Initial-Value Problems for Ordinary Differential Equations

CONTENTS

7.1	Euler'	's Method	177
	7.1.1	Euler's Explicit Method	177
	7.1.2	Euler's Implicit Method	179
	7.1.3	Trapezoidal method	180
	7.1.4	Modified Euler's Method	180
	7.1.5	Global Truncation Error	182
7.2	Runge-Kutta Methods		
	7.2.1	Second-order Runge-Kutta Methods	184
	7.2.2	High-order Runge-Kutta method	186
	7.2.3	Implicit Runge-Kutta Method	187
7.3	Stabil	ity and Convergence of One-step Method	188
7.4	Multis	tep Methods	190
	7.4.1	Adams Methods	191
	7.4.2	Taylor Methods	196
7.5	Exercis	se	200

Differential equations are used to model problems in science and engineering that involve the change of some variable with respect to another. Most of these problems require the solution of an initial-value problem, that is, the solution to a differential equation that satisfies a given initial condition.

In common real-life situations, the differential equation that models the problem is too complicated to solve exactly, and one of two approaches is taken to approximate the solution. The first approach is to modify the problem by simplifying the differential equation to one that can be solved exactly and then use the solution of the simplified equation to approximate the solution to the original problem. The other approach, which we will examine in this chapter, uses methods for approximating the solution of the original problem. This is the approach that is most commonly taken because the approximation methods give more accurate results and realistic error information.

The methods that we consider in this chapter do not produce a continuous approximation to the solution of the initial-value problem. Rather, approximations are found at certain specified, and often equally spaced points.

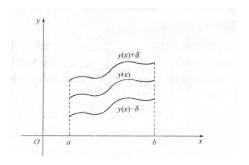


FIGURE 7.1

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We need some definitions and results from the theory of ordinary differential equations before considering methods for approximating the solutions to initial-value problems.

In this chapter, we consider the following initial-value problem

$$\begin{cases} y' = f(x,y) & (a \leqslant x \leqslant b) \\ y(a) = \eta \end{cases}$$
 (7.1)

Suppose Eq. (7.1) has a unique solution y(x) on [a,b] and y(x) is smooth enough on [a,b]. Let

$$D_{\delta} = \{(x, y) \mid a \leqslant x \leqslant b, y(x) - \delta \leqslant y \leqslant y(x) + \delta\}$$

$$(7.2)$$

which can be seen in Fig. 7.1.

Suppose f(x,y) and $\frac{\partial f(x,y)}{\partial y}$ are continuous on D_{δ} and let

$$M_0 = \max_{(x,y)\in D_{\delta}} |f(x,y)|, \quad M_1 = \max_{(x,y)\in D_{\partial}} \left| \frac{\partial f(x,y)}{\partial y} \right|. \tag{7.3}$$

A continuous approximation to the solution y(x) will not be obtained; instead, approximations to y will be generated at various values, called **mesh points**, in the interval [a, b]. Once the approximate solution is obtained at the points, the approximate solution at other points in the interval can be found by interpolation.

We first make the stipulation that the mesh points are equally distributed throughout the interval [a, b]. This condition is ensured by selecting the mesh points

$$a = x_0 < x_1 < \dots < x_i < x_{i+1} < \dots < x_n = b$$

The common distance between the points $h_i = x_{i+1} - x_i (0 \le i \le n-1)$ is called **step size**. For simplicity, equally-spaced points are considered, i.e.

$$x_i = a + ih \quad \left(0 \leqslant i \leqslant n, h = \frac{b - a}{n}\right).$$

Let y_i is an approximation to $y(x_i)$ $(i = 1, 2, \dots, n)$ and $y_0 = \eta$. If y_{i+1} is obtained from y_i , this method is called **one-step method**; If y_{i+1} is obtained by the r values of $y_i, y_{i+1}, \dots, y_{i-r+1}$, this is called r-step method.

7.1 Euler's Method

Euler's method is the most elementary approximation technique for solving initial-value problems. Although it is seldom used in practice, the simplicity of its derivation can be used to illustrate the techniques involved in the construction of some of the more advanced techniques, without the cumbersome algebra that accompanies these constructions.

7.1.1 Euler's Explicit Method

Integrating the Eq. (7.1) over the interval $[x_i, x_{i+1}]$, we have

$$\int_{x_i}^{x_{i+1}} y'(x) dx = \int_{x_i}^{x_{i+1}} f(x, y(x)) dx,$$

i.e.

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x)) dx.$$
 (7.4)

By left-side rectangle rule, there is

$$y(x_{i+1}) = y(x_i) + hf(x_i, y(x_i)) + R_{i+1}^{(1)},$$
(7.5)

where

$$R_{i+1}^{(1)} = \frac{1}{2} \frac{\mathrm{d}f(x, y(x))}{\mathrm{d}x} \bigg|_{x=\xi_i} h^2 = \frac{1}{2} y''(\xi_i) h^2 \quad (x_i < \xi_i < x_{i+1}).$$
 (7.6)

Neglecting $R_{i+1}^{(1)}$ in Eq. (7.5), then

$$y(x_{i+1}) \approx y(x_i) + hf(x_i, y(x_i)).$$
 (7.7)

Noting

$$y(x_0) = y(a) = \eta,$$

we obtain

$$y(x_{i+1}) \approx y(x_i) + hf(x_i, y(x_i)) \approx y_i + hf(x_i, y_i) \equiv y_{i+1}$$
.

Taking $y_0 = \eta$, we obtain Euler's method or Euler's explicit method

$$y_{i+1} = y_i + hf(x_i, y_i) \quad (i = 0, 1, \dots, n-1).$$
 (7.8)

The geometric interpretation of Euler's method can be seen in Fig. 7.2.

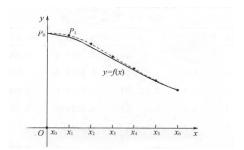


FIGURE 7.2

The geometric interpretation of Euler's method

TABLE 7.1 Computed results by Euler's method

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	i	x_i	y_i	$y\left(x_{i}\right)$	$\left y\left(x_{i}\right)-y_{i}\right $
Ī	1	0.1	1.000000	0.990099	0.009901
	2	0.2	0.980000	0.961538	0.018462
	3	0.3	0.941584	0.917431	0.024153
	4	0.4	0.888389	0.862069	0.026320
	5	0.5	0.825250	0.800000	0.025250
	6	0.6	0.757147	0.735294	0.021852
	7	0.7	0.688354	0.671141	0.017213
	8	0.8	0.622018	0.609756	0.012262
	9	0.9	0.560113	0.552486	0.007626
	10	1.0	0.503642	0.500000	0.003642
	11	1.1	0.452911	0.452489	0.000422
_	12	1.2	0.407783	0.409836	0.002053

Exercise 7.1. Apply Euler's method with h = 0.1 to approximate the solutions for the initial-value problem

$$\left\{ \begin{array}{ll} y'=-2xy^2 & (0\leqslant x\leqslant 1.2) \\ y(0)=1 \end{array} \right.$$

Solution The Euler's method is

$$\begin{cases} y_{i+1} = y_i - 2hx_iy_i^2 & (i = 0, 1, \dots, 11) \\ y_0 = 1 \end{cases}$$

where $x_i = 0.1i$. The computed results are listed in Table 7.1.

The initial-value problem has exact solution $y(x) = 1/(1+x^2)$. Table 7.1 shows the comparison between the approximate values at x_i and the actual values.

From Eq. (7.8), y_{i+1} can be obtained by y_i explicitly. So it is said one-step

explicit formula and can be expressed

$$\begin{cases} y_{i+1} = y_i + h\varphi(x_i, y_i, h) & (i = 0, 1, \dots, n-1), \\ y_0 = \eta. \end{cases}$$
 (7.9)

Generally,

$$y(x_{i+1}) \neq y(x_i) + h\varphi(x_i, y(x_i), h),$$

or

$$y(x_{i+1}) - [y(x_i) + h\varphi(x_i, y(x_i), h)] \neq 0.$$

Definition 41.

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\varphi(x_i, y(x_i), h)]$$

is said local truncation error or one-step error.

