

Thus the solution of the difference equation (3.58) is given by

$$y_n = \bar{c}_1 e^{n\bar{h}} + \bar{c}_2 (-1)^n e^{-1/3n\bar{h}}$$

It is obvious that for $\lambda > 0$, ξ_{1h} behaves as the exact solution and ξ_{2h} dies out since $|\xi_{2h}| < 1$, but for $\lambda < 0$, ξ_{1h} decreases as does the exact solution but ξ_{2h} oscillates with increasing amplitude. This behaviour is independent of h . Therefore, Milne's method is stable for $\bar{h} = 0$ but unstable for $\bar{h} < 0$. It is a weakly stable method.

3.5.5 Propagated error estimates

The constants A_1, A_2, \dots, A_k in (3.47) are chosen so that the initial conditions are satisfied; thus

$$\begin{aligned} E_0 &= A_1 + A_2 + \dots + A_k \\ E_1 &= A_1 \xi_{1h} + A_2 \xi_{2h} + \dots + A_k \xi_{kh} \\ &\vdots \\ E_{k-1} &= A_1 \xi_{1h}^{k-1} + A_2 \xi_{2h}^{k-1} + \dots + A_k \xi_{kh}^{k-1} \end{aligned}$$

where
$$E_j = \epsilon_j - \frac{T}{h\lambda\rho'(1)}, \quad j = 0, 1, 2, \dots, k-1$$

The principal root ξ_{1h} of the characteristic equation for sufficiently small λh is approximately equal to $e^{\lambda h}$. The other roots $\xi_{2h}, \xi_{3h}, \dots, \xi_{kh}$ are extraneous roots. The stability of the numerical method requires that these extraneous roots have magnitude less than unity so that the corresponding components of the error are negligible. For stable methods we therefore do not need to know A_2, \dots, A_k . To find A_1 , we use *Cramer's rule* and obtain

$$A_1 = \frac{\begin{vmatrix} E_0 & 1 & \dots & 1 \\ E_1 & \xi_{2h} & \dots & \xi_{kh} \\ \vdots & \vdots & \ddots & \vdots \\ E_{k-1} & \xi_{2h}^{k-1} & \dots & \xi_{kh}^{k-1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \dots & 1 \\ \xi_{1h} & \xi_{2h} & \dots & \xi_{kh} \\ \vdots & \vdots & \ddots & \vdots \\ \xi_{1h}^{k-1} & \xi_{2h}^{k-1} & \dots & \xi_{kh}^{k-1} \end{vmatrix}} \quad (3.61)$$

Substituting

$$C(\xi_{1h}) = c_{k-1} \xi_{1h}^{k-1} + c_{k-2} \xi_{1h}^{k-2} + \dots + c_0,$$

in Equation (3.61), we can write

$$A_1 = \frac{c_{k-1} E_{k-1} + c_{k-2} E_{k-2} + \dots + c_0 E_0}{C(\xi_{1h})}$$

which, if the initial errors ϵ_i are constant and equal to ϵ , becomes

$$A_1 = \left(\epsilon - \frac{T}{h\lambda\rho'(1)} \right) \frac{C(1)}{C(\xi_{1h})}$$

In (3.47) we now substitute this last expression for A_1 and put $\xi_{1h} = e^{\lambda h}$. Substituting $nh = t_n - t_0$ and neglecting the factor $C(1)/C(\xi_{1h})$ which is close to unity, since ξ_{1h} as $h \rightarrow 0$ is equal to 1, we get the estimate of the propagated error for any stable formula as

$$\epsilon_n \approx \left(\epsilon - \frac{T}{h\lambda\rho'(1)} \right) \exp(\lambda(t_n - t_0)) + \frac{T}{h\lambda\rho'(1)} \quad (3.62)$$

The first term is dominant when $\lambda > 0$, while the second term is dominant when $\lambda < 0$. For small λ it is worth noting the existence of the limit in (3.62) as $\lambda \rightarrow 0$. It yields an expression which increases linearly with $(t_n - t_0)$.

3.6 PREDICTOR-CORRECTOR METHODS

We now discuss the application of the multistep methods for the solution of the initial value problems.

3.6.1 Use of implicit multistep methods

Let us assume that the values of the ordinates and slopes are given at k points. We are required to determine y_{n+1} from the formula

$$y_{n+1} = h b_0 f(t_{n+1}, y_{n+1}) + \sum_{i=1}^k [a_i y_{n-i+1} + h b_i f_{n-i+1}]$$

As we cannot solve y_{n+1} directly, we use an iterative procedure:

P: Predict some value $y_{n+1}^{(0)}$ for y_{n+1}

E: Evaluate $f(t_{n+1}, y_{n+1}^{(0)})$

C: Correct $y_{n+1}^{(0)}$ to obtain a new $y_{n+1}^{(1)}$ for y_{n+1}

$$y_{n+1}^{(1)} = h b_0 f(t_{n+1}, y_{n+1}^{(0)}) + \sum_{i=1}^k [a_i y_{n-i+1} + h b_i f_{n-i+1}]$$

E: Evaluate $f(t_{n+1}, y_{n+1}^{(1)})$

C: Correct $y_{n+1}^{(1)}$

$$y_{n+1}^{(2)} = h b_0 f(t_{n+1}, y_{n+1}^{(1)}) + \sum_{i=1}^k [a_i y_{n-i+1} + h b_i f_{n-i+1}]$$

⋮

The sequence of operations

PECECE...

determines for y_{n+1} a sequence of values

$$y_{n+1}^{(0)}, y_{n+1}^{(1)}, y_{n+1}^{(2)}, \dots \quad (3.63)$$

Let us examine the convergence of this sequence.

