SEVENTH EDITION

ADVANCED ENGINEERING MATHEMATICS

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20.1 Methods for First-Order Differential Equations

From Chap. 1 we know that a *differential equation of the first order* is of the form $F(x, y, y') = 0$, and often it will be possible to write the equation in the *explicit form* $y' = f(x, y)$. An **initial value problem** consists of a differential equation and a condition the solution must satisfy (or several conditions referring to the same value of x if the equation is of higher order). In this section we shall consider initial value problems of the form

(1) $$\boxed{y' = f(x, y), \quad y(x_0) = y_0}$$

assuming f to be such that the problem has a unique solution on some interval containing x_0.

We shall discuss methods for computing numerical values of the solutions, which are needed if a formula for the solution of an equation is not available or is too complicated to be of practical use.

These methods are **step-by-step methods**, that is, we start from the given $y_0 = y(x_0)$ and proceed stepwise, computing approximate values of the solution $y(x)$ at the *"mesh points"*

$$x_1 = x_0 + h, \quad x_2 = x_0 + 2h, \quad x_3 = x_0 + 3h, \quad \cdots,$$

where the **step size** h is a fixed number, for instance 0.2 or 0.1 or 0.01, whose choice we discuss later in this section.

The computation in each step is done by the same formula. Such formulas are suggested by the Taylor series

(2) $$y(x + h) = y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \cdots.$$

Now for a small value of h, the higher powers $h^2, h^3, \cdots$ are very small. This suggests the crude approximation

$$y(x + h) \approx y(x) + hy'(x) = y(x) + hf(x, y)$$

(with the right side obtained from the given differential equation) and the following iteration process. In the first step we compute

$$y_1 = y_0 + hf(x_0, y_0)$$

which approximates $y(x_1) = y(x_0 + h)$. In the second step we compute

$$y_2 = y_1 + hf(x_1, y_1)$$

which approximates $y(x_2) = y(x_0 + 2h)$, etc., and in general

(3) $$\boxed{y_{n+1} = y_n + hf(x_n, y_n)} \qquad (n = 0, 1, \cdots).$$

This is called the **Euler method** or **Euler–Cauchy method**. Geometrically it is an approximation of the curve of $y(x)$ by a polygon whose first side is tangent to the curve at x_0 (see Fig. 422).

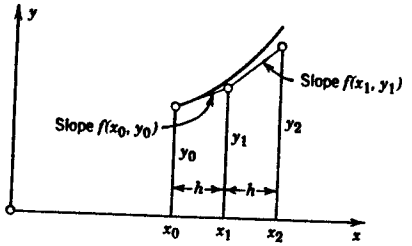

Fig. 422. Euler method

This crude method is hardly ever used in practice, but since it is simple, it nicely explains the principle of methods based on the Taylor series.

Euler's method is called a **first-order method**, because in (2) we take only the constant terms and the term containing the first power of h. The omission of the further terms in (2) causes an error, which is called the **truncation error** of the method. For small h, the third and higher powers of h will be small compared with h^2 in the first neglected term in (2), and we therefore say that the **truncation error per step** (or *local truncation error*) is of **order** h^2. In addition there are **round-off errors** in this and other methods, which may affect the accuracy of the values $y_1, y_2, \cdots$ more and more as n increases; we shall return to this point in the next section.

Table 20.1
Euler Method Applied to (4) in Example 1 and Error

n	x_n	y_n	$0.2(x_n + y_n)$	Exact Values	Error
0	0.0	0.000	0.000	0.000	0.000
1	0.2	0.000	0.040	0.021	0.021
2	0.4	0.040	0.088	0.092	0.052
3	0.6	0.128	0.146	0.222	0.094
4	0.8	0.274	0.215	0.426	0.152
5	1.0	0.489		0.718	0.229

EXAMPLE 1 Euler method

Apply the Euler method to the following initial value problem, choosing $h = 0.2$ and computing $y_1, \cdots, y_5$:

(4) $$y' = x + y, \qquad y(0) = 0.$$

Solution. Here $f(x, y) = x + y$, and we see that (3) becomes

$$y_{n+1} = y_n + 0.2(x_n + y_n).$$

Table 20.1 shows the computations, the values of the exact solution

$$y(x) = e^x - x - 1$$

obtained from (4) in Sec. 1.7, and the error. In practice the exact solution is unknown, but an indication of the accuracy of the values can be obtained by applying the Euler method once more with step $2h = 0.4$ and comparing corresponding approximations. This computation is:

x_n	y_n	$0.4(x_n + y_n)$	y_n in Table 20.1	Difference
0.0	0.000	0.000	0.000	0.000
0.4	0.000	0.160	0.040	0.040
0.8	0.160		0.274	0.114

