Applying (3.119) to $y'' = \lambda y$, we get the characteristic equation

$$\rho(\xi) - \bar{h}\sigma(\xi) = 0 \qquad (3.126)$$

where $\lambda h^2 = \bar{h}$.

The two roots of (3.126) tend to be the double principal root $\xi = 1$ as $h \to 0$. Let ξ_{jh}, $j = 1, 2, \ldots, k$ be the roots of (3.126). The linear k-step method (3.119) is called *absolutely stable* if

$$| \xi_{jh} | \leqslant 1, j = 1, 2, \ldots, k \qquad (3.127)$$

and it is called relatively stable if

$$| \xi_{jh} | \leqslant \min (| \xi_{1h} | \xi_{2h} |), j = 3, 4, \ldots, k \qquad (3.128)$$

DEFINITION 3.14 A multistep method of the form (3.119) when applied to the problem $y'' = -\lambda y$, $\lambda > 0$ is said to have interval of periodicity $(0, h_0)$, $\bar{h} \in (0, h_0)$, $\bar{h} = \lambda h^2$, if all the roots of $\rho(\xi) + \bar{h}\sigma(\xi) = 0$ are complex and lie on the unit circle.

DEFINITION 3.15 A multistep method is said to be P-stable if its interval of periodicity is $(0, \infty)$.

The main result about the P-stable linear multistep method is the following:

THEOREM 3.9 *The order p of a P-stable method cannot exceed 2 and the method must be implicit.*

For $k = 2$, we write (3.119) as

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h^2 (b_0 y''_{n+1} + b_1 y''_n + b_2 y''_{n-1}) \qquad (3.129)$$

where a_i's and b_i's are arbitrary.

From (3.120), we find that the formula (3.129) is of first order when

$$a_1 = 2, a_2 = -1, b_2 = 1 - b_0 - b_1 \qquad (3.130)$$

second order when, in addition,

$$b_0 - b_2 = 0 \qquad (3.131)$$

and third order when in addition to (3.130) and (3.131),

$$b_0 + b_2 = \frac{1}{6} \qquad (3.132)$$

To study the stability of the linear multistep method (3.129) we apply it to the test equation $y'' = -\lambda y$, $\lambda > 0$. We write the characteristic equation as

$$(1 + b_0\bar{h})\xi^2 - (2 - b_1\bar{h})\xi + 1 + b_2\bar{h} = 0 \qquad (3.133)$$

Substituting $\xi = (1+z)/(1-z)$ in (3.133), we get

$$[4 + \bar{h}(1 - 2b_1)]z^2 + 2(2b_0 + b_1 - 1)\bar{h}z + \bar{h} = 0 \qquad (3.134)$$

Using the Routh-Hurwitz criterion in (3.134), we find that the roots of (3.133) will lie within the unit circle if

(i) $b_1 \leqslant \frac{1}{2}$, $2b_0 + b_1 > 1$, $\bar{h} > 0$

or

$$\text{(ii) } b_1 > \tfrac{1}{2},\ 2b_0+b_1 > 1,\ \bar{h} \leqslant \frac{4}{2b_1-1} = h_0 \tag{3.135}$$

The stability interval $(0, h_0)$ as function of the parameters b_0 and b_1 is shown in Figure 3.11. The values $b_1 = 0$, $b_2 = 0$, $b_0 = 1$ give a first order formula

$$y_{n+1} = 2y_n - y_{n-1} + h^2 y''_{n+1} \tag{3.136}$$

The roots of the characteristic equation (3.133) are complex and their magnitude is

$$|\xi| = \frac{1}{\sqrt{1+\bar{h}}}$$

which shows that the formula (3.136) is A-stable. For $b_1 \leqslant 1/2$, $b_0 = (1-b_1)/2$, $b_2 = (1-b_1)/2$, we obtain a second order stable formula

$$y_{n+1} = 2y_n - y_{n-1} + \frac{h^2}{2}[(1-b_1)y''_{n+1} + 2b_1 y''_n + (1-b_1)y''_{n-1}] \tag{3.137}$$

The roots of the characteristic equation (3.133) are for all $\bar{h}$-values on the unit circle. Thus the formula (3.137) is P-stable for all values $b_1 \leqslant 1/2$.

For $b_1 = \frac{1}{2}$, we obtain the *Dahlquist* method

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{4}(y''_{n+1} + 2y''_n + y''_{n-1}) \tag{3.138}$$

which is P-stable and second order with minimum truncation error. The value $b_1 = \frac{2}{3}$ gives a second order method

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{6}(y''_{n+1} + 4y''_n + y''_{n-1}) \tag{3.139}$$

with interval of periodicity (0, 12). Finally, when we choose $b_1 = \frac{5}{6}$, the difference scheme (3.129) becomes the fourth order Numerov method (3.125) and it has interval of periodicity (0, 6).

The $P(EC)^m E$ mode discussed in Section 3.6.2 can easily be written here with h replaced by h^2. Similarly, the modified predictor-corrector mode in Section 3.6.4 is also adaptable here.

Example 3.7 Use the Numerov method to determine $y(0.6)$, where $y(t)$ denotes the solution of the initial value problem

$$y'' + ty = 0,\ y(0) = 1,\ y'(0) = 0$$

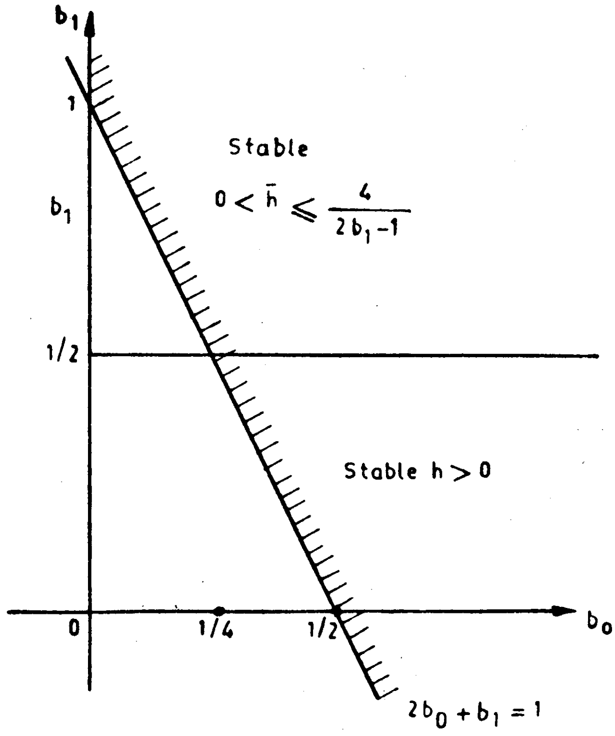

Fig. 3.11 Stability boundaries in the (b_0, b_1) plane

The Numerov method is given by

$$y_{n+1}-2y_n-2y_{n-1} = \frac{h^2}{12}(y''_{n+1}+10y''_n+y''_{n-1}), \quad n \geqslant 1$$

Here, we require the values y_0 and y_1 to start the computation. The Numerov method has order four and we use a fourth order singlestep method to determine the value y_1. The Taylor series method gives

$$y(h) = 1-\frac{h^3}{6}+\frac{h^6}{180}+\cdots$$

For $h = .2$, we get

$$y_1 = 1-\frac{(.2)^3}{6} = .9986667$$

We obtain,

for $n = 1$;

$$y_2 = 2y_1-y_0+\frac{h^2}{12}(y''_2+10y''_1+y''_0)$$

The parameters β_1 and β_2 are determined such that the method (3.146) is P-stable. Applying the method (3.146) to the test equation $y'' = -\lambda y$, $\lambda > 0$, we obtain

$$A\, y_{n+1} - 2B\, y_n + A\, y_{n-1} = 0 \tag{3.148}$$

where

$$\begin{aligned} A &= 1 + \beta_1 \bar{h} - \frac{1}{2}\left(\frac{1}{12} - \beta_1 - \beta_2\right)\bar{h}^2 \\ B &= 1 - \left(\frac{1}{2} - \beta_1\right)\bar{h} + \frac{1}{2}\beta_2\, \bar{h}^2 \end{aligned} \tag{3.149}$$

It is easily verified that the characteristic equation

$$A\xi^2 - 2B\xi + A = 0 \tag{3.150}$$

associated with the method (3.146) will have all its roots complex and are of unit modulus if and only if

$$\begin{aligned} &\text{(i)}\ \beta_2 + \frac{3}{4}\beta_1 - \frac{1}{2}\beta_1^2 - \frac{7}{96} \geqslant 0 \\ &\text{(ii)}\ \beta_1 \geqslant \frac{1}{12} \end{aligned} \tag{3.151}$$

For the values $\beta_1 = \frac{1}{12}$ and $\beta_2 = \frac{1}{72}$, we get the *Hairer* method

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(y''_{n+1} + 10y''_n + y''_{n-1}) - \frac{h^4}{144}(y^{(iv)}_{n+1} - 2y^{(iv)}_n + y^{(iv)}_{n-1}) \tag{3.152}$$

with the minimum truncation error

$$T_n = \frac{1}{360} h^6 y^{(iv)}_{(\xi_1)}$$

3.8.3 Adaptive numerical methods

We write (3.117) in the form

$$y'' + py = \phi(t, y) \tag{3.153}$$

where

$$\phi(t, y) = py + f(t, y) \tag{3.154}$$

and $p > 0$ is an arbitrary parameter to be determined. From application view point, the perturbing force $\phi(t, y)$ is assumed to be small with respect to the restoring force py, we may therefore approximate $\phi(t, y)$ by a polynomial $g(t)$ of an appropriate degree. Integrating (3.153) between the limits t_{n-1} to t_{n+1}, we get

$$y(t_{n+1})-2\cos\sqrt{p}\,h\,y(t_n)+y(t_{n-1})$$
$$=\frac{1}{\sqrt{p}}\int_{t_n}^{t_{n+1}}\sin\sqrt{p}\,(t_{n+1}-\tau)[g(\tau)+g(2t_n-\tau)]\,d\tau \tag{3.155}$$

We now approximate $g(\tau)$ in (3.155) by the Newton backward difference formula (3.7) and (3.14) to get the explicit and implicit multistep methods. We have the explicit methods

$$y_{n+1}-2\cos 2\sigma\, y_n+y_{n-1}$$
$$=h^2\frac{\sin^2\sigma}{\sigma^2}[\phi_n+\lambda\nabla^2\phi_n+\lambda\nabla^3\phi_n$$
$$+\left(\lambda+\frac{1}{4\sigma^2}\left(\frac{1}{12}-\lambda\right)\right)\nabla^4\phi_n+\ldots] \tag{3.156}$$

where

$$\sigma=\frac{\sqrt{p}\,h}{2}$$
$$\lambda=\frac{1}{4}\left(\frac{1}{\sin^2\sigma}-\frac{1}{\sigma^2}\right)$$
$$\phi_n=py_n+f_n \tag{3.157}$$

