Numerical Solution of Differential Equations

(Second Edition)

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NEW AGE INTERNATIONAL (P) LIMITED, PUBLISHERS
New Delhi · Bangalore · Calcutta · Chennai · Guwahati
Hyderabad · Lucknow · Mumbai

Reprint, 2002

NEW AGE INTERNATIONAL (P) LIMITED, PUBLISHERS
4835/24, Ansari Road, Daryaganj,
New Delhi - 110 002

Offices at:
Bangalore, Chennai, Guwahati, Hyderabad, Kolkata,
Lucknow and Mumbai

ISBN : 0 85226 432 1

5 6 7 8 9 10

Published by K.K. Gupta for New Age International (P) Ltd.,
4835/24, Ansari Road, Daryaganj, New Delhi-110 002 and
printed in India at Sarasgraphics, New Delhi-110 064.

TO MY TEACHERS

Professor Bhoj Raj Seth
on his seventy-first birthday

Professor Lothar Collatz
on his sixty-eighth birthday

Professor Jagat Narain Kapur
on his fifty-fifth birthday

AND

TO MY PARENTS

Muni Lal Jain & Manbhari Jain
whose memory lingers

FOREWORD

It is now nearly thirty years since the advent of the high speed electronic digital computer transformed numerical analysis from a somewhat esoteric science to a practical discipline of immense importance. For twenty-five of those years Professor Jain has been studying the numerical solution of differential equations, a study culminating in the present book. There used to be an academic custom that a Professor, having professed his subject for a sizeable proportion of a lifetime, should crown his work by producing a definitive book on the subject. The custom has sadly fallen into disuse of late, and it is pleasant to see Professor Jain revive it.

Jowett of Balliol was epitomised in the couplet:

"I am the Master of this College
What I don't know isn't knowledge"

Readers can be assured that, so far as the numerical solution of differential equation is concerned, that which is not in this book isn't knowledge either.

D.W. Barron

University of Southampton
Southampton, U.K.

PREFACE TO THE SECOND EDITION

Of the number of different approximation methods for solving differential equations, the most important are the methods of finite difference and finite element. The fundamental requirements common to these two methods are: consistency, stability and convergence. With the development of high-speed computers, it has been realized that numerical methods with strong stability are economical (from computational view-point). The stability requirements to be satisfied are: the stiff system in the left-half plane, the high oscillatory system on the imaginary axis and the convection-diffusion system in the right-half plane.

In this second edition nearly all present-day methods of solving differential equations are presented, and the convergence and stability of the methods are derived. Chapters 1—4 deal with numerical methods for the initial and boundary value problems of ordinary differential equations. The adaptive methods developed to stabilize the numerical methods for a particular problem have been discussed in Chapters 2 and 3. The variable step methods to solve stiff differential equations of singular perturbation problems have been presented in Chapters 3 and 4. The cubic spline and the compact implicit methods for the general second order differential equation, and the convergence analysis for the eigenvalues of the Sturm-Liouville problem are discussed in Chapter 4. Chapters 5—7 are concerned with difference methods for the partial differential equations of three types, parabolic, hyperbolic and elliptic. The difference methods for time-dependent convection-diffusion and cylindrical symmetric equations are given in Chapter 5. The system of conservation laws in one and two space dimensions is included in Chapter 6. The elliptic equations with convection terms have been presented in Chapter 7. Chapter 8 on 'Finite Element Methods' has been enlarged to include in detail the solution of ordinary and partial differential equations.

Also included in this edition are additional 78 references and 120 problems including BIT Problems. A number of problems have been solved to illustrate the methods currently used. The advantages and disadvantages of the methods have been discussed from the computational view-point. A bibliography at the end of the book and a bibliographical note at the end of each chapter are given. Answers and hints to the problems are listed at the end of the book.

Numerical Solution of Differential Equations will be appropriate as a text for at least two courses, for first year graduate students and possibly advanced undergraduates in mathematics, engineering, computer science and physical sciences such as biophysics, meteorology, physics and geosciences. The book will also be useful as a reference tool for researchers using finite difference and finite element methods.

This edition has incorporated the suggestions received from teachers teaching courses on numerical solution of ordinary differential equations and partial differential equations. In particular I am indebted to the reviewers, Prof. D. Greenspan, Prof. B.A. Finlayson, Prof. A. Iserles, Prof. Dr M.N. Spijker, Prof. A. Vander Sluis and Dr. W.H. Mills for advice on additions, corrections and deletions. Thanks are also due to Prof. C.E. Froberg for allowing the use of BIT Problems. I am grateful to Prof. S.R.K. Iyengar and Dr R.K. Jain for suggesting several important improvements in the manuscript. My thanks are also due to the Director, IIT Delhi for providing facilities for writing this book. I express my sincere thanks to Mr. Ranjit Kumar for his assistance in the preparation of the manuscript. Finally, I wish to thank my mother Manbhari, wife Usha and son Rabindra for their tolerance and understanding while this book was in preparation.

New Delhi
September 1983

M.K. JAIN

PREFACE TO THE FIRST EDITION

It is a well-known fact that the majority of differential equations in science and engineering cannot be integrated analytically. In these cases it is necessary to apply some method of approximation. There exists a large number of different approximation methods for solving differential equations; the most important of which are the methods of finite difference and finite element.

This book is based on a series of lectures given to undergraduate and postgraduate students, and at short-term courses under the Quality Improvement Programme at the Indian Institute of Technology, Delhi, during the last six years. The book is intended to serve as a text for students of mathematics, science and engineering who have acquired some knowledge of advanced calculus and elementary numerical analysis. Chapter 1 provides an introduction to the problem of numerical integration of differential equations. Chapter 2 contains discussion on the Runge-Kutta and allied single step methods. Chapter 3 presents a detailed treatment of multistep methods. Chapter 4 gives the derivation and implementation of the numerical algorithms for two point boundary value problems. Chapters 5, 6 and 7 contain numerical methods for the solution of parabolic, hyperbolic and elliptic differential equations. Chapter 8 includes a brief discussion on finite element methods. The problems given at the end of Chapters 2—8 are mainly theoretical, and may be supplemented by programming and running some examples by the methods discussed in the text. A short bibliographical note at the end of each chapter is given to guide the reader to a few standard books and research papers which may be profitably consulted either along with the present book or subsequently for a more rigorous and detailed study.

I gratefully acknowledge the generous help I have received from many colleagues and students in the preparation of this book. I am particularly grateful to Dr S.R.K. Iyengar and Dr R.K. Arora for Chapters 2—3, to Professor M.M. Chawla, Dr J.S.V. Saldanha and Dr R.G. Gupta for Chapter 4, to Dr A.G. Lone for Chapter 5, and Dr (Mrs) Raj Ahuja for Chapter 6. I am also thankful to Dr R.K. Jain for suggesting several important improvement in the manuscript. My thanks are also due to Mr U. Anantha

Krishnaiah for working out the problems in the book and Mr J.K. Jain and Mr J. Kurian for the computational work. I am deeply obliged to Mr M.P. Jain for critically reading the manuscript. I am thankful to Professor P.G. Reddy and Professor K.D. Sharma for helpful discussions. My thanks also go to Mr R.S. Yadav and Mr D.R. Joshi for their assistance. Finally, I express my sincere thanks to Miss Neelam Dhody and Mr Ranjit Kumar who patiently typed the manuscript over the last five years as it progressed from year to year.

New Delhi
December 1978

M.K. JAIN

CONTENTS

1

Elements of Ordinary Differential Initial Value Problem Approximation

1.1 INTRODUCTION

To obtain accurate numerical solutions to differential equations governing physical systems has always been an important problem with scientists and engineers. These differential equations basically fall into two classes, *ordinary* and *partial*, depending on the number of independent variables present in the differential equations: one for ordinary and more than one for partial.

The general form of the ordinary differential equation can be written as

$$L[y] = r \tag{1.1}$$

where L is a *differential operator* and r is a given function of the independent variable t. The order of the differential equation is the order of its highest derivative and its degree is the degree of the derivative of the highest order after the equation has been rationalized. If no product of the dependent variable $y(t)$ with itself or any of its derivatives occur, the equation is said to be linear, otherwise it is nonlinear. A linear differential equation of order m can be expressed in the form

$$L[y] = \sum_{p=0}^{m} f_p(t)\, y^{(p)}(t) = r(t) \tag{1.2}$$

in which $f_p(t)$ are known functions. The general nonlinear differential equation of order m can be written as

$$F(t, y, y', \ldots, y^{(m-1)}, y^{(m)}) = 0 \tag{1.3}$$

or

$$y^{(m)}(t) = f(t, y, y', \ldots, y^{(m-1)}) \tag{1.4}$$

which is called a canonical representation of differential equation (1.3). In such a form, the highest order derivative is expressed in terms of the lower order derivatives and the independent variable. The general solution of the mth order ordinary differential equation contains m independent arbitrary constants. In order to determine the arbitrary constants in the general solution if the m conditions are prescribed at one point, these are called *initial conditions*. The differential equation together with the initial conditions is called the *initial value problem*. Thus, the mth order initial value problem can be expressed as

$$y^{(m)}(t) = f(t, y, y', \ldots, y^{(m-1)})$$
$$y^{(p)}(t_0) = y_0^{(p)}, \; p = 0, 1, 2, \ldots, m-1 \tag{1.5}$$

If the m conditions are prescribed at more than one point, these are called *boundary conditions*. The differential equation together with the boundary conditions is known as the *boundary value problem*. We shall now discuss the basic concepts needed for the solution of initial value problems.