Since the error is of order h^2, in a switch from h to $2h$ it is multiplied by $2^2 = 4$, but since we then need only half as many steps as before, it will only be multiplied by $4/2 = 2$. Hence the difference $2\epsilon_2 - \epsilon_2 = 0.040$ indicates the error ϵ_2 of y_2 in Table 20.1 (which actually is 0.052), and 0.114 that of y_4 (actual: 0.152). ∎

Improved Euler Method (Heun's Method)

By taking more terms in (2) into account we obtain numerical methods of higher order and precision. But there is a practical problem. If we substitute $y' = f(x, y(x))$ into (2), we have

(2*) $$y(x + h) = y(x) + hf + \tfrac{1}{2}h^2f' + \tfrac{1}{6}h^3f'' + \cdots$$

where, since y in f depends on x,

$$f' = f_x + f_y y' = f_x + f_y f$$

and the further derivatives f'', f''' become even much more cumbersome. The ***general strategy*** now is to avoid their computation and replace it by computing f for one or several suitably chosen auxiliary values of (x, y), where "suitably" means that they are chosen to make the order of the method as high as possible (to have high accuracy). Let us discuss two such methods that are of practical importance.

The first method is the so-called **improved Euler method** or **improved Euler–Cauchy method** (sometimes also called **Heun's method**). In each step of this method we compute first the auxiliary value

(5a) $$\boxed{y^*_{n+1} = y_n + hf(x_n, y_n)}$$

and then the new value

(5b) $$\boxed{y_{n+1} = y_n + \tfrac{1}{2}h[f(x_n, y_n) + f(x_{n+1}, y^*_{n+1})].}$$

This method has a simple geometric interpretation. In fact, we may say that in the interval from x_n to $x_n + \frac{1}{2}h$ we approximate the solution y by the straight line through (x_n, y_n) with slope $f(x_n, y_n)$, and then we continue along the straight line with slope $f(x_{n+1}, y^*_{n+1})$ until x reaches x_{n+1} (see Fig. 423, where $n = 0$).

The improved Euler–Cauchy method is a **predictor–corrector method,** because in each step we first predict a value by (5a) and then correct it by (5b).

In algorithmic form, using the notations $k_1 = hf(x_n, y_n)$ in (5a) and $k_2 = hf(x_{n+1}, y^*_{n+1})$ in (5b) we can write this method as shown in Table 20.2 on the next page.

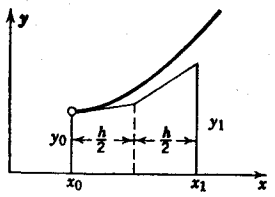

Fig. 423. Improved Euler method

Table 20.2
Improved Euler Method (Heun's Method)

ALGORITHM EULER (f, x_0, y_0, h, N)
This algorithm computes the solution of the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$ at equidistant points $x_1 = x_0 + h$, $x_2 = x_0 + 2h, \cdots, x_N = x_0 + Nh$; here f is such that this problem has a unique solution on the interval $[x_0, x_N]$ (see Sec. 1.11).

INPUT: Initial values x_0, y_0, step size h, number of steps N
OUTPUT: Approximation y_{n+1} to the solution $y(x_{n+1})$ at $x_{n+1} = x_0 + (n + 1)h$, where $n = 0, \cdots, N - 1$

For $n = 0, 1, \cdots, N - 1$ do:

$$x_{n+1} = x_n + h$$
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_{n+1}, y_n + k_1)$$
$$y_{n+1} = y_n + \tfrac{1}{2}(k_1 + k_2)$$
OUTPUT x_{n+1}, y_{n+1}

End
Stop
End EULER

XAMPLE 2 Improved Euler method

Apply the improved Euler method to the initial value problem (4), choosing $h = 0.2$, as before.

Solution. For the present problem,

$$k_1 = 0.2(x_n + y_n)$$
$$k_2 = 0.2(x_n + 0.2 + y_n + 0.2(x_n + y_n))$$
$$y_{n+1} = y_n + \frac{0.2}{2}(2.2x_n + 2.2y_n + 0.2)$$
$$= y_n + 0.22(x_n + y_n) + 0.02.$$

Table 20.3 shows that our present results are more accurate than those in Example 1; see also Table 20.6 on p. 1041. ∎

Table 20.3
Improved Euler Method Applied to (4) and Error

n	x_n	y_n	$0.22(x_n + y_n) + 0.02$	Exact Values	Error
0	0.0	0.0000	0.0200	0.0000	0.0000
1	0.2	0.0200	0.0684	0.0214	0.0014
2	0.4	0.0884	0.1274	0.0918	0.0034
3	0.6	0.2158	0.1995	0.2221	0.0063
4	0.8	0.4153	0.2874	0.4255	0.0102
5	1.0	0.7027		0.7183	0.0156