THEOREM 3.7 Let $y_{n+1}^{(p)}$ be a sequence of approximations to y_{n+1} . If for all values of y close to y_{n+1} and including the values $y = y_{n+1}^{(0)}, y_{n+1}^{(1)}, \dots$, we have

$$\left| \frac{\partial f}{\partial y}(t_n, y) \right| \leq L \tag{3.64}$$

where L satisfies $L < |1/hb_0|$, then the sequence $\{y_{n+1}^{(p)}\}$ converges to y_{n+1} .

For the Adams-Moulton methods, we have

$$\begin{aligned} |hL| < 2 &= 2.0 \text{ for second order method,} \\ |hL| < \frac{12}{5} &= 2.4 \text{ for third order method,} \\ |hL| < \frac{8}{3} &= 2.67 \text{ for fourth order method,} \\ |hL| < \frac{720}{251} &= 2.87 \text{ for fifth order method.} \end{aligned}$$

3.6.2 P(EC)^m E scheme

The determination of y_{n+1} at t_{n+1} from an implicit multistep method with an assumed value $y_{n+1}^{(0)}$ requires the procedure Predict-Estimate-Correct-... (PECECE...) which converges to y_{n+1} if $|hLb_0| < 1$.

A simple way to find $y_{n+1}^{(0)}$ is to use an explicit method. Thus, a predictor formula (explicit multistep formula) is used to obtain a first estimate of the next value of the dependent variable and the corrector formula is applied iteratively until convergence is obtained. This we shall denote by P(EC)^m E. The predictor-corrector scheme

$$y_{n+1}^{(0)} = \sum_{i=1}^k (a_i^{(0)} y_{n-i+1} + h b_i^{(0)} f_{n-i+1}) \tag{3.65}$$

$$y_{n+1}^{(\mu)} = \sum_{i=1}^k (a_i y_{n-i+1} + h b_i f_{n-i+1}) + h b_0 f_{n+1}^{(\mu-1)} \quad \mu = 1 (1) m \tag{3.66}$$

$$y_{n+1} = y_{n+1}^{(m)} \tag{3.67}$$

is a P(EC)^m E scheme if $f_{n+1} = f_{n+1}^{(m)}$

where $f_{n+1}^{(\mu)} = f(t_{n+1}, y_{n+1}^{(\mu)})$

Let us illustrate P(EC)^mE scheme for the equation $y' = \lambda y$;

$$P : y_{n+1}^{(0)} = \sum_{i=1}^k (a_i^{(0)} + h\lambda b_i^{(0)}) y_{n-i+1}$$

$$E : y_{n+1}^{(0)} = \lambda y_{n+1}^{(0)}$$

$$C : y_{n+1}^{(1)} = \sum_{i=1}^k (a_i + h\lambda b_i) y_{n-i+1}$$

$$+ h\lambda b_0 \sum_{i=1}^k (a_i^{(0)} + h\lambda b_i^{(0)}) y_{n-i+1}$$

The $P(EC)^mE$ scheme can be written as

$$\begin{aligned} y_{n+1}^{(0)} &= y_n + hf_n \\ y_{n+1}^{(\mu)} &= y_n + \frac{h}{2} (f_{n+1}^{(\mu-1)} + f_n), \quad \mu = 1(1)m \\ y_{n+1} &= y_{n+1}^{(m)} \\ f_{n+1} &= f_{n+1}^{(m)} \end{aligned} \quad (3.72)$$

where $f_{n+1}^{(\mu)} = f(t_{n+1}, y_{n+1}^{(\mu)})$

Let us examine the equation $y' = \lambda y$. The true solution is $y(t) = c \exp(\lambda t)$, so that $y(t_{n+1}) = e^{\lambda h} y(t_n)$.

The above $P(EC)^mE$ scheme becomes

$$\begin{aligned} y_{n+1}^{(0)} &= (1 + \lambda h) y_n \\ y_{n+1}^{(1)} &= y_n + \frac{h}{2} [\lambda(1 + \lambda h) y_n + \lambda y_n] \\ &= \left(1 + \lambda h + \frac{(\lambda h)^2}{2} \right) y_n \\ y_{n+1}^{(2)} &= y_n + \frac{h}{2} \left[\lambda \left(1 + \lambda h + \frac{(\lambda h)^2}{2} \right) y_n + \lambda y_n \right] \\ &= \left(1 + \lambda h + \frac{(\lambda h)^2}{2} + \frac{(\lambda h)^3}{4} \right) y_n \\ y_{n+1}^{(m)} &= \left(1 + \lambda h + \frac{(\lambda h)^2}{2} + \frac{(\lambda h)^3}{4} + \dots + \frac{(\lambda h)^{m+1}}{2^m} \right) y_n \\ &= \left(1 + \lambda h + \frac{(\lambda h)^2 \left(1 - \left(\frac{\lambda h}{2} \right)^m \right)}{1 - \frac{\lambda h}{2}} \right) y_n \\ &= \left(\frac{1 + \frac{\lambda h}{2} - 2 \left(\frac{\lambda h}{2} \right)^{m+2}}{1 - \frac{\lambda h}{2}} \right) y_n \\ \text{Therefore, } y_{n+1} &= \left(\frac{1 + \frac{\lambda h}{2} - 2 \left(\frac{\lambda h}{2} \right)^{m+2}}{1 - \frac{\lambda h}{2}} \right) y_n \end{aligned} \quad (3.73)$$

If the corrector is iterated to converge, i.e. $m \rightarrow \infty$, Equation (3.73) will converge if $|\lambda h| < 2$, which is the required condition.

