ریاضیات عالی پیشرفته

Numerical Methods for Engineers

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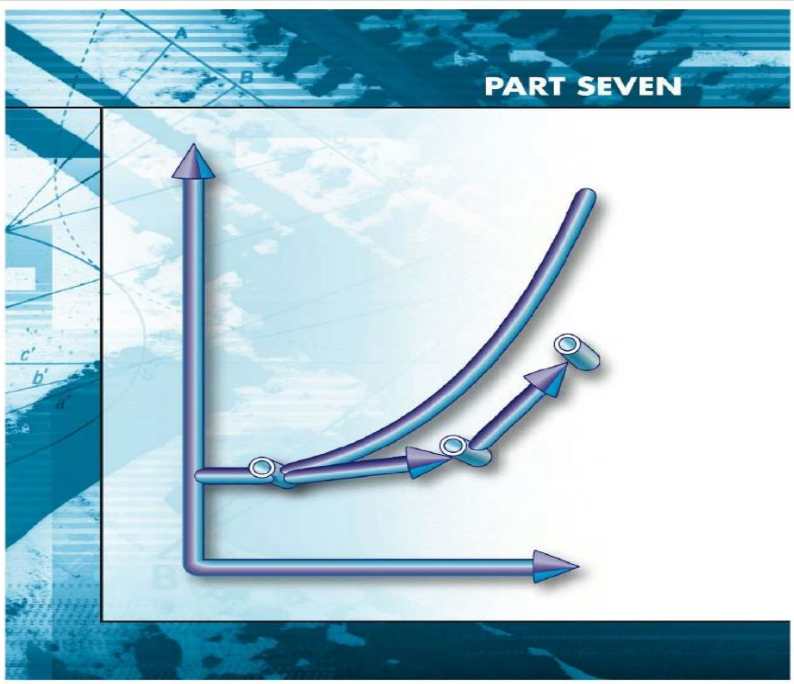

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$$\frac{dv}{dt} = g - \frac{c}{m} v$$

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0$$

Higher-order equations can be reduced to a system of first-order equations. For Eq. (PT7.2), this is done by defining a new variable y, where

$$y = \frac{dx}{dt} \quad \text{(PT7.3)}$$

which itself can be differentiated to yield

$$\frac{dy}{dt} = \frac{d^2x}{dt^2} \quad \text{(PT7.4)}$$

Equations (PT7.3) and (PT7.4) can then be substituted into Eq. (PT7.2) to give

$$m\frac{dy}{dt} + cy + kx = 0 \quad \text{(PT7.5)}$$

TABLE PT7.1 Examples of fundamental laws that are written in terms of the rate of change of variables (t = time and x = position).

Law	Mathematical Expression	Variables and Parameters
Newton's second law of motion	$\frac{dv}{dt} = \frac{F}{m}$	Velocity (v), force (F), and mass (m)
Fourier's heat law	$q = -k'\frac{dT}{dx}$	Heat flux (q), thermal conductivity (k') and temperature (T)
Fick's law of diffusion	$J = -D\frac{dc}{dx}$	Mass flux (J), diffusion coefficient (D), and concentration (c)
Faraday's law (voltage drop across an inductor)	$\Delta V_L = L\frac{di}{dt}$	Voltage drop (ΔV_L), inductance (L), and current (i)

