3

Multistep Methods

3.1 INTRODUCTION

The numerical methods for the solution of the differential equation

$$y' = f(t, y),\ y(t_0) = y_0,\ t \in [t_0, b] \tag{3.1}$$

are called multistep methods if the value of $y(t)$ at $t = t_{n+1}$ uses the values of the dependent variable and its derivative at more than one grid or mesh points. Let us suppose that we have already obtained approximate values of of y and $y' = f(t, y)$ at the points $t_m = t_0+mh$, $m = 1, 2, \ldots, n$. We denote the approximate values at these points by

$$y(t_m) = y_m,\ f(t_m, y(t_m)) = f_m,\ m = 0, 1, \ldots, n$$

Then the general multistep or k-step method for the solution of (3.1) may be written as

$$\begin{aligned} y_{n+1} = a_1 y_n + a_2 y_{n-1} + \cdots + a_k y_{n-k+1} + h\, \Phi\, (t_{n+1}, t_n, \ldots, t_{n-k+1}, \\ y'_{n+1}, y'_n, \cdots y'_{n-k+1}; h) \end{aligned} \tag{3.2}$$

where h is the constant stepsize and $a_1, a_2, \ldots a_k$ are real given constants. If Φ is independent of y'_{n+1}, then the general multistep method is called an *explicit*, open or predictor method; otherwise an *implicit*, closed or corrector method.

The truncation or discretization error of the method (3.2) at $t = t_n$ is given by

$$\begin{aligned} T(y(t_n), h) = y(t_{n+1}) - a_1\, y(t_n) - \cdots - a_k\, y(t_{n-k+1}) \\ - h\, \Phi\, (t_{n+1}, t_n, \ldots, t_{n-k+1}, y'(t_{n+1}), \\ y'(t_n), \ldots, y'(t_{n-k+1})) \end{aligned} \tag{3.3}$$

If p is the largest integer such that

$$|\, h^{-1}\, T(y(t_n), h)\,| = 0(h^p), \tag{3.4}$$

then p is said to be the order of the general multistep method.

A linear form

$$\begin{aligned} y_{n+1} = a_1\, y_n + a_2\, y_{n-1} + \cdots + a_k\, y_{n-k+1} \\ + h\, (b_0\, y'_{n+1} + b_1\, y'_n + \cdots + b_k y'_{n-k+1}) \end{aligned} \tag{3.5}$$

of (3.2) is called the general linear multistep method. The constants a_i's and b_i's are real and known. The $k-1$ values $y_1, y_2, \ldots, y_{k-1}$ required to start the computation in (3.5) are obtained, using the single step methods. The special cases of the linear multistep method (3.5) are used for solving the initial value problem (3.1).

3.2 EXPLICIT MULTISTEP METHODS

By integrating the differential equation $y' = f(t, y)$ between the limits t_{n-j} and t_{n+1}, we get

$$y(t_{n+1}) = y(t_{n-j}) + \int_{t_{n-j}}^{t_{n+1}} f(t, y)\, dt \tag{3.6}$$

To carry out integration in (3.6), we can approximate $f(t, y)$ by a polynomial which interpolates $f(t, y)$ at k points $t_n, t_{n-1}, \ldots, t_{n-k+1}$. We will use the Newton backward difference formula of degree $(k-1)$ for this purpose. If $f(t, y)$ has k continuous derivatives, then we have

$$\begin{aligned} P_{k-1}(t) = f_n &+ (t-t_n)\frac{\nabla f_n}{h} + \frac{(t-t_n)(t-t_{n-1})}{2!}\frac{\nabla^2 f_n}{h^2} + \ldots \\ &+ \frac{(t-t_n)(t-t_{n-1})\ldots(t-t_{n-k+2})}{(k-1)!}\frac{\nabla^{k-1} f_n}{h^{k-1}} \\ &+ \frac{(t-t_n)(t-t_{n-1})\ldots(t-t_{n-k+1})}{k!} f^{(k)}(\xi) \end{aligned} \tag{3.7}$$

where $f^{(k)}(\xi)$ is the kth derivative of f evaluated at some ξ in an interval containing t, t_{n-k+1} and t_n.