The improved Euler method is a **second-order method,** *because the truncation error per step is of order h^3.*

Proof. Setting $\tilde{f}_n = f(x_n, y(x_n))$ and using (2*), we have

(6a) $$y(x_n + h) - y(x_n) = h\tilde{f}_n + \tfrac{1}{2}h^2\tilde{f}_n' + \tfrac{1}{6}h^3\tilde{f}_n'' + \cdots.$$

Approximating the expression in the brackets in (5b) by $\tilde{f}_n + \tilde{f}_{n+1}$ and again using the Taylor expansion, we obtain from (5b)

(6b) $$y_{n+1} - y_n \approx \tfrac{1}{2}h[\tilde{f}_n + \tilde{f}_{n+1}]$$
$$= \tfrac{1}{2}h[\tilde{f}_n + (\tilde{f}_n + h\tilde{f}_n' + \tfrac{1}{2}h^2\tilde{f}_n'' + \cdots)].$$

Subtraction of (6a) from (6b) gives the truncation error per step

$$\frac{h^3}{4}\tilde{f}_n'' - \frac{h^3}{6}\tilde{f}_n'' + \cdots = \frac{h^3}{12}\tilde{f}_n'' + \cdots.$$

This proves the assertion. ∎

Choice of step size. This is an important matter in any step-by-step method. h should not be too small, to avoid excessively many steps and corresponding round-off error accumulation. But h should not be too large either, to avoid a large truncation error per step and an additional error, call it φ_n, caused by the evaluation of f at (x_n, y_n) instead of $(x_n, y(x_n))$. Now φ_n would be zero if f were independent of y; thus it will matter the more the faster f varies with y, that is, the larger the absolute value of the partial derivative $f_y = \partial f/\partial y$ is. More precisely, by the definition of φ_n and the mean value theorem we get

$$\varphi_n = f(x_n, y(x_n)) - f(x_n, y_n) = f_y(x_n, \tilde{y})\eta_n$$

where $\eta_n = y(x_n) - y_n$ is the error of y_n and $\tilde{y}$ lies between $y(x_n)$ and y_n. Hence the contribution of φ_n to the error of y_{n+1} is approximately $h\varphi_n = hf_y(x_n, \tilde{y})\eta_n$. This suggests to take a close upper bound K of $|f_y|$ in the region of interest and to choose h such that

$$\kappa = hK$$

is not too large. We see that if $|f_y|$ is large (strong dependence of f on y), then K is large and h must be small, which is understandable. (In Examples 1 and 2, $f_y = 1$, $K = 1$, $hK = 0.2$.) If f_y varies very much, we may choose a close upper bound K_n of $|f_y(x_n, \tilde{y})|$ and choose two or even three different values of h in different regions, to keep

$$\kappa_n = hK_n$$

within a certain interval (for example, $0.05 \leqq \kappa_n \leqq 0.1$), which depends on the desired accuracy; of course, because of the truncation error per step, we cannot let h increase beyond a certain value.

Runge–Kutta Method

A still more accurate method of great practical importance is the **Runge–Kutta method,**[1] shown in Table 20.4. We see that in each step we first compute four auxiliary quantities k_1, k_2, k_3, k_4 and then the new value y_{n+1}. These formulas look complicated at first sight, but they are in fact very easy to program.

It can be shown that the truncation error per step is of the order h^5 (see Ref. [E2] in Appendix 1) and the method is, therefore, a fourth-order method.

Table 20.4
Runge–Kutta Method (of Fourth Order)

ALGORITHM RUNGE–KUTTA (f, x_0, y_0, h, N).
This algorithm computes the solution of the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$ at equidistant points

$$x_1 = x_0 + h, x_2 = x_0 + 2h, \cdots, x_N = x_0 + Nh;$$

here f is such that this problem has a unique solution on the interval $[x_0, x_N]$ (see Sec. 1.11).

INPUT: Initial values x_0, y_0, step size h, number of steps N
OUTPUT: Approximation y_{n+1} to the solution $y(x_{n+1})$ at $x_{n+1} = x_0 + (n + 1)h$, where $n = 0, 1, \cdots, N - 1$

For $n = 0, 1, \cdots, N - 1$ do:

$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1)$$
$$k_3 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2)$$
$$k_4 = hf(x_n + h, y_n + k_3)$$
$$x_{n+1} = x_n + h$$
$$y_{n+1} = y_n + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$
OUTPUT x_{n+1}, y_{n+1}

End
Stop
End RUNGE–KUTTA

[1]Named after the German mathematicians CARL DAVID TOLMÉ RUNGE (1856—1927), professor of applied mathematics at Göttingen, and WILHELM KUTTA (1867—1944).
Without much historical justification, the improved Euler method is sometimes called a **second-order Runge–Kutta method.** The Runge–Kutta method discussed here is often called the **fourth-order Runge–Kutta method** because there are Runge–Kutta methods of still higher order based on the same principle of replacing the computation of derivatives by the computation of auxiliary values (values of f at certain points). For details, see Ref. [E21] in Appendix 1.