Similarly, we obtain the implicit methods

$$y_{n+1}-2\cos 2\sigma y_n+y_{n-1}$$
$$=h^2\frac{\sin^2\sigma}{\sigma^2}[\phi_{n+1}-\nabla\phi_{n+1}+\lambda\nabla^2\phi_{n+1}$$
$$+\frac{1}{4\sigma^2}\left(\frac{1}{12}-\lambda\right)(\nabla^4\phi_{n+1}+\nabla^5\phi_{n+1})+\ldots] \tag{3.158}$$

The coefficient of the third difference is zero in (3.158) and therefore the use of second or third difference gives the same accuracy. Retaining up to the second differences, we have the *Stiefel-Bettis* formula

$$y_{n+1}-2\cos 2\sigma\, y_n+y_{n-1}$$
$$=h^2\frac{\sin^2\sigma}{\sigma^2}[\phi+\lambda\nabla^2\phi_{n+1}]$$

which may be written as

$$y_{n+1}-2y_n+y_{n-1}=h^2[\lambda f_{n+1}+(1-2\lambda)f_n+\lambda f_{n-1}] \tag{3.159}$$

This formula (3.159) is the stabilized Numerov method. It is of order two for arbitrary σ and of order four for $\sigma\to 0$. With (3.159) we associate a difference operator

$$L[y(t),h]=y(t_{n+1})-2\,y(t_n)+y(t_{n-1})$$
$$-h^2[\lambda f(t_{n+1},y(t_{n+1}))+(1-2\lambda)f(t_n,y(t_n))$$
$$+\lambda f(t_{n-1},y(t_{n-1}))] \tag{3.160}$$

DEFINITION 3.16 The method (3.118) is said to be of trigonometric order p relative to the frequency w if

$$L_w[1, h] = 0, \; L_w[\cos rwt, h] = 0, \; L_w[\sin rwt, h] = 0$$

$$L_w[\cos (r+1) wt, h] \neq 0, \; L_w[\sin (r+1) wt, h] \neq 0, \; r = 1, 2, \ldots, p$$

where p is the largest integer and $L[y(t), h]$ is the difference operator.

Substituting $y(t) = e^{iwt}$, $w = \frac{2\sigma}{h}$, in the difference operator (3.160) we find

$$L[e^{iwt}, h] = 0$$

which shows that the method (3.159) is of trigonometric order one. Thus, the method (3.159) is of polynomial order two and trigonometric order one.

3.8.4 Results from computation

We use the Dahlquist method (3.138), the Numerov method (3.125) and the Stiefel-Bettis method (3.159) to find the numerical solution of the following initial value problems:

$$\text{(i)} \quad y'' + \left(100 + \frac{1}{4t^2}\right) y = 0 \qquad (3.161)$$

the initial conditions at $t = 1$ are chosen such that

$$y(t) = \sqrt{t}\, J_0(10t)$$

is the exact solution.

$$\text{(ii)} \quad x'' = -\frac{x}{r^3}, \qquad y'' = -\frac{y}{r^3} \qquad (3.162)$$

where $r^2 = x^2 + y^2$.

The initial conditions are chosen such that $x = \cos t$, $y = \sin t$ is the exact solution of the nonlinear system.

(iii) The undamped *Duffing* equation

$$y'' + y + y^3 = B \cos \Omega t \qquad (3.163)$$

forced by a harmonic function where $B = 0.002$ and $\Omega = 1.01$. The exact solution computed by the *Galerkin* method (see Section 8.2.3) with a precision 10^{-12} of the coefficients is given by

$$y(t) = A_1 \cos \Omega t + A_3 \cos 3\Omega t + A_5 \cos 5\Omega t + A_7 \cos 7\Omega t + A_9 \cos 9\Omega t$$

where

$$A_1 = 0.200179477536$$
$$A_3 = 0.000246946143$$
$$A_5 = 0.000000304014$$
$$A_7 = 0.000000000374$$
$$A_9 = 0.000000000000$$

For problem (3.161), we take $p_n = 100+\frac{1}{4t_n^2}$ and the steplengths $h = 0.2$, 0.5. The absolute error values $E = | y_n - y(t_n) |$ are found for $t = 1$ to $t = 6$ and the values E at $t = 6$ are presented in Table 3.16.

For problem (3.162), we take $p = \frac{1}{r_n^3}$ the the steplegths $h = \frac{\pi}{18}, \frac{\pi}{10}$. The absolute error values in radius R given by $E = | 1 - R_n |$ where $R_n^2 = x_n^2 + y_n^2$, x_n and y_n being computed values, are calculated from $t = 0$ to $t = 12\pi$ and the values E at $t = 12\pi$ are presented in Table 3.16. In solving the non-linear problem (3.162), the initial approximations are obtained from the exact solution. We used the *Picard* iteration and the formula is corrected to converge with tolerance $\epsilon = 1.0 \times 10^{-10}$.

For problem (3.163), we take $p = 1$, $1+y_n^2$ and 1.01, and steplengths $h = \frac{\pi}{18}, \frac{\pi}{10}$. The absolute error values $E = | y_n - y(t_n) |$ are calculated from $t = 0$ to $t = 12\pi$ and the values E for $p = 1$ at $t = 40\pi$ are listed in Table 3.16.

The numerical results show that the Numerov method (3.125) produces good results whenever the stability conditions are satisfied. For large steplengths, the Stiefel-Bettis method (3.159) gives the best results. It is obvious from the numerical results that *P*-stability is an important requirement for determining the numerical solutions of periodic initial value problems.

TABLE 3.16 COMPARISON OF ERRORS IN THE NUMERICAL SOLUTIONS

h\ *Method*	*Dahlquist*	*Numerov*	*Stiefel-Bettis*
	P-stable	$p \to 0$	p_n
	$y'' + \left(100+\frac{1}{4t^2}\right) y = 0,$	$t = 6$	$100+\frac{1}{4t_n^2}$
0.2	0.2774	0.2790	0.1240−03
0.5	0.4400	0.5585+06	0.5568−03
$x'' = -\frac{x}{r^3},$	$y'' = -\frac{y}{r^3},$	$t = 12\pi$	$\frac{1}{r_n^3}$
$\frac{\pi}{18}$	0.2631−02	0.6650−08	0.3740−08
$\frac{\pi}{10}$	0.3770−01	0.1514−06	0.2970−10
	$y''+y+y^3 = B \cos \Omega t$	$\Omega = 1.01$ $t = 40\pi$	$B = 0.002$ 1
$\frac{\pi}{18}$	0.4324−01	0.3337−04	0.6116−06
$\frac{\pi}{10}$	0.1350	0.3512−03	0.6418−05

In practice, we use a grid system in which each interval is a constant multiple of the preceding one, i.e.

$$h_{j+1} = \sigma h_j,\ j = 1(1)N-1 \tag{3.172}$$

with $\sigma > 1$, this gives more mesh points at small t, while $\sigma < 1$ gives more mesh points at large values of t.

3.9.3 Results from computation

We use the trapezoidal method (3.169) to find the numerical solution of the following initial value problem

$$u' = -2000u+999.75v+1000.25$$
$$v' = u-v$$

with initial conditions

$$u(0) = 0,\ v(0) = -2 \text{ over the interval } [0, 10]$$

The exact solution is given by

$$u(t) = -1.499875 \exp(-0.5t) +0.499875 \exp(-2000.5t)+1$$
$$v(t) = -2.99975 \exp(-0.5t) -0.00025 \exp(-2000.5t)+1$$

From (3.172), we write as

$$h_1+h_2+\dots+h_N = b-t_0$$

or

$$h_1 = (b-t_0)(\sigma-1)/(\sigma^N-1) \tag{3.173}$$

where $\sigma > 1$.

From equation (3.173), choosing $\sigma = 1.5$ and $N = 25$ we determine h_1 and then use the trapezoidal method to calculate the numerical solution. The solution values are listed in Table 3.17. The graph of the solution is shown in Figure 3.12.

TABLE 3.17 SOLUTION VALUES FOR STIFF SYSTEM USING TRAPEZOIDAL METHOD WITH VARIABLE STEP

t_n	u_n	v_n	$u(t_n)$	$v(t_n)$
0.1609−02	−0.4849+00	−0.1997+01	−0.4787+00	−0.1997+01
0.9754−02	−0.4926+00	−0.1985+00	−0.4926+00	−0.1985+01
0.5099−01	−0.4621+00	−0.1924+01	−0.4621+00	−0.1924+01
0.2597+00	−0.3172+00	−0.1634+01	−0.3172+00	−0.1634+01
0.1317+01	0.2244+01	−0.5512+01	0.2234+00	−0 5531+00
0.6666+01	0.9559+00	0.9118+00	0.9465+00	0.8930+00
0.1000+02	0.9960+00	0.9920+00	0.9899+00	0.9798+00

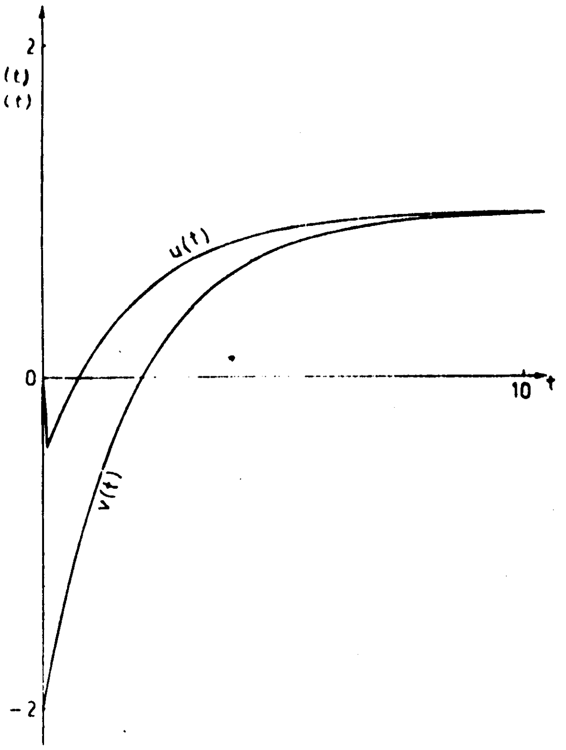

Fig. 3.12 Solution of a stiff problem using trapezoidal method with variable steps

Bibliographical note

The explicit and implicit multistep methods are discussed in detail in the books 33, 93, 113, 161 and 163. Further 93 and 113 include an extensive bibliography.