The local truncation error of Euler's method can be derived by Taylor's theorem

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + hf(x_i, y(x_i))]$$

$$= y(x_i) + hy'(x_i) + \frac{1}{2}h^2y''(\xi_i) - [y(x_i) + hy'(x_i)]$$

$$= \frac{1}{2}h^2y''(\xi_i) \quad (x_i < \xi_i < x_{i+1}).$$

7.1.2 Euler's Implicit Method

In Eq.(7.4), applying right-side rectangle rule, we have

$$y(x_{i+1}) = y(x_i) + hf(x_{i+1}, y(x_{i+1})) + R_{i+1}^{(2)},$$
(7.10)

where

$$R_{i+1}^{(2)} = -\frac{1}{2} \frac{\mathrm{d}f(x, y(x))}{\mathrm{d}x} \bigg|_{x=\xi_i} h^2 = -\frac{1}{2} y''(\xi_i) h^2 \quad (x_i < \xi_i < x_{i+1}). \quad (7.11)$$

Neglecting $R_{i+1}^{(2)}$ in Eq. (7.11) and using y_i and y_{i+1} to approximate $y(x_i)$ and $y(x_{i+1})$, we have

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1}) \quad (i = 0, 1, 2, \dots, n-1),$$
 (7.12)

which is called Euler's Implicit method.

And y_{i+1} is obtained implicitly by y_i . So it is called **one-step implicit method** which can be expressed

$$\begin{cases} y_{i+1} = y_i + h\psi(x_i, y_i, y_{i+1}, h) & (i = 0, 1, 2, \dots, n-1) \\ y_0 = \eta & \end{cases}$$
 (7.13)

180

In general,

$$y(x_{i+1}) \neq y(x_i) + h\psi(x_i, y(x_i), y(x_{i+1}), h),$$

or

$$y(x_{i+1}) - [y(x_i) + h\psi(x_i, y(x_i), y(x_{i+1}), h)] \neq 0.$$

Definition 42.

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\psi(x_i, y(x_i), y(x_{i+1}), h)]$$
(7.14)

is called local truncation error of Eq. (7.4).

The local truncation error of Euler's implicit method is

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + hf(x_{i+1}, y(x_{i+1}))] = R_{i+1}^{(2)}$$
$$= -\frac{1}{2}y''(\xi_i)h^2.$$

7.1.3 Trapezoidal method

Applying Trapezoidal rule, we have

$$y(x_{i+1}) = y(x_i) + \frac{h}{2} \left[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1})) \right] + R_{i+1}^{(3)}, \quad (7.15)$$

where

$$R_{i+1}^{(3)} = -\frac{h^3}{12} \frac{\mathrm{d}^2 f(x, y(x))}{\mathrm{d}x^2} \bigg|_{x=\xi_i} = -\frac{1}{12} y''(\xi_i) h^3 \quad (x_i < \xi_i < x_{i+1}). \quad (7.16)$$

Neglecting $R_{i+1}^{(3)}$ in Eq.(7.15) and using y_i, y_{i+1} to approximate $y(x_i)$ and $y(x_{i+1})$, we have

$$y_{i+1} = y_i + \frac{h}{2} [f(x_i, y_i) + f(x_{i+1}, y_{i+1})] \quad (i = 0, 1, \dots, n-1),$$
 (7.17)

which is called **Trapezoidal method**. The local truncation error is

$$R_{i+1} = y(x_{i+1}) - \left\{ y(x_i) + \frac{h}{2} \left[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1})) \right] \right\}$$

$$= R_{i+1}^{(3)} = -\frac{1}{12} y'''(\xi_i) h^3 \quad (x_i < \xi_i < x_{i+1}).$$
(7.18)

7.1.4 Modified Euler's Method

The local truncation error of Trapezoid method is proportion to h^3 , but the method is implicit. In practice, implicit methods are not used rather are used to improve approximations obtained by explicit methods. The combination of an explicit and implicit technique is called **predictor-corrector method**. The explicit method predicts an approximation, and the implicit method corrects this prediction. So $y(x_{i+1})$ in Trapezoid method is predicted by Euler's explicit method

$$y_i^{(p)} = y_i + hf(x_i, y_i).$$

Then

$$y_{i+1} = y_i + \frac{h}{2} \left[f(x_i, y_i) + f(x_{i+1}, y_i^{(p)}) \right],$$

i.e.

$$\begin{cases} y_i^{(p)} = y_i + h f(x_i, y_i) \\ y_{i+1} = y_i + \frac{h}{2} \left[f(x_i, y_i) + f\left(x_{i+1}, y_i^{(p)}\right) \right]. \end{cases}$$
 (7.19)

The above formula can be rewritten as

$$\begin{cases} y_{i+1}^{(p)} = y_i + hf(x_i, y_i) \\ y_{i+1}^{(c)} = y_i + hf(x_{i+1}, y_{i+1}^{(p)}) \\ y_{i+1} = \frac{1}{2} (y_{i+1}^{(p)} + y_{i+1}^{(c)}) \end{cases}$$
(7.20)

which is called Modified Euler's Method.

Exercise 7.2. Use modified Euler's method with h = 0.1 to approximate the solutions for the problem in Example 7.1.

Solution The computed results by modified Euler's method are listed in Table 7.2. Compared with the Example 7.1, modified Euler's method is more accuracy than Euler's method.

Modified Euler's method can also be expressed in the form

$$y_{i+1} = y_i + \frac{h}{2} [f(x_i, y_i) + f(x_{i+1}, y_i + hf(x_i, y_i))],$$
 (7.21)

or

$$\begin{cases} y_{i+1} = y_i + \frac{h}{2} (k_1 + k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_{i+1}, y_i + hk_1) \end{cases}$$
 (7.22)

TABLE 7.2
The computed results by modified Euler's method

\overline{i}	x_i	y_i	$y_i^{(ho)}$	$y_{i+1}^{(c)}$	$ y\left(x_{i}\right)-y_{i} $
0	0.0	1.000000	1.000000	0.980000	0.000000
1	0.1	0.990000	0.970398	0.952333	0.000099
2	0.2	0.961366	0.924397	0.910095	0.000173
3	0.3	0.917246	0.866765	0.857143	0.000185
4	0.4	0.861954	0.802517	0.797551	0.000115
5	0.5	0.800034	0.736029	0.735025	0.000034
6	0.6	0.735527	0.670607	0.672567	0.000233
7	0.7	0.671587	0.608443	0.612355	0.000446
8	0.8	0.610399	0.550785	0.555793	0.000643
9	0.9	0.553289	0.498186	0.503651	0.000803
10	1.0	0.500919	0.450735	0.456223	0.000919
11	1.1	0.453479	0.408237	0.413481	0.000990
12	1.2	0.410859			0.001023

So it is one-step explicit method and the local truncation error is

$$R_{i+1} = y(x_{i+1}) - y(x_i) - \frac{h}{2} [f(x_i, y(x_i)) + f(x_{i+1}, y(x_i) + hf(x_i, y(x_i)))]$$

$$= y(x_{i+1}) - y(x_i) - \frac{h}{2} [f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))]$$

$$+ \frac{h}{2} [f(x_{i+1}, y(x_{i+1})) - f(x_{i+1}, y(x_i) + hf(x_i, y(x_i)))].$$
(7.23)

Since Eqs. (7.15) and (7.16), there is

$$y(x_{i+1}) - y(x_i) - \frac{h}{2} [f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))] = -\frac{1}{12} y'''(\xi_i) h^3$$

where $x_i < \xi_i < x_{i+1}$. From Eqs. (7.5) and (7.6), we have

$$f(x_{i+1}, y(x_{i+1})) - f(x_{i+1}, y(x_i) + hf(x_i, y(x_i)))$$
 (7.24)

$$= \frac{\partial f(x_{i+1}, \eta_{i+1})}{\partial y} [y(x_{i+1}) - y(x_i) - hf(x_i, y(x_i))]$$
 (7.25)

$$= \frac{1}{2} \frac{\partial f(x_{i+1}, \eta_{i+1})}{\partial y} y''\left(\widetilde{\xi}_i\right) h^2$$
(7.26)

where $x_i < \xi_i < x_{i+1}, \eta_{i+1}$ is between $y(x_{i+1})$ and $y(x_i) + hf(x_i, y(x_i))$. Then the local truncation error is

$$R_{i+1} = \left[-\frac{1}{12} y'''(\xi_i) + \frac{1}{4} \frac{\partial f(x_{i+1}, \eta_{i+1})}{\partial y} y''(\xi_i) \right] h^3.$$
 (7.27)

7.1.5 Global Truncation Error

The values of the approximations y_1, y_2, \dots, y_n , are related with step size h, so we let

$$y_1^{[h]}, y_2^{[h]}, \cdots, y_n^{[h]}.$$

To be precise, let us define

$$\left| y\left(x_{i}\right) -y_{i}^{\left[h\right] }\right| \quad \left(i=1,2,\cdots,n\right)$$

Definition 43. Suppose $y_1^{[h]}, y_2^{[h]}, \dots, y_n^{[h]}$ are approximations to $y(x_1), y(x_2), \dots, y(x_n)$ which are the values of the solutions for Eq. (7.1) on mesh nodes. The global truncation error is defined

$$E(h) = \max_{1 \le i \le n} \left| y(x_i) - y_i^{[h]} \right|. \tag{7.28}$$

The method is said to be convergent if

$$\lim_{h \to 0} E(h) = 0$$

Under some conditions, if the local truncation error is $O(h^{p+1})$, the global truncation error is $O(h^p)$.