1.2 INITIAL VALUE PROBLEMS

The mth order initial value problem of Equation (1.5) is equivalent to the following system of m first order equations:

$$\begin{aligned}
y' = v_1' &= v_2 & v_1(t_0) &= y_0 \\
v_2' &= v_3 & v_2(t_0) &= y_0' \\
&\;\vdots & &\;\vdots \\
v_{m-1}' &= v_m & v_{m-1}(t_0) &= y_0^{(m-2)} \\
v_m' &= f(t, v_1, v_2, \ldots, v_m) & v_m(t_0) &= y_0^{(m-1)}
\end{aligned} \tag{1.6}$$

In vector notations it can be written as

$$\frac{d\mathbf{v}}{dt} = \mathbf{f}(t, \mathbf{v}), \; \mathbf{v}(t_0) = \boldsymbol{\eta} \tag{1.7}$$

where
$$\mathbf{v} = [v_1 \, v_2 \, \ldots \, v_m]^T,$$
$$\mathbf{f}(t, \mathbf{v}) = [v_2 \, v_3 \, \ldots \, f(t, v_1, v_2, \ldots, v_m)]^T,$$
$$\boldsymbol{\eta} = [y_0 \, y_0' \ldots \, y_0^{(m-1)}]^T$$

We shall, therefore, be concerned with methods for finding out numerical approximations to the solution of the equation

$$\frac{dy}{dt} = f(t, y), \; y(t_0) = y_0 \tag{1.8}$$

However, before attempting to approximate the solution numerically, we must ask if the problem has any solution. This can be answered easily in the case of initial value problem for ordinary differential equation by Theorem 1.1.

THEOREM 1.1 *We assume that $f(t, y)$ satisfies the following conditions:*

(i) *$f(t, y)$ is a real function,*

(ii) *$f(t, y)$ is defined and continuous in the strip*

$$t \in [t_0, b], \; y \in (-\infty, \infty),$$

(iii) *there exists a constant L such that for any $t \in [t_0, b]$ and for any two numbers y_1 and y_2*

$$| f(t, y_1) - f(t, y_2) | \leqslant L \, | y_1 - y_2 | ,$$

where L is called the Lipschitz constant.

Then, for any y_0 the initial value problem (1.8) *has a unique solution $y(t)$ for $t \in [t_0, b]$.*

We will always assume the existence and uniqueness of the solution and also that $f(t, y)$ has continuous partial derivatives with respect to t and y of as high an order as we desire.

1.3 DIFFERENCE EQUATIONS

In order to develop approximations to differential equations, we define the following operators:

$Ey(t) = y(t+h)$	The shift operator
$\Delta y(t) = y(t+h) - y(t)$	The forward-difference operator
$\nabla y(t) = y(t) - y(t-h)$	The backward-difference operator
$\delta y(t) = y\left(t + \frac{h}{2}\right) - y\left(t - \frac{h}{2}\right)$	The central-difference operator
$\mu y(t) = \frac{1}{2}\left[y\left(t + \frac{h}{2}\right) + y\left(t - \frac{h}{2}\right)\right]$	The average operator
$Dy(t) = y'(t)$	The differential operator

where h is the difference interval.

Repeated applications of the difference operators lead to the following higher order differences:

$$\Delta^n y(t) = \sum_{k=0}^{n} (-1)^k \frac{n!}{k!\,(n-k)!} \, y(t+(n-k)h) \tag{1.9}$$

$$\nabla^n y(t) = \sum_{k=0}^{n} (-1)^k \frac{n!}{k!\,(n-k)!} \, y(t-kh) \tag{1.10}$$

$$\delta^{2n} y(t) = \sum_{k=0}^{2n} (-1)^k \frac{(2n)!}{k!\,(2n-k)!} y(t+(n-k)h) \tag{1.11}$$

For linking the difference operators with the differential operator we consider Taylor's formula

$$y(t+h) = y(t) + hy'(t) + \frac{h^2}{2!} y''(t) + \dots \tag{1.12}$$

In operator notations we can write

$$Ey(t) = \left(1 + hD + \frac{(hD)^2}{2!} + \dots \right) y(t)$$

The series in parentheses is the expression for the exponential and hence we have (formally)

$$E = e^{hD} \tag{1.13}$$

Treating Equation (1.13) as an identity, we may derive expressions for any order derivative in terms of the various difference operators. In Table 1.1, we list the relations between the operators. There are many difference approximations possible for a given differential equation. The selection of a particular difference relation is usually determined by the nature of the truncation error associated with the approximation.

As an example, let us develop expressions for the first order derivative in terms of the forward, backward, and central difference operators. We assume that the function $y(t)$ may be expanded in a Taylor series in the closed interval $t-h \leqslant t \leqslant t+h$. We have

$$y(t \pm h) = y(t) \pm hy'(t) + \frac{h^2}{2!}y''(t) \pm \dots + \frac{(\pm 1)^n}{n!}h^n y^{(n)}(t) + \dots$$

where a prime denotes differentiation with respect to t. We have then

$$\frac{y(t+h)-y(t)}{h} = y'(t) + \frac{h}{2}y''(t) + 0(h^2)$$

or

$$\frac{\Delta y(t)}{h} = \frac{dy}{dt} + 0(h)$$

where the notation $0(h)$ means that the first term neglected is of order h.

Similarly we obtain

$$\frac{\nabla y(t)}{h} = \frac{dy}{dt} + 0(h)$$

However,

$$\frac{\mu\,\delta y(t)}{h} = \frac{dy}{dt} + 0(h^2)$$

The forward and backward differences are accurate to order h; the average central difference is accurate to order h^2.

Thus replacing the derivatives in a differential equation by the difference approximations results in an equation which may be considered as relating differences of an unknown function and may be called a *difference equation*. The order of a difference equation is the number of intervals separating the largest and the smallest arguments of the dependent variable. A *linear* difference equation is one in which no product of the dependent variable with itself or any of its differences appear. A difference equation is *homogeneous* if all nonzero terms involve the dependent variable; otherwise it is *inhomogeneous*. Furthermore, a difference equation may have coefficients which are constants or functions of the independent variable. If the coefficients are constants, we call it a difference equation with *constant coefficients*, otherwise we call it an equation with *variable coefficients*.

TABLE 1.1 Relationship between the Operators

	E	Δ	∇	δ	hD
E	E	$\Delta+1$	$(1-\nabla)^{-1}$	$1+\frac{1}{2}\delta^2+\delta\sqrt{\left(1+\frac{\delta^2}{4}\right)}$	e^{hD}
Δ	$E-1$	Δ	$(1-\nabla)^{-1}-1$	$\frac{1}{2}\delta^2+\delta\sqrt{\left(1+\frac{\delta^2}{4}\right)}$	$e^{hD}-1$
∇	$1-E^{-1}$	$1-(1+\Delta)^{-1}$	∇	$-\frac{1}{2}\delta^2+\delta\sqrt{\left(1+\frac{\delta^2}{4}\right)}$	$1-e^{-hD}$
δ	$E^{1/2}-E^{-1/2}$	$\Delta(1+\Delta)^{-1/2}$	$\nabla(1-\nabla)^{-1/2}$	δ	$2\sinh\left(\frac{hD}{2}\right)$
μ	$\frac{1}{2}(E^{1/2}+E^{-1/2})$	$\left(1+\frac{\Delta}{2}\right)(1+\Delta)^{-1/2}$	$\left(1-\frac{\nabla}{2}\right)(1-\nabla)^{-1/2}$	$\sqrt{\left(1+\frac{\delta^2}{4}\right)}$	$\cosh\left(\frac{hD}{2}\right)$
hD	$\log E$	$\log(1+\Delta)$	$-\log(1-\nabla)$	$2\sinh^{-1}\left(\frac{\delta}{2}\right)$	hD

A kth order linear inhomogeneous difference equation with constant coefficients is of the form

$$a_0 y_{n+k}+a_1 y_{n+k-1}+ \dots +a_k y_n = g_n \tag{1.14}$$

where $a_j, j = 0, 1, \dots, k$, are constants independent of n, and $a_0 \neq 0$, $a_k \neq 0$.

The solution y_n of Equation (1.14) consists of a solution to the homogeneous equation, say $y_n^{(H)}$, and a particular solution, say $y_n^{(P)}$ of the inhomogeneous part.

Substituting $g_n = 0$ in (1.14), we get the homogeneous difference equation

$$a_0 y_{n+k}+a_1 y_{n+k-1}+ \cdots +a_k y_n = 0 \tag{1.15}$$

To find the solution of (1.15), we use the trial solution

$$y_n = A\xi^n \tag{1.16}$$

where $A \neq 0$ is a constant and ξ is a number to be determined.

Inserting (1.16) in (1.15), we find that nontrivial solutions exist if ξ is a root of the polynomial

$$a_0 \xi^k+a_1 \xi^{k-1}+ \dots +a_k = 0 \tag{1.17}$$

This equation is called the *characteristic equation* of the difference equation (1.15).

Thus, if ξ_j are the distinct roots of (1.17), then we may write

$$y_n^{(H)} = \sum_{j=1}^{k} b_j \xi_j^n = \sum_{j=1}^{k} b_j \exp(n \log \xi_j) \tag{1.18}$$

where b_j are the arbitrary constants.

Let us assume now that $\xi_1(= \xi_2)$ is a double root of (1.17), and that all other roots ξ_j, $j = 3, 4, \dots, k$, are distinct. Then we would get $k-1$ solutions of the form $\xi_1^n, \xi_3^n, \dots, \xi_k^n$. However, it can easily be verified by substitution that if ξ_1 is a double root, then $n\xi_1^n$ is also a solution of (1.15). Thus the general solution of (1.15) becomes

$$y_n^{(H)}= b_1 \xi_1^n+b_2 n \xi_1^n+ \sum_{j=3}^{k} b_j \xi_j^n \tag{1.19}$$

In general, if the characteristic Equation (1.17) has roots $\xi_j, j = 1, 2, \dots, p$, and the roots ξ_j has multiplicity γ_j, where $\sum_{j=1}^{p} \gamma_j = k$, ther the general solution of (1.15) is given by

$$\begin{aligned} y_n^{(H)} =& [b_{11}+b_{12} n+b_{13} n(n-1)+ \dots +b_{1\gamma_1} n(n-1)\dots(n-\gamma_1+2)]\xi_1^n \\ &+[b_{21}+b_{22} n+b_{23} n(n-1)+\dots+b_{2\gamma_2} n(n-1)\dots \\ &\dots(n-\gamma_2+2)]\xi_2^n \\ &\dots+[b_{p1}+b_{p2} n+b_{p3} n(n-1)+\dots+b_{p\gamma_p} n(n-1)\dots \\ &\dots(n-\gamma_p+2)]\xi_p^n \end{aligned} \tag{1.20}$$

where k constants b_{jm}, $m = 1, 2, \ldots, \gamma_j$, $j = 1, 2, \ldots, p$, are arbitrary.