The reference 186 gives an iterated *Adams* Corrector method. The methods with minimum truncation error and those with extended stability region are obtained in 54 and 119 respectively. The stability analysis of the multistep methods has been examined in 18, 19, 32, 35, 68, 106, 122 and 228. The convergence and error bounds are studied in 57and 58. The hybrid methods are developed in 20, 26, 62, 91 and 101. The implicit methods to solve stiff differential equations are discussed in the following references; *A*-stable, 11, 59, 74, 144, 171 and 187; stiffly stable, 92, 141, 200 and 255.

The multistep methods for undamped second order equation of motion are given in 60, 110, 137, 162, 229, 230 and 250.

The adaptive methods for second order differential equations are given in 135.

Problems

1. Show that the linear explicit and implicit multistep methods given in the text for the initial value problem $y' = f(t, y)$, $y(t_0) = y_0$, are, respectively, in terms of operators
$$[-(1-\nabla)\log(1-\nabla)]\, y_{n+1} = h\, y'_n$$
$$[-\log(1-\nabla)]\, y_{n+1} = h\, y'_{n+1}$$
and hence obtain the expansions given.
2. Find the order of the method of the form
$$y_{n+1} = y_n + h\,(b_0\, y'_{n+1} + b_1\, y'_n + b_2\, y'_{n-1} + b_3\, y'_{n-2})$$
Determine the influence function and calculate the explicit form of the error term.
3. Construct the influence function for Milne-Simpson's method
$$y_{n+2} = y_n + \frac{h}{3}\,(y'_{n+2} + 4y'_{n+1} + y'_n)$$
and show that it does not change sign in [0, 2].
4. Show that the order of the linear multistep method
$$y_{n+1} + (a-1)\, y_n - a\, y_{n-1} = \frac{1}{4}\, h\,[(a+3)\, y'_{n+1} + (3a+1)\, y'_{n-1}]$$
is 2 if $a \neq -1$ and it is 3 if $a = -1$.
5. Find the constant c in the following methods so that the truncation error is minimum:

(i) $$y_{n+1} = (1-2c)\, y_n + (2c-c^2)\, y_{n-1} + c^2\, y_{n-2} + \frac{h}{24}\,[(c^2-2c+9)\, y'_{n+1} + (-5c^2+26c+19)\, y'_n + (19c^2+26c-5)\, y'_{n-1} + (9c^2-2c+1)\, y'_{n-2}]$$

(ii) $$y_{n+1} = (1-c)\, y_n + (c-c^2)\, y_{n-1} + c^2\, y_{n-2} + \frac{h}{24}\,[(c^2-c+9)\, y'_{n+1} + (-5c^2+13c+19)\, y'_n + (19c^2+13c-5)\, y'_{n-1} + (9c^2-c+1)\, y'_{n-2}]$$

6. If
$$\rho(\xi) = \xi^3 - \xi^2 + \tfrac{1}{4}\xi - \tfrac{1}{4},$$
find a $\sigma(\xi)$ such that:

(i) $\sigma(\xi)$ is of second degree and the method has third order;
(ii) $\sigma(\xi)$ is of third degree and the method has fourth order.

What are the coefficients of the principal term of the truncation error for these two methods?

7. If $\sigma(\xi) = \xi^2$, find $\rho(\xi)$ such that:

   (i) $\rho(\xi)$ is of second degree and the order is two;
   (ii) $\rho(\xi)$ is of third degree and the order is three.
   Are these methods stable?

8. Find values of the constants such that the truncation error of the corrector

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h\,(b_0 y'_{n+1} + b_1 y'_n + b_2 y'_{n-1})$$

   is of order h^3.
   Show that the use of this corrector is unstable for all values of h for solving the equation $y' = \lambda y$, $\lambda < 0$.

9. Find the maximum interval for stability with which the equation $y' = \lambda y$, $\lambda < 0$ may be integrated by the corrector

$$y_{n+1} = \frac{1}{8}[9y_n - y_{n-2} + 3h\,(y'_{n+1} + 2y'_n - y'_{n-1})]$$

   Find also the maximum interval with which the method may be used to integrate the system

$$y' = -3y + 2z$$
$$z' = 3y - 4z$$

10. Find the range of α for which the linear multistep method

$$y_{n+1} + \alpha\,(y_n - y_{n-1}) - y_{n-2} = \tfrac{1}{2}\,(3+\alpha)\,h(y'_n + y'_{n-1})$$

   is stable. Show that there exists a value of α for which the method has order 4.

11. Using the Routh-Hurwitz criterion, find the interval of absolute stability of the methods:

   (*i*) $y_{n+1} = y_n + \dfrac{h}{12}(23y'_n - 16y'_{n-1} + 5y'_{n-2})$;

   (*ii*) $y_{n+1} = y_n + \dfrac{h}{24}(9y'_{n+1} + 19y'_n - 5y'_{n-1} + y'_{n-2})$

12. Calculate the growth parameters for the following multistep methods:

   (i) $y_{n+1} = y_n + \dfrac{h}{2}(3y'_n - y'_{n-1})$

   (ii) $y_{n+1} = y_{n-1} + \dfrac{h}{3}(7y'_n - 2y'_{n-1} + y'_{n-2})$

13. Show that the error $\epsilon_n = y_n - y(t_n)$ in the k-step Adams-Bashforth formula

$$y_{n+1} = y_n + h \sum_{i=1}^{k} b_i\, y'_{n-i+1} + C_k\, h^{k+1}\, y^{(k+1)}_{(\xi)}$$

is bounded by

$$|\epsilon_n| \leqslant \delta \exp((t_n-t_0)b_k L)+ |C_k| h^k M_{k+1}\left\{\frac{\exp((t_n-t_0)B_kL)-1}{B_k L}\right\}$$

where $\quad |\epsilon_i| \leqslant |y_i-y(t_i)| \leqslant \delta,\ i=0,1,2,\ldots,k-1,$

$$B_k = \sum_{i=1}^{k} |b_i|$$

$$|y^{(k+1)}(t)| \leqslant M_{k+1}$$

$$|f(t,z_1)-f(t,z_2)| \leqslant L\,|z_1-z_2|$$

14. Assuming that the starting values are exact, show that the error ϵ_n of the Adams-Bashforth methods satisfy

$$\epsilon_n = \delta(t_n)\,h^k+0(h^{k+1})$$

where $\delta(t_n)$ denotes the solution of the initial value problem

$$\delta' = f_y(t, y(t))\,\delta - C_k\, y^{(k+1)}_{(t)}$$

$$\delta(t_0) = 0$$

15. The formula

$$y_{n+1} = y_{n-2}+\frac{3}{8}h(y'_{n+1}+3y'_n+3y'_{n-1}+y'_{n-2})$$

with a small step length h is used for solving the equation $y' = -y$. Investigate the convergence of the metnod. (BIT 7 (1967),247)

16. Show that the following two-step method

$$y_{n+1} = \frac{4}{3}\,y_n-\frac{1}{3}\,y_{n-1}+\frac{2}{3}\,hy'_{n+1}$$

is A-stable.

Determine also the error constant.

17. Find the conditions on a and b for which the following linear multistep methods

(i) $$y_{n+1}-(1+a)\,y_n+a\,y_{n-1} = h\Big[\Big(\frac{1}{2}(1+a)+b\Big)\,y'_{n+1} + \Big(\frac{1}{2}(1-3a)-2b\Big)y'_n+b\,y'_{n-1}\Big]$$

(ii) $$y_{n+1} = y_n+\frac{h}{2}[(1-a)\,y'_n+(1+a)\,y'_{n+1}]+\frac{h^2}{4}[(b-a)\,y''_n - (b+a)y''_{n+1}]$$

are A-stable.

18. Determine the multistep methods of the form

$$y_{n+1} = y_n+h\sum_{i=0}^{k} b_i\,y'_{n-i+1}+h^2\,c_0\,y''_{n+1}$$

for $k=1, 2, 3$ and show that the methods are stiffly stable.

19. Find the multistep methods for the form

$$y_{n+1} = \sum_{l=1}^{k} a_l\, y_{n-l+1} + h\, b_0\, h y'_{n+1} + h^2 c_0\, y''_{n+1}$$

for $k = 2, 3$. Prove that the methods are stiffly stable.

20. Consider the predictor P and the two correctors $C^{(1)}$, $C^{(2)}$, defined as follows, by their characteristic polynomials:

$$P: \rho^{(0)}(\xi) = \xi^4 - 1 \qquad \sigma^{(0)}(\xi) = \frac{4}{3}(2\xi^3 - \xi^2 + 2\xi),$$

$$C^{(1)}: \rho_1(\xi) = \xi^3 - 1 \qquad \sigma_1(\xi) = \frac{1}{3}(\xi^3 + 4\xi + 1)$$

$$C^{(2)}: \rho_2(\xi) = \xi^3 - \frac{9}{8}\xi^2 + \frac{1}{8} \qquad \sigma_2(\xi) = \frac{3}{8}(\xi^3 + 2\xi^2 - \xi)$$

Find the interval of absolute stability of (i) $P-C^{(1)}$, (ii) $P-C^{(2)}$ predictor-corrector pair in $P-M_p-C-M_c$ mode. Compare with the results for the same pairs in $PECE$ mode and show that the addition of modifiers almost halves the stability interval for $P-C^{(1)}$ set and almost doubles it for the $P-C^{(2)}$ set.

21. Consider the following $P-C$ set:

$$P: y_{n+1} + 4y_n - 5y_{n-1} = h(4y'_n + 2y'_{n-1})$$

$$C: y_{n+1} = y_{n-1} + \frac{h}{3}(y'_{n+1} + 4y'_n + y'_{n-1})$$

Form the characteristic polynomial for the $PECE$ algorithm. Hence show that for small negative λh, the algorithm is relatively stable according to the definition

$$|\xi_{jh}| < |\xi_{1h}|, j = 2, 3, \ldots, k$$

22. Let ξ_{j0} be the root of $\rho(\xi) = 0$ of multiplicity $m \geqslant 1$. Prove that for sufficiently small h the root ξ_{jh} of $\rho(\xi) - \lambda h \sigma(\xi) = 0$ can be written as

$$\xi_{jh} = \xi_{j0} + \left(\frac{m!\,\sigma(\xi_{j0})}{\rho^{(m)}(\xi_{j0})}\lambda h\right)^{1/m} + 0\,(h^{2/m})$$

23. Consider the two predictors P_v, P_k, and the hybrid corrector C_H defined as follows:

$$P_v: y_{n+1/2} = y_{n-1} + \frac{3h}{8}(3y'_n + y'_{n-1})$$

$$P_k: y_{n+1} + 4y_n - 5y_{n-1} = h(4y'_n + 2y'_{n-1})$$

$$C_H: y_{n+1} - y_n = \frac{h}{6}(y'_{n+1} + y'_n + 4y'_{n+1/2})$$

Find the interval of absolute stability of $P_v\,EP_k\,EC_H\,E$ algorithm. Determine the local truncation error of $P_v\,EP_k\,EC_H E$ mode.