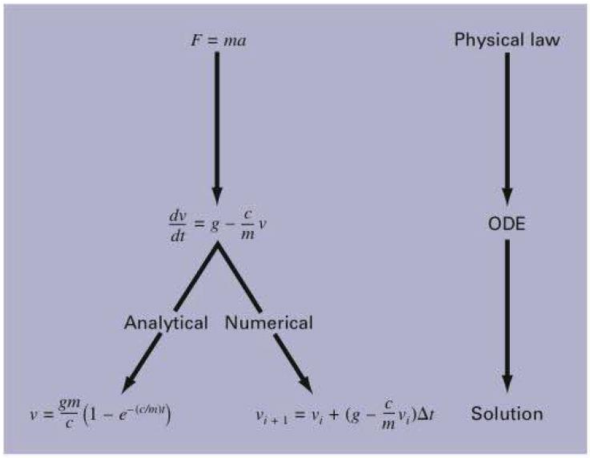


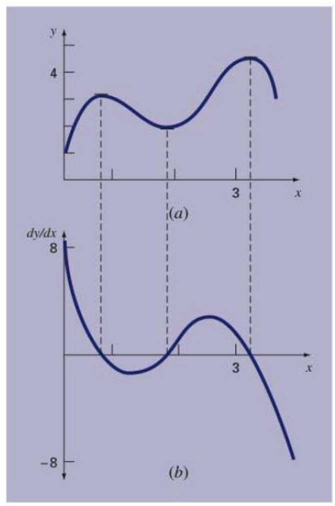
FIGURE PT7.2
The sequence of events in the application of ODEs for engineering problem solving. The example shown is the velocity of a falling parachutist.

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1 \qquad \text{(PT7.12)}$$

which is a fourth-order polynomial (Fig. PT7.3*a*). Now, if we differentiate Eq. (PT7.12), we obtain an ODE:

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

FIGURE PT7.3
Plots of (*a*) *y* versus *x* and (*b*) *dy*/*dx* versus *x* for the function $y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$.



$$y = \int (-2x^3 + 12x^2 - 20x + 8.5)\,dx$$

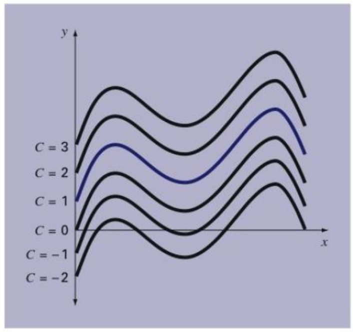
Applying the integration rule (recall Table PT6.2)

$$\int u^n\,du = \frac{u^{n+1}}{n+1} + C \qquad n \neq -1$$

to each term of the equation gives the solution

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + C$$

FIGURE PT7.4
Six possible solutions for the integral of $-2x^3 + 12x^2 - 20x + 8.5$. Each conforms to a different value of the constant of integration C.



Runge-Kutta Methods

This chapter is devoted to solving ordinary differential equations of the form

$$\frac{dy}{dx} = f(x, y)$$

In Chap. 1, we used a numerical method to solve such an equation for the velocity of the falling parachutist. Recall that the method was of the general form

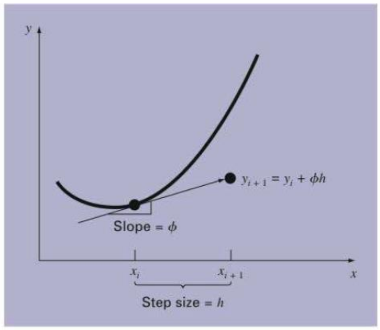
New value = old value + slope × step size

or, in mathematical terms,

$$y_{i+1} = y_i + \phi h \tag{25.1}$$

According to this equation, the slope estimate of ϕ is used to extrapolate from an old value y_i to a new value y_{i+1} over a distance h (Fig. 25.1). This formula can be applied step by step to compute out into the future and, hence, trace out the trajectory of the solution.

FIGURE 25.1
Graphical depiction of a one-step method.



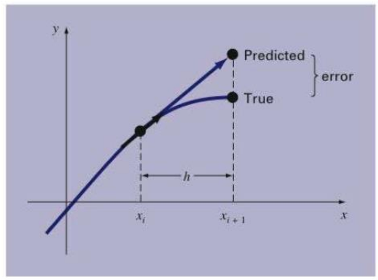


FIGURE 25.2
Euler's method.

EULER'S METHOD

The first derivative provides a direct estimate of the slope at x_i (Fig. 25.2):

$$\phi = f(x_i, y_i)$$

where $f(x_i, y_i)$ is the differential equation evaluated at x_i and y_i. This estimate can be substituted into Eq. (25.1):

$$y_{i+1} = y_i + f(x_i, y_i)h \qquad (25.2)$$

This formula is referred to as *Euler's* (or the *Euler-Cauchy* or the *point-slope*) *method.* A new value of y is predicted using the slope (equal to the first derivative at the original value of x) to extrapolate linearly over the step size h (Fig. 25.2).