To find the particular solution $y_n^{(P)}$ of (1.14), we shall confine ourselves to the case when g_n $(= g)$ is independent of n. If $\sum_{j=0}^{k} a_j \neq 0$, we can then choose as particular solution

$$y_n^{(P)} = \frac{g}{\sum_{j=0}^{k} a_j} \tag{1.21}$$

The general solution of (1.14) becomes

$$y_n = y_n^{(H)} + \frac{g}{\sum_{j=0}^{k} a_j} \tag{1.22}$$

The k arbitrary parameters in $y_n^{(H)}$ can be determined in such a way that for $n = 0, 1, 2, \ldots, k-1$, the variable y takes the assigned values $y_0, y_1, \ldots, y_{k-1}$.

1.4 NUMERICAL METHODS

The numerical methods for the solution of the differential Equation (1.8) are the algorithms which will produce a table of approximate values of $y(t)$ at certain equally spaced points called *grid*, *nodal*, *net* or *mesh points* along the t coordinate. Each grid point in terms of the previous point is given by the relationship

$$t_{n+1} = t_n + h, \quad n = 0, 1, 2, \ldots, N-1$$
$$t_N = b$$

where h is called the step size.

Alternatively, we may write

$$t_n = t_0 + nh, \quad n = 1, \ldots, N$$

We shall now discuss the numerical methods and related basic concepts with reference to a simple differential equation

$$\frac{dy}{dt} = \lambda y, \; y(t_0) = y_0, \quad t \in [t_0, b] \tag{1.23}$$

The exact solution of the above equation is given by

$$y(t) = c\, e^{\lambda t} \tag{1.24}$$

where c is an arbitrary constant. Using the initial condition $y(t_0) = y_0$, we can write (1.24) in the form

$$y(t) = y(t_0)\, e^{\lambda(t-t_0)}$$

In order to compute the values of $y(t)$ at the nodal points $t = t_0 + kh$, $k = 1, 2, \ldots, N$, we write a recurrence relation between the values of $y(t)$ at t_{n+1} and t_n as

$$y(t_{n+1}) = e^{\lambda h}\, y(t_n), \quad n = 0, 1, 2, \ldots, N-1 \tag{1.25}$$

This gives an algorithm for determining the values of $y(t_1), y(t_2), \ldots, y(t_N)$ from the given value $y(t_0)$ at $t = t_0$. However, from the computation viewpoint each value has to be multiplied by $e^{\lambda h}$, which is an exponential function and difficult to calculate exactly. We, therefore, take suitable approximation to $e^{\lambda h}$. For example, for sufficiently small $|\lambda h|$, the polynomials approximation to $e^{\lambda h}$ can be written

$$e^{\lambda h} = 1+\lambda h+0(|\lambda h|^2)$$

$$e^{\lambda h} = 1+\lambda h+\frac{1}{2}(\lambda h)^2+0(|\lambda h|^3)$$

$$e^{\lambda h} = 1+\lambda h+\frac{1}{2!}(\lambda h)^2+\ldots+\frac{1}{p!}(\lambda h)^p+0(|\lambda h|^{p+1})$$

We can also take other types of approximation to $e^{\lambda h}$. The Padé approximations are

$$e^{\lambda h} = \frac{1}{1-\lambda h}+0(|\lambda h|^2)$$

$$e^{\lambda h} = \frac{1+\frac{1}{2}\lambda h}{1-\frac{1}{2}\lambda h}+0(|\lambda h|^3)$$

$$e^{\lambda h} = \frac{1+\frac{1}{2}\lambda h+\frac{1}{12}(\lambda h)^2}{1-\frac{1}{2}\lambda h+\frac{1}{12}(\lambda h)^2}+0(|\lambda h|^5)$$

$$e^{\lambda h} = \frac{1+\frac{1}{2}\lambda h+\frac{1}{10}(\lambda h)^2+\frac{1}{120}(\lambda h)^3}{1-\frac{1}{2}\lambda h+\frac{1}{10}(\lambda h)^2-\frac{1}{120}(\lambda h)^3}+0(|\lambda h|^7)$$

Let us denote the approximation to $e^{\lambda h}$ by $E(\lambda h)$. The numerical method for obtaining the approximate values y_n of $y(t_n)$ can be written as

$$y_{n+1} = E(\lambda h)\, y_n,\ n = 0, 1, 2, \ldots, N-1 \tag{1.26}$$

The approximate values of $y(t)$ may contain the following errors.

DEFINITION 1.1 The *round-off error* is the quantity R which must be added to a finite representation of a computed number in order to make it the exact representation of that number.

$$y\text{ (machine representation)}+R = y\text{ (true representation)}$$

DEFINITION 1.2 The *truncation error* is the quantity T which must be added to the true representation of the computed quantity in order that the result be exactly equal to the quantity we are seeking to generate.

$$y\text{ (true representation)}+T = y\text{ (exact)}$$

If, $$E(\lambda h) = 1 + \lambda h + \frac{1}{2!}(\lambda h)^2 + \dots + \frac{(\lambda h)^p}{p!}$$

then (1.26) becomes

$$y_{n+1} = y(t_{n+1}) + 0\,(h^{p+1}) \tag{1.27}$$

The integer p is called the order of the method (1.26). The remainder term

$$\frac{(\lambda h)^{p+1}}{(p+1)!} e^{\theta\lambda h}, \; 0 < \theta < 1$$

which is neglected, is the *relative discretization* or *local truncation error.*

The numerical methods for finding solution of the initial value problem of Equation (1.8) may broadly be classified into the following two types:

(i) *Singlestep methods* These methods enable us to find approximation to the true solution $y(t)$ at t_{n+1} if y_n, y'_n and h are known.

(ii) *Multistep methods* These methods use recurrence relations, which express the function value $y(t)$ at t_{n+1} in terms of the function values $y(t)$ and derivative values $y'(t)$ at t_{n+1} and at previous nodal points.

It is obvious from (1.27) that the numerical methods of order p will produce exact results for all differential equations whose solutions are polynomials of degree p or less. If

$$y(t) = a_0 + a_1 t$$

where a_0 and a_1 are arbitrary constants, then the singlestep method of order one will be recurrence relation between the values y_{n+1}, y_n and y'_n. We may write

$$\begin{aligned} y_{n+1} &= a_0 + a_1 t_{n+1} \\ y_n &= a_0 + a_1 t_n \\ y'_n &= a_1 \end{aligned}$$

Eliminating a_0 and a_1, we obtain

$$y_{n+1} = y_n + h y'_n$$

Thus the singlestep numerical method of order one for Equation (1.8) will be of the form

$$y_{n+1} = y_n + h f_n, \; n = 0, 1, 2, \dots, N-1$$

where $$y'_n = f_n = f(t_n, y_n)$$

The exact values of $y(t)$ will satisfy

$$y(t_{n+1}) = y(t_n) + hf(t_n, y(t_n)) + T_n \tag{1.28}$$

where T_n is the local truncation error of the form

$$T_n = C_2 h^2 y''(\xi_2), \; t_n < \xi_2 < t_{n+1}$$

To determine C_2, we substitute $y(t) = t^2$ in (1.28), and get $C_2 = 1/2$.

Next, we construct a multistep numerical method that will produce exact results whenever $y(t)$ is a polynomial of degree three or less. Consider

$$y(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$$

where a_0, a_1, a_2 and a_3 are arbitrary constants.

A simple third order multistep method uses a recurrence relation between the values y_{n+1}, y_n, y'_n, y'_{n-1} and y'_{n-2}. Eliminating a_0, a_1, a_2 and a_3 from the equations

$$\begin{aligned}
y_{n+1} &= a_0 + a_1 t_{n+1} + a_2 t_{n+1}^2 + a_3 t_{n+1}^3 \\
y_n &= a_0 + a_1 t_n + a_2 t_n^2 + a_3 t_n^3 \\
y'_n &= a_1 + 2a_2 t_n + 3a_3 t_n^2 \\
y'_{n-1} &= a_1 + 2a_2 t_{n-1} + 3a_3 t_{n-1}^2 \\
y'_{n-2} &= a_1 + 2a_2 t_{n-2} + 3a_3 t_{n-2}^2
\end{aligned}$$

we obtain

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

The third order multistep method for Equation (1.8) becomes

$$y_{n+1} = y_n + \frac{h}{12}(23f_n - 16f_{n-1} + 5f_{n-2}), \quad n = 2, 3, \ldots, N-1 \tag{1.29}$$

Here we need y_0, y_1 and y_2 initially to start the computation. The exact values of $y(t)$ will satisfy

$$y(t_{n+1}) = y(t_n) + \frac{h}{12}[23f(t_n, y(t_n)) - 16f(t_{n-1}, y(t_{n-1})) + 5f(t_{n-2}, y(t_{n-2}))] + T_n \tag{1.30}$$

where T_n is the local truncation error given by

$$T_n = C_4 h^4 y^{(4)}(\xi), \quad t_{n-2} < \xi < t_{n+1} \tag{1.31}$$

Putting $y(t) = t^4$ in (1.30), we get $C_4 = 3/8$.

In an analogous manner, we may obtain numerical methods based on functions other than polynomials.

Example 1.1 Find the numerical solution of the initial value problem

$$\begin{aligned}
y' &= \lambda y, \quad \lambda = \pm 1, \\
y(0) &= 1, \quad 0 \leqslant t \leqslant 2
\end{aligned}$$

Use the first order method

$$y_{n+1} = (1 + \lambda h) y_n, \quad n = 0, 1, 2, \ldots, N-1$$

with $h = .1$.

We obtain

$$\begin{aligned}
y_1 &= (1 + .1\lambda) y_0 = (1 + .1\lambda) \\
y_2 &= (1 + .1\lambda) y_1 = (1 + .1\lambda)^2
\end{aligned}$$

$$y_3 = (1+.1\lambda)\,y_2 = (1+.1\lambda)^3$$
$$\vdots$$
$$y_N = (1+.1\lambda)\,y_{N-1} = (1+.1\lambda)^N$$

where $N = 20$.

