9.5 Runge-Kutta Methods

The Taylor methods in the preceding section have the desirable feature that the F.G.E. is of order $O(h^N)$, and N can be chosen large so that this error is small. However, the shortcomings of the Taylor methods are the a priori determination of N and the computation of the higher derivatives, which can be very complicated. Each Runge-Kutta method is derived from an appropriate Taylor method in such a way that the F.G.E. is of order $O(h^N)$. A trade-off is made to perform several function evaluations at each step and eliminate the necessity to compute the higher derivatives. These methods can be constructed for any order N. The Runge-Kutta method of order N = 4 is most popular. It is a good choice for common purposes because it is quite accurate, stable, and easy to program. Most authorities proclaim that it is not necessary to go to a higher-order method because the increased accuracy is offset by additional computational effort. If more accuracy is required, then either a smaller step size or an adaptive method should be used.

The fourth-order Runge-Kutta method (RK4) simulates the accuracy of the Taylor series method of order N = 4. The method is based on computing y_{k+1} as follows:

(1)
$$y_{k+1} = y_k + w_1k_1 + w_2k_2 + w_3k_3 + w_4k_4,$$

where k_1, k_2, k_3 , and k_4 have the form

(2)

$$k_{1} = hf(t_{k}, y_{k}),$$

$$k_{2} = hf(t_{k} + a_{1}h, y_{k} + b_{1}k_{1}),$$

$$k_{3} = hf(t_{k} + a_{2}h, y_{k} + b_{2}k_{1} + b_{3}k_{2}),$$

$$k_{4} = hf(t_{k} + a_{3}h, y_{k} + b_{4}k_{1} + b_{5}k_{2} + b_{6}k_{3}).$$

By matching coefficients with those of the Taylor series method of order N = 4 so that the local truncation error is of order $O(h^5)$, Runge and Kutta were able to obtain the

following system of equations:

$$b_{1} = a_{1},$$

$$b_{2} + b_{3} = a_{2},$$

$$b_{4} + b_{5} + b_{6} = a_{3},$$

$$w_{1} + w_{2} + w_{3} + w_{4} = 1,$$

$$w_{2}a_{1} + w_{3}a_{2} + w_{4}a_{3} = \frac{1}{2},$$

$$w_{2}a_{1}^{2} + w_{3}a_{2}^{2} + w_{4}a_{3}^{2} = \frac{1}{3},$$

$$w_{2}a_{1}^{3} + w_{3}a_{2}^{3} + w_{4}a_{3}^{3} = \frac{1}{4},$$

$$w_{3}a_{1}b_{3} + w_{4}(a_{1}b_{5} + a_{2}b_{6}) = \frac{1}{6},$$

$$w_{3}a_{1}a_{2}b_{3} + w_{4}(a_{1}^{2}b_{5} + a_{2}^{2}b_{6}) = \frac{1}{12},$$

$$w_{4}a_{1}b_{3}b_{6} = \frac{1}{24}.$$

The system involves 11 equations in 13 unknowns. Two additional conditions must be supplied to solve the system. The most useful choice is

(4)
$$a_1 = \frac{1}{2}$$
 and $b_2 = 0$.

Then the solution for the remaining variables is

(5)
$$a_2 = \frac{1}{2}, \quad a_3 = 1, \quad b_1 = \frac{1}{2}, \quad b_3 = \frac{1}{2}, \quad b_4 = 0, \quad b_5 = 0, \quad b_6 = 1,$$

 $w_1 = \frac{1}{6}, \quad w_2 = \frac{1}{3}, \quad w_3 = \frac{1}{3}, \quad w_4 = \frac{1}{6}.$

The values in (4) and (5) are substituted into (2) and (1) to obtain the formula for the standard Runge-Kutta method of order N = 4, which is stated as follows. Start with the initial point (t_0, y_0) and generate the sequence of approximations using