from $x = 0$ to $x = 4$ with a step size of 0.5. The initial condition at $x = 0$ is $y = 1$. Recall that the exact solution is given by Eq. (PT7.16):

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$$

Solution. Equation (25.2) can be used to implement Euler's method:

$$y(0.5) = y(0) + f(0, 1)0.5$$

where $y(0) = 1$ and the slope estimate at $x = 0$ is

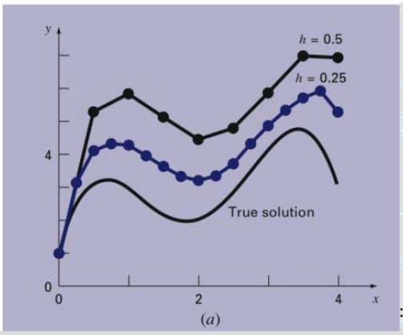
$$f(0, 1) = -2(0)^3 + 12(0)^2 - 20(0) + 8.5 = 8.5$$

Therefore,

$$y(0.5) = 1.0 + 8.5(0.5) = 5.25$$

TABLE 25.1 Comparison of true and approximate values of the integral of $y' = -2x^3 + 12x^2 - 20x + 8.5$, with the initial condition that $y = 1$ at $x = 0$. The approximate values were computed using Euler's method with a step size of 0.5. The local error refers to the error incurred over a single step. It is calculated with a Taylor series expansion as in Example 25.2. The global error is the total discrepancy due to past as well as present steps.

			Percent Relative Error	
x	y_{true}	y_{Euler}	Global	Local
0.0	1.00000	1.00000		
0.5	3.21875	5.25000	−63.1	−63.1
1.0	3.00000	5.87500	−95.8	−28.0
1.5	2.21875	5.12500	131.0	−1.41
2.0	2.00000	4.50000	−125.0	20.5
2.5	2.71875	4.75000	−74.7	17.3
3.0	4.00000	5.87500	46.9	4.0
3.5	4.71875	7.12500	−51.0	−11.3
4.0	3.00000	7.00000	−133.3	−53.0



(a)

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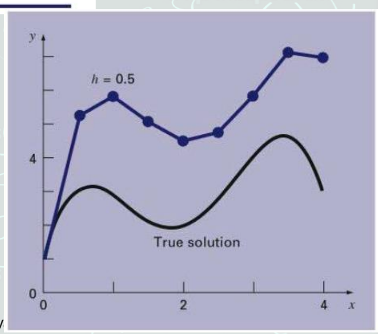


25.2.1 Heun's Method

One method to improve the estimate of the slope involves the determination of two derivatives for the interval—one at the initial point and another at the end point. The two derivatives are then averaged to obtain an improved estimate of the slope for the entire interval. This approach, called *Heun's method,* is depicted graphically in Fig. 25.9.

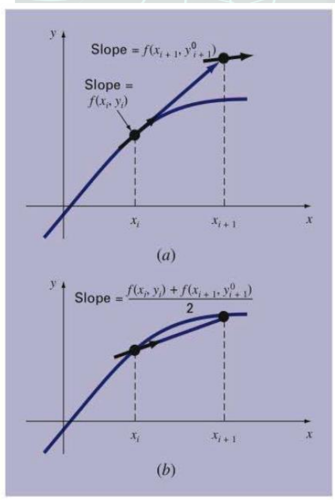
Recall that in Euler's method, the slope at the beginning of an interval

$$y_i' = f(x_i, y_i) \tag{25.12}$$

is used to extrapolate linearly to y_{i+1}:

$$y_{i+1}^0 = y_i + f(x_i, y_i)h \tag{25.13}$$

For the standard Euler method we would stop at this point. However, in Heun's method the y_{i+1}^0 calculated in Eq. (25.13) is not the final answer, but an intermediate prediction. This is why we have distinguished it with a superscript 0. Equation (25.13) is called a *predictor*



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equation. It provides an estimate of y_{i+1} that allows the calculation of an estimated slope at the end of the interval:

$$y'_{i+1} = f(x_{i+1}, y^0_{i+1}) \tag{25.14}$$

Thus, the two slopes [Eqs. (25.12) and (25.14)] can be combined to obtain an average slope for the interval:

$$\bar{y}' = \frac{y'_i + y'_{i+1}}{2} = \frac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1})}{2}$$