The values of y_n for $\lambda = \pm 1$ are listed in Table 1.2, together with the true values obtained from $y(t_n) = e^{\lambda nh}$. These values are plotted in Figure 1.1 and compared with the true values. We observe that for $\lambda = 1$, the approximate solution increases as fast as the exact solution whereas for $\lambda = -1$ the approximate solution decreases at least as fast as the exact solution.

TABLE 1.2 SOLUTION OF $y' = \lambda y$, $y(0) = 1$, $0 < t < 2$ WITH $h = 0.1$

	$\lambda = 1$		$\lambda = -1$	
t	First order method	Exact solution	First order method	Exact solution
0	1	1	1	1
0.2	1.21000	1.22140	0.81	0.81873
0.4	1.46410	1.49182	0.6561	0.67032
0.6	1.77156	1.82212	0.53144	0.54881
0.8	2.14359	2.22554	0.43047	0.44933
1.0	2.59374	2.71828	0.34868	0.36788
1.2	3.13843	3.32012	0.28243	0.30119
1.4	3.79750	4.05520	0.22877	0.24660
1.6	4.59497	4.95303	0.18530	0.20190
1.8	5.55992	6.04965	0.15009	0.16530
2.0	6.72750	7.38906	0.12158	0.13534

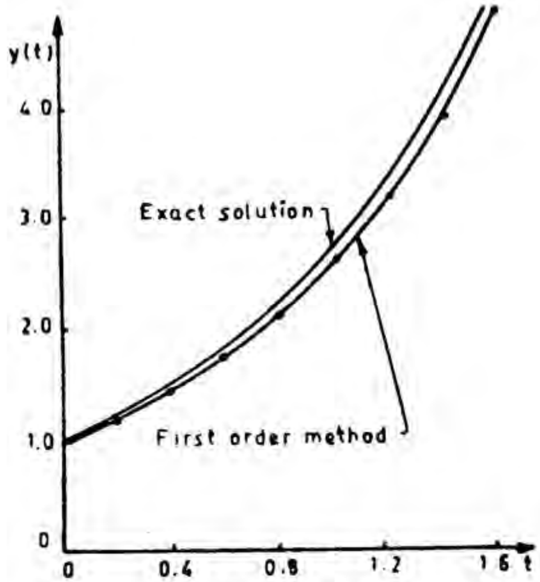


Fig. 1.1 (a) Numerical solution of $y' = y$, $y(0) = 1$

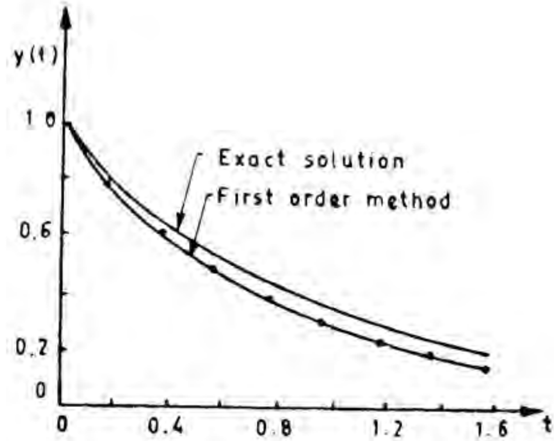


Fig. 1.1 (b) Numerical solution of $y' = -y$, $y(0) = 1$

1.5 STABILITY ANALYSIS

A numerical method is said to be stable if the effect of any single fixed round-off error is bounded, independent of the number of mesh points. More precisely, if for every $\epsilon > 0$ there exists a $\delta = \delta(\epsilon)$ such that difference between two different numerical solutions y_n and $\bar{y}_n$ is such that

$$| y_n - \bar{y}_n | < \epsilon, \quad | y_0 - \bar{y}_0 | < \delta(\epsilon)$$

for all $0 \leqslant h \leqslant h_0$.

Let us examine the stability of the numerical method (1.26). We can write as

$$\begin{aligned} y(t_{n+1}) + \epsilon_{n+1} &= E(\lambda h)[y(t_n) + \epsilon_n] \\ \epsilon_{n+1} &= E(\lambda h) y(t_n) + E(\lambda h)\epsilon_n - y(t_{n+1}) \\ \epsilon_{n+1} &= [E(\lambda h) - e^{\lambda h}] y(t_n) + E(\lambda h)\epsilon_n \end{aligned} \tag{1.32}$$

It is obvious from (1.32) that the error at t_{n+1} consists of two parts. The first part, $E(\lambda h) - e^{\lambda h}$ is the local truncation error, and can be made as small as we like by suitably determining $E(\lambda h)$. The second part $E(\lambda h)\epsilon_n$ is the propagation of the error from the previous step t_n to t_{n+1} (inherited error) and will not grow if $| E(\lambda h) | \leqslant 1$.

DEFINITION 1.3 A numerical method of the form (1.26) is called *absolutely stable* if

$$| E(\lambda h) | \leqslant 1 \tag{1.33}$$

Furthermore, we also observe from (1.25) that the exact value $y(t_n)$ increases $(\lambda > 0)$ or decreases $(\lambda < 0)$ with the factor $e^{\lambda h}$ whereas the approximate value y_n (see (1.26)) grows or dies out with the factor $E(\lambda h)$. In order to have meaningful numerical results, it is necessary that the growth factor of the numerical method either should not increase faster than the growth factor of the exact solution or should decay at least as fast as the growth factor of the exact solution.

DEFINITION 1.4 A numerical method of the form (1.26) is called *relatively stable* if

$$| E(\lambda h) | \leqslant e^{\lambda h} \tag{1.34}$$

For example, the methods based upon polynomial approximation are always relatively stable for $\lambda > 0$, as

$$E(\lambda h) < e^{\lambda h}, \ \lambda > 0$$

For $\lambda < 0$, the numerical methods will be absolutely stable if $| E(\lambda h) | \leqslant 1$, i.e.

$$| 1+\lambda h | \leqslant 1, \ -2 < \lambda h < 0, \qquad \text{first order method,}$$

$$\left| 1+\lambda h+\frac{1}{2}(\lambda h)^2 \right| \leqslant 1, \ -2 < \lambda h < 0, \qquad \text{second order method,}$$

$$\left| 1+\lambda h+\frac{1}{2}(\lambda h)^2+\frac{1}{6}(\lambda h)^3 \right| \leqslant 1, \ -2.5 < \lambda h < 0,$$

third order method,

$$\left| 1+\lambda h+\frac{1}{2}(\lambda h)^2+\frac{1}{6}(\lambda h)^3+\frac{1}{24}(\lambda h)^4 \right| \leqslant 1,$$

$$-2.78 < \lambda h < 0, \qquad \text{fourth order method}$$

Next, we consider the stability analysis of multistep methods. We shall do so by applying the third order method (1.29) to Equation (1.23). Ignoring the round-off errors, we obtain

$$y_{n+1} = y_n + \frac{h\lambda}{12}(23y_n - 16y_{n-1} + 5y_{n-2}) \tag{1.35}$$

The true solution will satisfy

$$y(t_{n+1}) = y(t_n) + \frac{h\lambda}{12}(23y(t_n) - 16y(t_{n-1}) + 5y(t_{n-2})) + T_n \tag{1.36}$$

where T_n is the local truncation error.

Subtracting (1.36) from (1.35) and using $\epsilon_n = y_n - y(t_n)$, we get

$$\epsilon_{n+1} = \epsilon_n + \frac{h\lambda}{12}(23\epsilon_n - 16\epsilon_{n-1} + 5\epsilon_{n-2}) - T_n \tag{1.37}$$

This is an inhomogeneous third order linear difference equation with constant coefficients. The general solution will consist of a particular solution of the inhomogeneous equation and a linear combination of the three independent solutions of the homogeneous equation with $T_n = 0$ in (1.37). The homogeneous equation becomes

$$\epsilon_{n+1} = \epsilon_n + \frac{\bar{h}}{12}(23\epsilon_n - 16\epsilon_{n-1} + 5\epsilon_{n-2}) \tag{1.38}$$

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

We look for the solution of this equation in the form

$$\epsilon_n = A\,\xi^n \tag{1.39}$$

where $A \neq 0$, ξ is an arbitrary number to be determined. Substituting (1.39) in (1.38) and simplifying, we obtain

$$\xi^3 - \left(1 + \frac{23}{12}\,\bar{h}\right)\xi^2 + \frac{4}{3}\bar{h}\xi - \frac{5}{12}\bar{h} = 0 \tag{1.40}$$

If ξ_{1h}, ξ_{2h} and ξ_{3h} are the three roots (distinct) of the characteristic equation, then the solution of the difference equation (1.38) is of the form

$$c_1\,\xi_{1h}^n + c_2\,\xi_{2h}^n + c_3\,\xi_{3h}^n$$

Suppose the characteristic equation has a double root,

$$\xi_{2h} = \xi_{3h},\ \xi_{1h} \neq \xi_{2h}$$

then the form of the above solution is modified to

$$c_1\,\xi_{1h}^n + (c_2 + c_3\,n)\xi_{2h}^n$$

If $\xi_{1h} = \xi_{2h} = \xi_{3h}$, then the solution of the difference equation is of the type

$$(c_1 + c_2\,n + c_3\,n^2)\xi_{1h}^n$$

To obtain the particular solution of the inhomogeneous equation (1.37), we assume $T_n = T$, a constant; then we find the particular solution as $T/\bar{h}$.

The general solution of (1.37) for distinct roots becomes

$$\epsilon_n = c_1\,\xi_{1h}^n + c_2\,\xi_{2h}^n + c_3\,\xi_{3h}^n + \frac{T}{\bar{h}} \tag{1.41}$$

where c_1, c_2 and c_3 are arbitrary constants to be determined from the initial errors. For stability, $|\epsilon_n| < \infty$ as $n \to \infty$ and if any $|\xi_{ih}| > 1$, the error $|\epsilon_n|$ increases unboundedly. If two or more ξ_{ih} are equal and equal to one, then also $|\epsilon_n|$ increases unboundedly.