Substituting $u = (t-t_n)/h$ in (3.7), we get

$$\begin{aligned} P_{k-1}(t_n+hu) &= f_n + u\,\nabla f_n + \frac{u(u+1)}{2!}\nabla^2 f_n + \ldots \\ &\quad + \frac{u(u+1)\ldots(u+k-2)}{(k-1)!}\nabla^{k-1} f_n \\ &\quad + \frac{u(u+1)\ldots(u+k-1)}{k!} h^k f^{(k)}(\xi) \\ &= \sum_{m=0}^{k-1} (-1)^m \binom{-u}{m} \nabla^m f_n + (-1)^k \binom{-u}{k} h^k f^{(k)}(\xi) \end{aligned} \tag{3.8}$$

where $$\binom{-u}{m} = (-1)^m \frac{u(u+1)\ldots(u+m-1)}{m!}$$

Inserting (3.8) into (3.6) and putting $dt = h\,du$, we obtain

$$y(t_{n+1}) = y(t_{n-j}) + h \int_{-j}^{1} \left[\sum_{m=0}^{k-1} (-1)^m \binom{-u}{m} \nabla^m f_n \right.$$

$$+(-1)^k\binom{-u}{k}h^k f^{(k)}(\xi)\Big]\,du$$

$$= y(t_{n-j})+h\sum_{m=0}^{k-1}\gamma_m^{(j)}\nabla^m f_n+T_k^{(j)} \tag{3.9}$$

where $$T_k^{(j)} = h^{k+1}\int_{-j}^{1}(-1)^k\binom{-u}{k}f^{(k)}(\xi)\,du$$

$$\gamma_m^{(j)} = \int_{-j}^{1}(-1)^m\binom{-u}{m}du \tag{3.10}$$

If we ignore the remainder term $T_m^{(j)}$ in (3.9), we get

$$y_{n+1} = y_{n-j}+h\sum_{m=0}^{k-1}\gamma_m^{(j)}\nabla^m f_n \tag{3.11}$$

On calculating a few of $\gamma_m^{(j)}$ from (3.10), we obtain

$$\gamma_0^{(j)} = \int_{-j}^{1}du = 1+j$$

$$\gamma_1^{(j)} = \int_{-j}^{1}u\,du = \frac{1}{2}(1-j)(1+j)$$

$$\gamma_2^{(j)} = \int_{-j}^{1}\frac{1}{2}u(u+1)\,du = \frac{1}{12}(5-3j^2+2j^3)$$

$$\gamma_3^{(j)} = \int_{-j}^{1}\frac{1}{6}u(u+1)(u+2)\,du = \frac{1}{24}(3-j)(3+j-j^2+j^3)$$

$$\gamma_4^{(j)} = \int_{-j}^{1}\frac{1}{24}u(u+1)(u+2)(u+3)\,du$$

$$= \frac{1}{720}(251-90j^2+110j^3-45j^4+6j^5)$$

$$\gamma_5^{(j)} = \int_{-j}^{1}\frac{1}{120}u(u+1)(u+2)(u+3)(u+4)\,du$$

$$= \frac{1}{1440}(5-j)(95+19j-25j^2+35j^3-14j^4+2j^5)$$

An alternative form of formula (3.11) can be obtained if the differences $\nabla^m f_n$ are expressed in terms of the function values f_m.

$$y_{10} = .5254828+\frac{.1}{12}[23\,(-.2761322)$$

$$-16\,(-.3076785)+5(-.3449723)]$$

$$y_{10} = .4992074$$

Example 3.2 Apply the Adams-Bashforth formula of order four to $y' = t+y$, $y(0) = 1$ to compute approximation to $y\,(1)$ with $h = .1$.

We need here the values of $y\,(t)$ at $t = .1, .2$ and $.3$ in order to start the computation. These values are determined by the Runge-Kutta method or Taylor's series method of the same order. The values have been obtained in Example 2.2. The exact solution is

$$y\,(t) = 2e^t-t-1$$

We have

$$y\,(0) = 1.0$$

$$y\,(.1) = 1.110342$$

$$y\,(.2) = 1.242806$$

$$y\,(.3) = 1.399718$$

and

$$f\,(t_0, y_0) = 1.000000$$

$$f\,(0.1, y(0.1)) = 1.210342$$

$$f\,(0.2, y(0.2)) = 1.442806$$

$$f\,(0.3, y(0.3)) = 1.699718$$

Then

$$y\,(.4) = 1.399718+\frac{.1}{24}[55\,(1.699718)-59\,(1.442806)$$

$$+37\,(1.210342)-9] = 1.583641$$

The computed value of $y\,(.4)$ is in error in the last figure. Using the local error estimate, we have

$$|\,T_4^{(0)}\,| \leqslant \frac{251}{720}h^5 \max_{0\leqslant t\leqslant 0.4} |\,f^{(4)}\,(t)\,|$$

where

$$f^{(4)}\,(\xi) = y^{(5)}\,(\xi) = 2e^{\xi}$$

Therefore

$$|\,T_4^{(0)}\,| \leqslant \frac{251}{720}\times 10^{-5}\times 2e^{.4}$$

$$= 3.48611\times 10^{-6}\times 2.98364$$

or

$$|\,T_4^{(0)}\,| \leqslant 0.11\times 10^{-4}$$

This bound is much larger than the actual error 0.8×10^{-5}. The complete solution is given in Table 3.2.

