global error:	$O(h^2)$	$O(h^3)$	$O(h^4)$	$O(h^{n-1})$	$O(h^{n-2})$	$O(h^{n-3})$

One way to compare the lower-order Runge-Kutta methods is described as follows: The Runge-Kutta method of order 4 requires four evaluations per step, so to be superior to Euler's method, which requires only one evaluation per step, it should give more accurate answers than when Euler's method uses one-fourth the Runge-Kutta step size. Similarly, if the Runge-Kutta method of order 4 is to be superior to the second-order Runge-Kutta methods, which require two evaluations per step, it should give more accuracy with step size h than a second-order method with step size $\frac{1}{2}h$. The following Illustration indicates the superiority of the Runge-Kutta method of order 4 by this measure.

Illustration For the problem

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

Euler's method with $h = 0.025$, the Midpoint method with $h = 0.05$, and the Runge-Kutta fourth-order method with $h = 0.1$ are compared at the common mesh points of these methods 0.1, 0.2, 0.3, 0.4, and 0.5. Each of these techniques requires 20 function evaluations to determine the values listed in Table 5.10 to approximate $y(0.5)$. In this example, the fourth-order method is clearly superior. □

Table 5.10

t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order 4 $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

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

EXERCISE SET 5.3

1. Use the Modified Euler method to approximate the solutions to each of the following initial-value problems, and compare the results to the actual values.
   a. $y' = te^{3t} - 2y, \quad 0 \le t \le 1, \quad y(0) = 0$, with $h = 0.5$; 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 $h = 0.5$; 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 $h = 0.25$; 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 $h = 0.25$; actual solution $y(t) = \frac{1}{2}\sin 2t - \frac{1}{3}\cos 3t + \frac{4}{3}$.
2. Use the Modified Euler method to approximate the solutions to each of the following initial-value problems, and 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 $y(t) = t/(1 + \ln t)$.
   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 $h = 0.2$; actual solution $y(t) = -3 + 2(1 + e^{-2t})^{-1}$.
   d. $y' = -5y + 5t^2 + 2t, \quad 0 \le t \le 1, \quad y(0) = \frac{1}{3}$, with $h = 0.1$; actual solution $y(t) = t^2 + \frac{1}{3}e^{-5t}$.
3. Use the Modified Euler method to approximate the solutions to each of the following initial-value problems, and 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 $y(t) = \dfrac{2t + 1}{t^2 + 1}$.
   b. $y' = \dfrac{y^2}{1 + t}, \quad 1 \le t \le 2, \quad y(1) = \frac{-1}{\ln 2}$, 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 $y(t) = \sqrt{4 - 3e^{-t^2}}$.

4. Repeat Exercise 1 using the Midpoint method.

5. Repeat Exercise 2 using the Midpoint method.

6. Repeat Exercise 3 using the Midpoint method.

7. Repeat Exercise 1 using Heun's method.

8. Repeat Exercise 2 using Heun's method.

9. Repeat Exercise 3 using Heun's method.

10. Repeat Exercise 1 using the Runge-Kutta method of order 4.

11. Repeat Exercise 2 using the Runge-Kutta method of order 4.

12. Repeat Exercise 3 using the Runge-Kutta method of order 4.

13. Use the results of Exercise 2 and linear interpolation to approximate values of $y(t)$, and compare the results to the actual values.

a. $y(1.25)$ and $y(1.93)$ **b.** $y(2.1)$ and $y(2.75)$

c. $y(1.3)$ and $y(1.93)$ **d.** $y(0.54)$ and $y(0.94)$

14. Use the results of Exercise 3 and linear interpolation to approximate values of $y(t)$, and compare the results to the actual values.

a. $y(0.54)$ and $y(0.94)$ **b.** $y(1.25)$ and $y(1.93)$

c. $y(1.3)$ and $y(2.93)$ **d.** $y(0.54)$ and $y(0.94)$

15. Use the results of Exercise 11 and Cubic Hermite interpolation to approximate values of $y(t)$, and compare the approximations to the actual values.

a. $y(1.25)$ and $y(1.93)$ **b.** $y(2.1)$ and $y(2.75)$

c. $y(1.3)$ and $y(1.93)$ **d.** $y(0.54)$ and $y(0.94)$

16. Use the results of Exercise 12 and Cubic Hermite interpolation to approximate values of $y(t)$, and compare the approximations to the actual values.

a. $y(0.54)$ and $y(0.94)$ **b.** $y(1.25)$ and $y(1.93)$

c. $y(1.3)$ and $y(2.93)$ **d.** $y(0.54)$ and $y(0.94)$

17. Show that the Midpoint method and the Modified Euler method give the same approximations to the initial-value problem

$$y' = -y + t + 1,\quad 0 \le t \le 1,\quad y(0) = 1,$$

for any choice of h. Why is this true?

18. Water flows from an inverted conical tank with a circular orifice at the rate

$$\frac{dx}{dt} = -0.6\pi r^2 \sqrt{2g}\,\frac{\sqrt{x}}{A(x)},$$

where r is the radius of the orifice, x is the height of the liquid level from the vertex of the cone, and $A(x)$ is the area of the cross-section of the tank x units above the orifice. Suppose $r = 0.1$ ft, $g = 32.1$ ft/s^2, and the tank has an initial water level of 8 ft and initial volume of $512(\pi/3)$ ft^3. Use the Runge-Kutta method of order 4 to find the following.

a. The water level after 10 min with $h = 20$ s

b. When the tank will be empty, to within 1 min.

19. The irreversible chemical reaction in which two molecules of solid potassium dichromate ($K_2Cr_2O_7$), two molecules of water (H_2O), and three atoms of solid sulfur (S) combine to yield three molecules of the gas sulfur dioxide (SO_2), four molecules of solid potassium hydroxide (KOH), and two molecules of solid chromic oxide (Cr_2O_3) can be represented symbolically by the *stoichiometric equation*:

$$2K_2Cr_2O_7 + 2H_2O + 3S \longrightarrow 4KOH + 2Cr_2O_3 + 3SO_2.$$

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