DEFINITION 1.5 A multistep method when applied to $y' = \lambda y$, $\lambda < 0$, is said to be absolutely stable if the roots of the characteristic equation of the homogeneous difference equation for the error are either inside the unit circle or on the unit circle and simple.

The roots of Equation (1.40) are plotted in Figure 1.2. In the graph the roots are displayed in the following fashion: for real roots the absolute value of the roots is plotted, and for conjugate complex roots the modulus of the pair is plotted as a single quantity (thus conjugate pair of roots are shown as a single curve). In Figure 1.2, it can be seen that $|\xi_{2h}|$ is greater than one at $\bar{h} = -0.55$ and in Equation (1.41) the term containing $|\xi_{2h}|$ grows without bound as n gets large. Thus the third order method (1.29) is absolutely stable for $-0.55 < \lambda h < 0$.

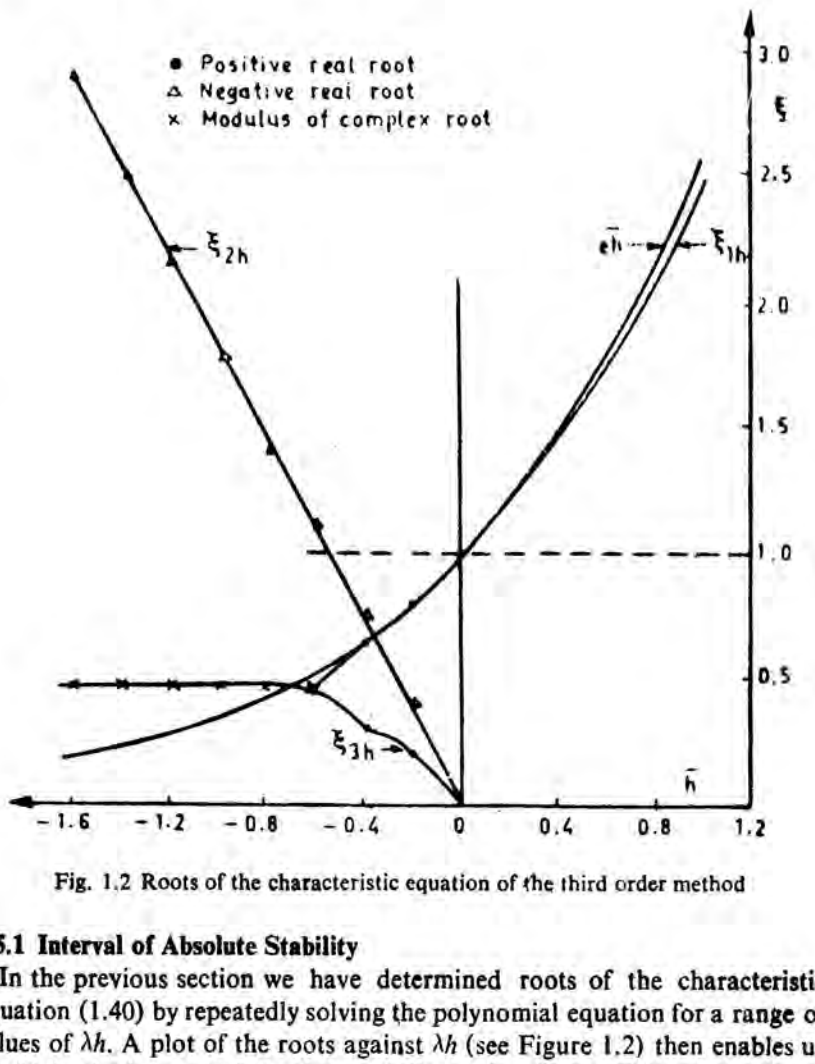


Fig. 1.2 Roots of the characteristic equation of the third order method

1.5.1 Interval of Absolute Stability

In the previous section we have determined roots of the characteristic equation (1.40) by repeatedly solving the polynomial equation for a range of values of λh. A plot of the roots against λh (see Figure 1.2) then enables us to obtain the interval of absolute stability as $(-.55, 0)$. This procedure is known as the *root locus method.*

An alternative to this procedure consists of applying to the characteristic equation (1.40) a transformation which maps the interior of the unit circle onto the left half-plane and then using the Routh-Hurwitz criterion which gives the necessary and sufficient conditions for the roots of the characteristic equation to have negative real part. The transformation

$$\xi = \frac{1+z}{1-z} \tag{1.42}$$

maps the interior of the unit circle onto the left half-plane and the unit circle onto the imaginary axis, the point $\xi = 1$ onto $z = 0$, and the point $\xi = -1$ onto $z = -\infty$. This is shown in Figure 1.3.

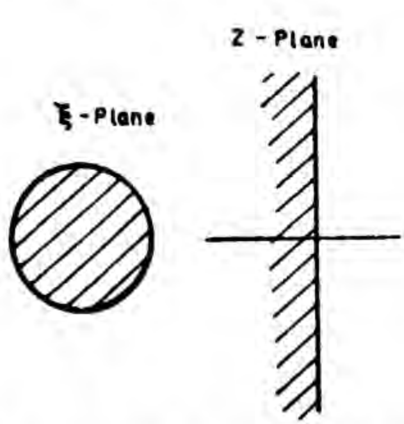


Fig. 1.3 Mapping of the unit circle onto left half-plane

THEOREM (*Hurwitz*) 1.2 *Let*

$$P(z) = a_0 z^k + a_1 z^{k-1} + \ldots + a_k$$

and

$$D = \begin{vmatrix} a_1 & a_3 & a_5 & \cdots & a_{2k-1} \\ a_0 & a_2 & a_4 & \cdots & a_{2k-2} \\ 0 & a_1 & a_3 & \cdots & a_{2k-3} \\ 0 & a_0 & a_2 & \cdots & a_{2k-4} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & a_k \end{vmatrix} \tag{1.43}$$

where $a_L > 0$ *for all j. Then, the real parts of the roots of* $P(z) = 0$ *are negative if and only if, the leading principal minors of D are positive.*

For $k = 3$, we have

$$\begin{gathered} a_0 > 0,\ a_1 > 0,\ a_2 > 0,\ a_3 > 0 \\ a_1 a_2 - a_3 a_0 > 0 \end{gathered} \tag{1.44}$$

as the necessary and sufficient conditions for the real parts of the roots to be negative.

Substituting (1.42) into (1.40), we get

$$a_0 z^3 + a_1 z^2 + a_2 z + a_3 = 0$$

where $$a_0 = 2+\frac{11}{3}\bar{h},\ a_1 = 4-\frac{2}{3}\bar{h},\ a_2 = 2(1-\bar{h}),\ a_3 = -\bar{h}$$

Conditions (1.44) are satisfied if $-.55 < \bar{h} < 0$. Thus the interval of absolute stability is given by $(-.55, 0)$.

Example 1.2 Find $y(t)$ at $t = 1$ with the help of the fourth order method for the initial value problem

$$y' = -10y,\ y(0) = 1,\ 0 \leqslant t \leqslant 1$$

using step lengths 2^{-m}, $m = 1(1)8$.

The exact value of $y(t)$ at $t = 1$ is obtained from the solution

$$y(t) = e^{-10t} \text{ as } y(1) = 0.45399930 \times 10^{-4}$$

The approximate value is given by

$$y_N = \left(1 - 10h + \frac{(10h)^2}{2!} - \frac{(10h)^3}{3!} + \frac{(10h)^4}{4!}\right)^N$$

where $Nh = 1$.

The values of y_N are listed as integers with an exponent (e.g., $43670-08 = 43670\times 10^{-8} = 4.3670\times 10^{-4}$) in Table 1.3.

TABLE 1.3 EFFECT OF ABSOLUTE STABILITY ON THE VALUES $y(1)$

N	h	$y(1)$
2	.5	0.18791840+03
4	.25	0.17679602
8	.125	0.79844684−04
16	.0625	0.46385288−04
32	.03125	0.45446811−04
64	.015625	0.45402499−04
128	.0078125	0.45400080−04
256	.00390625	0.45399939−04

The fourth order method is absolutely stable if $|\lambda h| < 2.78$. i.e. $10h < 2.78$ or $h < .278$. It is obvious from Table 1.3 that the results are reasonably good as soon as the absolute stability criterion is satisfied.

1.6 CONVERGENCE ANALYSIS

The difference approximation to the differential equation does not guarantee that the solution of the difference equation approximates the analytical solution of the differential equation. Here the convergence problem arises by way of the conditions for which the difference solutions converge to the analytical solution if the difference approximate is refined.

DEFINITION 1.6 A numerical method of the form (1.26) is said to be *convergent* if

$$\lim_{h \to 0} y_n = y(t_n) \text{ for all } t_n \in [t_0, b]$$
$$t_n = t_0 + nh$$

The true value $y(t_n)$ will satisfy

$$y(t_{n+1}) = E(\lambda h) y(t_n) + T_n \tag{1.45}$$

where T_n denotes the truncation error.

The approximate solution will satisfy

$$y_{n+1} = E(\lambda h) y_n - R_n \tag{1.46}$$

where R_n denotes the round-off error.

Subtracting (1.45) from (1.46) and by substituting $\epsilon_n = y_n - y(t_n)$, we get

$$\epsilon_{n+1} = E(\lambda h)\epsilon_n - R_n - T_n \tag{1.47}$$

Let us denote $\max\limits_{(t_0, t_N)} | R_n | = R$ and $\max\limits_{(t_0, t_N)} | T_n | = T$ and assume these as constants. Then (1.47) becomes

$$| \epsilon_{n+1} | \leqslant E(\lambda h) | \epsilon_n | + R + T, n = 0, 1, 2, \ldots \tag{1.48}$$

By induction, we can write (1.48) for $E(\lambda h) \neq 1$ as

$$| \epsilon_n | \leqslant E^n(\lambda h) | \epsilon_0 | + \frac{E^n(\lambda h) - 1}{E(\lambda h) - 1}(R + T) \tag{1.49}$$

Let $E(\lambda h)$ be the pth order approximation, then

$$e^{\lambda h} = E(\lambda h) + \frac{(\lambda h)^{p+1}}{(p+1)!} M_{p+1}$$

where M_{p+1} is a constant. Thus (1.49) becomes

$$| \epsilon_n | \leqslant | \epsilon_0 | e^{\lambda(t_n - t_0)} + \frac{e^{\lambda(t_n - t_0)} - 1}{\lambda\left(1 + \frac{\lambda h}{2!} + \frac{\lambda^2 h^2}{3!} + \ldots + \frac{\lambda^{p-1} h^{p-1}}{p!}\right)} \times \left(\frac{R}{h} + \frac{\lambda^{p+1} h^p}{(p+1)!} M_{p+1}\right) \tag{1.50}$$

It is obvious that in the absence of the initial and round-off errors, $| \epsilon_n | \to 0$ as $h \to 0$ like Ch^p where C is a constant, independent of h.