(c) If the scalar equation $y' = qy$ is integrated as above, which is the largest value of p for which $\lim_{h\to 0} \frac{y_n - e^{qx}y_0}{h^p}$, $x = nh$, x fixed, has a finite limit? (BIT 8 (1968), 138).

34. Let a linear multistep method for the initial value problem

$$y' = f(x, y),\ y(0) = y_0$$

be applied to the test equation $y' = -y$. If the resulting difference equation has at least one characteristic root $\alpha(h)$ such that $|\alpha(h)| > 1$ for arbitrary small values of h, then the method is called weakly stable. Which of the following methods are weakly stable?

(a) $y_{n+1} = y_{n-1} + 2h\, f(x_n, y_n)$

(b) $\bar{y}_n = -y_n + 2y_{n-1} + 2h\, f(x_n, y_n)$

$y_{n+1} = y_{n-1} + 2h\, f(x_n, \bar{y}_n)$

(c) $\bar{y}_{n+1} = -4y_n + 5y_{n-1} + 2h\,(2f_n + f_{n-1})$

$y_{n+1} = y_{n-1} + \frac{1}{3}h\,(f\,(x_{n+1}, \bar{y}_{n+1}) + 4f_n + f_{n-1})$

$f_n = f\,(x_n, y_n)$ (BIT 8 (1968), 343)

35. Use the two-step method

$$y_{n+1} = y_{n-1} + \frac{h}{3}(y'_{n+1} + 4y'_n + y'_{n-1})$$

to solve the test problem

$$y' = \alpha y,\ y(0) = y_0$$

where $\alpha < 0$.

Determine $\lim_{n\to\infty} |y_n|$ and $\lim_{n\to\infty} y(x_n)$ where $x_n = nh$, h fixed, and $y(x)$ is the exact solution of the test problem. (BIT 12 (1972), 272).

36. For the corrector formula

$$y_{n+1} - \alpha y_{n-1} = A\, y_n + B\, y_{n-2} + h\,(C\, y'_{n+1} + D\, y'_n + E\, y'_{n-1}) + R$$

we have $R = 0\,(h^5)$.

(a) Show that $A = \frac{9}{8}(1-\alpha)$, $B = -\frac{1}{8}(1-\alpha)$ and determine C, D and E.

(b) Show that the formula is not strongly unstable (that is the converse of stable in the sense of Dahlquist), if $-0.6 < \alpha \leqslant 1$.

(BIT 13 (1973), 375).

37. Consider the problem

$$\mathbf{y}' = \mathbf{A}\mathbf{y}\,,\ \mathbf{y}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} -2 & 1 \\ 1 & -20 \end{bmatrix}$$

(a) Show that the system is asymptotically stable.
(b) Examine the method

$$y_{i+1} = y_i + \frac{h}{2}(3f_{i+1} - f_i)$$

for the equation $y' = f(x, y)$.
What is its order of approximation?
Is it stable? Is it A-stable?
(c) Choose stepsizes $h = 0.2$ and $h = 0.1$ and compute approximation to $y(0.2)$ using the method in (*b*). Finally make a suitable extrapolation to $h = 0$. (BIT 15 (1975), 335)

38. A certain 4-step method for the numerical solution of the initial value problem

$$y' = f(x, y),\ y(0) = c$$

is given by

$$y_{n+4} = y_n + 4h(\beta_0 f_n + \beta_1 f_{n+1} + \beta_2 f_{n+2} + \beta_3 f_{n+3})$$
$$y_0 = c$$

where $\quad y_j = y(x_j),\ x_j = jh$

$$f_j = f(x_j, y_j),\ j = 0, 1, 2, \ldots$$

The coefficient β_0 is less than zero while the exact appearance of the remaining coefficients $\beta_1, \ldots, \beta_3$ is of no importance for this study. The truncation error $y_n - y(x_n)$ is a power series in h. An attempt has been made to determine the powers appearing in the series by using the method with different stepsizes, h, for the computation of $y(1)$ in the test equation $y' = -y$, $y(0) = 1$. The starting values were $y_0 = 1$, $y_1 = e^{-h}$, $y_2 = e^{-2h}$, and $y_3 = e^{-3h}$. The following results were obtained.

$h = 1/5$	$y = 0.367706,$	$h = 1/80$	$y = 0.36788$
$h = 1/10$	$y = 0.367846,$	$h = 1/160$	$y = 0.367879$
$h = 1/20$	$y = 0.367873,$	$h = 1/320$	$y = 0.367879$
$h = 1/40$	$y = 0.367879,$	$h = 1/640$	$y = 0.36788$

(a) How do you usually use this kind of information to determine the first powers in the series?

(b) Show that the approach in (a) does not work satisfactorily in this case.

(c) Analyse the 4-step method and show what makes the approach in (a) useless. (BIT 16 (1976), 111)

39. To solve the differential equation

$$y' = f(x, y),\ y(0) = y_0$$

the method

$$y_{n+1} = \frac{18}{19}(y_n - y_{n-2}) + y_{n-3} + \frac{6h}{19}(f_{n+1} + 4f_n + 4f_{n-2} + f_{n-3})$$

is suggested, where $f_n = f(x_n, y_n)$.

(a) What is the local truncation error of the method?

(b) Is the method stable? (BIT 20 (1980), 261)

40. The general solution of the differential equation $y' = 1 + a(1 + x + y)$ is $y = 1 + x + c\exp(-ax)$. We attempt to calculate the solution given by $y(0) = 1$ numerically. What happens to stability when

(a) $a < 0$; any method

(b) $a > 0$; the midpoint method

$$(y_{n+1} - y_{n-1})/2h = 1 + a(1 + x_n - y_n),$$
$$x_n = nh.$$

(BIT 21 (1981), 136)

4

Difference Methods for Boundary Value Problems in Ordinary Differential Equations

4.1 INTRODUCTION

A general boundary value problem can be represented symbolically as

$$L[y] = r$$
$$U_\mu[y] = r_\mu,\ \mu = 1, 2, \ldots, m \tag{4.1}$$

where L is an mth order differential operator, r is a given function and U_μ are the boundary conditions. We shall use x as an independent variable for the boundary value problem.

If L represents an mth order linear differential operator and $U_\mu[y]$ represent two point boundary conditions, then (4.1) can be expressed in the form

$$L[y] = \sum_{\nu=0}^{m} f_\nu(x)\, y^{(\nu)} = f_0(x)\, y + f_1(x)\, y' + \ldots + f_m(x) y^{(m)} = r(x),\ x \in [a, b] \tag{4.2}$$

$$U_\mu[y] = \sum_{k=0}^{m-1} (a_{\mu,k}\, y^{(k)}(a) + b_{\mu,k}\, y^{(k)}(b)) = \gamma_\mu,\ \mu = 1, 2, \ldots m$$

For $m = 2q$, the k boundary conditions which are linearly independent and contain only derivatives up to $(q-1)$th order are called the *essential* boundary conditions, and the remaining $(2q-k)$ boundary conditions are termed the *suppressible* boundary conditions.

The simplest boundary value problem is given by a second order differential equation

$$f_2(x)\, y'' + f_1(x)\, y' + f_0(x)\, y = r(x),\ x \in [a, b] \tag{4.3}$$

with one of the three boundary conditions given below.
The boundary conditions of the first kind are:

(i) $y(a) = \gamma_1,\ y(b) = \gamma_2$

When this approximation is used in (4.5), we find that the solution satisfies

$$-\frac{1}{h^2}[y(x_{n+1})-2y(x_n)+y(x_{n-1})]+f(x_n)y(x_n)$$
$$+0(h^2) = r(x_n) \qquad (4.7)$$

at the grid points $x_1, x_2, \ldots, x_N$.

Dropping the error term in (4.7) and defining approximations $y_1, y_2, \ldots, y_N$ to the values of the solution at the grid points x_j, we get the system of N equations

$$-y_{n-1}+2y_n-y_{n+1}+h^2 f_n y_n = h^2 r_n \qquad (4.8)$$

The boundary conditions become

$$y_0 = \gamma_1, \; y_{N+1} = \gamma_2$$

If

$$\mathbf{J} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ \cdot & \cdot & \cdot & & \\ & \cdot & \cdot & \cdot & \\ & -1 & 2 & -1 & \\ & & -1 & 2 \end{bmatrix}, \; \mathbf{F} = \begin{bmatrix} f_1 & & & \\ & \cdot & & \\ & & \cdot & \\ & & & f_N \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} \gamma_1+h^2r_1 \\ h^2r_2 \\ \vdots \\ \gamma_2+h^2r_N \end{bmatrix}, \; \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

then Equations (4.8), after incorporating the boundary conditions, can be written as

$$(\mathbf{J}+h^2 \mathbf{F})\,\mathbf{y} = \mathbf{C}$$

If $|\mathbf{J}+h^2 \mathbf{F}| \neq 0$, then the solution of the above system becomes

$$\mathbf{y} = (\mathbf{J}+h^2 \mathbf{F})^{-1}\mathbf{C}$$

The local truncation error is defined by

$$T_n = -(y(x_{n+1})-2y(x_n)+y(x_{n-1}))+h^2f(x_n)y(x_n)-h^2r(x_n)$$
$$= -\frac{h^4}{12}y^{(iv)}_{(\xi_n)}, \; \xi_n \in (x_{n-1}, x_{n+1}), \; n = 1(1)N$$

If $y \in C^{p+2}$, it means that the derivatives of y with respect to x are continuous up to orders $p+2$, then in the present case, it may be pointed out, we require $y \in C^4$ in order to find the truncation error.