Definition 44. The numerical method has **order p** if the local truncation error $R_{i+1} = O(h^{p+1})$.

So Euler's explicit and implicit methods have order 1 and the Trapezoidal method and modified Euler's method have order 2.

7.2 Runge-Kutta Methods

In Eq. (7.4), by Mean Value Theorem for Integrals, we have

$$y(x_{i+1}) = y(x_i) + hf(x_i + \theta h, y(x_i + \theta h)).$$
 (7.29)

where $0 \le \theta \le 1$. Denote

$$k^* = f(x_i + \theta h, yx_i + \theta h).$$

Thus it is important to construct an approximation to k^* . From this view, if $k^* \approx f(x_i, y_i)$, it is the Euler's method. The modified Euler's method can be constructed by $k^* \approx (k_1 + k_2)/2$, where $k_1 = f(x_i, y_i)$ and $k_2 = f(x_{i+1}, y_i + hk_1)$.

So the numerical solver is called Runge-Kutta methods defined by

$$\begin{cases} y_{i+1} = y_i + h \sum_{j=1}^{r} \alpha_j k_j \\ k_1 = f(x_i, y_i) \\ k_j = f\left(x_i + \lambda_j h, y_i + h \sum_{l=1}^{j-1} \mu_{jl} k_l\right) & (j = 2, 3, \dots, r) \end{cases}$$
 (7.30)

where α_j, λ_j and μ_{jl} are constants to be determined. The local truncation error of Eq. (7.30) is

$$R_{i+1} = y(x_{i+1}) - y(x_i) - h \sum_{j=1}^{r} \alpha_j K_j,$$
 (7.31)

where

$$K_{1} = f(x_{i}, y(x_{i})),$$

 $K_{j} = f\left(x_{i} + \lambda_{j}h, y(x_{i}) + h\sum_{l=1}^{j-1} \mu_{jl}K_{l}\right) \quad (j = 2, 3, \dots, r).$

By Taylor's Theorem, the local truncation error becomes

$$R_{i+1} = c_0 + c_1 h + \dots + c_p h^p + c_{p+1} h^{p+1} + \dots$$
 (7.32)

Choose α_j, λ_j and μ_{jl} , such that $c_0 = 0, c_1 = 0, \dots, c_p = 0$ while $c_{p+1} \neq 0$, then the Runge-Kutta method has order p. If r = 1, take $\alpha_1 = 1$, i.e.

$$y_{i+1} = y_i + hf(x_i, y_i).$$

It is just Euler's method.

Next we will give some useful formulas

$$y'(x) = f(x, y(x)), \qquad (7.33)$$

$$y''(x) = \frac{\partial f(x, y(x))}{\partial x} + y'(x) \frac{\partial f(x, y(x))}{\partial y}, \qquad (7.34)$$

$$y'''(x) = \frac{\partial^2 f(x, y(x))}{\partial x^2} + 2y'(x) \frac{\partial^2 f(x, y(x))}{\partial x \partial y} + (y'(x))^2 \frac{\partial^2 f(x, y(x))}{\partial y^2} + y''(x) \frac{\partial f(x, y(x))}{\partial y}, \qquad (7.35)$$

$$y^{(4)}(x) = \frac{\partial^3 f(x, y(x))}{\partial x^3} + 3y'(x) \frac{\partial^3 f(x, y(x))}{\partial x^2 \partial y} + 3(y'(x))^2 \frac{\partial^3 f(x, y(x))}{\partial x \partial y^2} + (y'(x))^3 \frac{\partial^3 f(x, y(x))}{\partial y^3} + 3y''(x) \frac{\partial^2 f(x, y(x))}{\partial x \partial y} + 3y'(x) \frac{\partial^2 f(x, y(x))}{\partial x \partial y}. \qquad (7.36)$$

7.2.1 Second-order Runge-Kutta Methods

If r = 2, Runge-Kutta method is

$$\begin{cases} y_{i+1} = y_i + h (\alpha_1 k_1 + \alpha_2 k_2) \\ k_1 = f (x_i, y_i) \\ k_2 = f (x_i + \lambda_2 h, y_i + h \mu_{21} k_1) \end{cases}$$
(7.37)

and the local truncation error is

$$\begin{cases}
R_{i+1} = y(x_{i+1}) - y(x_i) - h(\alpha_1 K_1 + \alpha_2 K_2) \\
K_1 = f(x_i, y(x_i)) \\
K_2 = f(x_i + \lambda_2 h, y(x_i) + h\mu_{21} K_1)
\end{cases} (7.38)$$

Taking

$$\begin{split} K_{1} &= f\left(x_{i}, y\left(x_{i}\right)\right) = y'\left(x_{i}\right), \\ K_{2} &= f\left(x_{i} + \lambda_{2}h, y\left(x_{i}\right) + h_{\mu 21}y'\left(x_{i}\right)\right) \\ &= f\left(x_{i}, y\left(x_{i}\right)\right) + \left(\lambda_{2}h\frac{\partial}{\partial x} + h\mu_{21}y'\left(x_{i}\right)\frac{\partial}{\partial y}\right)f\left(x_{i}, y\left(x_{i}\right)\right) \\ &+ \frac{1}{2}\left(\lambda_{2}h\frac{\partial}{\partial x} + h\mu_{21}y'\left(x_{i}\right)\frac{\partial}{\partial y}\right)^{2}f\left(x_{i}, y\left(x_{i}\right)\right) + O\left(h^{3}\right), \end{split}$$

into Eq. (7.38), and by Taylor's theorem and Eqs. (7.33),(7.34),(7.35), we have

$$R_{i+1} = hy'(x_i) + \frac{h^2}{2}y''(x_i) + \frac{1}{6}h^3y'''(x_i) + O(h^4) - h\alpha_1y'(x_i)$$

$$- h\alpha_2 \left[y'(x_i) + \lambda_2 h \frac{\partial f(x_i, y(x_i))}{\partial x} + h\mu_{21}y'(x_i) \frac{\partial f(x_i, y(x_i))}{\partial y} + \frac{1}{2}h^2 \left(\lambda_2 \frac{\partial}{\partial x} + \mu_{21}y'(x_i) \frac{\partial}{\partial y} \right)^2 f(x_i, y(x_i)) + O(h^3) \right]$$

$$= h(1 - \alpha_1 - \alpha_2)y'(x_i)$$

$$+ h^2 \left[\left(\frac{1}{2} - \alpha_2 \lambda_2 \right) \frac{\partial f(x_i, y(x_i))}{\partial x} + \left(\frac{1}{2} - \alpha_2 \mu_{21} \right) y'(x_i) \frac{\partial f(x_i, y(x_i))}{\partial y} \right]$$

$$+ h^3 \left[\frac{1}{6}y'''(x_i) - \frac{1}{2}\alpha_2 \left(\lambda_2 \frac{\partial}{\partial x} + \mu_{21}y'(x_i) \frac{\partial}{\partial y} \right)^2 f(x_i, y(x_i)) \right] + O(h^4)$$

For any function f, Eq. (7.37) has order two if and only if $\alpha_1, \alpha_2, \lambda_2$ and μ_{21} satisfy

$$\begin{cases} 1 - \alpha_1 - \alpha_2 = 0, \\ \frac{1}{2} - \alpha_2 \lambda_2 = 0, \\ \frac{1}{2} - \alpha_2 \mu_{21} = 0 \end{cases}$$

i.e.

$$\begin{cases} \alpha_1 + \alpha_2 = 1, \\ \alpha_2 \lambda_2 = \frac{1}{2}, \\ \alpha_2 \mu_{21} = \frac{1}{2} \end{cases}$$

The solutions of the above equation can be expressed

$$\begin{cases} \alpha_1 = 1 - \alpha_2 \\ \lambda_2 = \frac{1}{2\alpha_2}, \quad (\alpha_2 \neq 0) \\ \mu_{21} = \frac{1}{2\alpha_2} \end{cases}$$

Then the second-order Runge-Kutta method is

$$\begin{cases} y_{i+1} = y_i + h \left[(1 - \alpha_2) k_1 + \alpha_2 k_2 \right] \\ k_1 = f \left(x_i, y_i \right) \\ k_2 = f \left(x_i + \frac{1}{2\alpha_2} h, y_i + \frac{1}{2\alpha_2} h k_1 \right) \end{cases}$$
(7.39)

and the local truncation error is

$$R_{i+1} = \left[\left(\frac{1}{6} - \frac{1}{8\alpha_2} \right) y'''(x_i) + \frac{1}{8\alpha_2} y''(x_i) \frac{\partial f(x_i, y(x_i))}{\partial y} \right] h^3 + O(h^4).$$

If $\alpha_2 = \frac{1}{2}$, then

$$\begin{cases} y_{i+1} = y_i + \frac{h}{2} (k_1 + k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + h, y_i + hk_1) \end{cases}$$

or

$$y_{i+1} = y_i + \frac{h}{2} \left[f(x_i, y_i) + f(x_{i+1}, y_i + hf(x_i, y_i)) \right].$$

This is modified Euler's method.