For $| \epsilon_0 | = 0$ and $p = 1$, (1.50) becomes

$$| \epsilon_n | \leqslant \frac{e^{\lambda(t_n - t_0)} - 1}{\lambda}\left(\frac{R}{h} + \frac{\lambda^2 h}{2} M_2\right) \tag{1.51}$$

The dependence of $| \epsilon_n |$ on h is shown in Figure 1.4. Clearly, as $h \to 0$, the truncation error tends to zero whereas the round-off error becomes infinite. On the other hand as $h \to \infty$, the round-off error tends to zero but the

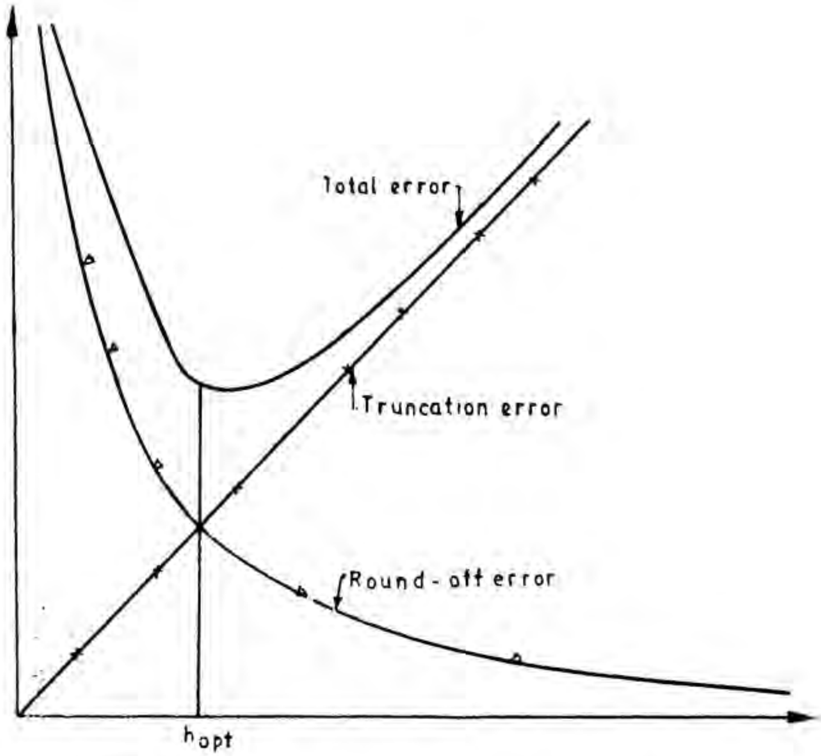


Fig. 1.4 Truncation and round-off errors as function of h

truncation error becomes infinitely large. The choice of h for which the bound (1.51) is minimum is obtained when

$$h = \sqrt{\frac{2R}{\lambda^2 M_2}}$$

We also observe from (1.51) that the first order method converges as $h \to 0$ if the round-off error is of order h^2.

To discuss the convergence of the multistep method (1.29), we determine the constants c_1, c_2, c_3 in (1.41). Let us denote

$$E_j = \epsilon_j - \frac{T}{h}, \quad j = 0, 1, 2$$

The constants c_1, c_2, c_3 can be found by solving the linear system

$$\begin{aligned} E_0 &= c_1 + c_2 + c_3, \\ E_1 &= c_1 \xi_{1h} + c_2 \xi_{2h} + c_3 \xi_{3h}, \\ E_2 &= c_1 \xi_{1h}^2 + c_2 \xi_{2h}^2 + c_3 \xi_{3h}^2 \end{aligned}$$

If we assume that the initial errors ϵ_0, ϵ_1, ϵ_2 are constant and equal to ϵ, then (1.41) becomes

$$\epsilon_n = \left(\epsilon - \frac{T}{h}\right)\left[\frac{(1-\xi_{3h})(1-\xi_{2h})}{(\xi_{1h}-\xi_{3h})(\xi_{1h}-\xi_{2h})}\xi_{1h}^n - \frac{(1-\xi_{1h})(1-\xi_{3h})}{(\xi_{1h}-\xi_{2h})(\xi_{2h}-\xi_{3h})}\xi_{2h}^n + \frac{(1-\xi_{1h})(1-\xi_{2h})}{(\xi_{1h}-\xi_{3h})(\xi_{2h}-\xi_{3h})}\xi_{3h}^n\right] + \frac{T}{h} \tag{1.52}$$

For the stable method, as $h \to 0$, $\xi_{1h} \to 1$, ξ_{2h} and ξ_{3h} approach to zero; for sufficiently small values of $|\lambda h|$, ξ_{1h} behaves like $e^{\lambda h}$ and, ξ_{2h} and ξ_{3h} are less than one.

Thus, (1.52) can be written as

$$\epsilon_n \leqslant \left(\epsilon - \frac{T}{h}\right)e^{\lambda nh} + \frac{T}{h}$$

or

$$\epsilon_n \leqslant \epsilon\, e^{\lambda(t_n - t_0)} + \frac{T}{h}(1 - e^{\lambda(t_n - t_0)}) \tag{1.53}$$

We may also write (1.53) as

$$|\epsilon_n| \leqslant \frac{3}{8} h^3 \frac{M_4}{\lambda}(1 - e^{\lambda(t_n - t_0)})$$

where we have put

$$|\epsilon| = 0$$
$$|T| \leqslant \frac{3}{8} h^4 M_4$$
$$M_4 = \max_{(t_{n-2},\, t_{n+1})} |y^{(4)}(\xi)|$$

This shows that $|\epsilon_n| \to 0$ as $h \to 0$ like Ch^3.

Further details of the stability and convergence for singlestep methods will be given in Chapter 2 and those of multistep methods in Chapter 3.

Example 1.3 Discuss the relation between stability and truncation error of the method

$$y_{n+1} = y_n + h\,[(1-b_2)\,y'_n + b_2\, y'_{n-1}]$$

where b_2 is an arbitrary parameter.

The truncation error T_n for this method may be written as

$$T_n = y(t_{n+1}) - y(t_n) - h\,[(1-b_2)y'(t_n) + b_2\, y'(t_{n-1})]$$
$$= \frac{1}{2}(1+2b_2)h^2 y''(t_n) + \frac{1}{6}(1-3b_2)h^3 y'''(t_n) + \cdots$$

The Lagrange form is given by

$$T_n = \frac{1}{2}(1+2b_2)h^2 y''(\xi_1),\ b_2 \neq -\frac{1}{2}, \qquad t_{n-1} < \xi_1 < t_{n+1}$$
$$T_n = \frac{5}{12}h^3 y'''(\xi_2),\ b_2 = -\frac{1}{2}, \qquad t_{n-1} < \xi_2 < t_{n+1}$$

Next we consider the stability by applying the method to the equation $y' = \lambda y$. The method will be stable if the roots of the characteristic equation

$$\xi^2-(1+\bar{h}(1-b_2))\,\xi-\bar{h}\,b_2 = 0$$

lie within the unit circle with roots of modulus one simple, where $\bar{h} = \lambda h$. Substituting $\xi = (1+z)/(1-z)$ into the characteristic equation we obtain

$$[2-\bar{h}(-1+2b_2)]z^2+2z(1+\bar{h}b_2)-\bar{h} = 0$$

The necessary and sufficient conditions that the roots of the transformed characteristic equation lie on the left-half plane are

$$\begin{aligned} 2-\bar{h}(-1+2b_2) &> 0 \\ (1+\bar{h}\,b_2) &> 0 \\ -\bar{h} &> 0 \end{aligned}$$

Therefore, the method is unstable when $\bar{h} > 0$. For $\bar{h} < 0$, $b_2 = \frac{1}{4}$, $\bar{h} \in (-4, 0)$, the above conditions are satisfied and the interval of absolute stability is $(-4, 0)$. We now study the relation of stability to truncation error. We have

$$2b_2-1 < \frac{2}{h\lambda_{\max}}$$

$$T_n = \left(\frac{1}{2}+b_2\right)h^2\,y'',\ \ b_2 \neq -\frac{1}{2}$$

where $h\lambda_{\max}$ means the signed $h\lambda$ value corresponding to $|\,h\lambda\,|_{\max}$.

We wish to compare $(\frac{1}{2}+b_2)$ to $h\lambda_{\max}$ as $h\lambda_{\max}$ decreases in magnitude from 4 to 0. We write as

$$\frac{1}{2}+b_2 = 1+\frac{1}{h\lambda_{\max}} = C_2$$

The values of $h\lambda_{\max}$, b_2 and C_2 are listed in Table 1.4.

TABLE 1.4 VALUES OF $h\lambda_{\max}$ AND C_2

b_2	$h\lambda_{\max}$	C_2
$\frac{1}{4}$	-4	$\frac{3}{4}$
$\frac{1}{6}$	-3	$\frac{2}{3}$
0	-2	$\frac{1}{2}$
$-\frac{1}{2}$	-1	0
$-\frac{3}{2}$	$-\frac{1}{2}$	-1

These results show that for this method, the magnitude of the truncation error coefficient C_2 decreases towards zero (from the right) and then increases negatively as the magnitude of $h\lambda_{max}$ decreases to zero. The values of C_2 and $h\lambda_{max}$ are shown in Figure 1.5.