This average slope is then used to extrapolate linearly from y_i to y_{i+1} using Euler's method:

$$y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1})}{2}h$$

which is called a *corrector equation.*

The Heun method is a *predictor-corrector approach.* All the multistep methods to be discussed subsequently in Chap. 26 are of this type. The Heun method is the only one-step predictor-corrector method described in this book. As derived above, it can be expressed concisely as

Predictor (Fig. 25.9*a*): $$y^0_{i+1} = y_i + f(x_i, y_i)h \tag{25.15}$$

Corrector (Fig. 25.9*b*): $$y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1})}{2}h \tag{25.16}$$

Heun's Method

Problem Statement. Use Heun's method to integrate $y' = 4e^{0.8x} - 0.5y$ from $x = 0$ to $x = 4$ with a step size of 1. The initial condition at $x = 0$ is $y = 2$.

Solution. Before solving the problem numerically, we can use calculus to determine the following analytical solution:

$$y = \frac{4}{1.3}(e^{0.8x} - e^{-0.5x}) + 2e^{-0.5x} \tag{E25.5.1}$$

This formula can be used to generate the true solution values in Table 25.2.

First, the slope at (x_0, y_0) is calculated as

$$y'_0 = 4e^0 - 0.5(2) = 3$$

This result is quite different from the actual average slope for the interval from 0 to 1.0, which is equal to 4.1946, as calculated from the differential equation using Eq. (PT6.4).

The numerical solution is obtained by using the predictor [Eq. (25.15)] to obtain an estimate of y at 1.0:

$$y^0_1 = 2 + 3(1) = 5$$

Note that this is the result that would be obtained by the standard Euler method. The true value in Table 25.2 shows that it corresponds to a percent relative error of 19.3 percent.

Now, to improve the estimate for y_{i+1}, we use the value y^0_1 to predict the slope at the end of the interval

$$y'_1 = f(x_1, y^0_1) = 4e^{0.8(1)} - 0.5(5) = 6.402164$$

which can be combined with the initial slope to yield an average slope over the interval from $x = 0$ to 1

$$\bar{y}' = \frac{3 + 6.402164}{2} = 4.701082$$

which is closer to the true average slope of 4.1946. This result can then be substituted into the corrector [Eq. (25.16)] to give the prediction at $x = 1$

$$y_1 = 2 + 4.701082(1) = 6.701082$$

which represents a percent relative error of −8.18 percent. Thus, the Heun method without iteration of the corrector reduces the absolute value of the error by a factor of 2.4 as compared with Euler's method.

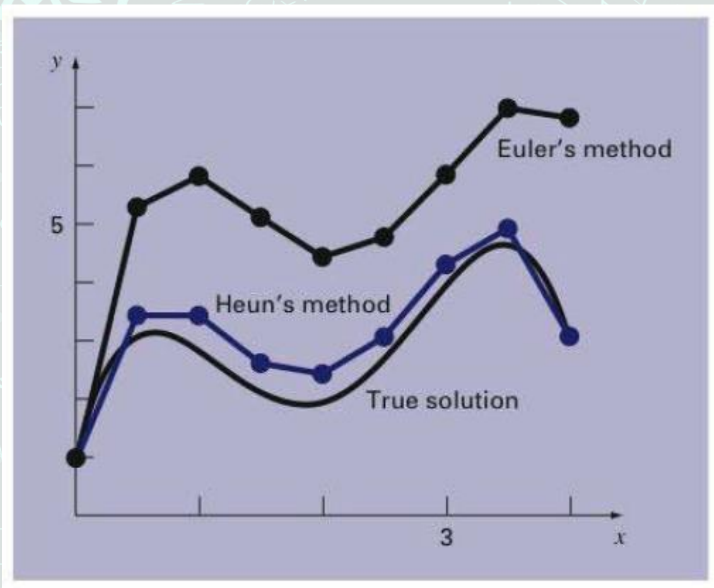
Now this estimate can be used to refine or correct the prediction of y_1 by substituting the new result back into the right-hand side of Eq. (25.16):