(6)
$$y_{k+1} = y_k + \frac{h(f_1 + 2f_2 + 2f_3 + f_4)}{6}$$

where

(7)

$$f_{1} = f(t_{k}, y_{k}),$$

$$f_{2} = f\left(t_{k} + \frac{h}{2}, y_{k} + \frac{h}{2}f_{1}\right),$$

$$f_{3} = f\left(t_{k} + \frac{h}{2}, y_{k} + \frac{h}{2}f_{2}\right),$$

$$f_{4} = f(t_{k} + h, y_{k} + hf_{3}).$$

Discussion about the Method

The complete development of the equations in (7) is beyond the scope of this book and can be found in advanced texts, but we can get some insights. Consider the graph of the solution curve y = y(t) over the first subinterval $[t_0, t_1]$. The function values in (7) are approximations for slopes to this curve. Here f_1 is the slope at the left, f_2 and f_3 are two estimates for the slope in the middle, and f_4 is the slope at the right (see Figure 9.9(a)). The next point (t_1, y_1) is obtained by integrating the slope function

(8)
$$y(t_1) - y(t_0) = \int_{t_0}^{t_1} f(t, y(t)) dt$$

If Simpson's rule is applied with step size h/2, the approximation to the integral in (8) is

(9)
$$\int_{t_0}^{t_1} f(t, y(t)) dt \approx \frac{h}{6} (f(t_0, y(t_0)) + 4f(t_{1/2}, y(t_{1/2})) + f(t_1, y(t_1))),$$

where $t_{1/2}$ is the midpoint of the interval. Three function values are needed; hence we make the obvious choice $f(t_0, y(t_0)) = f_1$ and $f(t_1, y(t_1)) \approx f_4$. For the value in the middle we chose the average of f_2 and f_3 :

$$f(t_{1/2}, y(t_{1/2})) \approx \frac{f_2 + f_3}{2}.$$

These values are substituted into (9), which is used in equation (8) to get y_1 :

(10)
$$y_1 = y_0 + \frac{h}{6} \left(f_1 + \frac{4(f_2 + f_3)}{2} + f_4 \right).$$

When this formula is simplified, it is seen to be equation (6) with k = 0. The graph for the integral in (9) is shown in Figure 9.9(b).

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Figure 9.9 The graphs y = y(t) and z = f(t, y(t)) in the discussion of the Runge-Kutta method of order N = 4.

Step Size versus Error

The error term for Simpson's rule with step size h/2 is

(11)
$$-y^{(4)}(c_1)\frac{h^5}{2880}.$$

. .

If the only error at each step is that given in (11), after M steps the accumulated error for the RK4 method would be

(12)
$$-\sum_{k=1}^{M} y^{(4)}(c_k) \frac{h^5}{2880} \approx \frac{b-a}{5760} y^{(4)}(c) h^4 \approx \boldsymbol{O}(h^4).$$

The next theorem states the relationship between F.G.E. and step size. It is used to give us an idea of how much computing effort must be done when using the RK4 method.

Theorem 9.7 (Precision of the Runge-Kutta Method). Assume that y(t) is the solution to the I.V.P. If $y(t) \in C^{5}[t_{0}, b]$ and $\{(t_{k}, y_{k})\}_{k=0}^{M}$ is the sequence of approximations generated by the Runge-Kutta method of order 4, then

(13)
$$\begin{aligned} |e_k| &= |y(t_k) - y_k| = \boldsymbol{O}(h^4), \\ |\epsilon_{k+1}| &= |y(t_{k+1}) - y_k - hT_N(t_k, y_k)| = \boldsymbol{O}(h^5) \end{aligned}$$

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In particular, the F.G.E. at the end of the interval will satisfy

(14)
$$E(y(b), h) = |y(b) - y_M| = O(h^4).$$

Examples 9.10 and 9.11 illustrate Theorem 9.7. If approximations are computed using the step sizes h and h/2, we should have

(15)
$$E(y(b), h) \approx Ch^4$$

for the larger step size, and

(16)
$$E\left(y(b), \frac{h}{2}\right) \approx C\frac{h^4}{16} = \frac{1}{16}Ch^4 \approx \frac{1}{16}E(y(b), h).$$

Hence the idea in Theorem 9.7 is that if the step size in the RK4 method is reduced by a factor of $\frac{1}{2}$ we can expect that the overall F.G.E. will be reduced by a factor of $\frac{1}{16}$.