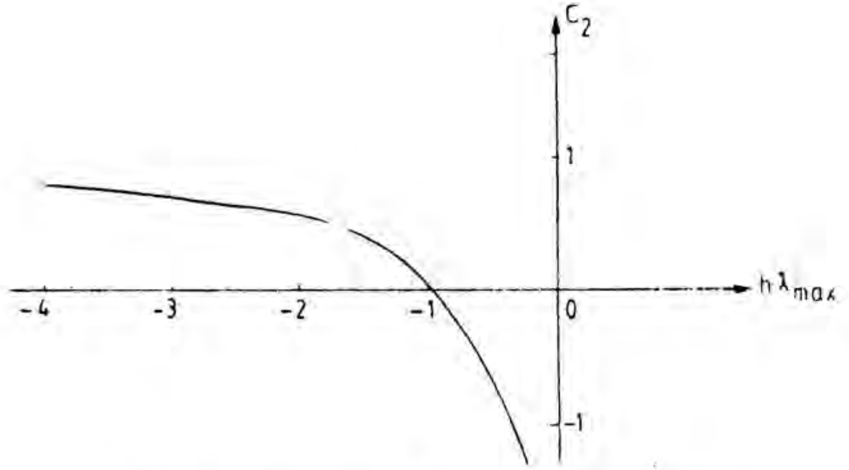


Fig. 1.5 Truncation error coefficient C_2 as function of $h\lambda_{max}$

Bibliographical Note

There are many numerical analysis books having chapters concerning numerical solution of ordinary differential equations, e.g. 61, 103, 114, 121 and 237. Some useful books which deal with the numerical methods for ordinary differential equations in detail are 33, 93, 113, 161 and 163. The difference methods for ordinary and partial differential equations are given in 46, 88 and 147.

Problems

1. Prove that each of the following ordinary differential equation has a unique solution on the interval indicated:

   (i) $y' = t^2 \exp(-y^2)$, $y(0) = 1$ on $[0, 10]$

   (ii) $y' = ty+t^2$, $y(0) = 0$ on $[0, \frac{1}{2}]$

2. Verify that the function

$$y(t) = y_0 \exp\left(\int_{t_0}^{t} p(\tau)\, d\tau\right) + \exp\left(\int_{t_0}^{t} p(\tau)\, d\tau\right) \int_{t_0}^{t} \left[g(\tau) \exp\left(-\int_{t_0}^{\tau} p(s)\, ds\right)\right] d\tau$$

satisfies the initial value problem

$$\frac{dy}{dt} = p(t)y+g(t), \ y(t_0) = y_0$$

3. (i) Solve the initial value problem
$y'-ky = A \sin wt, \ y(0) = y_0$
where k, A, w and y_0 are given constants.
(ii) Assuming that $k < 0$ show that the steady-state response is equal to $A_0 \sin (wt-\phi)$ where $A_0 = \dfrac{A}{\sqrt{k^2+w^2}}$ and $\tan \phi = \dfrac{w}{k}$. $\dfrac{A_0}{A}$ is called the *amplification factor*, and ϕ is called the *phase angle.*

4. Consider a system of first order ordinary differential equations

$$\frac{dv_i}{dt} = f_i(t, v_1, v_2, \ldots, v_m)$$

$$v_i(t_0) = v_{i0} \qquad\qquad i = 1(1)m$$

Assume that each of the functions $f_i(t, v_1, v_2, \ldots, v_m)$ is continuous and bounded and satisfies a Lipschitz condition in

$v_1, v_2, \ldots, v_m$ for $t \in [t_0, b]$ and $-\infty < v_1, v_2, \ldots, v_m < \infty$

Then the system of the first order equations has a unique solution on $[t_0, b]$.
Investigate the existense and uniqueness of a solution to the following system on [0, 2]:

$$v_1' = 3t+4tv_1-v_2+v_3, \qquad v_1(0) = 1$$

$$v_2' = t \exp(-v_2^2), \qquad v_2(0) = -1$$

$$v_3' = t^2+\frac{1}{(t-4)}(v_1+v_2+v_3), \qquad v_3(0) = 1$$

5. Consider the following system of two simultaneous second order equations

$$u'' = g_1(t, u, v, u', v')$$

$$v'' = g_2(t, u, v, u', v')$$

$$u(t_0) = u_0, u'(t_0) = u_0'$$

$$v(t_0) = v_0, v'(t_0) = v_0'$$

(i) Convert the above system into a system of first order equations.
(ii) State the number of first order equations in the system.

6. Find y_n from the difference equation
$\Delta^2 y_{n+1}+\frac{1}{2}\Delta^2 y_n = 0, \ n = 0, 1, 2, \ldots$
when $\quad y_0 = 0, y_1 = \frac{1}{2}, y_2 = \dfrac{1}{4}.$ (BIT7 (1967), 81)

7. Consider

$y_n = \sqrt{3}[(1+\sqrt{3})^{n+1}-(1-\sqrt{3})^{n+1}]/6$

(i) State a difference equation for y_n and calculate $y_0, y_1, \cdots, y_6$.

(ii) Determine $\lim\limits_{n\to\infty} [y_{n+1}/y_n]$. (BIT21 (1981), 242)

8. We wish to use the difference equation

$$y_{n+3} = 0.8\,y_{n+2}+1.19y_{n+1}-0.99y_n$$

to calculate $y_3, y_4, \cdots, y_{100}$, when $y_0 = 1$, $y_1 = 0.95$, $y_2 = 0.905$. Using exact arithmetic obtain the value of y_{100}. (BIT20 (1980), 124)

9. Consider the difference equation

$$y_n = y_{n-1}+y_{n-2}$$
$$y_0 = 0,\ y_1 = 1$$

Show that

$$y_n^2+y_{n+1}^2 = y_{2n+1}$$ (BIT16 (1976), 344)

10. Assuming the function $\dfrac{(2x+7)}{x^2+5x+6}$ has an expansion of the form $a_0+a_1x+a_2x^2+\cdots$,
show that

$$a_n+5a_{n+1}+6a_{n+2} = 0,\ n \geqslant 0$$

Solve the difference equation. (BIT13 (1973), 123)

11. The sequence $\{y_n\}$ is defined by

$$y_0 = 1,\ y_1 = 1.6,\ y_2 = 2.05$$
$$y_{n+1} = \frac{1}{100}\,(280y_n-261y_{n-1}+81y_{n-2}),\ n \geqslant 2$$

Show that $\lim\limits_{n\to\infty} y_n = -2$. (BIT17 (1977), 494)

12. For which values of a and b do the solutions of the difference equation

$$y_{n+3}-y_{n+2}\left(\frac{1}{b}+a+1\right)+y_{n+1}\left(\frac{a}{b}+\frac{1}{b}+a\right)-\frac{a}{b}\,y_n = 0$$

remain finite. (BIT19 (1979), 425)

13. Show that the functions

$$y_n(t) = \int_0^\pi \frac{\cos ns-\cos nt}{\cos s-\cos t}\,ds,\ n \text{ integer},\ n \geqslant 0$$

satisfy the recurrence relation

$$y_{n+2}(t) = 2\cos t\,y_{n+1}(t)-y_n(t)$$

and hence obtain an explicit expression for $y_n(t)$. (BIT4 (1964), 61)

14. Show that all solutions of the difference equation

$$y_{n+1}-2\lambda y_n+y_{n-1} = 0$$

are bounded, when $n \to \infty$ if $|\lambda| < 1$, while for all other complex values of λ there is at least one unbounded solution. **(BIT4 (1964), 261)**

15. Find the general solution of the recurrence relation
$$y_{n+2}+2by_{n+1}+cy_n = 0$$
where b and c are real constants.
Show that all solutions tend to zero as $n \to \infty$, if and only if, the point (b, c) lies in the interior of a certain region in the b-c plane, and determine this region.

16. Find the general solution of the difference equation
$$[1+\alpha(1+\xi)]y_{j-1}-2[1+\alpha\xi]y_j+[1-\alpha(1-\xi)]y_{j+1} = 0$$
Determine the conditions under which there are no oscillations in the solution.

17. Determine a_0, b_0, a_2 and b_2 such that the relation
$$y'((a+b)/2) = a_0y(a)+b_0y(b)+a_2y''(a)+b_2y''(b)$$
is of $0((b-a)^4)$. The truncation error tends to
$$(-(b-a)^4/2880)y^{(v)}((a+b)/2) \text{ as } |b-a| \to 0$$ **(BIT16 (1976) 111)**

18. Define $S(h) = [-y(t+2h)+4y(t+h)-3y(t)]/2h$
Show that
$$y'(t)-S(h) = c_1h^2+c_2h^3+c_3h^4+\dots \text{and state } c_1.$$ **(BIT19 (1979), 285)**

19. Determine the exponents k_i in the difference formula
$$y''(t_0) = \frac{y(t_0+h)-2y(t_0)+y(t_0-h)}{h^2}+\sum_{i=1}^{\infty} a_ih^{k_i}$$
assuming that $y(t)$ has a convergent Taylor expansion in a sufficiently large interval around t_0. **(BIT13 (1973), 123)**

20. Consider the method of the form
$$y_{n+1} = y_n+h(b_0y'_{n+1}+b_1y'_n)$$
where b_0 and b_1 are arbitrary constants.
Determine the coefficients b_0 and b_1 for $y(t)$ to be of the following form:
(i) $\{1, t, t^2\}$
(ii) $\{1, t, \exp(\lambda t)\}$
(iii) $\{1, t, t\exp(\lambda t)\}$
Also show that the boundary of the stability of these methods is a circle with the centre at point $(1/(b_0-b_1), 0)$ if $b_0 \neq b_1$. If $b_0 = b_1$ the stability region is the left half plane, $\lambda < 0$.

21. Determine the coefficients in the method
$$y_{n+1} = y_n+h(b_0y'_{n+1}+b_1y'_n)$$
by assuming the function $y(t) = \{1, \cos wt, \sin wt\}$, where w is a parameter.