$$y_1 = 2 + \frac{\left[3 + 4e^{0.8(1)} - 0.5(6.701082)\right]}{2}1 = 6.275811$$

which represents an absolute percent relative error of 1.31 percent. This result, in turn, can be substituted back into Eq. (25.16) to further correct:

$$y_1 = 2 + \frac{\left[3 + 4e^{0.8(1)} - 0.5(6.275811)\right]}{2}1 = 6.382129$$

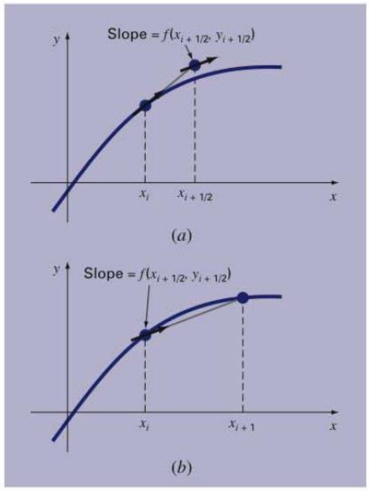
which represents an $|\varepsilon_t|$ of 3.03%. Notice how the errors sometimes grow as the iterations proceed. Such increases can occur, especially for large step sizes, and they prevent us from drawing the general conclusion that an additional iteration will always improve the result. However, for a sufficiently small step size, the iterations should eventually converge on a single value. For our case, 6.360865, which represents a relative error of 2.68 percent, is attained after 15 iterations. Table 25.2 shows results for the remainder of the computation using the method with 1 and 15 iterations per step.



25.2.2 The Midpoint (or Improved Polygon) Method

Figure 25.12 illustrates another simple modification of Euler's method. Called the *midpoint method* (or the *improved polygon* or the *modified Euler*), this technique uses Euler's method to predict a value of y at the midpoint of the interval (Fig. 25.12*a*):

$$y_{i+1/2} = y_i + f(x_i, y_i)\frac{h}{2}$$



(b) Midpoint Method

```
SUB Midpoint (x, y, h, ynew)
  CALL Derivs(x, y, dydx)
  ym = y + dydx · h/2
  CALL Derivs (x + h/2, ym, dymdx)
  ynew = y + dymdx · h
  x = x + h
END SUB
```

Then, this predicted value is used to calculate a slope at the midpoint:

$$y'_{i+1/2} = f(x_{i+1/2}, y_{i+1/2})$$

which is assumed to represent a valid approximation of the average slope for the entire interval. This slope is then used to extrapolate linearly from x_i to x_{i+1} (Fig. 25.12*b*):

$$y_{i+1} = y_i + f(x_{i+1/2}, y_{i+1/2})h \qquad (25.27)$$

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25.3 RUNGE-KUTTA METHODS

Runge-Kutta (*RK*) methods achieve the accuracy of a Taylor series approach without requiring the calculation of higher derivatives. Many variations exist but all can be cast in the generalized form of Eq. (25.1):

$$y_{i+1} = y_i + \phi(x_i, y_i, h)h \qquad (25.28)$$

where $\phi(x_i, y_i, h)$ is called an *increment function,* which can be interpreted as a representative slope over the interval. The increment function can be written in general form as

$$\phi = a_1k_1 + a_2k_2 + \cdots + a_nk_n \qquad (25.29)$$

where the a's are constants and the k's are

$$k_1 = f(x_i, y_i) \qquad (25.29a)$$

$$k_2 = f(x_i + p_1h, y_i + q_{11}k_1h) \qquad (25.29b)$$

$$k_3 = f(x_i + p_2h, y_i + q_{21}k_1h + q_{22}k_2h) \qquad (25.29c)$$

$$\vdots$$

$$k_n = f(x_i + p_{n-1}h, y_i + q_{n-1,1}k_1h + q_{n-1,2}k_2h + \cdots + q_{n-1,n-1}k_{n-1}h) \qquad (25.29d)$$

where the p's and q's are constants. Notice that the k's are recurrence relationships. That is, k_1 appears in the equation for k_2, which appears in the equation for k_3, and so forth. Because each k is a functional evaluation, this recurrence makes RK methods efficient for computer calculations.