Note that if f depends only on x, this method reduces to Simpson's rule of integration (Sec. 18.5).

In hand calculations, the frequent calculation of $f(x, y)$ is laborious. On a computer this does not matter too much, and the method is well suited because it needs no special starting procedure, makes light demands on storage, requires no estimation, and repeatedly uses the same straightforward computational procedure.

EXAMPLE 3 Runge–Kutta method

Apply the Runge–Kutta method to the initial value problem (4) in Example 1, choosing $h = 0.2$, as before, and computing five steps.

Solution. For the present problem we have $f(x, y) = x + y$. Hence

$$k_1 = 0.2(x_n + y_n), \qquad k_2 = 0.2(x_n + 0.1 + y_n + 0.5k_1),$$
$$k_3 = 0.2(x_n + 0.1 + y_n + 0.5k_2), \qquad k_4 = 0.2(x_n + 0.2 + y_n + k_3).$$

Since these expressions are so simple, we find it convenient to insert k_1 into k_2, obtaining $k_2 = 0.22(x_n + y_n) + 0.02$, insert this into k_3, finding $k_3 = 0.222(x_n + y_n) + 0.022$, and finally insert this into k_4, finding $k_4 = 0.2444(x_n + y_n) + 0.0444$. If we use these expressions, the formula for y_{n+1} in Table 20.4 becomes

(7) $$y_{n+1} = y_n + 0.2214(x_n + y_n) + 0.0214.$$

Of course, our present inserting process is *not typical* of the Runge–Kutta method and should not be tried in general. Table 20.5 shows the computations. From Table 20.6 we see that the values are much more accurate than those in Examples 1 and 2. ∎

Table 20.5
Runge–Kutta Method Applied to (4); Computations by the Use of (7)

n	x_n	y_n	$0.2214(x_n + y_n) + 0.0214$	Exact Values $y = e^x - x - 1$	$10^6 \times$ Error of y_n
0	0.0	0	0.021 400	0.000 000	0
1	0.2	0.021 400	0.070 418	0.021 403	3
2	0.4	0.091 818	0.130 289	0.091 825	7
3	0.6	0.222 107	0.203 414	0.222 119	11
4	0.8	0.425 521	0.292 730	0.425 541	20
5	1.0	0.718 251		0.718 282	31

Table 20.6
Comparison of the Accuracy of the Three Methods Under Consideration in the Case of the Initial Value Problem (4), with $h = 0.2$

x	$y = e^x - x - 1$	Error		
		Euler Method (Table 20.1)	Improved Euler (Table 20.3)	Runge–Kutta (Table 20.5)
0.2	0.021 403	0.021	0.0014	0.000 003
0.4	0.091 825	0.052	0.0034	0.000 007
0.6	0.222 119	0.094	0.0063	0.000 011
0.8	0.425 541	0.152	0.0102	0.000 020
1.0	0.718 282	0.229	0.0156	0.000 031

Step size h. The step size h should not be greater than a certain value H, which depends on the desired accuracy, and should otherwise be such that

$$\kappa = hK \qquad (K \text{ a close upper bound for } |\partial f/\partial y|)$$

lies about between 0.01 and 0.05; this is similar to the case of the improved Euler method discussed before.

It is an advantage of the Runge–Kutta method that we may **control h** by means of k_1, k_2, k_3, because from the definition of f_y we have

$$\kappa = hK \approx h|f_y| \approx h\left|\frac{f(x, y^*) - f(x, y^{**})}{y^* - y^{**}}\right|,$$

and if in the numerator we choose

$$hf(x, y^*) = k_3 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2), \quad \text{thus,} \quad y^* = y_n + \tfrac{1}{2}k_2,$$

$$hf(x, y^{**}) = k_2 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1), \quad \text{thus,} \quad y^{**} = y_n + \tfrac{1}{2}k_1,$$

we have in the denominator $y^* - y^{**} = \frac{1}{2}(k_2 - k_1)$ and get the desired formula for κ in terms of computed quantities,

$$\kappa \approx 2\left|\frac{k_3 - k_2}{k_2 - k_1}\right|. \tag{8}$$

We may now make provision to leave h unchanged if, say, $0.01 \leqq \kappa_n \leqq 0.05$, to decrease h by 50% if $\kappa_n > 0.05$, and to double h if $\kappa_n < 0.01$ (if doubling is possible without increasing h beyond a suitably chosen number H, which depends on the desired accuracy).