If $\alpha_2 = 1$, then

$$\begin{cases} y_{i+1} = y_i + hk_2 \\ k_1 = f(x_i, y_i) \\ k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1\right) \end{cases}$$

or

$$y_{i+1} = y_i + hf\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hf(x_i, y_i)\right).$$

If $\alpha_2 = \frac{3}{4}$, then

$$\begin{cases} y_{i+1} = y_i + \frac{h}{4} (k_1 + 3k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f\left(x_i + \frac{2}{3}h, y_i + \frac{2}{3}hk_1\right) \end{cases}$$

or

$$y_{i+1} = y_i + \frac{h}{4} \left[f(x_i, y_i) + 3f\left(x_i + \frac{2}{3}h, y_i + \frac{2}{3}hf(x_i, y_i)\right) \right].$$

7.2.2 High-order Runge-Kutta method

Similarly as the above derivation, two commonly used third-order Runge-Kutta methods are Heun's method and Kutta's method

$$\begin{cases} y_{i+1} = y_i + \frac{h}{4}(k_1 + 3k_3) \\ k_1 = f(x_i, y_i) \\ k_2 = f\left(x_i + \frac{1}{3}h, y_i + \frac{1}{3}hk_1\right) \\ k_3 = f\left(x_i + \frac{2}{3}h, y_i + \frac{2}{3}hk_2\right) \end{cases}$$

$$\begin{cases} y_{i+1} = y_i + \frac{h}{6}(k_1 + 4k_2 + k_3) \\ k_1 = f(x_i, y_i) \\ k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1\right) \\ k_3 = f(x_i + h, y_i - hk_1 + 2hk_2) \end{cases}$$

And two Runge-Kutta methods of order four are RK_4 method and Gill's method:

$$\begin{cases} y_{i+1} = y_i + \frac{h}{6} \left(k_1 + 2k_2 + 2k_3 + k_4 \right) \\ k_1 = f \left(x_i, y_i \right) \\ k_2 = f \left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1 \right) \\ k_3 = f \left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_2 \right) \\ k_4 = f \left(x_i + h, y_i + hk_3 \right) \end{cases}$$

$$\begin{cases} y_{i+1} = y_i + \frac{h}{6} \left[k_1 + (2 - \sqrt{2})k_2 + (2 + \sqrt{2})k_3 + k_4 \right] \\ k_1 = f \left(x_i, y_i \right) \\ k_2 = f \left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_1 \right) \\ k_3 = f \left(x_i + \frac{h}{2}, y_i + \frac{\sqrt{2}-1}{2}hk_1 + \left(1 - \frac{\sqrt{2}}{2} \right)hk_2 \right) \\ k_4 = f \left(x_i + h, y_i - \frac{\sqrt{2}}{2}hk_2 + \left(1 + \frac{\sqrt{2}}{2} \right)hk_3 \right) \end{cases}$$

RK4 method is the most common used method.

Let $p^*(r)$ be the highest order of Runge-Kutta method. Butcher found the relation between r and $p^*(r)$ in 1965:

Exercise 7.3. Apply RK4 method with h = 0.1 to approximate the solutions for the initial-value problem in Example 7.1.

Soltion The RK₄ method is

$$\begin{cases} y_{i+1} = y_i + \frac{h}{6} \left(k_1 + 2k_2 + 2k_3 + 2k_4 \right) \\ k_1 = -2x_i y_i^2 \\ k_2 = -2 \left(x_i + \frac{h}{2} \right) \left(y_i + \frac{h}{2} k_1 \right)^2, \quad (i = 0, 1, \dots, 11) \\ k_3 = -2 \left(x_i + \frac{h}{2} \right) \left(y_i + \frac{h}{2} k_2 \right)^2 \\ k_4 = -2x_{i+1} \left(y_i + hk_3 \right)^2 \end{cases}$$

The computing results are listed in Table 7.3.

TABLE 7.3 The computing results by RK₄

~		•		
	$\overline{x_i}$	y_i	$y\left(x_{i}\right)$	$y\left(x_{i}\right)-y_{i}$
	0.0	1.000000	1.000000	0.000000
	0.1	0.990099	0.990099	0.000000
	0.2	0.961538	0.961538	0.000000
	0.3	0.917431	0.971431	0.000001
	0.4	0.862068	0.862069	0.000001
	0.5	0.799999	0.800000	0.000001
	0.6	0.735294	0.735294	0.000001
	0.7	0.671141	0.671141	0.000000
	0.8	0.609756	0.609756	0.000000
	0.9	0.552487	0.552486	0.000000
	1.0	0.500001	0.500000	0.000001
	1.1	0.452489	0.452489	0.000001
	1.2	0.409837	0.409836	0.000001

7.2.3 Implicit Runge-Kutta Method

In the above section, the Runge-Kutta is explicit. As we know, the implicit method is of better stability. So the implicit Runge-Kutta method is also used for the stiff problem. The commonly used second-order, fourth-order and sixth-order methods are as follows

$$(1) \begin{cases} y_{i+1} = y_i + hk_1 \\ k_1 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1h\right), \end{cases}$$

$$(2) \begin{cases} y_{i+1} = y_i + \frac{h}{2}\left(k_1 + k_2\right) \\ k_1 = f\left(x_i + \frac{3-\sqrt{3}}{6}h, y_i + \frac{1}{4}k_1h + \frac{3-2\sqrt{3}}{12}k_2h\right) \\ k_2 = f\left(x_i + \frac{3+\sqrt{3}}{6}h, y_i + \frac{3+2\sqrt{3}}{12}k_1h + \frac{1}{4}k_2h\right) \end{cases}$$

$$(3) \begin{cases} y_{i+1} = y_i + \frac{h}{18} \left(5k_1 + 8k_2 + 5k_3 \right) \\ k_1 = f \left(x_i + \frac{5 - \sqrt{15}}{10} h, y_i + \left(\frac{5}{36} k_1 + \frac{10 - 3\sqrt{15}}{45} k_2 + \frac{25 - 6\sqrt{15}}{180} k_3 \right) h \right), \\ k_2 = f \left(x_i + \frac{1}{2} h, y_i + \left(\frac{10 + 3\sqrt{15}}{72} k_1 + \frac{2}{9} k_2 + \frac{10 - 3\sqrt{15}}{72} k_3 \right) h \right) \\ k_3 = f \left(x_i + \frac{5 + \sqrt{15}}{10} h, y_i + \left(\frac{25 + 6\sqrt{15}}{180} k_1 + \frac{10 + 3\sqrt{15}}{45} k_2 + \frac{5}{36} k_3 \right) h \right) \end{cases}$$

7.3 Stability and Convergence of One-step Method

Suppose the initial-value problem

$$\begin{cases} y' = f(x, y) & (a \leqslant x \leqslant b) \\ y(a) = \eta \end{cases}$$
 (7.40)

is approximated by a one-step difference method in the form

$$\begin{cases} y_{i+1} = y_i + h\varphi(x_i, y_i, h) & (i = 0, 1, \dots, n-1) \\ y_0 = \eta & \end{cases}$$
 (7.41)

The local truncation error is

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\varphi(x_i, y(x_i), h)] \quad (i = 0, 1, \dots, n-1).$$
 (7.42)

Definition 45. A one-step difference-equation method with local truncation error $R_{i+1}(h)$ at the ith step is said to be **consistent** with the differential equation it approximates if

$$\lim_{h \to 0} R_{i+1}(h) = 0.$$

Theorem 47. Suppose y(x) is the solution of Eqs. (7.40) and $\{y_i\}_{i=0}^n$ is the solution of Eq. (7.41). If

 1° the constant c_0 exists with

$$|R_{i+1}| \le c_0 h^{p+1} \quad (i = 0, 1, 2, \dots, n-1);$$
 (7.43)

 2° the constant $h_0 > 0$ exists with

$$\max_{\substack{(x,y)\in D_{\delta}\\0\leqslant h\leqslant h_0}} \left| \frac{\partial \varphi(x,y,h)}{\partial y} \right| \leqslant L \tag{7.44}$$

where D_{δ} is defined in Eq. (7.2);

$$E(h) \leqslant ch^p, \tag{7.45}$$

when $h \leqslant \min \left\{ h_0, \sqrt[p]{\frac{\delta}{c}} \right\}$ where $c = \frac{c_0}{L} \left[e^{L(b-a)} - 1 \right]$.