Example 9.10. Use the RK4 method to solve the I.V.P. y' = (t - y)/2 on [0, 3] with y(0) = 1. Compare solutions for $h = 1, \frac{1}{2}, \frac{1}{4}$, and $\frac{1}{8}$.

Table 9.8 gives the solution values at selected abscissas. For the step size h = 0.25, a sample calculation is

$$f_{1} = \frac{0.0 - 1.0}{2} = -0.5,$$

$$f_{2} = \frac{0.125 - (1 + 0.25(0.5)(-0.5))}{2} = -0.40625,$$

$$f_{3} = \frac{0.125 - (1 + 0.25(0.5)(-0.40625))}{2} = -0.4121094,$$

$$f_{4} = \frac{0.25 - (1 + 0.25(-0.4121094))}{2} = -0.3234863,$$

$$y_{1} = 1.0 + 0.25 \left(\frac{-0.5 + 2(-0.40625) + 2(-0.4121094) - 0.3234863}{6}\right)$$

$$= 0.8974915.$$

Example 9.11. Compare the F.G.E. when the RK4 method is used to solve y' = (t - y)/2 over [0, 3] with y(0) = 1 using step sizes 1, $\frac{1}{2}$, $\frac{1}{4}$, and $\frac{1}{8}$.

Table 9.9 gives the F.G.E. for the various step sizes and shows that the error in the approximation to y(3) decreases by about $\frac{1}{16}$ when the step size is reduced by a factor of 1/2.

$$E(y(3), h) = y(3) - y_M = O(h^4) \approx Ch^4$$
 where $C = -0.000614$.

A comparison of Examples 9.10 and 9.11 and Examples 9.8 and 9.9 shows what is meant by the statement "The RK4 method simulates the Taylor series method of order N = 4." For these examples, the two methods generate identical solution sets { (t_k, y_k) }

t_k	h = 1	$h = \frac{1}{2}$	$h = \frac{1}{4}$	$h = \frac{1}{8}$	$y(t_k)$ Exact	
0	1.0	1.0	1.0	1.0	1.0	
0.125				0.9432392	0.9432392	
0.25			0.8974915	0.8974908	0.8974917	
0.375				0.8620874	0.8620874	
0.50		0.8364258	0.8364037	0.8364024	0.8364023	
0.75			0.8118696	0.8118679	0.8118678	
1.00	0.8203125	0.8196285	0.8195940	0.8195921	0.8195920	
1.50		0.9171423	0.9171021	0.9170998	0.9170997	
2.00	1.1045125	1.1036826	1.1036408	1.1036385	1.1036383	
2.50		1.3595575	1.3595168	1.3595145	1.3595144	
3.00	1.6701860	1.6694308	1.6693928	1.6693906	1.6693905	

Table 9.8 Comparison of the RK4 Solutions with Different Step Sizes for y' = (t - y)/2 over [0, 3] with y(0) = 1

Table 9.9 Relation between Step Size and F.G.E. for the RK4 Solutions to y' = (t - y)/2 over [0, 3] with y(0) = 1

Step size, <i>h</i>	Number of steps, <i>M</i>	Approximation to $y(3)$, y_M	F.G.E. Error at $t = 3$, $y(3) - y_M$	$O(h^4) \approx Ch^4$ where C = -0.000614
1	3	1.6701860	-0.0007955	-0.0006140
$\frac{1}{2}$	6	1.6694308	-0.0000403	-0.0000384
$\frac{1}{4}$	12	1.6693928	-0.0000023	-0.0000024
$\frac{1}{8}$	24	1.6693906	-0.0000001	-0.0000001

over the given interval. The advantage of the RK4 method is obvious; no formulas for the higher derivatives need to be computed nor do they have to be in the program.

It is not easy to determine the accuracy to which a Runge-Kutta solution has been computed. We could estimate the size of $y^{(4)}(c)$ and use formula (12). Another way is to repeat the algorithm using a smaller step size and compare results. A third way is to adaptively determine the step size, which is done in Program 9.5. In Section 9.6 we will see how to change the step size for a multistep method.