Another control of h results from performing the computation simultaneously with step $2h$, which corresponds to increasing the truncation error per step by a factor $2^5 = 32$, but since the number of steps decreases, the actual increase is by a factor $2^5/2 = 16$. Hence the error ϵ of an approximation $\bar{y}$ obtained with step h equals about 1/15 times the difference $\delta = \bar{y} - \bar{\bar{y}}$ of corresponding approximations obtained with steps h and $2h$, respectively,

$$\epsilon \approx \frac{1}{15}(\bar{y} - \bar{\bar{y}}). \tag{9}$$

We may now choose a number ϵ (for example, 1 unit of the last digit that is supposed to be significant) and leave h unchanged if $0.2\epsilon \leqq |\delta| \leqq 10\epsilon$, decrease h by 50% if $|\delta| > 10\epsilon$, and double h if $|\delta| < 0.2\epsilon$; of course, in doubling we must take care that the step does not become larger than a suitable number H; this is as before.

Let us illustrate the error estimate (9) by a simple example.

EXAMPLE 4 **Runge–Kutta method (of fourth order), error estimate**
Solve the initial value problem

$$y' = (y - x - 1)^2 + 2, \qquad y(0) = 1$$

by the Runge–Kutta method for $0 \leqq x \leqq 0.4$ with step $h = 0.1$ and estimate the error by (9).

Solution. The numerical results are shown in Table 20.7. They also illustrate how the accuracy increases with decreasing step (from $2h = 0.2$ to $h = 0.1$). The error estimates (9) are close to the actual error. Although we cannot always expect this, formula (9) will certainly give information about the order of magnitude of the error. ∎

It can be shown that the methods discussed in this section are *numerically stable* (definition in Sec. 18.1). They are **one-step methods** because in each step we use the data of just one preceding step, in contrast to **multistep methods,** which in each step use data from several preceding steps, as we shall see in the next section.

Table 20.7
Runge–Kutta Method Applied to the Initial Value Problem in Example 4 and Error Estimate

x	$\bar{y}$ (Step h)	$\bar{\bar{y}}$ (Step $2h$)	Error Estimate (9)	Actual Error	Exact Solution (9D)
0.0	1.000 000 000	1.000 000 000	0.000 000 000	0.000 000 000	1.000 000 000
0.1	1.200 334 589			0.000 000 083	1.200 334 672
0.2	1.402 709 878	1.402 707 341	0.000 000 181	0.000 000 157	1.402 710 036
0.3	1.609 336 039			0.000 000 210	1.609 336 250
0.4	1.822 792 993	1.822 788 917	0.000 000 291	0.000 000 226	1.822 793 219

Problem Set 20.1

Apply the Euler method to the following initial value problems. Do 10 steps. Solve the problem exactly. Compute the errors.

1. $y' = y$, $y(0) = 1$, $h = 0.1$
2. $y' = y$, $y(0) = 1$, $h = 0.01$
3. $y' + 5x^4y^2 = 0$, $y(0) = 1$, $h = 0.1$
4. $y' = (y + x)^2$, $y(0) = 0$, $h = 0.1$

Apply the improved Euler method to the following initial value problems. Do 10 steps with $h = 0.1$. Solve the problem exactly. Compute the errors.

5. $y' = y$, $y(0) = 1$
6. $y' = 1 + y^2$, $y(0) = 0$
7. $y' + y \tan x = \sin 2x$, $y(0) = 1$
8. $y' = y - y^2$, $y(0) = 0.5$

Apply the Runge–Kutta method (of fourth order) to the following initial value problems. Do 5 steps with $h = 0.2$. Solve the problem exactly. Compute the errors.

9. $y' = xy$, $y(0) = 1$
10. $y' = y - y^2$, $y(0) = 0.5$
11. $y' = (1 + x^{-1})y$, $y(1) = e$
12. $y' = \frac{1}{2}(y/x - x/y)$, $y(2) = 2$