(1) For Euler's method, $\varphi(x, y, h) = f(x, y)$, and

$$\max_{\substack{(x,y)\in D_{\delta}\\0\leq h\leq h_0}}\left|\frac{\partial \varphi(x,y,h)}{\partial y}\right|=\max_{(x,y)\in D_{\delta}}\left|\frac{\partial f(x,y)}{\partial y}\right|=M_1\equiv L.$$

(2) For modified Euler's method,

$$\begin{split} \varphi(x,y,h) &= \frac{1}{2}[f(x,y) + f(x+h,y+hf(x,y))], \\ \left| \frac{\partial \varphi(x,y,h)}{\partial y} \right| &= \frac{1}{2} \left[\frac{\partial f(x,y)}{\partial y} + \frac{\partial f(x+h,y+hf(x,y))}{\partial y} \left(1 + h \frac{\partial f(x,y)}{\partial y} \right) \right]. \end{split}$$

Let $h_0 = \frac{\delta}{4M_0} (M_0$ defined in Eq. (7.3)), there is

$$\max_{(x,y)\in D_{\delta/2}} \left| \frac{\partial \varphi(x,y,h)}{\partial y} \right| \leqslant \frac{1}{2} \left\{ \max_{\substack{(x,y)\in D_{\delta/2} \\ 0\leqslant h\leqslant h_0}} \left| \frac{\partial f(x,y)}{\partial y} \right| + \max_{\substack{(x,y)\in D_{\delta/2} \\ 0\leqslant h\leqslant h_0}} \left| \frac{\partial f(x+h,y+hf(x,y))}{\partial y} \right| \right\} \\
\cdot \left(1 + h \max_{(x,y)\in D_{\delta/2}} \left| \frac{\partial f(x,y)}{\partial y} \right| \right) \right\} \\
\leqslant \frac{1}{2} \left[M_1 + M_1 \left(1 + h M_1 \right) \right] \leqslant M_1 \left(1 + \frac{h_0}{2} M_1 \right) \equiv L$$

when $h \leq h_0$.

7.4 Multistep Methods

The methods discussed to this point in the chapter are called one-step methods because the approximation for the mesh point x_{i+1} involves information from only one of the previous mesh points, x_i . Although these methods might use function evaluation information at points between x_i and x_{i+1} , they do not retain that information for direct use in future approximations. All the information used by these methods is obtained within the subinterval over which the solution is being approximated.

The approximate solution is available at each of the mesh points x_0, x_1, \dots, x_i before the approximation at x_{i+1} is obtained, and because the error $|y_i - y(x_i)|$ tends to increase with i, so it seems reasonable to develop methods that use these more accurate previous data when approximating the solution at x_{i+1} .

Methods using the approximation at more than one previous mesh point to determine the approximation at the next point are called **multistep methods**

An **k-step multistep method** for solving the initial-value problem has a difference equation for finding the approximation y_{i+1} at the mesh point x_{i+1} represented by the following equation, where a k is an integer greater than 1:

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}), \qquad (7.46)$$

where a_j, b_j are independent with j and $|a_{k-1}| + |b_{k-1}| \neq 0$. When $b_{-1} = 0$, the method is called **explicit**, or **open**, because Eq. (7.46) then gives y_{i+1} explicitly in terms of previously determined values. When $b_{-1} \neq 0$, the method is called **implicit** or **closed**, because y_{i+1} occurs on both sides of Eq. (7.46), so y_{i+1} is specified only implicitly. If $k = 1, a_0 = b_0 = 1, b_{-1} = 0$, it is Euler's method; If $k = 1, a_0 = 1, b_0 = b_{-1} = \frac{1}{2}$, it is Trapezoidal method.

The local truncation error is

$$R_{i+1} = y\left(x_{i+1}\right) - \left[\sum_{j=0}^{k-1} a_j y\left(x_{i-j}\right) + h \sum_{j=-1}^{k-1} b_j f\left(x_{i-j}, y\left(x_{i-j}\right)\right)\right].$$

The method (7.46) has order p if

$$R_{i+1} = O\left(h^{p+1}\right).$$

By y'(x) = f(x, y(x)), the local truncation error can be expressed

$$R_{i+1} = y(x_{i+1}) - \left[\sum_{j=0}^{k-1} a_j y(x_{i-j}) + h \sum_{j=-1}^{k-1} b_j y'(x_{i-j}) \right].$$

In computation, $y_0 = \eta$, and y_1, y_2, \dots, y_{k-1} is given by the same order methods.

7.4.1 Adams Methods

Integrating the equation over the interval $[x_i, x_{i+1}]$

$$y' = f(x, y),$$

we have

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x)) dx.$$
 (7.47)

The function f(x, y(x)) is approximated by the interpolating polynomial of degree r about the nodes $x_i, x_{i-1}, \dots, x_{i-r}$. Then

$$f(x,y(x)) = \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \prod_{\substack{l=0\\l\neq j}}^{r} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}$$

$$+ \frac{1}{(r+1)!} \frac{d^{r+1} f(x, y(x))}{dx^{r+1}} \Big|_{x=\eta_i} \prod_{j=0}^{r} (x - x_{i-j})$$

$$= \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \prod_{\substack{l=0\\l\neq j}}^{r} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}$$

$$+ \frac{1}{(r+1)!} y^{(r+2)} (\eta_i) \prod_{j=0}^{r} (x - x_{i-j})$$

$$(7.48)$$

192

where

$$\eta_i = \eta_i(x) \in (\min\{x, x_{i-r}\}, \max\{x, x_i\}).$$

Taking Eq. (7.48) to Eq. (7.47) and letting $x = x_i + th$, there is

$$y(x_{i+1}) = y(x_i) + \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{\substack{l=0 \ l \neq j}}^{r} \frac{x - x_{i-l}}{x_i - x_{i-l}} dx$$

$$+ \frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)} (\eta_i) \prod_{j=0}^{r} (x - x_{i-j}) dx$$

$$= y(x_i) + h \sum_{j=0}^{r} f(x_{i-j}, y(x_i)) \int_{0}^{1} \prod_{\substack{l=0 \ l \neq j}}^{r} \frac{l+t}{l-j} dt$$

$$+ h^{r+2} y^{(r+2)} (\xi_i) \frac{1}{(r+1)!} \int_{0}^{1} \prod_{j=0}^{r} (j+t) dt,$$

where $\xi_{i-r} \in (x_i, x_{i+1})$.

Let

$$\begin{cases}
\beta_{rj} = \int_0^1 \prod_{\substack{l=0 \ l \neq j}}^r \frac{l+t}{l-j} dt & (j=0,1,\dots,r) \\
\alpha_{r+1} = \frac{1}{(r+1)!} \int_0^1 \prod_{j=0}^r (j+t) dt
\end{cases}$$
(7.49)

then

$$y(x_{i+1}) = y(x_i) + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j})) + \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i).$$

Neglecting $\alpha_{r+1}h^{r+2}y^{(r+2)}(\xi_i)$, and using y_i to approximate $y(x_i)$, the (r+1)-step method is constructed

$$y_{i+1} = y_i + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y_{i-j}).$$
 (7.50)

and the local truncation error of (7.50) is

$$R_{i+1} = y(x_{i+1}) - \left[y(x_i) + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j})) \right]$$
$$= \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i).$$

which is called (r+1)-step explicit Adams method. From the above equation, the (r+1)-step Adams explicit method has order (r+1).