TABLE 3.2 SOLUTION OF $y' = t+y$, $y(0) = 1$, $0 \leq t \leq 1$ BY FOURTH ORDER ADAMS-BASHFORTH METHOD, $h = 0.1$

t_n	y_n	$y(t_n)$
0	1	1
0.1	1.1103418	1.1103418
0.2	1.2428055	1.2428055
0.3	1.3997176	1.3997176
0.4	1.5836409	1.5836494
0.5	1.7974227	1.7974425
0.6	2.0442050	2.0442376
0.7	2.3274574	2.3275054
0.8	2.6510155	2.6510819
0.9	3.0191182	3.0192062
1.0	3.4364501	3.4365637

3.2.2 Nystrom formulas ($j = 1$)

Substituting $j = 1$ in formula (3.11), we get

$$y_{n+1} = y_{n-1}+h\left[2f_n+\frac{1}{3}\nabla^2 f_n+\frac{1}{3}\nabla^3 f_n+\frac{29}{90}\nabla^4 f_n+\frac{14}{45}\nabla^5 f_n+\dots\right]$$

In order to obtain the formula of order k, we retain the terms in the bracket upto $\nabla^{k-1} f_n$ inclusive. Nystrom's formula ($j = 1$) in terms of function values is given by (3.13). The coefficient $\gamma_m^{*(1)}$ are given in Table 3.3.

TABLE 3.3 COEFFICIENTS FOR THE FORMULA

$$y_{n+1} = y_{n-1}+h\sum_{m=0}^{k-1}\gamma_m^{*(1)} f_{n-m}$$

k	$\gamma_0^{*(1)}$	$\gamma_1^{*(1)}$	$\gamma_2^{*(1)}$	$\gamma_3^{*(1)}$	$\gamma_4^{*(1)}$	$\gamma_5^{*(1)}$
1	2					
2	2	0				
3	$\frac{7}{3}$	$-\frac{2}{3}$	$\frac{1}{3}$			
4	$\frac{8}{3}$	$-\frac{5}{3}$	$\frac{4}{3}$	$-\frac{1}{3}$		
5	$\frac{269}{90}$	$-\frac{266}{90}$	$\frac{294}{90}$	$-\frac{146}{90}$	$\frac{29}{90}$	
6	$\frac{279}{90}$	$-\frac{406}{90}$	$\frac{574}{90}$	$-\frac{426}{90}$	$\frac{169}{90}$	$-\frac{28}{90}$

3.2.3 Formulas for $j = 0, 1, 3, 5$

The formula we get with j odd and with j differences retained in (3.11) are of particular interest since in these cases it can be seen that the coefficient of the jth difference is zero, and the use of $j-1$ or j differences gives the same accuracy. The coefficients $\gamma_m^{(j)}$, $j = 0, 1, 3, 5$ are given in Table 3.4.

TABLE 3.4 COEFFICIENTS FOR THE FORMULA

$$y_{n+1} = y_{n-j} + h \sum_{m=0}^{k-1} \gamma_m^{(j)} \nabla^m f_n, \; j = 0, 1, 3, 5$$

j	$\gamma_0^{(j)}$	$\gamma_1^{(j)}$	$\gamma_2^{(j)}$	$\gamma_3^{(j)}$	$\gamma_4^{(j)}$	$\gamma_5^{(j)}$
0	1	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{475}{1440}$
1	2	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{29}{90}$	$\frac{14}{45}$
3	4	-4	$\frac{8}{3}$	0	$\frac{14}{45}$	$\frac{14}{45}$
5	6	-12	15	-9	$\frac{33}{10}$	0

3.2.4 Results from computation for predictor methods

We have used the Adams-Bashforth and Nystrom formulas of order two to five to solve numerically the following initial value problems:

(i) $y' = -y, \qquad y(0) = 1,$

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

(iii) $y' = -t\,(y+y^2), \qquad y(0) = 1,$

with stepsizes 2^{-m}, $m = 5\,(1)\,8$.

Determining the starting values from the analytical solution, the computation has been carried out in double precision and the error values ϵ_n at $t = 5$ are tabulated in Tables 3.5 and 3.6.

From Table 3.5, we find that the high order Adams-Bashforth predictor methods are best suited if high degree of accuracy is desired and the low order predictor methods are best suited if accuracy requirements are low.

The Nystrom methods (see Table 3.6) produce inferior results in comparison to the Adams-Bashforth methods. The error values for the high order Nystrom methods are grossly inconsistent with the one for low order methods. This indicates that the high order methods are not suitable with respect to stability.