13. Apply the Euler method and the improved Euler method with $h = 0.1$ and 10 steps to the initial value problem $y' = 2 - 2y$, $y(0) = 0$, and determine and compare the errors.
14. Apply the Runge–Kutta method with $h = 0.1$ and 10 steps to Prob. 13 and determine and compare the errors with those in Prob. 13.
15. Solve $y' = 2x^{-1}\sqrt{y - \ln x} + x^{-1}$, $y(1) = 0$ for $1 \leqq x \leqq 1.8$ by Euler's method with $h = 0.1$. Verify that the exact solution is $y = (\ln x)^2 + \ln x$ and compute the error.
16. Solve Prob. 15 by the improved Euler method with $h = 0.2$, determine the error, compare with Prob. 15, and comment. Note that this is a fair comparison because here we evaluate $f(x, y)$ eight times (4 steps with 2 evaluations each), just as in Prob. 15.
17. Solve Prob. 15 by the Runge–Kutta method with $h = 0.4$, determine the error, and compare with Prob. 15. (Note that these 2 Runge–Kutta steps require 8 evaluations of $f(x, y)$, just as many as in Prob. 15.)
18. Solve Prob. 15 by the Runge–Kutta method with $h = 0.1$ and compare the error with that in Prob. 15.
19. Another Euler–Cauchy type method is given by

$$y_{n+1} = y_n + hf(x_n + \tfrac{1}{2}h, y^*_{n+1}),$$

where $y^*_{n+1} = y_n + \frac{1}{2}hf(x_n, y_n)$. Give a geometric motivation of the method. Apply it to (4), choosing $h = 0.2$ and calculating 5 steps.

20. **Kutta's third-order method** is defined by

$$y_{n+1} = y_n + \tfrac{1}{6}(k_1 + 4k_2 + k_3^*)$$

where k_1 and k_2 are as in Table 20.4 and $k_3^* = hf(x_{n+1}, y_n - k_1 + 2k_2)$. Apply this method to (4) in Example 1. Choose $h = 0.2$ and do 5 steps. Compare with Table 20.6.

20.2 Multistep Methods

A **one-step method** is a method that in each step uses only values obtained in a single step, namely, in the preceding step. Examples are the Runge–Kutta method and all the other methods in the last section. In contrast, a method that uses values from more than one preceding step is called a **multistep method**. We shall explain the idea of obtaining such methods in terms of the derivation of the **Adams–Moulton method**, which is of great practical importance. The initial value problem is as before,

(1) $$y' = f(x, y), \quad y(x_0) = y_0$$

where f is assumed to be such that the problem has a unique solution in some interval containing x_0 as well as all the x-values at which we shall compute approximate values of the solution.

M.D. Greenberg, Foundations of Applied Mathematics, Prentice Hall, 1978

2.4. TAYLOR SERIES

Starting with the identity

$$\int_a^x f'(x)\,dx = f(x) - f(a),$$

we have

$$f(x) = f(a) + \int_a^x f'(x)\,dx. \tag{2.20}$$

Since $f(x)$ is arbitrary, (2.20) should also hold with $f(x)$ replaced by the function $f'(x)$,[10]

$$f'(x) = f'(a) + \int_a^x f''(x)\,dx. \tag{2.21}$$

Using this expression for $f'(x)$ in the integral in (2.20), we obtain

$$\begin{aligned} f(x) &= f(a) + \int_a^x \left\{ f'(a) + \int_a^x f''(x)\,dx \right\} dx \\ &= f(a) + f'(a)(x-a) + \int_a^x \int_a^x f''(x)\,dx\,dx. \end{aligned} \tag{2.22}$$

But just as we obtained (2.21) from (2.20) by replacing $f(x)$ with $f'(x)$, we can replace $f'(x)$ in (2.21) by $f''(x)$, so that

$$f''(x) = f''(a) + \int_a^x f'''(x)\,dx. \tag{2.23}$$

Using this result in (2.22),

$$\begin{aligned} f(x) &= f(a) + f'(a)(x-a) + \int_a^x \int_a^x \left\{ f''(a) + \int_a^x f'''(x)\,dx \right\} dx\,dx \\ &= f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \int_a^x \int_a^x \int_a^x f'''(x)\,dx\,dx\,dx. \end{aligned} \tag{2.24}$$

Repeating this process, under the assumption that $f(x)$ is sufficiently differentiable of course,[11] we find

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(n-1)}(a)}{(n-1)!}(x-a)^{n-1} + R_n \tag{2.25a}$$

[10] This step is *not* the same as differentiating (2.20).

[11] Whereas the function $xH(x)$ (where H is the Heaviside function) is not even once differentiable over any interval containing the origin (because of its kink at $x = 0$), the function $x \sin(x^2)$, for example, is differentiable over $-\infty < x < \infty$ as many times as we like; we say that it is *infinitely differentiable*. As one more example, the function $x^3H(x)$ is twice differentiable over any interval containing the origin (Exercise 2.23).

where

$$R_n = \int_a^x \cdots \int_a^x f^{(n)}(x)(dx)^n \tag{2.25b}$$

and $(dx)^n$ means $dx \ldots dx$, n times. Equation (2.25) is known as **Taylor's formula with remainder,** where the remainder is expressed in *integral* form by (2.25b).