An important special case of (4.5) is

$$L[y] = y''+\lambda y = 0.$$
$$y(a) = y(b) = 0 \qquad (4.9)$$

in which $r(x) = 0$, $\gamma_1 = 0$, $\gamma_2 = 0$ and $f(x) = -\lambda$, so that the boundary value problem is a simple type of eigenvalue problem. The difference Equation (4.8) and the boundary conditions become

$$-y_{n-1}+2y_n-y_{n+1}-\Lambda y_n = 0,$$
$$y_0 = 0,\ y_{N+1} = 0 \tag{4.10}$$

where $\Lambda = h^2\lambda$. Thus $h^{-2}\Lambda$ determines the required characteristic parameter in (4.9). The general solution of (4.10) can be written as

$$y_n = c_1 \cos n\alpha + c_2 \sin n\alpha \tag{4.11}$$

where c_1, c_2 are arbitrary constants and we have substituted $\Lambda = 2-2\cos\alpha = 4\sin^2\alpha/2$ in (4.10). The boundary condition $y_0 = 0$ gives

$$c_1 = 0$$

while the second boundary condition $y_{N+1} = 0$ leads to the condition

$$c_2 \sin\alpha(N+1) = 0$$

As $c_2 = 0$ gives a trivial solution, we take

$$\sin\alpha(N+1) = 0$$

This yields

$$\alpha(N+1) = k\pi,\ k = 1, 2\ldots, N$$

With this value of α, the N characteristic values of the quantity Λ are

$$\Lambda_k = 4\sin^2\frac{k\pi}{2(N+1)},\ k = 1, 2, \ldots, N$$

The corresponding N characteristic functions are given by

$$y_{n,k} = \sin n\frac{k\pi}{N+1},\ k = 1, 2, \ldots, N \tag{4.12}$$

Again, we take a special case of (4.3),

$$y''+\mu y' = 0$$
$$y(a) = 1,\ y(b) = 0 \tag{4.13}$$

where we have put $r(x) = 0, f_2(x) = 1, f_1(x) = \mu$ a constant, $f_0(x) = 0$, $\gamma_1 = 1$ and $\gamma_2 = 0$, so that the boundary value problem may be regarded a simple type of second order differential equation with a significant first derivative. Three different approximations for (4.13) in which the first derivative is replaced by central, backward or forward difference, respectively are

(i) $\frac{1}{h^2}(y_{n+1}-2y_n+y_{n-1})+\frac{\mu}{2h}(y_{n+1}-y_{n-1}) = 0$

(ii) $\frac{1}{h^2}(y_{n+1}-2y_n+y_{n-1})+\frac{\mu}{h}(y_n-y_{n-1}) = 0$

(iii) $\frac{1}{h^2}(y_{n+1}-2y_n+y_{n-1})+\frac{\mu}{h}(y_{n+1}-y_n) = 0$. (4.14)

$$h^4 y_n^{(iv)} = \begin{cases} \Delta^4 y_n - 2\Delta^5 y_n + \frac{17}{6}\Delta^6 y_n - \frac{7}{2}\Delta^7 y_n + \dots \\ \nabla^4 y_n + 2\nabla^5 y_n + \frac{17}{6}\nabla^6 y_n + \frac{7}{2}\nabla^7 y_n + \dots \\ \delta^4 y_n - \frac{1}{6}\delta^6 y_n + \frac{7}{240}\delta^8 y_n - \dots \end{cases}$$

4.3 NONLINEAR BOUNDARY VALUE PROBLEM $y'' = f(x, y)$

Let us consider the numerical solution of the nonlinear differential equation (4.4)

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

subject to the boundary conditions

$$y(a) = A,\ y(b) = B \tag{4.17}$$

The differential equation (4.4) together with (4.17) has a unique solution provided $f_y(x, y) \geq 0$, $x \in [a, b]$, i.e., it is class M problem. We introduce a finite set of grid points

$$x_n = a + nh,\ n = 0, 1, 2, \dots, N+1$$

where $x_0 = a$, $x_{N+1} = b$ and $h = (b-a)/(N+1)$.

We approximate (4.4) by the difference scheme of the form

$$-y_{n-1} + 2y_n - y_{n+1} + h^2(\beta_0 y''_{n-1} + \beta_1 y''_n + \beta_2 y''_{n+1}) = 0,\ 1 \leq n \leq N \tag{4.18}$$

where $\beta_0 + \beta_1 + \beta_2 = 1$, $\beta_0 = \beta_2$, $y_0 = A$, $y_{N+1} = B$

The difference scheme (4.18) represents a system of nonlinear equations in the unknowns y_n, $1 \leq n \leq N$, which in matrix form can be written as

$$\mathbf{J}\,\mathbf{y} + h^2\,\mathbf{B}\mathbf{f}(\mathbf{y}) + \alpha = 0 \tag{4.19}$$

where
$$\mathbf{J} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} \beta_1 & \beta_2 & & & \\ \beta_0 & \beta_1 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_0 & \beta_1 & \beta_2 \\ & & & \beta_0 & \beta_1 \end{bmatrix}$$

$$\mathbf{f(y)} = \begin{bmatrix} f(x_1, y_1) & & & \\ & f(x_2, y_2) & & \\ & & \ddots & \\ & & & f(x_N, y_N) \end{bmatrix}$$

$$\boldsymbol{\alpha} = \begin{bmatrix} -A+\beta_0 h^2 f(x_0, A) \\ 0 \\ \vdots \\ -B+\beta_2 h^2 f(x_{N+1}, B) \end{bmatrix}$$

The system of nonlinear equations (4.19) is generally solved by *Newton's* method. If the first approximation is called $\mathbf{y}^{(0)}$, then the formulas for the *Newton* method are in this case,

$$\mathbf{r}(\mathbf{y}^{(l)}) = \mathbf{J}\,\mathbf{y}^{(l)}+h^2\,\mathbf{B}\,\mathbf{f}(\mathbf{y}^{(l)})+\boldsymbol{\alpha}$$

$$\Delta\mathbf{y}^{(l)} = -(\mathbf{J}+h^2\,\mathbf{B}\,\mathbf{F}(\mathbf{y}^{(l)}))^{-1}\,\mathbf{r}(\mathbf{y}^{(l)})$$

and finally

$$\mathbf{y}^{(l+1)} = \mathbf{y}^{(l)}+\Delta\mathbf{y}^{(l)}$$

where $\mathbf{r(y)}$ is a residual vector, $\mathbf{F(y)}$ being a diagonal matrix of order N,

$$\mathbf{F(y)} = \begin{bmatrix} f_{y_1} & & & \\ & f_{y_2} & & \\ & & \ddots & \\ & & & f_{y_N} \end{bmatrix}$$

and $\quad f_{y_j} = f_y(x_j, y_j)$

The Newton method has quadratic convergence, i.e., the number of correct decimal places is doubled in the numerical solution at each iteration. The iteration is repeated until the convergence is achieved.

4.3.1 Difference scheme based on quadrature formulas

We convert the original differential equation into an equivalent integro-difference equation and then apply the quadrature formulas to evaluate the integral in the equation. We illustrate this technique by finding the difference equations for the second order differential equation $y'' = f(x, y)$.

Let us consider the identity

$$\delta^2 y(x_n) = \int_{x_n}^{x_{n+1}} (x_{n+1}-t)\,[y''(t)+y''(2x_n-t)]\,dt \tag{4.20}$$

We also note from (4.30) that if $r^2 = 13/42$, the truncation error of formula (4.29) vanishes and we obtain an eighth order formula with only one off-step point. Thus the optimal difference scheme with one off-step point is found as

$$\delta^2 y_n = h^2\left[\frac{199}{390} y''_n + \frac{19}{1740}(y''_{n-1}+y''_{n+1}) + \frac{441}{1885}(y''_{n-r}+y''_{n+r})\right],\ r^2 = \frac{13}{42} \tag{4.33}$$

with the truncation error

$$T^*_n = -\frac{23}{237081600} h^{10} y^{(10)}(\xi_8),\ x_{n-1} < \xi_8 < x_{n+1}$$

We put $v = 3$ into (4.26) to get hybrid difference schemes with two off-step points.

The difference scheme is given by

$$\delta^2 y_n = h^2 [W_0 y''_n + W_1 (y''_{n-1}+y''_{n+1}) + W_2 (y''_{n-r}+y''_{n+r}) + W_3 (y''_{n-s}+y''_{n+s})] \tag{4.34}$$

where we have put $\theta_2 = r$ and $\theta_3 = s$.

The two parameter families of sixth order methods can be obtained for the two cases (i) $W_0 \neq 0$, $W_1 = 0$, and (ii) $W_0 = 0$, $W_1 \neq 0$.

$$\delta^2 y_n = h^2 [W_0 y''_n + W_2 (y''_{n-r} + y''_{n+r}) + W_3 (y''_{n-s}+y''_{n+s})] \tag{4.35}$$

where
$$W_0 = \frac{30 r^2 s^2 - 5(r^2+s^2)+2}{30 r^2 s^2}$$

$$W_2 = \frac{2-5s^2}{60 r^2 (r^2-s^2)} \text{ and } W_3 = \frac{2-5r^2}{60 s^2 (s^2-r^2)}$$

The truncation error in this case is

$$T^*_n = \frac{70 r^2 s^2 - 28 (r^2+s^2)+15}{302400} h^8 y^{(8)}(\xi_9),\ x_{n-1} < \xi_9 < x_{n+1} \tag{4.36}$$

The value $r^2 = 2/5$ in (4.35) gives the formula (4.31). If we take

$$r = \frac{5-\sqrt{5}}{10},\ s = \frac{5+\sqrt{5}}{10}$$

then formula (4.35) becomes (4.24).

The values $W_0 = 0$, $W_1 \neq 0$ give the two parameter family of method as

$$\delta^2 y_n = h^2 [W_1 (y''_{n-1}+y''_{n+1}) + W_2 (y''_{n-r}+y''_{n+r}) + W_3 (y''_{n-s}+y''_{n+s})] \tag{4.37}$$

where
$$W_1 = \frac{30 r^2 s^2 - 5(r^2+s^2)+2}{60(1-r^2)(1-s^2)}$$

$$W_2 = \frac{3-25 s^2}{60(1-r^2)(r^2-s^2)}$$

$$W_3 = \frac{3-25 r^2}{60(1-r^2)(s^2-r^2)}$$

The truncation error of method (4.37) is given by

$$T_n^* = -\frac{(350\,r^2s^2-42\,(r^2+s^2)+13)}{302400}\,h^8\,y^{(8)}\,(\xi_{10}),\; x_{n-1} < \xi_{10} < x_{n+1}$$

The most general two parameter family of order eight formula is given by

$$\begin{aligned}\delta^2 y_n = h^2\,[W_0\,y_n''+W_1\,(y_{n-1}''+y_{n+1}'')\\ +W_2\,(y_{n-r}''+y_{n+r}'')+W_3\,(y_{n-s}''+y_{n+s}'')]\end{aligned} \tag{4.38}$$

where $$W_0 = \frac{350\,r^2s^2-42\,(r^2+s^2)+13}{420\,r^2s^2}$$

$$W_1 = \frac{70r^2s^2-28\,(r^2+s^2)+15}{840\,(1-r^2)\,(1-s^2)}$$

$$W_2 = \frac{13-42\,s^2}{840r^2\,(1-r^2)\,(r^2-s^2)}$$

and $$W_3 = \frac{13-42r^2}{840s^2\,(1-s^2)\,(s^2-r^2)}$$

The truncation error of this formula is

$$T_n^* = -\frac{126r^2s^2-39\,(r^2+s^2)+17}{50803200}\,h^{10}\,y^{(10)}\,(\xi_{11}),\; x_{n-1} < \xi_{11} < x_{n+1}$$