The truncation error and the stability of $P(EC)^mE$ scheme can be determined if we substitute $y_n = y(t_n) + \epsilon_n$ in (3.73). We find

$$\epsilon_{n+1} + y(t_{n+1}) = \left(\frac{1 + \frac{\lambda h}{2} - 2 \left(\frac{\lambda h}{2} \right)^{m+2}}{1 - \frac{\lambda h}{2}} \right) (y(t_n) + \epsilon_n)$$

or

$$\begin{aligned} \epsilon_{n+1} &= \left(\frac{1 + \frac{\lambda h}{2} - 2 \left(\frac{\lambda h}{2} \right)^{m+2}}{1 - \frac{\lambda h}{2}} - e^{\lambda h} \right) y(t_n) \\ &\quad + \left(\frac{1 + \frac{\lambda h}{2} - 2 \left(\frac{\lambda h}{2} \right)^{m+2}}{1 - \frac{\lambda h}{2}} \right) \epsilon_n \end{aligned} \quad (3.74)$$

The first term on the right hand side of (3.74) is the local truncation error while the second term is the contribution to the error from the previous step. The relative local truncation error given by

$$\frac{1 + \frac{\lambda h}{2} - 2 \left(\frac{\lambda h}{2} \right)^{m+2}}{1 - \frac{\lambda h}{2}} - e^{\lambda h}$$

becomes

- $-\frac{1}{2}(\lambda h)^2 + O(|\lambda h|^3)$ for 0 corrector
- $-\frac{1}{6}(\lambda h)^3 + O(|\lambda h|^4)$ for 1 corrector
- $\frac{1}{12}(\lambda h)^3 + O(|\lambda h|^4)$ for 2 corrector
- $\frac{1}{12}(\lambda h)^3 + O(|\lambda h|^4)$ for 3 corrector

We thus see that the application of the corrector more than twice does not improve the result because the minimum local truncation error is obtained at this stage.

3.6.3 Results from computation for Adams $P-C$ methods

The following initial value problems

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

Assume that ϵ_i changes slowly from step to step and that $h\epsilon_i$ is small compared to the truncation error. Subtracting (3.80) from (3.79), we get

$$y_{n+1}^{(P)} - y_{n+1}^{(C)} = (C_{p+1} - C_{p+1}^*) h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}) \quad (3.81)$$

Thus the estimates of the truncation error in predictor and corrector formula can be written as

$$\begin{aligned} & C_{p+1}^* h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}) \\ &= C_{p+1}^* (C_{p+1} - C_{p+1}^*)^{-1} (y_{n+1}^{(P)} - y_{n+1}^{(C)}) \end{aligned}$$

and $C_{p+1} h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2})$

$$= C_{p+1} (C_{p+1} - C_{p+1}^*)^{-1} (y_{n+1}^{(P)} - y_{n+1}^{(C)})$$

The above estimates enable us to control and adjust the step size in $P-C$ set. However, if we assume that the predicted and corrected values at each step change slowly, we can write

$$m_{n+1} = p_{n+1} + C_{p+1}^* (C_{p+1} - C_{p+1}^*)^{-1} (p_n - c_n)$$

which will be a modified value of the predicted value. Similarly the modified value of the corrected value will be

$$y_{n+1} = c_{n+1} + C_{p+1} (C_{p+1} - C_{p+1}^*)^{-1} (p_{n+1} - c_{n+1})$$

where m_{n+1} and y_{n+1} denote the modified predicted and corrected values of y_{n+1} .

Thus the modified $P-C$ scheme becomes

$$\text{Predict : } p_{n+1} = \sum_{i=1}^k (a_i^{(0)} y_{n-i+1} + h b_i^{(0)} y'_{n-i+1})$$

$$\text{Modify : } m_{n+1} = p_{n+1} + C_{p+1}^* (C_{p+1} - C_{p+1}^*)^{-1} (p_n - c_n)$$

$$\text{Correct : } c_{n+1} = \sum_{i=1}^{k-1} (a_i y_{n-i+1} + h b_i y'_{n-i+1}) + h b_0 m_{n+1}$$

Final value :

$$y_{n+1} = c_{n+1} + C_{p+1} (C_{p+1} - C_{p+1}^*)^{-1} (p_{n+1} - c_{n+1}) \quad (3.82)$$