Various types of Runge-Kutta methods can be devised by employing different numbers of terms in the increment function as specified by n. Note that the first-order RK method with $n = 1$ is, in fact, Euler's method. Once n is chosen, values for the a's, p's, and q's are evaluated by setting Eq. (25.28) equal to terms in a Taylor series expansion (Box 25.1). Thus, at least for the lower-order versions, the number of terms, n, usually represents the order of the approach. For example, in the next section, second-order RK methods use an increment function with two terms ($n = 2$). These second-order methods will be exact if the solution to the differential equation is quadratic. In addition, because terms with h^3 and higher are dropped during the derivation, the local truncation error is $O(h^3)$ and the global error is $O(h^2)$. In subsequent sections, the third- and fourth-order RK methods ($n = 3$ and 4, respectively) are developed. For these cases, the global truncation errors are $O(h^3)$ and $O(h^4)$, respectively.

25.3.1 Second-Order Runge-Kutta Methods

The second-order version of Eq. (25.28) is

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h \tag{25.30}$$

where

$$k_1 = f(x_i, y_i) \tag{25.30a}$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \tag{25.30b}$$

As described in Box 25.1, values for a_1, a_2, p_1, and q_{11} are evaluated by setting Eq. (25.30) equal to a Taylor series expansion to the second-order term. By doing this, we derive three equations to evaluate the four unknown constants. The three equations are

$$a_1 + a_2 = 1 \tag{25.31}$$

$$a_2 p_1 = \frac{1}{2} \tag{25.32}$$

$$a_2 q_{11} = \frac{1}{2} \tag{25.33}$$

Because we have three equations with four unknowns, we must assume a value of one of the unknowns to determine the other three. Suppose that we specify a value for a_2. Then Eqs. (25.31) through (25.33) can be solved simultaneously for

$$a_1 = 1 - a_2 \tag{25.34}$$

$$p_1 = q_{11} = \frac{1}{2a_2} \tag{25.35}$$

Heun Method with a Single Corrector ($a_2 = 1/2$). If a_2 is assumed to be 1/2, Eqs. (25.34) and (25.35) can be solved for $a_1 = 1/2$ and $p_1 = q_{11} = 1$. These parameters, when substituted into Eq. (25.30), yield

$$y_{i+1} = y_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h \tag{25.36}$$

where

$$k_1 = f(x_i, y_i) \tag{25.36a}$$

$$k_2 = f(x_i + h, y_i + k_1 h) \tag{25.36b}$$

Note that k_1 is the slope at the beginning of the interval and k_2 is the slope at the end of the interval. Consequently, this second-order Runge-Kutta method is actually Heun's technique without iteration.

The Midpoint Method ($a_2 = 1$). If a_2 is assumed to be 1, then $a_1 = 0$, $p_1 = q_{11} = 1/2$, and Eq. (25.30) becomes

$$y_{i+1} = y_i + k_2 h \qquad (25.37)$$

where

$$k_1 = f(x_i, y_i) \qquad (25.37a)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \qquad (25.37b)$$

This is the midpoint method.

Ralston's Method ($a_2 = 2/3$). Ralston (1962) and Ralston and Rabinowitz (1978) determined that choosing $a_2 = 2/3$ provides a minimum bound on the truncation error for the second-order RK algorithms. For this version, $a_1 = 1/3$ and $p_1 = q_{11} = 3/4$ and yields

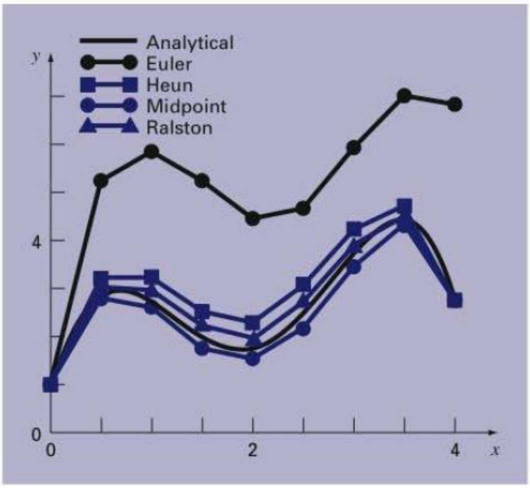
$$y_{i+1} = y_i + \left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)h \qquad (25.38)$$

where

$$k_1 = f(x_i, y_i) \qquad (25.38a)$$

$$k_2 = f\left(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h\right) \qquad (25.38b)$$

FIGURE 25.14
Comparison of the true solution with numerical solutions using three second-order RK methods and Euler's method.