If $r^2 = 13/42$, we get the eighth order method (4.33). Thus corresponding to every replacement of the right-hand side of (4.21) by an expression of the form (4.25), we get a difference scheme involving one or more off-step points. Furthermore, we also note that the difference scheme (4.26) will be of computational value only if we have accurate estimates of the values of $y(x)$ at these off-step points. Therefore, for obtaining methods of order six, we take one of the two following fourth order approximations to $y_{n\pm\theta_j}$

Approximation I

$$\begin{aligned}y_{n+q} = (1-q)\,y_n+q\,y_{n+1}+\frac{h^2}{12}\,[(1-4q+4q^2-q^3)y_n''\\ +q\,(q^2+q-1)\,y_{n+1}''+(q^2-q-1)\,y_{n+q}'']\end{aligned} \tag{4.39}$$

$$\begin{aligned}y_{n-q} = (1-q)\,y_n+q\,y_{n-1}+\frac{h^2}{12}[(1-4q+4q^2-q^3)\,y_n''\\ +q\,(q^2+q-1)y_{n-1}''+(q^2-q-1)\,y_{n-q}'']\end{aligned} \tag{4.40}$$

where $\theta_j = q$. The truncation error in (4.39) and (4.40) are respectively

$$T_n^{(I)} = -R_5h^5y^{(5)}\,(x_n)-R_6h^6y^{(6)}\,(\xi_1),\; x_n < \xi_1 < x_{n+1}$$

$$T_n^{*(I)} = R_5h^5y^{(5)}\,(x_n)\;-R_6h^6y^{(6)}\,(\xi_2),\; x_{n-1} < \xi_2 < x_n \tag{4.41}$$

$$R_5 = \frac{1}{360}\,(2q^5-5q^4+5q^2-2q)$$

$$R_6 = \frac{1}{1440}\,(3q^6-5q^5-5q^4+5q^3+5q^2-3q) \tag{4.42}$$

The approximate values y_n, $1 \leqslant n \leqslant N$ can be determined by solving the system of linear equations (4.52).

4.3.3 Solution of tridiagonal system

The solution of the differential equation (4.46) subject to the boundary conditions (4.47) leads to the solution of the system of algebraic equations in N unknowns whose coefficients give rise to a special case of the tridiagonal system

$$-b_j y_{j-1}+a_j y_j-c_j y_{j+1} = d_j \tag{4.54}$$

for $1 \leqslant j \leqslant N$, where y_0 and y_{N+1} are known from the boundary conditions.

If
$$b_j > 0,\ a_j > 0,\ c_j > 0$$
and
$$a_j \geqslant (b_j+c_j)$$

for $1 \leqslant j \leqslant N$, then we can construct a very efficient algorithm for solving a tridiagonal system. Let us consider the difference relation

$$y_j = w_j y_{j+1}+g_j \tag{4.55}$$

for $0 \leqslant j \leqslant N$, from which we get

$$y_{j-1} = w_{j-1}y_j+g_{j-1} \tag{4.56}$$

Eliminating y_{j-1} from equations (4.54) and (4.56), we obtain

$$y_j = \frac{c_j}{a_j-b_j w_{j-1}} y_{j+1}+\frac{d_j+b_j g_{j-1}}{a_j-b_j w_{j-1}} \tag{4.57}$$

Thus

$$w_j = \frac{c_j}{a_j-b_j w_{j-1}},\ g_j = \frac{d_j+b_j g_{j-1}}{a_j-b_j w_{j-1}}$$

If $y_0 = A$, then $w_0 = 0$, $g_0 = A$, so that the difference relation

$$y_0 = w_0 y_1+g_0$$

holds for any y_1. The remaining $w_j, g_j, j = 1, \ldots, N$ can now be calculated from

$$w_1 = \frac{c_1}{a_1}, \qquad g_1 = \frac{d_1+b_1A}{a_1}$$

$$w_2 = \frac{c_2}{a_2-b_2w_1}, \qquad g_2 = \frac{d_2+b_2g_1}{a_2-b_2w_1}$$

$$\vdots \qquad\qquad \vdots$$

$$w_N = \frac{c_N}{a_N-b_N w_{N-1}},\ g_N = \frac{d_N+b_N g_{N-1}}{a_N-b_N w_{N-1}}$$

If $y_{N+1} = B$, then $y_1, y_2, \ldots, y_N$ are calculated from

$$\begin{aligned} y_N &= w_N B + g_N \\ y_{N-1} &= w_{N-1} y_N + g_{N-1} \\ &\vdots \\ y_1 &= w_1 y_2 + g_1 \end{aligned}$$

The convergence of this method is ensured by the condition

$$|w_n| \leqslant 1, n = 1, 2, \ldots, N$$

Example 4.1 Solve the first boundary value problem

$$y'' = \frac{2}{x^2} y - \frac{1}{x}, \; y(2) = y(3) = 0$$

by the Numerov method with $h = 1/4$.

The interval [2, 3] is subdivided into four subintervals with $h = 1/4$; the nodal points are given by

$$x_i = 2 + ih, \; 0 \leqslant i \leqslant 4$$

Applying the Numerov method at the nodal points x_1, x_2 and x_3, we obtain the following system of equations:

$$y_0 - 2y_1 + y_2 - \frac{1}{192}(y_0'' + 10y_1'' + y_2'') = 0, \; \left(\text{for } x_1 = \frac{9}{4}\right)$$

$$y_1 - 2y_2 + y_3 - \frac{1}{192}(y_1'' + 10y_2'' + y_3'') = 0, \; \left(\text{for } x_2 = \frac{10}{4}\right)$$

$$y_2 - 2y_3 + y_4 - \frac{1}{192}(y_2'' + 10y_3'' + y_4'') = 0, \; \left(\text{for } x_3 = \frac{11}{4}\right)$$

Using the boundary conditions $y_0 = y_4 = 0$ and $y_i'' = 2x_i^{-2}y_i - x_i^{-1}$, $0 \leqslant i \leqslant 4$, in the previous equations and simplifying, we get

$$\begin{aligned} \frac{491}{243} y_1 - \frac{599}{600} y_2 \qquad\qquad &= \frac{481}{17280} \\ -\frac{485}{486} y_1 + \frac{121}{60} y_2 - \frac{725}{726} y_3 &= \frac{119}{4752} \\ -\frac{599}{600} y_2 + \frac{731}{363} y_3 &= \frac{721}{31680} \end{aligned}$$

The solution of these equations together with the exact values obtained from

$$y(x) = \frac{1}{38}\left(19x - 5x^2 - \frac{36}{x}\right)$$

is given in Table 4.1.

TABLE 4.1 SOLUTION OF $y'' = 2x^{-2}y - x^{-1}$, $y(2) = y(3) = 0$, $h = 1/4$

x_n	y_n	$y(x_n)$
2.25	0.378314−01	0.378289−01
2.50	0.486868−01	0.486842−01
2.75	0.354382−01	0.354366−01

4.3.4 Mixed boundary conditions

The boundary conditions (4.47) are modified to

$$y'(a) - cy(a) = A$$
$$y'(b) + dy(b) = B \qquad (4.58)$$

where we have assumed $c \geqslant 0$, $d \geqslant 0$, $c+d > 0$.

The differential equation (4.46) subject to the mixed boundary conditions (4.58) will have a unique solution if $f(x) \geqslant 0$, $x \in [a, b]$. The system (4.48) contains N equations in $N+2$ unknowns y_i, $0 \leqslant i \leqslant N+1$. We need to find two more equations corresponding to the boundary conditions (4.58). For example, for the sixth order method, we proceed as follows

$$y(x_1) = y(x_0) + h\,y'(x_0) + h^2 \int_0^1 (1-t)\,y''(x_0+ht)\,dt \qquad (4.59)$$

and

$$y(x_N) = y(x_{N+1}) - h\,y'(x_{N+1}) + h^2 \int_0^1 (1-t)\,y''(x_{N+1}-ht)\,dt \qquad (4.60)$$

Replacing the integral in (4.59) by the four point Lobatto quadrature formula, we get

$$y(x_1) = y(x_0) + h\,y'(x_0) + \frac{h^2}{24}[2y''(x_0) + (5+\sqrt{5})\,y''(x_0+rh) + (5-\sqrt{5})\,y''(x_0+sh)] + \frac{h^7}{252000}\,y^{(6)}(\xi)$$

where $r = \dfrac{5-\sqrt{5}}{10}$, $s = \dfrac{5+\sqrt{5}}{10}$ and $x_0 < \xi < x_1$

Substituting the fourth order approximations of $y(x_0+rh)$ and $y(x_0+sh)$ given by (4.39), neglecting the truncation error, and using (4.46) and (4.58), we obtain

$$(1+B_0)\,y_0 + (-1+C_0)\,y_1 = D_0 \qquad (4.61)$$

where

$$B_0 = ch + \frac{h^2}{12}f_0 + \frac{h^2}{720}[(30(3+\sqrt{5}) + (1+\sqrt{5})\,h^2 f_0)P_r + (30(3-\sqrt{5}) + (1-\sqrt{5})\,h^2 f_0)\,P_s]$$

$$C_0 = \frac{h^2}{720}\,[(60-(1+\sqrt{5})\,h^2f_1)\,P_r+(60-(1-\sqrt{5})\,h^2f_1)\,P_s]$$

$$D_0 = -hA-\frac{h^2}{720}[(60g_0+30)\,((5+\sqrt{5})\,g_r+(5-\sqrt{5})\,g_s)$$
$$+h^2((1+\sqrt{5})\,(g_0-g_1)-3(5+\sqrt{5})\,g_r)\,P_r$$
$$+h^2((1-\sqrt{5})\,(g_0-g_1)-3(5-\sqrt{5})\,g_s)\,P_s]$$

The corresponding equation in y_N and y_{N+1} obtained from (4.60) is

$$(-1+A_{N+1})\,y_N+(1+B_{N+1})\,y_{N+1} = D_{N+1} \tag{4.62}$$

where
$$A_{N+1} = \frac{h^2}{720}\,[(60-(1+\sqrt{5})\,h^2f_N)\,P_{N+1-r}$$
$$+(60-(1-\sqrt{5})\,h^2f_N)P_{N+1-s}]$$

$$B_{N+1} = hd+\frac{h^2}{112}\,f_{N+1}+\frac{h^2}{720}\,[(30(3+\sqrt{5})$$
$$+(1+\sqrt{5})\,h^2f_{N+1})\,P_{N+1-r}+(30(3-\sqrt{5})$$
$$+(1-\sqrt{5})\,h^2f_{N+1})P_{N+1-s}]$$

$$D_{N+1} = h\,B-\frac{h^2}{720}\,[60g_{N+1}+30((5+\sqrt{5})\,g_{N+1-r}$$
$$+(5-\sqrt{5})\,g_{N+1-s})+h^2((1+\sqrt{5})\,(g_{N+1}-g_N)$$
$$-3\,(5+\sqrt{5})\,g_{N+1-r})\,P_{N+1-r}+h^2\,((1-\sqrt{5})\,(g_{N+1}-g_N)$$
$$-3\,(5-\sqrt{5})\,g_{N+1-s})\,P_{N+1-s}]$$

Grouping Equations (4.61), (4.48) and (4.62), we get

$$(1+B_0)\,y_0+(-1+C_0)\,y_1 = D_0$$
$$(-1+A_n)\,y_{n-1}+(2+B_n)\,y_n+(-1+C_n)\,y_{n+1} = D_n,\ 1 \leqslant n \leqslant N$$
$$(-1+A_{N+1})\,y_N+(1+B_{N+1})\,y_{N+1} = D_{N+1} \tag{4.63}$$

The above equations can be written as tridiagonal system as in (4.53), and can be solved by the method given in Section 4.3.3.