The Runge-Kutta method may be used to calculate the starting values, i.e. y_1, y_2, \dots, y_n . The quantity $p_n - c_n$ that is needed for the modification on the first step is generally put

$$p_n - c_n = 0$$

The characteristic equation can be obtained if we substitute $y' = \lambda y$ and $p_n = A_1 \xi^n, y_n = A_2 \xi^n, m_n = A_3 \xi^n, c_n = A_4 \xi^n$ in (3.82). We find a system of four simultaneous linear homogeneous equations in the constants A_1, A_2, A_3 and A_4 . For this system to have a nonzero solution it is necessary that the determinant of the coefficient matrix vanishes. This leads to

$$\left| \begin{array}{cccc}
 \xi^k & -\xi^k + (\rho^{(0)}(\xi)) & 0 & 0 \\
 & -h\lambda\sigma^{(0)}(\xi) & & \\
 \xi + \frac{C_{p+1}^*}{C_{p+1} - C_{p+1}^*} & 0 & -\xi & -\frac{C_{p+1}^*}{C_{p+1} - C_{p+1}^*} \\
 0 & \xi^k - (\rho(\xi) - h\lambda\sigma(\xi)) & h\lambda b_0 \xi^k & -\xi^k \\
 & -h\lambda b_0 \xi^k & & \\
 \frac{C_{p+1}}{C_{p+1} - C_{p+1}^*} & -1 & 0 & -\frac{C_{p+1}^*}{C_{p+1} - C_{p+1}^*}
 \end{array} \right| = 0 \tag{3.83}$$

where $\rho^{(0)}(\xi)$, $\sigma^{(0)}(\xi)$, $\rho(\xi)$ and $\sigma(\xi)$ are defined in (3.69). Simplifying, (3.83), we get

$$\left[h\lambda b_0 (\xi - 1) - \frac{C_{p+1}}{C_{p+1}^*} \xi \right] (\rho^{(0)}(\xi) - h\lambda\sigma^{(0)}(\xi)) + \xi^{k-k+1} (\rho(\xi) - h\lambda\sigma(\xi)) = 0 \tag{3.84}$$

as the characteristic equation of the modified predictor-corrector method.

On simplifying the characteristic equation (3.84) for the Adams predictor-corrector methods, we find

$$\sum_{i=0}^{k+2} c_i \xi^{k+2-i} = 0 \tag{3.85}$$

where the coefficients c_i are given by

$$\begin{aligned}
 c_0 &= 1 - R \\
 c_1 &= (R - \theta)(1 + \bar{h}b_1^{(0)}) - \theta - (1 + \bar{h}b_1) \\
 c_2 &= (R - \theta)\bar{h}b_2^{(0)} + \theta(1 + \bar{h}b_1^{(0)}) - \bar{h}b_2 \\
 c_j &= (R - \theta)\bar{h}b_j^{(0)} + \theta\bar{h}b_{j-1}^{(0)} - \bar{h}b_j, \quad j = 3, \dots, k+2
 \end{aligned} \tag{3.86}$$

$$\begin{aligned}
 \text{and } b_{k+1} &= 0 & R &= \frac{C_{k+1}}{C_{k+1}^*} \\
 b_{k+2} &= 0 & \bar{h} &= \lambda h \\
 b_{k+2}^{(0)} &= 0 & \theta &= \bar{h}b_0
 \end{aligned}$$

Equation (3.85) is a $(k+2)$ th degree polynomial and will have one principal root, and $k+1$ extraneous roots.

The principal root will approximate the true solution $e^{\bar{h}}$ of the differential equation $y' = \lambda y$, $y(0) = 1$, $\bar{h} \leq 0$. We are concerned with the rate of growth of the extraneous roots as n gets large. The extraneous roots will not produce undesirable effects on the numerical solution if the predictor-corrector is stable and convergent, that is $|\theta| < 1$. The predictor-corrector is stable if and only if the roots of (3.85) are inside the unit circle; it is also

The absolute value of the largest root of Equation (3.85) is shown in Figure 3.9.

Example 3.5 Solve the initial value problem

$$y' = t + y, y(0) = 1, t \in [0, 1]$$

using second order Adams modified predictor-corrector method for step length $h = .1$.

In order to apply the second order Adams modified $P-C$ method

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

$$m_{n+1} = p_{n+1} - \frac{5}{6} (p_n - c_n)$$

$$c_{n+1} = y_n + \frac{h}{2} (m'_{n+1} + y'_n)$$

$$y_{n+1} = c_{n+1} + \frac{1}{6} (p_n - c_n), n = 1, 2, \dots$$

we need the values of $y(t)$ and $y'(t)$ for $n = 1$.

The exact values are

$$y_0 = 1, \quad y'_0 = 1,$$

$$y_1 = 1.11034184, \quad y'_1 = 1.21034184$$

For $n = 1$

$$\begin{aligned} p_2 &= y_1 + \frac{h}{2} (3y'_1 - y'_0) \\ &= 1.11034184 + \frac{.1}{2} (3 \times 1.21034184 - 1) \\ &= 1.241893116 \end{aligned}$$

$$m_2 = p_2 - \frac{5}{6} (p_1 - c_1)$$

Taking, $p_1 - c_1 = 0$, we obtain

$$\begin{aligned} m_2 &= p_2 = 1.241893116 \\ m'_2 &= t_2 + m_2 = .2 + 1.241893116 \\ &= 1.441893116 \end{aligned}$$

$$\begin{aligned} c_2 &= y_1 + \frac{h}{2} (m'_2 + y'_1) \\ &= 1.11034184 + \frac{.1}{2} (1.441893116 + 1.21034184) \end{aligned}$$

$$\begin{aligned}
 &= 1.2429535878 \\
 p_2 - c_2 &= 1.241893116 - 1.2429535878 \\
 &= -0.0010604718 \\
 y_2 &= c_2 + \frac{1}{6}(p_2 - c_2) \\
 &= 1.2429535878 - \frac{1}{6}(0.0010604718) \\
 &= 1.2427768425
 \end{aligned}$$