25.3.2 Third-Order Runge-Kutta Methods

For $n = 3$, a derivation similar to the one for the second-order method can be performed. The result of this derivation is six equations with eight unknowns. Therefore, values for two of the unknowns must be specified a priori in order to determine the remaining parameters. One common version that results is

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h \quad (25.39)$$

where

$$k_1 = f(x_i, y_i) \quad (25.39a)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \quad (25.39b)$$

$$k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h) \quad (25.39c)$$

Note that if the derivative is a function of x only, this third-order method reduces to Simpson's 1/3 rule. Ralston (1962) and Ralston and Rabinowitz (1978) have developed an alternative version that provides a minimum bound on the truncation error. In any case, the third-order RK methods have local and global errors of $O(h^4)$ and $O(h^3)$, respectively, and yield exact results when the solution is a cubic. When dealing with polynomials, Eq. (25.39) will also be exact when the differential equation is cubic and the solution is quartic. This is because Simpson's 1/3 rule provides exact integral estimates for cubics (recall Box 21.3).

25.3.3 Fourth-Order Runge-Kutta Methods

The most popular RK methods are fourth order. As with the second-order approaches, there are an infinite number of versions. The following is the most commonly used form, and we therefore call it the *classical fourth-order RK method:*

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \quad (25.40)$$

where

$$k_1 = f(x_i, y_i) \quad (25.40a)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \quad (25.40b)$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right) \quad (25.40c)$$

$$k_4 = f(x_i + h, y_i + k_3 h) \quad (25.40d)$$

Notice that for ODEs that are a function of x alone, the classical fourth-order RK method is similar to Simpson's 1/3 rule. In addition, the fourth-order RK method is similar to the Heun approach in that multiple estimates of the slope are developed in order to come up with an improved average slope for the interval. As depicted in Fig. 25.15, each of the k's represents a slope. Equation (25.40) then represents a weighted average of these to arrive at the improved slope.

Classical Fourth-Order RK Method

Problem Statement.

(a) Use the classical fourth-order RK method [Eq. (25.40)] to integrate

$$f(x, y) = -2x^3 + 12x^2 - 20x + 8.5$$

using a step size of $h = 0.5$ and an initial condition of $y = 1$ at $x = 0$.

(b) Similarly, integrate

$$f(x, y) = 4e^{0.8x} - 0.5y$$

using $h = 0.5$ with $y(0) = 2$ from $x = 0$ to 0.5.

Solution.

(a) Equations (25.40*a*) through (25.40*d*) are used to compute $k_1 = 8.5$, $k_2 = 4.21875$, $k_3 = 4.21875$ and $k_4 = 1.25$, which are substituted into Eq. (25.40) to yield

$$y(0.5) = 1 + \left\{\frac{1}{6}[8.5 + 2(4.21875) + 2(4.21875) + 1.25]\right\} 0.5$$
$$= 3.21875$$

which is exact. Thus, because the true solution is a quartic [Eq. (PT7.16)], the fourth-order method gives an exact result.

(b) For this case, the slope at the beginning of the interval is computed as

$$k_1 = f(0, 2) = 4e^{0.8(0)} - 0.5(2) = 3$$

This value is used to compute a value of y and a slope at the midpoint,

$$y(0.25) = 2 + 3(0.25) = 2.75$$
$$k_2 = f(0.25, 2.75) = 4e^{0.8(0.25)} - 0.5(2.75) = 3.510611$$

This slope in turn is used to compute another value of y and another slope at the midpoint,

$$y(0.25) = 2 + 3.510611(0.25) = 2.877653$$
$$k_3 = f(0.25, 2.877653) = 4e^{0.8(0.25)} - 0.5(2.877653) = 3.446785$$

Next, this slope is used to compute a value of y and a slope at the end of the interval,

$$y(0.5) = 2 + 3.071785(0.5) = 3.723392$$
$$k_4 = f(0.5, 3.723392) = 4e^{0.8(0.5)} - 0.5(3.723392) = 4.105603$$