When r = 0, it is Euler's method

$$y_{i+1} = y_i + hf(x_i, y_i)$$
 (7.51)

$$R_{i+1} = \frac{1}{2}h^2y''(\xi_i), \quad \xi_i \in (x_i, x_{i+1}).$$
 (7.52)

When r = 1, it is

$$y_{i+1} = y_i + \frac{h}{2} \left[3f(x_i, y_i) - f(x_{i-1}, y_{i-1}) \right]$$
 (7.53)

$$R_{i+1} = \frac{5}{12} h^3 y^{(3)}(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1})$$
 (7.54)

When r=2, that is

$$y_{i+1} = y_i + \frac{h}{12} \left[23f(x_i, y_i) - 16f(x_{i-1}, y_{i-1}) + 5f(x_{i-2}, y_{i-2}) \right]$$
 (7.55)

$$R_{i+1} = \frac{3}{8} h^4 y^{(4)}(\xi_i), \quad \xi_i \in (x_{i-2}, x_{i+1})$$
 (7.56)

When r = 3, it is an explicit four-step method known as the **fourth-order** Adams-Bashforth technique (AB4)

$$y_{i+1} = y_i + \frac{h}{24} \left[55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1}) + 37f(x_{i-2}, y_{i-2}) - 9f(x_{i-3}, y_{i-3}) \right]$$
(7.57)

$$R_{i+1} = \frac{251}{720} h^5 y^{(5)}(\xi_i), \quad \xi_i \in (x_{i-3}, x_{i-r+1}).$$
(7.58)

If we use the interpolating polynomial of degree r to approximate f(x, y(x)) about distinct nodes $x_{i+1}, x_i, \dots, x_{i+1}$, then

$$f(x,y(x)) = \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \prod_{\substack{l=-1\\l\neq j}}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}$$

$$+ \frac{1}{(r+1)!} \frac{d^{r+1} f(x, y(x))}{dx^{r+1}} \Big|_{x=\bar{\eta}_i} \prod_{\substack{l=-1\\l\neq j}}^{r-1} (x - x_{i-j})$$

$$= \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \prod_{\substack{l=-1\\l\neq j}}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}}$$

$$+ \frac{1}{(r+1)!} y^{(r+2)} (\bar{\eta}_i) \prod_{j=-1}^{r-1} (x - x_{i-j})$$

$$(7.59)$$

where $\bar{\eta}_i = \bar{\eta}_i(x) \in (\min\{x, x_{i-r+1}\}, \max\{x, x_{i+1}\})$. Similarly as the above

derivation, we have

$$y(x_{i+1}) = y(x_i) + \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{\substack{l=-1\\l\neq j}}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - x_{i-l}} dx$$

$$+ \frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)} (\bar{\eta}_i) \prod_{j=-1}^{r-1} (x - x_{i-j}) dx$$

$$= y(x_i) + h \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \int_0^1 \prod_{\substack{l=-1\\l\neq j}}^{r-1} \frac{l+t}{l-j} dt$$

$$+ h^{r+2} y^{(r+2)} (\bar{\xi}_i) \frac{1}{(r+1)!} \int_0^1 \prod_{j=-1}^{r-1} (j+t) dt,$$

where $\bar{\xi}_i \in (x_{i-r+1}, x_{i+1})$. Let

$$\begin{cases} \bar{\beta}_{r,j} = \int_0^1 \prod_{\substack{l=-1\\l\neq j}}^{r-1} \frac{l+t}{l-j} dt & (j=-1,0,1,\cdots,r-1) \\ \bar{\alpha}_{r+1} = \frac{1}{(r+1)!} \int_0^1 \prod_{j=-1}^{-1} (j+t) dt \end{cases}$$

Then

$$y(x_{i+1}) = y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y(x_{i-j})) + \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)} (\bar{\xi}_i).$$
(7.60)

Neglecting $\bar{\alpha}_{r+1}h^{r+2}y^{(r+2)}\left(\bar{\xi}_{i}\right)$, and using y_{i} to approximate $y\left(x_{i}\right)$, we have the r-step method

$$y_{i+1} = y_i + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y_{i-j}), \qquad (7.61)$$

and the local truncation error is

$$R_{i+1} = y(x_{i+1}) - \left[y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y(x_{i-j})) \right]$$
$$= \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)} (\bar{\xi}_i)$$

which is called r-step Adams implicit method and it has order (r + 1). When r = 1, it is Trapezoidal method

$$y_{i+1} = y_i + \frac{h}{2} \left[f(x_{i+1}, y_{i+1}) + f(x_i, y_i) \right]$$
 (7.62)

$$R_{i+1} = -\frac{1}{12}h^3y'''(\bar{\xi}_i), \quad \bar{\xi}_i \in (x_i, x_{i+1})$$
 (7.63)

When r=2, it is

$$y_{i+1} = y_i + \frac{h}{12} \left[5f(x_{i+1}, y_{i+1}) + 8f(x_i, y_i) - f(x_{i-1}, y_{i-1}) \right]$$
 (7.64)

$$R_{i+1} = -\frac{1}{24} h^4 y^{(4)} \left(\bar{\xi}_i\right), \quad \bar{\xi}_i \in (x_{i-1}, x_{i+1})$$
 (7.65)

When r = 3, that is an implicit three-step method known as the **fourth-order Adams-Moulton technique** (AM4)

$$y_{i+1} = y_i + \frac{h}{24} \left[9f(x_{i+1}, y_{i+1}) + 19f(x_i, y_i) - 5f(x_{i-1}, y_{i-1}) + f(x_{i-2}, y_{i-2}) \right]$$
(7.66)

$$R_{i+1} = -\frac{19}{720} h^5 y^{(5)} \left(\bar{\xi}_i\right), \quad \bar{\xi}_i \in (x_{i-2}, x_{i+1})$$
(7.67)

The predictor-corrector method of AB₄ and AM₄ is

$$\begin{cases} y_{i}^{(p)} = y_{i} + \frac{h}{24} \left[55f\left(x_{i}, y_{i}\right) - 59f\left(x_{i-1}, y_{i-1}\right) + 37f\left(x_{i-2}, y_{i-2}\right) - 9f\left(x_{i-3}, y_{i-3}\right) \right] \\ y_{i+1} = y_{i} + \frac{h}{24} \left[9f\left(x_{i+1}, y_{i}^{(p)}\right) + 19f\left(x_{i}, y_{i}\right) - 5f\left(x_{i-1}, y_{i-1}\right) + f\left(x_{i-2}, y_{i-2}\right) \right] \end{cases}$$

$$(7.68)$$

and the local truncation error is

$$R_{i+1} = y(x_{i+1}) - y(x_i) - \frac{h}{24} \left\{ 9f\left(x_{i+1}, y(x_i) + \frac{h}{24} \left[55f\left(x_i, y(x_i)\right) \right. \right. \right. \\ \left. - 59f\left(x_{i-1}, y\left(x_{i-1}\right)\right) + 37f\left(x_{i-2}, y\left(x_{i-2}\right)\right) - 9f\left(x_{i-3}, y\left(x_{i-3}\right)\right) \right] \right) \\ \left. + 19f\left(x_i, y\left(x_i\right)\right) - 5f\left(x_{i-1}, y\left(x_{i-1}\right)\right) + f\left(x_{i-2}, y\left(x_{i-2}\right)\right) \right\} \right. \\ \left. = y\left(x_{i+1}\right) - y\left(x_i\right) - \frac{h}{24} \left\{ 9f\left(x_{i+1}, y\left(x_{i+1}\right)\right) + 19f\left(x_i, y\left(x_i\right)\right) \right. \\ \left. - 5f\left(x_{i-1}, y\left(x_{i-1}\right)\right) + f\left(x_{i-2}, y\left(x_{i-2}\right)\right) \right\} \right. \\ \left. + \frac{9h}{24} \left\{ f\left(x_{i+1}, y\left(x_{i+1}\right)\right) - f\left(x_{i+1}, y\left(x_i\right) + \frac{h}{24} \left[55f\left(x_i, y\left(x_i\right)\right) \right. \right. \\ \left. - 59f\left(x_{i-1}, y\left(x_{i-1}\right)\right) + 37f\left(x_{i-2}, y\left(x_{i-2}\right)\right) - 9f\left(x_{i-3}, y\left(x_{i-3}\right)\right) \right] \right\} \right. \\ \left. = y\left(x_{i+1}\right) - y\left(x_i\right) - \frac{h}{24} \left[9f\left(x_{i+1}, y\left(x_{i+1}\right)\right) + 19f\left(x_i, y\left(x_i\right)\right) \right. \\ \left. - 5f\left(x_{i-1}, y\left(x_{i-1}\right)\right) + f\left(x_{i-2}, y\left(x_{i-2}\right)\right) \right] \right. \\ \left. + \frac{9h}{24} \frac{\partial f\left(x_{i+1}, \eta_i\right)}{\partial y} \left\{ y\left(x_{i+1}\right) - \left[y\left(x_i\right) + \frac{h}{24} \left(55f\left(x_i, y\left(x_i\right)\right) \right. \\ \left. - 59f\left(x_{i-1}, y\left(x_{i-1}\right)\right) + 37f\left(x_{i-2}, y\left(x_{i-2}\right)\right) - 9f\left(x_{i-3}, y\left(x_{i-3}\right)\right) \right) \right] \right\} \right.$$