For $n=2$

$$\begin{aligned}
 p_3 &= y_2 + \frac{h}{2}(3y_2' - y_1') \\
 &= 1.2427768425 + \frac{.1}{2}(4.3283305275 - 1.21034184) \\
 &= 1.398676276875 \\
 m_3 &= p_3 - \frac{5}{6}(p_2 - c_2) \\
 &= 1.398676276875 - \frac{5}{6}(-0.0010604718) \\
 &= 1.399560003375 \\
 m_3' &= t_3 + m_3 \\
 &= .3 + 1.399560003375 \\
 &= 1.699560003375 \\
 c_3 &= y_2 + \frac{h}{2}(m_3' + y_2') \\
 &= 1.2427768425 + \frac{.1}{2}(1.699560003375 + 1.4427768425) \\
 &= 1.39989368479375 \\
 p_3 - c_3 &= 1.398676276875 - 1.39989368479375 \\
 &= -0.00121740791875 \\
 y_3 &= c_3 + \frac{1}{6}(p_3 - c_3) \\
 &= 1.39989368479375 + \frac{1}{6}(-0.0012740791875) \\
 &= 1.39969078347396
 \end{aligned}$$

The exact solution is given by

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

The computed solution is tabulated in Table 3.12.

TABLE 3.12 SOLUTION OF $y' = t + y$, $y(0) = 1$, $h = 0.1$ BY THE SECOND ORDER ADAMS MODIFIED P-C METHOD

t	y_n	$p_n - c_n$	$y(t_n)$
0	1		1
0.1	1.1103418		1.1103418
0.2	1.2427768	-0.0010604720	1.2428055
0.3	1.3996908	-0.0012174079	1.3997176
0.4	1.5836270	-0.0013457670	1.5836494
0.5	1.7974259	-0.0014872370	1.7974425
0.6	2.0442281	-0.0016436510	2.0442376
0.7	2.3275048	-0.0018165196	2.3275054
0.8	2.6510921	-0.0020075696	2.6510819
0.9	3.0192296	-0.0022187130	3.0192062
1.0	3.4366029	-0.0024520631	3.4365637

3.7 HYBRID METHODS

These methods are also called multistep methods with nonstep points. The linear k -step method (3.26) contains $2k+1$ arbitrary parameters. We can determine these parameters by satisfying $2k+1$ relations of the type (3.30) in which case the order of the method will be $2k$. However, the stability requirements restrict this order to $k+1$ if k is odd and to $k+2$ if k is even. The k -step methods based on numerical differentiation have order k and stable methods are obtained for $k \leq 6$. To increase the order of the stable k -step methods, we modify (3.26) by including a linear combination of the slopes at several points between t_n and t_{n+1} . The modified k -step method with v slopes is given by

$$y_{n+1} = \sum_{j=1}^k a_j y_{n-j+1} + h \sum_{j=0}^k b_j f_{n-j+1} + h \sum_{j=1}^v c_j f_{n-\theta_j+1} \quad (3.88)$$

where a_j 's, b_j 's, c_j 's and θ_j 's are $2k+2v+1$ arbitrary parameters. Furthermore, $0 < \theta_j < 1$, $j = 1, 2, \dots, v$.

If $b_0 = 0$, the formula (3.88) is called an explicit hybrid method, otherwise an implicit hybrid method. The consistency conditions for (3.88) are found to be

$$\rho(1) = 0, \rho'(1) = \sigma(1) + \sum_{j=1}^v c_j \quad (3.89)$$

where $\rho(\xi)$ and $\sigma(\xi)$ are defined by

$$\rho(\xi) = \xi^k - \sum_{j=1}^k a_j \xi^{k-j}, \quad \sigma(\xi) = \sum_{j=0}^k b_j \xi^{k-j}$$

The formula (3.88) is called stable if $\rho(\xi)$ has no zeros outside the unit circle and no multiple zeros on the unit circle; it is of order p if for any $y(t) \in C^{(p+2)}$ and for some non-zero C_{p+1} , we have

$$\begin{aligned} y(t_{n+1}) - \sum_{j=1}^k a_j y(t_{n-j+1}) - h \sum_{j=0}^k b_j f(t_{n-j+1}, y(t_{n-j+1})) \\ - h \sum_{j=1}^v c_j f(t_{n-\theta_j+1}, y(t_{n-\theta_j+1})) \\ = \frac{1}{(p+1)!} C_{p+1} h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}) \end{aligned} \quad (3.90)$$

where $y'(t) = f(t, y)$. In practice, we use one or two non-step points in (3.88).

The k -step method with one non-step point can be written in the form

$$y_{n+1} = \sum_{j=1}^k a_j y_{n-j+1} + h \sum_{j=0}^k b_j f_{n-j+1} + hc_1 f_{n-\theta_1+1} \quad (3.91)$$

where a_j 's, b_j 's, c_1 and θ_1 are arbitrary and $0 < \theta_1 < 1$.

We now discuss in detail a few special cases of (3.91).

3.7.1 One step hybrid methods

For $k = 1$, we write (3.91) as

$$y_{n+1} = a_1 y_n + h(b_0 f_{n+1} + b_1 f_n) + hc_1 f_{n-\theta_1+1} \quad (3.92)$$

where a_1, b_0, b_1, c_1 and θ_1 are arbitrary and $\theta_1 \neq 0$ or 1 .