Suppose next that $m \le f^{(n)}(x) \le M$ over $[a, x]$,[12] where m and M are constants. Then

$$\int_a^x \cdots \int_a^x m(dx)^n \le R_n \le \int_a^x \cdots \int_a^x M(dx)^n.$$

Integrating, we have

$$m\frac{(x-a)^n}{n!} \le R_n \le M\frac{(x-a)^n}{n!} \tag{2.26}$$

If we assume that $f^{(n)}(x)$ is continuous over $[a, x]$, then (it can be shown that) it must take on all values between its minimum m and its maximum M over the interval. It follows from (2.26) that we must be able to express

$$R_n = \frac{f^{(n)}(\xi)}{n!}(x-a)^n, \tag{2.27}$$

where ξ is *some* suitable point in $[a, x]$; this is the *Lagrange* form of R_n. For the special case $n = 1$, Taylor's formula with Lagrange remainder is simply

$$f(x) = f(a) + f'(\xi)(x-a)$$

or

$$\frac{f(x) - f(a)}{x-a} = f'(\xi) \qquad (a \le \xi \le x) \tag{2.28}$$

which is known as the **mean value theorem of the differential calculus.**

Assuming that f is infinitely differentiable at the point a, let us formally write down the infinite series

$$f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \cdots \tag{2.29}$$

and call it **the Taylor series of $f(x)$**[13] about the point a. Hoping that (2.29) is *equal* to $f(x)$, we are tempted to make the tentative claim that if (2.29) converges, it converges to $f(x)$, and so we can write

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots \tag{2.30}$$

But

Example 2.11. The Taylor expansion of $f(x) = e^{-1/x^2}$ about $x = 0$,[14] also called

[12] It is standard practice to denote a *closed* interval $\alpha \le x \le \beta$ by the symbol $[\alpha, \beta]$ and an *open* interval $\alpha < x < \beta$ by (α, β). Similarly, $[\alpha, \beta)$ means $\alpha \le x < \beta$ and so on.

[13] Introduced by Brook Taylor (1685–1731) in 1715, although apparently known to James Gregory at least 45 years earlier, its importance was not fully recognized until 1755 when Euler applied it in his development of the differential calculus.

[14] If we were fussy, we would note that $f(0)$ is not actually defined by $f(x) = e^{-1/x^2}$, since $1/0$ is not defined. To complete the definition of f let us define $f(x) = e^{-1/x^2}$ for $x \neq 0$, and $f(0) = 0$. Incidentally, you should sketch this function. Note how *extremely* flat it is in the neighborhood of $x = 0$, since $f'(0) = f''(0) = f'''(0) = \cdots = 0$, and yet is does eventually rise toward its asymptotic value of unity as $|x| \to \infty$.

its *Maclaurin expansion* (i.e., the Taylor expansion about $x = 0$), is (Exercise 2.22)

$$0 + 0 + 0 + \cdots$$

which certainly converges (to zero) but *not* to the given $f(x)$ (except at $x = 0$, where $f(0) = 0$). The difficulty is that R_n, which gets "lost" when we go from (2.25) to (2.30), does not tend to zero as $n \to \infty$ but is, in fact, equal to e^{-1/x^2} for all n! ∎

What we need to show is that $R_n \to 0$ if we want to be certain of the equality in (2.30). Let us illustrate the procedure.

Example 2.12. Let $f(x) = e^x$ and $a = 0$. The resulting Taylor series

$$1 + x + \frac{x^2}{2!} + \cdots + \frac{x^n}{n!} + \cdots \tag{2.31}$$

is seen (e.g., by the ratio test) to converge for all x. Now examine R_n. Consider $x > 0$. From (2.27)

$$R_n = \frac{e^\xi}{n!}x^n,$$

Where $0 \le \xi \le x$. Actually, we don't know the value of ξ, but since $0 \le \xi \le x$, it follows that $R_n \le e^x x^n/n!$, which tends to zero (for x fixed) as $n \to \infty$. [If you're not sure why $x^n/n! \to 0$ as $n \to \infty$, recall that (2.31) converges, by the ratio test, and hence the nth term, $x^n/n!$, *must* $\to 0$ as $n \to \infty$.] A similar argument applies for $x < 0$. So not only does the Taylor series of e^x converge for all x, it also converges to e^x. We therefore have the equality

$$e^x = 1 + x + \frac{x^2}{2!} + \cdots \qquad (-\infty < x < \infty). \quad ∎$$

Example 2.13. The expansion of $f(x) = 1/x$ about $x = a$ $(a \neq 0)$,

$$\sum_0^\infty \frac{(-1)^n}{a^{n+1}}(x - a)^n, \tag{2.32}$$

is seen (e.g., by the ratio test) to converge in $|x - a| < a$—that is, in $0 < x < 2a$. We state (this time without proof) that $R_n \to 0$ as $n \to \infty$, and so the sum function coincides, in fact, with $1/x$. ∎