Example 4.2 Obtain numerical solution of the mixed boundary value problem

$$y'' = y-4x\,e^x$$
$$y'\,(0)-y\,(0) = 1,\ y'\,(1)+y\,(1) = -e$$

with step length $h = 1/4$.

The analytic solution is given by

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

We subdivide the interval [0, 1] into four subintervals, the nodal points are $x_n = nh$, $0 \leqslant n \leqslant 4$ and $h = 1/4$. The Numerov method gives the following system of equations

$$-191y_{n-1}+394y_n-191y_{n+1}$$
$$= 4x_{n-1}\, e^{x_{n-1}}+40x_n e^{x_n}+4x_{n+1}\, e^{x_{n+1}},\ 1 \leqslant n \leqslant 3$$

The boundary conditions become

$$y_0'-y_0 = 1,\ y_4'+y_4 = -e$$

In order to approximate the boundary conditions, we consider the indentity

$$y(x_1) = y(x_0)+hy'(x_0)+h^2P\, D^2y(x_0)$$

where the operator P is given by

$$P = (E-1-hD)(hD)^{-2}$$
$$= (\Delta-\log(1+\Delta))\left(\Delta-\frac{1}{2}\Delta^2+\frac{1}{3}\Delta^3-\ldots\right)^{-2}$$
$$=\frac{1}{2}\left(1+\frac{1}{3}\Delta-\frac{1}{12}\Delta^2+\frac{2}{45}\Delta^3-\frac{7}{240}\Delta^3+\ldots\right)$$

Thus, we have

$$y(x_1) = y(x_0)+hy'(x_0)+\frac{h^2}{2}\left(1+\frac{1}{3}\Delta-\frac{1}{12}\Delta^2+\frac{2}{45}\Delta^3-\ldots\right)y''(x_0)$$

Similarly, we get for the second boundary condition

$$y(x_3) = y(x_4)-hy'(x_4)+\frac{h^2}{2}\left(1-\frac{1}{3}\nabla-\frac{1}{12}\nabla^2-\frac{2}{45}\nabla^3-\ldots\right)y''(x_4)$$

We can now obtain various order approximations to the boundary conditions. The Numerov method has local truncation error of order h^6. Therefore, in order to approximate the boundary conditions to the same order, we retain third difference in the previous expressions and get

$$7297\, y_0-5646\, y_1-39\, y_2+8\, y_3$$
$$= -1440+4\,(8\, x_3\, e^{x_3}-39\, x_2\, e^{x_2}+112\, x_1\, e^{x_1}+97\, x_0\, e^{x_0})$$
$$8\, y_1-39\, y_2-5646\, y_3+7297\, y_4$$
$$= -\ 1440\, e+4\,(97\, x_4\, e^{x_4}+114\, x_3\, e^{x_3}-39\, x_2\, e^{x_2}+8\, x_1\, e^{x_1})$$

The solution of the linear system of equations and the exact values of $y(x)$ at x_i, $0 \leqslant i \leqslant 4$ are given in Table 4.2.

TABLE 4.2 Solution of $y'' = y-4x\, e^x$, $y'(0)-y(0) = 1$, $y'(1)+y(1) = -e$ with $h = 1/4$

x_n	$y(x_n)$	y_n	$e_n = y(x_n)-y_n$
0	0	0.622525−03	−0.622525−03
1	0.240754	0.241416	−0.661249−03
2	0.412180	0.412886	−0.706125−03
3	0.396937	0.397682	−0.744520−03
4	0	0.759196−03	−0.759196−03

4.3.5 Boundary condition at infinity

We consider now a boundary value problem as given by (4.46) and (4.47) but with the second boundary condition replaced by $y(x) \to 0$ as $b \to \infty$. The boundary conditions become

$$y(a) = A,\ y(\infty) = 0 \tag{4.64}$$

A typical method to solve the boundary value problem (4.46) and (4.64) is to apply the boundary condition at a finite point or at several finite points. Let us replace the second condition in (4.64) by

$$y(b^{(N)}) = 0 \tag{4.65}$$

where

$$b^{(N)} = a+(N+1)\,h \tag{4.66}$$

and N is an unknown number to be determined.

We denote the approximate value of $y(x)$ at $x = x_n$ by $y_n^{(N)}$ when $b^{(N)}$ is given by (4.66). The difference equations (4.48) and the boundary conditions (4.64) can be written as

$$(-1+A_n)\,y_{n-1}^{(N)}+(2+B_n)\,y_n^{(N)}+(-1+C_n)\,y_{n+1}^{(N)} = D_n,\ 1 \leqslant n \leqslant N \tag{4.67}$$

$$y_0^{(N)} = A,\ y_{N+1}^{(N)} = 0$$

As in Section 4.3.3, we write (4.67) in the form

$$y_n^{(N)} = w_n\, y_{n+1}^{(N)}+l_n \tag{4.68}$$

where

$$w_0 = 0,\ l_0 = A$$

The equation (4.68) can now be used to express $y_2^{(N)}, y_3^{(N)},\ldots,$ as functions of $y_1^{(N)}$; the first unknown nodal value is then determined by the boundary condition $y_{N+1}^{(N)} = 0$. Thus an approximate value for $y_1^{(N)}$ and hence also for $y_2^{(N)}, y_3^{(N)}, \ldots, y_N^{(N)}$ are obtained depending on N. The values of $y_1^{(N)}$, for a series of values of N will have differences which approximate closely to a geometric sequence, and a suitable value of N will be reached as soon as the criterion

$$|\, y_n^{(N+1)}-y_n^{(N)}\,| < \epsilon,\ 1 \leqslant n \leqslant N$$

is satisfied for a given ϵ.

This procedure for determining the value of N is not well suited for high speed computation and is rather time consuming. We now give a simple algorithm by which we can test the suitability of N without computing $y_n^{(N)}$, $1 \leqslant n \leqslant N$. Evidently, the $y_n^{(N)}$, $1 \leqslant n \leqslant N$, are obtained by back substitution from (4.68). The values of w_n and l_n are given by

$$w_n = -\frac{-1+C_n}{2+B_n+(-1+A_n)\,w_{n-1}},$$

$$l_n = \frac{D_n-(-1+A_n)\,l_{n-1}}{2+B_n+(-1+A_n)\,w_{n-1}},\ 1 \leqslant n \leqslant N \tag{4.69}$$

and truncate it with $\delta^4 y''(x_n)$.

The required sixth order difference scheme is obtained as

$$-y_{n-1}+2y_n-y_{n+1}+\frac{h^2}{240}\left[-y''_{n-2}+24y''_{n-1}+194y''_n+24y''_{n+1}-y''_{n+2}\right]=0 \tag{4.75}$$

The difference equation (4.75) has to be satisfied at the N points $x_1, x_2, \ldots, x_N$ inside (a, b). It is obvious that equation (4.75) associated with x_n involves not only the values of y'' at nodal points x_{n-1}, x_n and x_{n+1} but also at points x_{n-2} and x_{n+2}. Hence, when $n = 1$ or $n = N$, the difference equation (4.75) would involve a *fictitious* quantity $y''_{-1} = y''(a-h)$ or $y''_{N+2} = y''(b+h)$ so that a supplementary relation then would be required in correspondence with each of those values of n. Generally, in such cases we take a lower order difference equation near the end points. For example, if we satisfy the *Numerov* difference scheme (4.23) near the boundary points then the required system of nonlinear equations is given by

$$2y_1-y_2+\frac{h^2}{12}(10y''_1+y''_2) = A-\frac{h^2}{12}y''_0,\ n=1,$$

$$-y_{n-1}+2y_n-y_{n+1}+\frac{h^2}{240}(-y''_{n-2}+24y''_{n-1}+194y''_n+24y''_{n+1}-y''_{n+2})=0,$$

$$2 \leqslant n \leqslant N-1,$$

$$-y_{N-1}+2y_N+\frac{h^2}{12}(y''_{N-1}+10y''_N) = B-\frac{h^2}{12}y''_{N+1},\ n=N, \tag{4.76}$$

and hence can be written in matrix form

$$\mathbf{Jy}+\frac{h^2}{240}\mathbf{Bf(y)}-\boldsymbol{\alpha}=0, \tag{4.77}$$

where $\mathbf{J}$ is defined in (4.19), $\mathbf{B}$ and $\boldsymbol{\alpha}$ are given by

$$\mathbf{B}=\begin{bmatrix} 200 & 20 & & & & \\ 24 & 194 & 24 & -1 & & \\ -1 & 24 & 194 & 24 & -1 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & -1 & 24 & 194 & 24 \\ & & & & 20 & 200 \end{bmatrix}$$

$$\boldsymbol{\alpha} = \begin{bmatrix} A - \frac{h^2}{12} y_0'' \\ \frac{h^2}{240} y_0'' \\ 0 \\ \vdots \\ 0 \\ \frac{h^2}{240} y_{N+1}'' \\ B - \frac{h^2}{12} y_{N+1}'' \end{bmatrix}$$

The local truncation error of the method (4.75) is $0\,(h^8)$ but in application it is only $0\,(h^6)$ due to the first and the last equations in (4.76).