Expanding each term in (3.92) in Taylor's series about t_n and equating the coefficients of like powers of h , we obtain a family of third order methods if the following equations are satisfied:

$$\begin{aligned} a_1 &= 1 \\ b_1 + b_0 + c_1 &= 1 \\ b_0 + (1 - \theta_1)c_1 &= \frac{1}{2} \\ \frac{1}{2}b_0 + \frac{1}{2}(1 - \theta_1)^2 c_1 &= \frac{1}{6} \end{aligned} \quad (3.93)$$

The principal term of the truncation error is given by

$$\frac{1}{4!} C_4 h^4 y^{(4)}(t_n) + O(h^5)$$

where

$$C_4 = 1 - 4b_0 - 4c_1(1 - \theta_1)^3$$

Retaining b_1 as arbitrary, we find the solution of the equation in (3.93) as

$$a_1 = 1, \quad b_0 = \frac{1 - 4b_1}{4(1 - 3b_1)}$$

$$c_1 = \frac{3(1 - 2b_1)^2}{4(1 - 3b_1)}$$

$$\theta_1 = \frac{2(1 - 3b_1)}{3(1 - 2b_1)}$$

Thus for arbitrary $\theta_1 \neq 0, 1, \text{ or } 2$, we get methods of order 5 and the truncation error is given by

$$\frac{h^6}{6!} \frac{(16 - 48\theta_1 + 24\theta_1^2)}{(23 - 15\theta_1)} y_{(t_n)}^{(6)} + O(h^7) \quad (3.98)$$

If we take $b_0 = 0$, i.e. $\theta_1 = (9 - \sqrt{41})/10$, we have an explicit hybrid method of order 5. The value $\theta_1 = 1/2$ gives an implicit hybrid method of order 5 as

$$y_{n+1} = \frac{1}{31} (32y_n - y_{n-1}) + \frac{h}{93} (15f_{n+1} + 12f_n - f_{n-1} + 64f_{n+1/2})$$

The principal term of the truncation error vanishes for $\theta_1 = 1 - 1/\sqrt{3}$, and for this value of θ_1 , we get a sixth order method with the following values for the parameters :

$$\begin{aligned} a_1 &= 16/(8+5\sqrt{3}), a_2 = -(8-5\sqrt{3})/(8+5\sqrt{3}) \\ b_0 &= (\sqrt{3}+1)/[(8+5\sqrt{3})(3-\sqrt{3})] \\ b_1 &= 8\sqrt{3}/[3(8+5\sqrt{3})] \\ b_2 &= (\sqrt{3}-1)/[(8+5\sqrt{3})(3+\sqrt{3})] \\ c_1 &= 6\sqrt{3}/(8+5\sqrt{3}), \theta_1 = 1 - 1/\sqrt{3} \end{aligned} \quad (3.99)$$

Substituting the values of the parameters from (3.99) into (3.96), we obtain the principal term of the truncation error

$$-8\sqrt{3}/[9(8+5\sqrt{3})] \frac{h^7}{7!} y_{(t_n)}^{(7)} + O(h^8)$$

Thus the maximum attainable order of two step method with one nonstep point is 6.

3.7.3 Implementation of hybrid predictor-corrector methods

The values of the ordinates and the slopes are known at the k points and we wish to determine the ordinate y_{n+1} from the formula

$$y_{n+1} = \sum_{j=1}^k a_j y_{n-j+1} + h \sum_{j=0}^k b_j f_{n-j+1} + h c_1 f_{n-\theta_1+1} \quad (3.100)$$

We cannot determine y_{n+1} directly from (3.100) even if it is explicit, i.e. $b_0 = 0$, since it contains on the right side the term $f_{n-\theta_1+1}$. Therefore, we use a predictor $P^{(0)}$ to determine $y_{n-\theta_1+1}$ and then evaluate $f(t, y)$ to get $f_{n-\theta_1+1}$. Thus, if (3.100) is an explicit hybrid formula, then we use the following sequence of operations to find y_{n+1} .

$$P^{(0)} : y_{n-\theta_1+1} = \sum_{j=1}^k \bar{a}_j y_{n-j+1} + h \sum_{j=1}^k \bar{b}_j f_{n-j+1}$$

$$E : f_{n-\theta_1+1} = f(t_{n-\theta_1+1}, y_{n-\theta_1+1})$$

$$P^{(H)} : y_{n+1} = \sum_{j=1}^k a_j y_{n-j+1} + h \sum_{j=1}^k b_j f_{n-j+1} + h c_1 f_{n-s_1+1}$$

$$E : f_{n+1} = f(t_{n+1}, y_{n+1}) \tag{3.101}$$

The above sequence of operations may be called $P^{(s)} E P^{(H)} E$ mode. If we use the implicit hybrid method (3.100) to find y_{n+1} , then in addition to the predictor $P^{(s)}$, we also require a predictor to predict y_{n+1} . The value y_{n+1} can be predicted in two ways, either we use $P^{(k)}$, a predictor which does not contain the term at a nonstep point or we use a hybrid predictor $P^{(H)}$ which contains a term at a nonstep point. Thus we have two types of modes, either

$$(i) \quad P^{(s)} E P^{(k)} E C^{(H)} E \tag{3.102}$$

$$(ii) \quad P^{(s)} E P^{(H)} E C^{(H)} E \tag{3.103}$$

where $C^{(H)}$ denotes the implicit hybrid method (3.100). We shall now illustrate the various predictor-corrector modes by applying to a few simple cases.