If the equality (2.30) holds over $|x - a| < \delta$ for some $\delta > 0$, we say that $f(x)$ is **analytic** *at $x = a$.* For instance, recalling that the Taylor series (2.32) of $1/x$ about $x = a$ converges to $1/x$ within $|x - a| < a$ for all $a \neq 0$, it follows that $1/x$ is analytic for all $x \neq 0$. The Taylor series about $x = 0$, however, does *not* converge in any interval $|x| < \delta$ [in fact, the terms $f(0), f'(0), f''(0), \ldots$ in the series do not exist]; therefore $1/x$ is not analytic at $x = 0$. We say that it is **singular** there or that $x = 0$ is a **singular point** of $1/x$. The singular point $x = 0$ is significant not only in regard to the failure of the Taylor expansion about this point but also in that it limits the interval of convergence of the Taylor expansion about any other point $a \neq 0$. For example, the interval of convergence of the expansion about $a = 2$ is $|x - 2| < 2$ or $0 < x <$

4; that is, the interval of convergence "spreads out equally to the left and right until one end bumps up against a singularity," in this case at $x = 0$.

The function e^{-1/x^2} of Example 2.11 also happens to have a singular point at $x = 0$, since the Taylor series $0 + 0 + 0 + \ldots$ does not converge to e^{-1/x^2} in $|x| < \delta$ for any $\delta > 0$. Why? What's wrong? The function seems to be nicely behaved at $x = 0$; in fact, $f(0), f'(0), f''(0), \ldots$ all exist (and are zero). Although complex variable theory is not discussed until Part II, let us anticipate a little and consider $f(z) = e^{-1/z^2} = e^{-1/(x+iy)^2}$; in other words, we extend the domain off the real axis into the complex z plane. As $x \to 0$ along the real axis $(y = 0)$, $f = e^{-1/x^2} \to 0$, which looks fine. But if we approach the origin along the *imaginary* axis $(x = 0)$, then $f = e^{-1/(iy)^2} = e^{1/y^2} \to \infty$ as $y \to 0$, and the singular nature of $f(z)$ at $z = 0$ now comes into view!

The fact is that we are not going to understand Taylor series and analyticity fully until we study complex variable theory. As a final example, we note that the Taylor expansion $1/(1 + x^2) = 1 - x^2 + x^4 - x^6 + \ldots$ holds in the interval of convergence $|x| < 1$. Why the restriction $|x| < 1$? The function $1/(1 + x^2)$ is beautifully smooth and well behaved for *all* $-\infty < x < \infty$. Quite so, but $f(z) = 1/(1 + z^2)$ is singular at $z = \pm i$, and these singularities limit the region of convergence to the unit disk $|z| < 1$ or, putting our "blinders" back on and just looking at f on the x axis, to the interval $|x| < 1$. Again, a detailed discussion must wait until Part II.

Having discussed both power series and Taylor series, we point out (without proving it) the following fundamental connection: namely, that *every power series with nonzero radius of convergence is the Taylor series of its sum function.* Suppose that we have

$$\sum_0^\infty a_n(x - a)^n = \sum_0^\infty b_n(x - a)^n \tag{2.33}$$

over some common interval of convergence, say $|x - a| < R$; that is, the two series converge to the same sum function, say $f(x)$, over that interval. Then the previous statement (italics) implies that $a_n = f^{(n)}(a)/n!$ and that $b_n = f^{(n)}(a)/n!$, so that $a_n = b_n$. We rely on this important result quite often—in the power series solution of differential equations, for instance. It is stated below as a theorem for reference.

THEOREM 2.13. Equation (2.33) holds over some common interval of convergence $|x - a| < R$ if and only if $a_n = b_n$ for all n.

COROLLARY.

$$\sum_0^\infty a_n(x - a)^n = 0 \tag{2.34}$$

over $|x - a| < R$ if and only if all the a_n's $= 0$.

Let us close the present discussion with an elementary look at (2.30). Basically, the problem is one of extrapolation: given data at some point $x = a$—namely, the values of f and all its derivatives—can we predict what f will be at some other point x? The first partial sum provides the simplest extrapolation, simply $f(x) = f(a)$. The second and third partial sums provide tangent-line and parabolic fits and so on (Exercise 2.25).