The nonlinear differential equation (4.4) subject to the mixed boundary conditions (4.58) can be replaced by the following system of equations:

$$\begin{aligned} &(1+hc)\,y_0 - y_1 + h^2\left(\frac{1}{3}f_0 + \frac{1}{6}f_1\right) + hA = 0, \\ &-y_{n-1} + 2y_n - y_{n+1} + h^2(\beta_0 f_{n-1} + \beta_1 f_n + \beta_2 f_{n+1}) = 0,\ 1 \leqslant n \leqslant N, \\ &-y_N + (1+hd)\,y_{N+1} + h^2\left(\frac{1}{6}f_N + \frac{1}{3}f_{N+1}\right) - hB = 0 \end{aligned} \qquad (4.78)$$

The sixth order difference scheme based on two off-step points can be applied to the nonlinear mixed boundary value problem as follows:

The system of nonlinear equations for the differential equation (4.4) is given by (4.72) for $1 \leqslant n \leqslant N$. The values of y at the points $x_{n\pm r}$ and $x_{n\pm s}$ can be obtained by using *Approximation II.* On substituting in (4.72) the values of $y_{n\pm r}$ and $y_{n\pm s}$ as given by (4.43) and (4.44), we get N nonlinear equations in $(N+2)$ unknown y_n, $0 \leqslant n \leqslant N+1$. The two more relations needed can be obtained by replacing the integrals in (4.59) and (4.60) by the four-point *Lobatto* quadrature formula and neglecting the truncations. We get

$$y_1 = y_0 + h\,y_0' + \frac{h^2}{12}\,[y_0'' + 5\,(s\,y_r'' + r\,y_s'')] \qquad (4.79)$$

and $$y_N = y_{N+1} - h\,y_{N+1}' + \frac{h^2}{12}\,[y_{N+1}'' + 5(s\,y_{N-r+1}'' + r\,y_{N-s+1}'')] \qquad (4.80)$$

Here the values of y_r, y_s, y_{N-r+1} and y_{N-s+1} are obtained from *Approximation III.*

Approximation III

$$y_q = (1-2q^3+q^4)\, y_0+(2q^3-q^4)\, y_1+(q-2q^3+q^4)\, h\, y_0'$$
$$+\frac{h^2}{6}\,[(2q^4-5q^3+3q^2)\, y_0'' +(q^4-q^3)\, y_1''\,] \qquad (4.81)$$

$$y_{N-q+1} = (1-2q^3+q^4)\, y_{N+1}+(2q^3-q^4)\, y_N-(q-2q^3+q^4)\, h\, y_{N+1}'$$
$$+\frac{h^2}{6}\,[(2q^4-5q^3+3q^2)\, y_{N+1}'' +(q^4-q^3)\, y_N''] \qquad (4.82)$$

The truncation error in (4.81) and (4.82) are respectively

$$T_q = Qh^5\, y^{(5)}(\xi_6^*),\ x_0 < \xi_6^* < x_1$$
$$T_q^* = -Qh^5 y^{(5)}\,(\xi^*),\ x_N < \xi_7^* < x_{N+1}$$
$$Q = \frac{1}{360}\,(3q^5-7q^4+4q^3)$$

The required two relations are given by

$$(1+ch)\, y_0-y_1+\frac{h^2}{12}\,[f(x_0,\, y_0)+5(sf(x_r,\, y_r)+rf(x_s,\, y_s)]+hA = 0 \qquad (4.83)$$

$$-y_N+ (1+dh)\, y_{N+1} +\frac{h^2}{12}\,[\,f(x_{N+1},\, y_{N+1})+5(sf(x_{N-r+1},\, y_{N-r+1})$$
$$+rf(x_{N-s+1},\, y_{N-s+1}))]-hB = 0 \qquad (4.84)$$

Thus, (4.72), (4.83) and (4.84) give the required $(N+2)$ nonlinear equations in the unknowns y_n, $0 \leqslant n \leqslant N+$ The truncation error is obtained as

$$T_n^* = \begin{cases} \left[\dfrac{1}{252000}\, y^{(8)}\,(x_n)+\dfrac{11}{108000}\, f_y\, y^{(5)}\,(x_n)+\ \dfrac{7}{3600}\, f_n\, f_{yyyy}\, y'\right]h^7 \\ \quad +0(h^8),\ n = 0,\ N+1 \\ \left[\dfrac{1}{302400}\, y^{(8)}\,(x_n)-\dfrac{1}{8640}\, f_y\, y^{(6)}\,(x_n)-\ \dfrac{1}{720}(\,f_{xy}+y'f_{yy})\, y^{(5)}\,(x_n)\right]h^8 \\ \quad +0(h^{10}),\ 1 \leqslant n \leqslant N \end{cases} \qquad (4.85)$$

We can again solve the nonlinear system by *Newton* method or by the iteration method given in Section 3.6.1. If pth approximation to the vector $\mathbf{y} = [y_0\, y_1\, \cdots\, y_{N+1}]^T$ is denoted by $\mathbf{y}^{(p)} = [y_0^{(p)}\ y_1^{(p)}\ \ldots\ y_{N+1}^{(p)}]^T$, then the iteration process for (4.77) can be described by the equations

$$\mathbf{J}\ \mathbf{y}^{(p+1)} = -\ \frac{h^2}{240}\ \mathbf{Bf}\,(\mathbf{y}^{(p)})+\boldsymbol{\alpha},\ p = 0,\ 1,\ 2,\ \ldots \qquad (4.86)$$

where $\mathbf{y}^{(0)}$ is the initial approximation of $\mathbf{y}$.

Example 4.4 Obtain the numerical solution of the nonlinear boundary value problem

$$y'' = \frac{1}{2}(1+x+y)^3$$

$$y'(0)-y(0) = -\frac{1}{2},\ y'(1)+y(1) = 1$$

with $h = \frac{1}{2}$ and $\frac{1}{64}$.

The analytical solution of the boundary value problem is

$$y(x) = \frac{2}{2-x}-x-1$$

We define the nodal points x_i

$$x_i = ih,\ h = 1/(N+1),\ i = 0, 1, 2, \ldots, N+1$$

Applying (4.78) with $\beta_0 = \beta_2 = 0$, $\beta_1 = 1$, to the boundary value problem, we get

$$(1+h)\,y_0-y_1+\frac{h^2}{2}\left[\frac{1}{3}(1+x_0+y_0)^3+\frac{1}{6}(1+x_1+y_1)^3\right]-\frac{h}{2} = 0$$

$$-y_{n-1}+2y_n-y_{n+1}+\frac{1}{2}h^2(1+x_n+y_n)^3 = 0,\ 1 \leqslant n \leqslant N$$

$$-y_N+(1+h)\,y_{N+1}+\frac{h^2}{2}\left[\frac{1}{6}(1+x_N+y_N)^3+\frac{1}{3}(1+x_{N+1}+y_{N+1})^3\right]-h = 0$$

The system of nonlinear equations has been solved by the *Newton* method. For $N = 1$, i.e., $h = 1/2$, we get

$$\frac{3}{2}y_0-y_1+\frac{1}{8}\left(\frac{1}{3}(1+y_0)^3+\frac{1}{6}\left(\frac{3}{2}+y_1\right)^3\right)-\frac{1}{4} = 0$$

$$-y_0+2y_1-y_2+\frac{1}{8}\left(\frac{3}{2}+y_1\right)^3 = 0$$

$$-y_1+\frac{3}{2}y_2+\frac{1}{8}\left(\frac{1}{6}\left(\frac{3}{2}+y_1\right)^3+\frac{1}{3}(2+y_2)^3\right)-\frac{1}{2} = 0$$

The Newton method gives the following linear equations

$$\begin{bmatrix} \frac{3}{2}+\frac{1}{8}(1+y_0^{(p)})^2 & -1+\frac{1}{16}\left(\frac{3}{2}+y_1^{(p)}\right)^2 & 0 \\ -1 & 2+\frac{3}{8}\left(\frac{3}{2}+y_1^{(p)}\right)^2 & -1 \\ 0 & -1+\frac{1}{16}\left(\frac{3}{2}+y_1^{(p)}\right)^2 & \frac{3}{2}+\frac{1}{8}(2+y_2^{(p)})^2 \end{bmatrix} \begin{bmatrix} \Delta y_0^{(p)} \\ \Delta y_1^{(p)} \\ \Delta y_2^{(p)} \end{bmatrix}$$

$$+\begin{bmatrix} \frac{3}{2}y_0^{(p)} - y_1^{(p)} + \frac{1}{8}\left[\frac{1}{3}(1+y_0^{(p)})^3 + \frac{1}{6}\left(\frac{3}{2}+y_1^{(p)}\right)^3\right] - \frac{1}{4} \\ -y_0^{(p)} + 2y_1^{(p)} - y_2^{(p)} + \frac{1}{8}\left(\frac{3}{2}+y_1^{(p)}\right)^3 \\ -y_1^{(p)} + \frac{3}{2}y_2^{(p)} + \frac{1}{8}\left[\frac{1}{6}\left(\frac{3}{2}+y_1^{(p)}\right)^3 + \frac{1}{3}(2+y_2^{(p)})^3\right] - \frac{1}{2} \end{bmatrix} = 0$$

where

$$y_0^{(p+1)} = y_0^{(p)} + \Delta y_0^{(p)}$$
$$y_1^{(p+1)} = y_1^{(p)} + \Delta y_1^{(p)}$$
$$y_2^{(p+1)} = y_2^{(p)} + \Delta y_2^{(p)}$$

Using $y_0^{(0)} = 0.001$, $y_1^{(0)} = -0.1$, $y_2^{(0)} = 0.001$, we get, after three iterations

$$y_0^{(3)} = -0{,}0023,\ y_1^{(3)} = -0.1622,\ y_2^{(3)} = -0.0228.$$

The numerical results with $h = 1/64$ at the interval of $1/4$ are given in Table 4.4.

TABLE 4.4 SOLUTION OF $y'' = \frac{1}{2}(1+x+y)^3$, $y'(0)-y(0) = -1/2$, $y'(1)+y(1) = 1$, $h = 1/64$

x_i	y_i	$y(x_i)$
0.0	0.000028	0.0
0.25	−0.107106	−0.107143
0.50	−0.166622	−0.166667
0.75	−0.149948	−0.15
1.00	0.000048	0.0

4.4 NONLINEAR BOUNDARY VALUE PROBLEM $y'' = f(x, y, y')$

We consider the general second order nonlinear differential equation

$$y'' = f(x, y, y'),\ x \in [a, b] \tag{4.87}$$

subject to appropriate boundary conditions. Letting $y' = z$, we assume that, for $x \in [a, b]$ and $-\infty < y, z < \infty$,

(i) $f(x, y, z)$ is continuous,

(ii) $\frac{\partial f}{\partial y}$ and $\frac{\partial f}{\partial z}$ exist and are continuous,

(iii) $\frac{\partial f}{\partial y} > 0$ and $\left|\frac{\partial f}{\partial z}\right| \leq W$, for some positive W.