Let us consider the following $P^{(s)} - P^{(H)}$ schemes

$$P^{(s)} : y_{n+2/3} = y_n + \frac{2}{3} h f_n$$

$$P^{(H)} : y_{n+1} = y_n + \frac{h}{4} (f_n + 3f_{n+2/3}) \tag{3.104}$$

Applying (3.104) to $y' = \lambda y$, then $P^{(s)} E P^{(H)} E$ mode becomes

$$P^{(s)} : y_{n+2/3} = y_n + \frac{2}{3} \lambda h y_n = \left(1 + \frac{2}{3} \lambda h\right) y_n$$

$$E : f(t_{n+2/3}, y_{n+2/3}) = \lambda y_{n+2/3}$$

$$P^{(H)} : y_{n+1} = y_n + \frac{\lambda h}{4} \left[y_n + 3 \left(1 + \frac{2}{3} \lambda h\right) y_n \right]$$

$$E : f(t_{n+1}, y_{n+1}) = \lambda \left(1 + \lambda h + \frac{(\lambda h)^2}{2}\right) y_n$$

The characteristic equation of the mode $P^{(s)} E P^{(H)} E$ is given by

$$\xi = 1 + \lambda h + \frac{(\lambda h)^2}{2} \tag{3.105}$$

We cannot talk about the stability of the predictor $P^{(s)}$, since it has the characteristic equation which is no longer a polynomial. However, from (3.105), the mode $P^{(s)} E P^{(H)} E$ will be stable for $-2 < \lambda h < 0$.

Next, we apply $P^{(H)} - C^{(H)}$ scheme

$$P^{(s)} : y_{n+1/2} = y_n + \frac{h}{2} f_n$$

$$P^{(H)} : \bar{y}_{n+1} = y_n + h (2f_{n+1/2} - f_n)$$

$$C^{(H)} : y_{n+1} = y_n + \frac{h}{6} (f_{n+1} + 4f_{n+1/2} + f_n) \tag{3.106}$$

equivalent first order system. However, if the higher order differential equation is free from lower order derivatives, it is advantageous to have direct methods of solution since it is not necessary then to determine the lower order derivatives during the course of computation.

We shall now describe the multistep methods for the second order initial value problem of the form

$$\begin{aligned} y'' &= f(t, y) \\ y(t_0) &= y_0 \\ y'(t_0) &= y'_0 \end{aligned} \quad (3.117)$$

A linear multistep method of the form (3.26) for (3.117) can be written as

$$y_{n+1} = \sum_{i=1}^k a_i y_{n-i+1} + h^2 \sum_{i=0}^k b_i y''_{n-i+1} \quad (3.118)$$

where a_i 's, b_i 's are arbitrary parameters.

Symbolically, we can write (3.118) in the form

$$\rho(E) y_{n-k+1} - h^2 \sigma(E) y''_{n-k+1} = 0 \quad (3.119)$$

where ρ and σ are the polynomials of degree k .

The formula (3.119) can only be used if we know the values of the solution at k successive points. These k values are assumed to be given.

Furthermore, it can be assumed without loss of generality that the polynomials $\rho(\xi)$ and $\sigma(\xi)$ have no common factors since in the general case (3.119) can be reduced to a difference equation of lower order.

DEFINITION 3.12 The method (3.119) will be said to be of order $p > 0$ if it fulfils the $p+2$ conditions

$$\sum_{i=1}^k a_i (1-i)^q + q(q-1) \sum_{i=0}^k b_i (1-i)^{q-2} = 1, \quad q = 0, 1, 2, \dots, p+1 \quad (3.120)$$

Thus the method is of order p if for any $y \in C^{(p+2)}$ and for some non-zero C_{p+2} , we get

$$y(t_{n+1}) = \sum_{i=1}^k a_i y(t_{n-i+1}) + h^2 \sum_{i=0}^k b_i y''(t_{n-i+1}) + C_{p+2} h^{p+2} y^{(p+2)}(\xi) \quad (3.121)$$

where $y^{(p+2)}(\xi)$ is the $(p+2)$ th derivative of y evaluated for some ξ between t_{n-k+1} and t_{n+1} . The last term represents the truncation error.

The consistency conditions for (3.119) can be obtained as

$$\rho(1) = 0, \quad \rho'(1) = 0, \quad \rho''(1) = 2\sigma(1) \quad (3.122)$$

DEFINITION 3.13 The multistep method of the form (3.119) is said to be stable if the modulus of no root of the polynomial $\rho(\xi)$ exceed 1, and that the multiplicity of the roots of modulus 1 be at most 2.