By Eqs. (7.58) and (7.67), we have the local truncation error of the explicit

TABLE 7.4
The computing results

compating receive						
	Explicit method		Predictor-corrector method			
$y(x_i)$	y_i	$ y(x_i)-y_i $	y_i	$ y(x_i)-y_i $		
0.862069	0.862389	0.000320	0.862027	0.000042		
0.800000	0.800527	0.000527	0.799928	0.000072		
0.735294	0.735944	0.000650	0.735212	0.000082		
0.671141	0.671754	0.000613	0.671066	0.000075		
0.609756	0.610267	0.000511	0.609698	0.000058		
0.552486	0.552850	0.000364	0.552448	0.000038		
0.500000	0.500237	0.000237	0.499979	0.000021		
0.452489	0.452618	0.000129	0.452481	0.000008		
0.409836	0.409896	0.000060	0.409836	0.000000		
	$\begin{array}{c} y(x_i) \\ 0.862069 \\ 0.800000 \\ 0.735294 \\ 0.671141 \\ 0.609756 \\ 0.552486 \\ 0.500000 \\ 0.452489 \end{array}$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		

method

$$R_{i+1} = -\frac{19}{720} h^5 y^{(5)} (\xi_i) + \frac{9h}{24} \frac{\partial f(x_{i+1}, \eta_i)}{\partial y} \cdot \frac{251}{720} h^5 y^{(5)} (\xi_i)$$
$$= -\frac{19}{720} h^5 y^{(5)} (\xi_i) + O(h^6)$$
(7.69)

Exercise 7.4. Use four-order Adams explicit method and the Adams predictor-corrector method to approximate the solutions for the initial-value problem in Example 7.1 with h = 0.1. The values of y_1, y_2, y_3 are given by RKA.

Solution The computing results are listed in Table 7.4.

From the table, the method by Eq. (7.68) is more accuracy than that of Eq. (7.57).

7.4.2 Taylor Methods

Try to confirm the constants a_j and b_j in the following linear k-step method

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}), \qquad (7.70)$$

with the highest order. By Taylor's Theorem, the local truncation error is

$$\begin{split} R_{i+1} &= y\left(x_{i+1}\right) - \left[\sum_{j=0}^{k-1} a_j y\left(x_{i-j}\right) + h \sum_{j=-1}^{k-1} b_j f\left(x_{i-j}, y\left(x_{i-j}\right)\right)\right] \\ &= y\left(x_{i+1}\right) - \sum_{j=0}^{k-1} a_j y\left(x_{i-j}\right) - h \sum_{j=-1}^{k-1} b_j y'\left(x_{i-j}\right) \\ &= \sum_{l=0}^{p+1} \frac{1}{l!} y^{(l)}\left(x_i\right) h^l + O\left(h^{p+2}\right) \\ &- \sum_{j=0}^{k-1} a_j \left[\sum_{l=0}^{+1} \frac{1}{l!} y^{(l)}\left(x_i\right) \left(-jh\right)^l + O\left(h^{p+2}\right)\right] \\ &- h \sum_{j=-1}^{k-1} \left[b_j \sum_{l=0}^{p} \frac{1}{l!} y^{(l+1)}\left(x_i\right) \left(-jh\right)^l + O\left(h^{p+1}\right)\right] \\ &= \left(1 - \sum_{j=0}^{k-1} a_j\right) y\left(x_i\right) \\ &+ \sum_{i=1}^{p+1} \frac{1}{l!} \left[1 - \sum_{i=0}^{k-1} (-j)^l a_j - l \sum_{i=1}^{k-1} (-j)^{l-1} b_j\right] h^l y^{(l)}\left(x_i\right) + O\left(h^{p+2}\right) \end{split}$$

If Eq. (7.70) has order p, then

$$\begin{cases} 1 - \sum_{j=0}^{k-1} a_j = 0 \\ 1 - \sum_{j=0}^{k-1} (-j)^l a_j - l \sum_{j=-1}^{k-1} (-j)^{l-1} b_j = 0 \quad (l = 1, 2, \dots, p) \end{cases}$$

i.e.

$$\begin{cases}
\sum_{j=0}^{k-1} a_j = 1 \\
\sum_{j=0}^{k-1} (-j)^l a_j + l \sum_{j=-1}^{k-1} (-j)^{l-1} b_j = 1 \quad (l = 1, 2, \dots, p).
\end{cases}$$
(7.71)

The local truncation error is

$$R_{i+1} = \frac{1}{(p+1)!} \left[1 - \sum_{j=0}^{k-1} (-j)^{p+1} a_j - (p+1) \sum_{j=-1}^{k-1} (-j)^p b_j \right]$$

$$\cdot h^{p+1} y^{(p+1)} (x_i) + O(h^{p+2})$$
(7.72)

Exercise 7.5. For the initial-value problem

$$\begin{cases} y'(x) = f(x, y(x)), \ a \le x \le b, \\ y(a) = \eta, \end{cases}$$

let h = (b-a)/n, $x_i = a+ih$, $0 \le i \le n$ where n is positive integer. Determine the values of the constants $\alpha, \beta_0, \beta_1, \beta_2$, in the following two-step method in the form

$$y_{i+1} = \alpha y_{i-1} + h \Big[\beta_0 f(x_{i+1}, y_{i+1}) + \beta_1 f(x_i, y_i) + \beta_2 f(x_{i-1}, y_{i-1}) \Big]$$

with highest order.

Solution The local truncation error is

$$\begin{split} R_{i+1} &= y(x_{i+1}) - \alpha y(x_{i-1}) - h[\beta_0 f(x_{i+1}, y(x_{i+1})) \\ &+ \beta_1 b f(x_i, y(x_i)) + \beta_2 f(x_{i-1}, y(x_{i-1}))] \\ &= y(x_{i+1}) - \alpha y(x_{i-1}) - \beta_0 h y'(x_{i+1}) - \beta_1 h y'(x_i) - \beta_2 h y'(x_{i-1}) \\ &= y(x_i) + h y'(x_i) + \frac{h^2}{2} y''(x_i) + \frac{h^3}{3!} y'''(x_i) + \frac{h^4}{4!} y^{(4)}(x_i) \\ &+ \frac{h^5}{5!} y^{(5)}(x_i) + O(h^6) \\ &- \alpha \Big[y(x_i) - h y'(x_i) + \frac{h^2}{2} y''(x_i) - \frac{h^3}{3!} y'''(x_i) + \frac{h^4}{4!} y^{(4)}(x_i) \\ &- \frac{h^5}{5!} y^{(5)}(x_i) + O(h^6) \Big] \\ &- \beta_0 h \Big[y'(x_i) + h y''(x_i) + \frac{h^2}{2} y'''(x_i) + \frac{h^3}{3!} y^{(4)}(x_i) \\ &+ \frac{h^4}{4!} y^{(5)}(x_i) + O(h^5) \Big] - \beta_1 h y'(x_i) \\ &- \beta_2 h \Big[y'(x_i) - h y''(x_i) + \frac{h^2}{2} y'''(x_i) - \frac{h^3}{3!} y^{(4)}(x_i) \\ &+ \frac{h^4}{4!} y^{(5)}(x_i) + O(h^5) \Big] \\ &= (1 - \alpha) y(x_i) + (1 + \alpha - \beta_0 - \beta_1 - \beta_2) h y'(x_i) \\ &+ \left(\frac{1}{2} - \frac{\alpha}{2} - \beta_0 + \beta_2 \right) h^2 y''(x_i) \\ &+ \left(\frac{1}{6} + \frac{\alpha}{6} - \frac{\beta_0}{2} - \frac{\beta_2}{2} \right) h^3 y'''(x_i) + \left(\frac{1}{24} - \frac{\alpha}{24} - \frac{\beta_0}{6} + \frac{\beta_2}{6} \right) h^4 y^{(4)}(x_i) \\ &+ \left(\frac{1}{120} + \frac{\alpha}{120} - \frac{\beta_0}{24} - \frac{\beta_2}{24} \right) h^5 y^{(5)}(x_i) + O(h^6). \end{split}$$

Then

$$1 - \alpha = 0$$

$$1 + \alpha - \beta_0 - \beta_1 - \beta_2 = 0$$

$$\frac{1}{2} - \frac{\alpha}{2} - \beta_0 + \beta_2 = 0$$

$$\frac{1}{6} + \frac{\alpha}{6} - \frac{\beta_0}{2} - \frac{\beta_2}{2} = 0$$

By solving the above linear system, we have $\alpha = 1, \beta_0 = \frac{1}{3}, \beta_1 = \frac{4}{3}, \beta_2 = \frac{1}{3}$. The local truncation error is

$$R_{i+1} = -\frac{1}{90}h^5y^{(5)}(x_i) + O(h^6).$$

It is the fourth-order method.

