where the $a_i$'s are constants and the $k_i$'s are

\[ k_1 = f(x_i, y_i) \]
\[ k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \]
\[ k_3 = f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h) \]
\[ k_n = f(x_i + p_{n-1} h, y_i + q_{n-1,1} k_1 h + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h) \]

where the $p_i$'s and $q_{ij}$'s are constants. Notice that the $k_i$'s are recurrence relationships. The $k_1$ appears in the equation for $k_2$, which appears in the equation for $k_3$, and so forth. Because each $k_i$ 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 method with $n = 1$ is, in fact, Euler's method. Once $n$ is chosen, values for the $a_i$'s, and $q_{ij}$'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 exact if the solution to the differential equation is quadratic. In addition, because terms $O(h^3)$ and higher are dropped during the derivation, the local truncation error is $O(h^2)$ and the global error is $O(h^3)$. 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

\[ y_{i+1} = y_i + (a_1 k_1 + a_2 k_2) h \]

where

\[ k_1 = f(x_i, y_i) \]
\[ k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \]

As described in Box 25.1, values for $a_1, a_2, p_1, a_2 q_{11}$ are evaluated by setting Eq. (25.4) 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

\[ a_1 + a_2 = 1 \]
\[ a_2 p_1 = \frac{1}{2} \]
\[ a_2 q_{11} = \frac{1}{2} \]
Box 25.1 Derivation of the Second-Order Runge-Kutta Methods

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

\[ y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h \]  

(B25.1.1)

where

\[ k_1 = f(x_i, y_i) \]  

(B25.1.2)

and

\[ k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \]  

(B25.1.3)

To use Eq. (B25.1.1) we have to determine values for the constants \( a_1, a_2, p_1, \) and \( q_{11}. \) To do this, we recall that the second-order Taylor series for \( y_{i+1} \) in terms of \( y_i \) and \( f(x_i, y_i) \) is written as [Eq. (25.11)]

\[ y_{i+1} = y_i + f(x_i, y_i)h + \frac{f(x_i, y_i)}{2!}h^2 \]  

(B25.1.4)

where \( f(x_i, y_i) \) must be determined by chain-rule differentiation [Sec. 25.1.3]:

\[ f(x_i, y_i) = \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y} \frac{dy}{dx} \]  

(B25.1.5)

Substituting Eq. (B25.1.5) into (B25.1.4) gives

\[ y_{i+1} = y_i + f(x_i, y_i)h + \left( \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y} \frac{dy}{dx} \right) \frac{h^2}{2!} \]  

(B25.1.6)

The basic strategy underlying Runge-Kutta methods is to use algebraic manipulations to solve for values of \( a_1, a_2, p_1, \) and \( q_{11} \) that make Eqs. (B25.1.1) and (B25.1.6) equivalent.

To do this, we first use a Taylor series to expand Eq. (25.1.3). The Taylor series for a two-variable function is defined as [recall Eq. (4.26)]

\[ g(x + r, y + s) = g(x, y) + r \frac{\partial g}{\partial x} + s \frac{\partial g}{\partial y} + \cdots \]

Applying this method to expand Eq. (B25.1.3) gives

\[ f(x_i + p_1 h, y_i + q_{11} k_1 h) = f(x_i, y_i) + p_1 h \frac{\partial f}{\partial x} \]

\[ + q_{11} k_1 h \frac{\partial f}{\partial y} \]  

\[ + O(h^3) \]

This result can be substituted along with Eq. (B25.1.2) into Eq. (B25.1.1) to yield

\[ y_{i+1} = y_i + a_1 h f(x_i, y_i) + a_2 h f(x_i, y_i) + a_2 p_1 h^2 \frac{\partial f}{\partial x} \]

\[ + a_2 q_{11} h^2 f(x_i, y_i) \frac{\partial f}{\partial y} \]  

\[ + O(h^3) \]

or, by collecting terms,

\[ y_{i+1} = y_i + [a_1 f(x_i, y_i) + a_2 f(x_i, y_i)]h \]

\[ + \left[ a_2 p_1 \frac{\partial f}{\partial x} + a_2 q_{11} f(x_i, y_i) \frac{\partial f}{\partial y} \right] h^2 + O(h^3) \]  

(B25.1.7)

Now, comparing like terms in Eqs. (B25.1.6) and (B25.1.7), we determine that for the two equations to be equivalent, the following must hold:

\[ a_1 + a_2 = 1 \]

\[ a_2 p_1 = \frac{1}{2} \]

\[ a_2 q_{11} = \frac{1}{2} \]

These three simultaneous equations contain the four unknown constants. Because there is one more unknown than the number of equations, there is no unique set of constants that satisfy the equations. However, by assuming a value for one of the constants, we can determine the other three. Consequently, there is a family of second-order methods rather than a single version.

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

\[ a_1 = 1 - a_2 \]  

(B25.34)

\[ p_1 = q_{11} = \frac{1}{2a_2} \]  

(B25.35)
Because we can choose an infinite number of values for $a_2$, there are an infinite number of second-order RK methods. Every version would yield exactly the same results if the solution to the ODE were quadratic, linear, or a constant. However, they yield different results when (as is typically the case) the solution is more complicated. We present three of the most commonly used and preferred versions:

**Heun Method with a Single Corrector ($a_2 = 1/2$).** If $a_2$ is assumed to be 1, 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

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

(25.3)

where

$$k_1 = f(x_i, y_i)$$
(25.36)

$$k_2 = f(x_i + h, y_i + k_1 h)$$
(25.36)

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

$$y_{i+1} = y_i + k_2 h$$
(25.57)

where

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

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

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

where

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

$$k_2 = f \left( x_i + \frac{3}{4} h, y_i + \frac{3}{4} k_1 h \right)$$
(25.38b)
4.1 Single, First Order ODE

Figure 4.5 Graphical representation of a fourth order Runge-Kutta method.

Solution
Using $\Delta X = 0.1$,

$$
K_1 = f(x_0, y_0) = 0
$$

$$
K_2 = f(x_0 + \frac{\Delta X}{2}, y_0 + \frac{K_1 \Delta X}{2}) = 0.05^2 \times 1 = 0.0025
$$

$$
K_3 = f(x_0 + \frac{\Delta X}{2}, y_0 + \frac{K_2 \Delta X}{2}) = 0.05^2 \times 1.000125 = 0.0025
$$

$$
K_4 = f(x_0 + \Delta X, y_0 + K_3 \Delta X) = 0.1^2 \times 1.000250 = 0.0100
$$

$$
Y_n = y_0 + \frac{K_1 + 2K_2 + 2K_3 + K_4}{6} \Delta X = 0.026
$$