The equations analogous to (3.32) and (3.33) for finding the specific methods for (3.117) are given by

$$\rho(\xi) - (\log \xi)^2 \sigma(\xi) = C_{p+2}(\xi-1)^{p+2} + O((\xi-1)^{p+3}) \quad (3.123)$$

$$\frac{\rho(\xi)}{(\log \xi)^2} - \sigma(\xi) = C_{p+2}(\xi-1)^p + O((\xi-1)^{p+1}) \quad (3.124)$$

If $\sigma(\xi)$ is specified, (3.123) can be used to determine a $\rho(\xi)$ of degree k , whereas (3.124) can be used to determine $\sigma(\xi)$ of degree $\leq k$, if $\rho(\xi)$ is specified. The $(\log \xi)^2 \sigma(\xi)$ or $(\log \xi)^{-2} \rho(\xi)$ are expanded as a power series in $(\xi-1)$ and terms up to $(\xi-1)^k$ can be used to give $\rho(\xi)$ or $\sigma(\xi)$ respectively. The linear k -step methods corresponding to $\rho(\xi) = \xi^{k-2}(\xi-1)^2$ are called *Stormer's method* if $\sigma(\xi)$ obtained from (3.124) is of degree $k-1$ and *Cowell's method* if $\sigma(\xi)$ is of degree k . A few special cases for $k = 2$ (1) 6 are listed in Tables 3.13 and 3.14. For $k = 2$ and if $\sigma(\xi)$ is of degree 2, we get a method of order 4 as

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(y''_{n+1} + 10y''_n + y''_{n-1}) \quad (3.125)$$

This is known as *Numerov's* or *royal road* method.

The methods for $\sigma(\xi) = \xi^k$ and $\rho(\xi)$, a polynomial of degree k determined from (3.123), are called implicit *differentiation type* methods. Table 3.15 contains a few special cases for $k = 2$ (1) 6.

THEOREM 3.8 *The order p of a stable linear k -step method cannot exceed $k+2$. A necessary and sufficient condition for $p=k+2$ is that k be even, and all roots of $\rho(\xi)$ have modulus 1. If k is odd, the order cannot exceed $k+1$.*

Example 3.6 Let $\rho(\xi) = (\xi-1)^2(\xi^2 + \lambda)$ where $-1 < \lambda \leq 1$, find $\sigma(\xi)$.
From equation (3.124), we get

$$\begin{aligned} \frac{\rho(\xi)}{(\log \xi)^2} &= \frac{(\xi-1)^2[(\xi-1)^2 + 2(\xi-1) + 1 + \lambda]}{[\log(1+(\xi-1))]^2} \\ \sigma(\xi) &= 1 + \lambda + (3+\lambda)(\xi-1) + (4+\lambda)(\xi-1)^2 \\ &\quad + \frac{7}{6}(\xi-1)^3 + \frac{1}{240}(19-\lambda)^2(\xi-1)^4 \\ &\quad + \frac{1}{240}(-1+\lambda)(\xi-1)^5 + O((\xi-1)^6) \end{aligned}$$

Thus we find that the values $-1 < \lambda < 1$ give methods of order 4 and the value $\lambda = 1$ gives a sixth order method. For $\lambda = 1$, we get

$$\sigma(\xi) = \frac{1}{120}(9\xi^4 + 104\xi^3 + 234\xi^2 - 336\xi + 229)$$

TABLE 3.13 COEFFICIENT FOR THE FORMULA

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

k	b_1	b_2	b_3	b_4	b_5	b_6
2	1					
3	$\frac{13}{12}$	$-\frac{2}{12}$	$\frac{1}{12}$			
4	$\frac{14}{12}$	$-\frac{5}{12}$	$\frac{4}{12}$	$-\frac{1}{12}$		
5	$\frac{299}{240}$	$-\frac{176}{240}$	$\frac{194}{240}$	$-\frac{96}{240}$	$\frac{19}{240}$	
6	$\frac{317}{240}$	$-\frac{266}{240}$	$\frac{374}{240}$	$-\frac{276}{240}$	$\frac{109}{240}$	$-\frac{18}{240}$

TABLE 3.14 COEFFICIENT FOR THE FORMULA

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

k	b_0	b_1	b_2	b_3	b_4	b_5	b_6
0	1						
2	$\frac{1}{12}$	$\frac{10}{12}$	$\frac{1}{12}$				
4	$\frac{19}{240}$	$\frac{204}{240}$	$\frac{14}{240}$	$\frac{4}{240}$	$-\frac{1}{240}$		
5	$\frac{18}{240}$	$\frac{209}{240}$	$\frac{4}{240}$	$\frac{14}{240}$	$-\frac{6}{240}$	$\frac{1}{240}$	
6	$\frac{4315}{60480}$	$\frac{53994}{60480}$	$-\frac{2307}{60480}$	$\frac{7948}{60480}$	$-\frac{4827}{60480}$	$\frac{1578}{60480}$	$-\frac{221}{60480}$

TABLE 3.15 COEFFICIENT FOR THE FORMULA

$$y_{n+1} = \sum_{i=1}^n a_i y_{n-i+1} + h^2 b_0 y''_{n+1}$$

k	b_0	a_1	a_2	a_3	a_4	a_5	a_6
2	1	2	-1				
3	$\frac{1}{2}$	$\frac{5}{2}$	-2	$\frac{1}{2}$			
4	$\frac{144}{420}$	$\frac{1248}{420}$	$-\frac{1368}{420}$	$\frac{672}{420}$	$-\frac{132}{420}$		
5	$\frac{12}{45}$	$\frac{154}{45}$	$-\frac{214}{45}$	$\frac{156}{45}$	$-\frac{61}{45}$	$\frac{10}{45}$	
6	$\frac{180}{812}$	$\frac{3132}{812}$	$-\frac{5265}{812}$	$\frac{5080}{812}$	$-\frac{2970}{812}$	$\frac{972}{812}$	$-\frac{137}{812}$