(1) For example, try to determine an explicit four-step explicit method $\hfill\Box$

$$y_{i+1} = a_0 y_i + a_1 y_{i-1} + a_2 y_{i-2} + h \left[b_0 f \left(x_i, y_i \right) + b_1 f \left(x_{i-1}, y_{i-1} \right) + b_2 f \left(x_{i-2}, y_{i-2} \right) + b_3 f \left(x_{i-3}, y_{i-3} \right) \right]$$

$$(7.73)$$

with order four.

By Eq. (7.71), the constants satisfy the following linear system

$$\begin{cases} a_0 + a_1 + a_2 = 1 \\ -a_1 - 2a_2 + b_0 + b_1 + b_2 + b_3 = 1 \\ a_1 + 4a_2 - 2b_1 - 4b_2 - 6b_3 = 1 \\ -a_1 - 8a_2 + 3b_1 + 12b_2 + 27b_3 = 1 \\ a_1 + 16a_2 - 4b_1 - 32b_2 - 108b_3 = 1 \end{cases}$$

If $a_1 = a_2 = 0$, then

$$a_0 = 1$$
, $b_0 = \frac{55}{24}$, $b_1 = -\frac{59}{24}$, $b_2 = \frac{37}{24}$, $b_3 = -\frac{9}{24}$.

The formula is AB₄ and the local truncation error is

$$R_{i+1} = \frac{251}{720} h^5 y^{(5)}(x_i) + O(h^6).$$

(2) Suppose

$$y_{i+1} = a_0 y_i + a_1 y_{i-1} + a_2 y_{i-2} + h \left[b_{-1} f\left(x_{i+1}, y_{i+1}\right) + b_0 f\left(x_i, y_i\right) + b_1 f\left(x_{i-1}, y_{i-1}\right) + b_2 f\left(x_{i-2}, y_{i-2}\right) \right]$$

$$(7.74)$$

has order four. The constants in Eq. (7.71) satisfy

$$\begin{cases}
 a_0 + a_1 + a_2 = 1 \\
 -a_1 - 2a_2 + b_{-1} + b_0 + b_1 + b_2 = 1 \\
 a_1 + 4a_2 + 2b_{-1} - 2b_1 - 4b_2 = 1 \\
 -a_1 - 8a_2 + 3b_{-1} + 3b_1 + 12b_2 = 1 \\
 a_1 + 16a_2 + 4b_{-1} - 4b_1 - 32b_2 = 1
\end{cases}$$
(7.75)

Let $a_1 = a_2 = 0$, then

$$a_0 = 1$$
, $b_{-1} = \frac{9}{24}$, $b_0 = \frac{19}{24}$, $b_1 = -\frac{5}{24}$, $b_2 = \frac{1}{24}$

and the local truncation error is

$$R_{i+1} = -\frac{19}{720} h^5 y^{(5)}(x_i) + O(h^6).$$

If $a_0 = 0, a_2 = 0$, then

$$a_1 = 1$$
, $b_{-1} = \frac{1}{3}$, $b_0 = \frac{4}{3}$, $b_1 = \frac{1}{3}$, $b_2 = 0$.

We derive the two-step implicit Simpson method

$$y_{i+1} = y_{i-1} + \frac{h}{3} \left[f(x_{i+1}, y_{i+1}) + 4f(x_i, y_i) + f(x_{i-1}, y_{i-1}) \right]$$

which local truncation error is

$$R_{i+1} = -\frac{1}{90}h^5y^{(5)}(x_i) + O(h^6).$$

(3) Considering

$$y_{i+1} = a_0 y_i + a_1 y_{i-1} + a_2 y_{i-2} + a_3 y_{i-3} + h \left[b_0 f(x_i, y_i) + b_1 f(x_{i-1}, y_{i-1}) + b_2 f(x_{i-2}, y_{i-2}) \right],$$

we can derive four-step explicit Milne Method

$$y_{i+1} = y_{i-3} + \frac{4h}{3} \left[2f(x_i, y_i) - f(x_{i-1}, y_{i-1}) + 2f(x_{i-2}, y_{i-2}) \right].$$

The local truncation error is

$$R_{i+1} = \frac{14}{45} h^5 y^{(5)} (x_i) + O(h^6)$$

(4) Considering

$$y_{i+1} = a_0 y_i + a_1 y_{i-1} + a_2 y_{i-2}$$

+ $h \left[b_{-1} f(x_{i+1}, y_{i+1}) + b_0 f(x_i, y_i) + b_1 f(x_{i-1}, y_{i-1}) \right],$

we can derive three-step implicit Hamming Method

$$y_{i+1} = \frac{1}{8} (9y_i - y_{i-2}) + \frac{3h}{8} [f(x_{i+1}, y_{i+1}) + 2f(x_i, y_i) - f(x_{i-1}, y_{i-1})].$$

The local truncation error is

$$R_{i+1} = -\frac{1}{40}h^5 y^{(5)}(x_i) + O(h^6).$$

If Milne method predicts an approximation, and the Simpson method corrects this prediction. We obtain the Milne-Simpson predictor-corrector method:

$$\begin{cases} y_i^{(p)} = y_{i-3} + \frac{4h}{3} \left[2f(x_i, y_i) - f(x_{i-1}, y_{i-1}) + 2f(x_{i-2}, y_{i-2}) \right] \\ y_{i+1} = y_{i-1} + \frac{h}{3} \left[f\left(x_{i+1}, y_i^{(p)}\right) + 4f(x_i, y_i) + f(x_{i-1}, y_{i-1}) \right] \end{cases}$$

of order four.

7.5 Exercise

1. Use Euler's method and modified Euler's method with h=0.2 to approximate the solutions for the initial-value problem

$$\left\{ \begin{array}{ll} y'=x+y & (0\leqslant x\leqslant 1) \\ y(0)=1 \end{array} \right.$$

and compare them with the exact solution $y = -x - 1 + 2e^x$ at mesh nodes.

2. Compute the approximations to

$$y(x) = \int_0^x e^{t^2} dt$$

at x = 0.5, 1, 1.5, 2 by Euler's method.

3. Determine the coefficient α such that the local truncation error of

$$y_{i+1} = y_i + h \left[\alpha f(x_i, y_i) + (1 - \alpha) f(x_{i+1}, y_{i+1}) \right]$$

with the highest order.

4. Use RK_4 method with h=0.1 to solve the initial-value problem:

(1)
$$y' = x^2 - y, 0 \le x \le 0.3, y(0) = 1;$$

(2)
$$y' = y^2/(1+x), 0 \le x \le 0.3, y(0) = 1.$$

5. Show the formula

$$\begin{cases} y_{i+1} = y_i + \frac{h}{6} \left(k_1 + 4k_2 + k_3 \right) \\ k_1 = f \left(x_i, y_i \right) \\ k_2 = f \left(x_i + \frac{h}{2}, y_i + \frac{1}{2} h k_1 \right) \\ k_3 = f \left(x_i + h, y_i - h k_1 + 2 h k_2 \right) \end{cases}$$

has order three.

6. Derive the two-step Euler's method

$$y_{i+1} = y_{i-1} + 2hf(x_i, y_i)$$

and the local truncation error.

7. Derive the two-step explicit Admas method

$$y_{i+1} = y_i + \frac{h}{2} \left[3f(x_i, y_i) - f(x_{i-1}, y_{i-1}) \right]$$

and show the local truncation error is

$$R_{i+1} = \frac{5}{12} h^3 y^{(3)}(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1}).$$

8. Derive the local truncation error of the predictor-corrector method

$$\begin{cases} y_i^{(p)} = y_i + \frac{h}{2} \left[3f(x_i, y_i) - f(x_{i-1}, y_{i-1}) \right] \\ y_{i+1} = y_i + \frac{h}{2} \left[f(x_i, y_i) + f(x_{i+1}, y_i^{(p)}) \right] \end{cases}$$

9. Use the RK₄, AB₄, and AB₄-AM₄ predictor-corrector method with h=0.1 to solve the initial-value problem

$$\left\{ \begin{array}{ll} y'=-x^2y^2 & (0\leqslant x\leqslant 1.5) \\ y(0)=3 \end{array} \right.$$

and compare the numerical solution with exact solutions $y(x) = 3/(1+x^3)$.