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Runge-Kutta Methods of Order N = 2

The second-order Runge-Kutta method (denoted RK2) simulates the accuracy of the Taylor series method of order 2. Although this method is not as good to use as the RK4 method, its proof is easier to understand and illustrates the principles involved. To start, we write down the Taylor series formula for y(t + h):

(17)
$$y(t+h) = y(t) + hy'(t) + \frac{1}{2}h^2y''(t) + C_Th^3 + \cdots,$$

where C_T is a constant involving the third derivative of y(t) and the other terms in the series involve powers of h^j for j > 3.

The derivatives y'(t) and y''(t) in equation (17) must be expressed in terms of f(t, y) and its partial derivatives. Recall that

(18)
$$y'(t) = f(t, y)$$

The chain rule for differentiating a function of two variables can be used to differentiate (18) with respect to t, and the result is

$$y''(t) = f_t(t, y) + f_y(t, y)y'(t).$$

Using (18), this can be written

(19)
$$y''(t) = f_t(t, y) + f_y(t, y)f(t, y).$$

The derivatives (18) and (19) are substituted in (17) to give the Taylor expression for y(t + h):

(20)
$$y(t+h) = y(t) + hf(t, y) + \frac{1}{2}h^2 f_t(t, y) + \frac{1}{2}h^2 f_y(t, y)f(t, y) + C_T h^3 + \cdots$$

Now consider the Runge-Kutta method of order N = 2, which uses a linear combination of two function values to express y(t + h):

(21)
$$y(t+h) = y(t) + Ahf_0 + Bhf_1,$$

where

(22)
$$f_0 = f(t, y), f_1 = f(t + Ph, y + Qhf_0).$$

Next the Taylor polynomial approximation for a function of two independent variables is used to expand f(t, y) (see the Exercises). This gives the following representation for f_1 :

(23)
$$f_1 = f(t, y) + Phf_t(t, y) + Qhf_y(t, y)f(t, y) + C_Ph^2 + \cdots,$$

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where C_P involves the second-order partial derivatives of f(t, y). Then (23) is used in (21) to get the RK2 expression for y(t + h):

(24)
$$y(t+h) = y(t) + (A+B)hf(t, y) + BPh^{2}f_{t}(t, y) + BQh^{2}f_{y}(t, y)f(t, y) + BC_{P}h^{3} + \cdots$$

A comparison of similar terms in equations (20) and (24) will produce the following conclusions:

$$hf(t, y) = (A + B)hf(t, y)$$
 implies that $1 = A + B$,

$$\frac{1}{2}h^2 f_t(t, y) = BPh^2 f_t(t, y)$$
 implies that $\frac{1}{2} = BP$,

$$\frac{1}{2}h^2 f_y(t, y)f(t, y) = BQh^2 f_y(t, y)f(t, y)$$
 implies that $\frac{1}{2} = BQ$.

Hence, if we require that A, B, P, and Q satisfy the relations

(25)
$$A + B = 1$$
 $BP = \frac{1}{2}$ $BQ = \frac{1}{2}$,

then the RK2 method in (24) will have the same order of accuracy as the Taylor's method in (20).

Since there are only three equations in four unknowns, the system of equations (25) is underdetermined, and we are permitted to choose one of the coefficients. There are several special choices that have been studied in the literature; we mention two of them.

Case (i): Choose $A = \frac{1}{2}$. This choice leads to $B = \frac{1}{2}$, P = 1, and Q = 1. If equation (21) is written with these parameters, the formula is

(26)
$$y(t+h) = y(t) + \frac{h}{2}(f(t,y) + f(t+h,y+hf(t,y))).$$

When this scheme is used to generate $\{(t_k, y_k)\}$, the result is Heun's method.

Case (ii): Choose A = 0. This choice leads to B = 1, $P = \frac{1}{2}$, and $Q = \frac{1}{2}$. If equation (21) is written with these parameters, the formula is

(27)
$$y(t+h) = y(t) + hf\left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y)\right).$$

When this scheme is used to generate $\{(t_k, y_k)\}$, it is called the *modified Euler-Cauchy method*.

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