Estimate the parameter w by requiring that the method be also exact for the following functions:

(i) $y(t) = \{1, t, t^2\}$

(ii) $y(t) = \{1, t, \exp(-wt)\}$

22. Consider the recursion formula:

$$y_{n+1} = y_{n-1} + 2hy_n$$
$$y_0 = 1$$
$$y_1 = 1 + h + h^2\left(\frac{1}{2} + \frac{h}{6} + \frac{h^2}{24}\right)$$

Show that

$y_n - e^{nh} = 0(h^2)$ as $h \to 0$, $nh =$ constant. (BIT14 (1974), 482)

23. Show that the general solution of the initial value problem
$y'' + y = r(t)$, $y(0) = y_0$, $y'(0) = y'_0$ can be written as

$$y(t) = y_0 \cos t + y'_0 \sin t + \int_0^t r(\tau) \sin(t-\tau)\, d\tau$$

24. Show that the numerical solution of the initial value problem

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

may be obtained by satisfying the formula

$$y_{n+1}^2 + y_{n+1}'^2 = y_n^2 + y_n'^2$$

25. Consider the following system of difference equations:

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = \begin{bmatrix} -1+\cos(h) & \sin(h) \\ -\sin(h) & -1+\cos(h) \end{bmatrix} \begin{bmatrix} u_{n-1} \\ v_{n-1} \end{bmatrix}$$

How small should h be chosen so that $u_n \to 0$ and $v_n \to 0$ when $n \to \infty$.

(BIT20 (1980), 389)

2

Singlestep Methods

2.1 INTRODUCTION

A singlestep method for the solution of the differential equation

$$\frac{dy}{dt} = f(t, y), y(t_0) = y_0, t \in [t_0, b] \tag{2.1}$$

is one in which the solution of the differential equation is approximated by calculating the solution of a related first order difference equation. Thus, a general singlestep method can be written in the form

$$y_{n+1} = y_n + h\phi(t_n, y_n, h), n = 0, 1, 2, \ldots, N-1 \tag{2.2}$$

where $\phi(t, y, h)$ is a function of the arguments t, y, h and, in addition, depends on the right-hand side of (2.1). The function $\phi(t, y, h)$ is called the *increment function*. If y_{n+1} can be obtained simply by evaluating the right-hand side of (2.2), then the singlestep method is called explicit otherwise it is called implicit. The true value $y(t_n)$ will satisfy

$$y(t_{n+1}) = y(t_n) + h\phi(t_n, y(t_n), h) + T_n, n = 0, 1, 2, \ldots, N-1 \tag{2.3}$$

where T_n is the truncation error.

The largest integer p such that $| h^{-1} T_n | = 0(h^p)$ is called the *order* of the singlestep method.

Before stating the main result about convergence, we introduce a few definitions.

DEFINITION 2.1 The singlestep method (2.2) is said to be *regular* if the function $\phi(t, y, h)$ is defined and continuous in the domain $t_0 \leqslant t \leqslant b$, $-\infty < y < \infty$, $0 \leqslant h \leqslant h_0$ (h_0 is a positive constant) and if there exists a constant L such that

$$| \phi(t, y, h) - \phi(t, z, h) | \leqslant L | y - z | \tag{2.4}$$

for every $t \in [t_0, b]$, $y, z \in (-\infty, \infty)$, $h \in (0, h_0)$.

DEFINITION 2.2 A singlestep method of the form (2.2) is said to be *consistent* if

$$\phi(t, y, 0) = f(t, y)$$

We must also ensure that the formula (2.2) be insensitive to small change in the local errors. This will be guaranteed by the stability condition. The main result of convergence is

THEOREM 2.1 *A necessary and sufficient condition for convergence of a regular singlestep method of order $p \geqslant 1$ is consistency.*

This result ensures that the approximate solution converges to the exact solution like $C h^p$.

For the application of the formula (2.2) to (2.1), we need a specific form of the increment function $\phi(t, y, h)$.

2.2 TAYLOR SERIES METHOD

Let us assume that the differential equation (2.1) has a unique solution $y(t)$ on $[t_0, b]$ and that $y(t) \in C^{(p+1)}[t_0, b]$ for $p \geqslant 1$. The solution $y(t)$ can be expanded in a Taylor series about any point t_n

$$y(t) = y(t_n)+(t-t_n)y'(t_n)+\frac{1}{2!}(t-t_n)^2 y''(t_n)+\cdots$$

$$+\frac{1}{p!}(t-t_n)^p y^{(p)}(t_n)+\frac{(t-t_n)^{p+1}}{(p+1)!}y^{(p+1)}(\xi_n) \tag{2.5}$$

This expansion holds good for $t \in [t_0, b]$; $t_n < \xi < t$. Substituting $t = t_{n+1}$ in (2.5), we get

$$y(t_{n+1}) = y(t_n)+hy'(t_n)+\frac{h^2}{2!}y''(t_n)+\cdots+\frac{h^p}{p!}y^{(p)}(t_n)+\frac{h^{p+1}}{(p+1)!}y^{(p+1)}(\xi_n)$$

We define

$$h\,\phi(t_n, y(t_n), h)=h\,y'(t_n)+\frac{h^2}{2!}y''(t_n)+\cdots+\frac{h^p}{p!}y^{(p)}(t_n)$$

and $h\,\phi(t_n, y_n, h)$ is to be obtained from $h\,\phi(t_n, y(t_n), h)$ by using an approximate value y_n in place of the exact value $y(t_n)$. We compute

$$y_{n+1} = y_n+h\phi(t_n, y_n, h),\ n = 0, 1, 2, \ldots, N-1 \tag{2.6}$$

to approximate $y(t_{n+1})$. This is called *Taylor's series method* of order p. Substituting $p = 1$ in (2.6), we get

$$y_{n+1} = y_n+hf(t_n, y_n),\ n = 0, 1, 2, \ldots, N-1 \tag{2.7}$$

which is known as *Euler's method*. To apply (2.6), it is necessary to know $y(t_n), y'(t_n), \ldots, y^{(p)}(t_n)$. If t_n and $y(t_n)$ were known, the derivatives can be calculated as follows:

First the known values t_n and $y(t_n)$ are substituted into the differential equation to give

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

Next, the differential equation (2.1) can be differentiated to obtain formulas for the higher derivatives of $y(t)$.

Thus
$$\begin{aligned}
y' &= f(t, y)\\
y'' &= f_t + f f_y\\
y''' &= f_{tt} + 2f f_{ty} + f^2 f_{yy} + f_y(f_t + f f_y)\\
&\vdots
\end{aligned}$$

where $f_t, f_y, \ldots$ represent the derivatives of f with respect to t and y.

The values $y''(t), y'''(t), \ldots$ can be computed by substituting $t = t_n$. Therefore, if t_n and $y(t_n)$ were known exactly, then (2.6) could be used to compute $y(t_{n+1})$ with an error

$$\frac{h^{p+1}}{(p+1)!}\, y^{(p+1)}(\xi_n),\ t_n < \xi_n < t_{n+1}$$

The number of terms to be included in (2.6) is fixed by the permissible error. If this error is ϵ and the series is truncated at the term $y^{(p)}(t_n)$, then

$$h^{p+1}\,|\,y^{(p+1)}(\xi_n)\,| < (p+1)!\,\epsilon$$

or
$$h^{p+1}\,|\,f^{(p)}(\xi_n)\,| < (p+1)!\,\epsilon \tag{2.8}$$

For given h, (2.8) will determine p, and if p is specified, it will give an upper bound on h. The value $|\,f^{(p)}(\xi_n)\,|$ in (2.8) may be replaced by max. $|\,f^{(p)}(t_n)\,|$ in $[t_0, b]$ for computational purposes.

Example 2.1 Solve the differential equation

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

by Taylor's series method, and determine the number of terms to be included in Taylor's series to obtain an accuracy of 10^{-10}.

The high order derivatives of $y(t)$ can be calculated by successively differentiating the differential equation

$$y' = t + y$$

We get
$$y'' = 1 + y'$$

and
$$y^{(r+1)} = y^{(r)},\ r = 2, 3, \ldots$$

Also we have

$$\begin{aligned}
y'(0) &= 1\\
y''(0) &= 2\\
y^{(r)}(0) &= 2,\ r = 3, 4 \ldots
\end{aligned}$$

Therefore, we obtain

$$y(t) = 1 + t + t^2 + \frac{2t^3}{3!} + \ldots + \frac{2t^p}{p!}$$

To get results accurate up to 10^{-10} for $t \leqslant 1$, we obtain from (2.8)

$$\frac{2e}{(p+1)!} < 5 \times 10^{-11}$$

which gives $p \cong 15$. Hence it follows that about 15 terms are required to achieve the accuracy in the range $t \leqslant 1$.

Example 2.2 Solve the initial value problem

$$y' = -y^2, y(0) = 1, t \in [0, 1]$$

by the Euler method with $h = .1$

The Euler method is given by

$$y_{n+1} = y_n + hf_n, n = 0, 1, 2, \ldots$$

Hence we have

$$f_n = -y_n^2 \text{ and } y_0 = 1$$

We obtain,

for $n = 0$;

$$y_1 = y_0 - h\,y_0^2$$
$$= 1-(.1)\times(1)^2 = 1-.1 = .9$$

for $n = 1$;

$$y_2 = y_1 - h\,y_1^2$$
$$= .9-(.1)\times(.9)^2$$
$$= .9-.081 = .819$$

for $n = 2$;

$$y_3 = y_2 - h\,y_2^2 = .819-(.1)\times(.819)^2$$
$$y_3 = .7519239$$

for $n = 9$;

$$y_{10} = y_9 - h\,y_9^2 = .5074649-(.1)\times(.5074649)^2$$
$$y_{10} = .4817128$$

2.2.1 Convergence

We now discuss the error $y_n - y(t_n)$ in Taylor's series method for an arbitrary initial value problem (2.1). We assume

(i) the solution $y(t)$ is a function such that $\phi(t, y, h)$ satisfies for some L

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

for all $t \in [t_0, b]$ and for all $z_1, z_2, -\infty < z_1, z_2 < \infty$,

(ii) $y^{(p+1)}(t)$ is continuous for $t \in [t_0, b]$ and

$$|y^{(p+1)}(t)| < M_{p+1}$$

To establish the convergence, we need the following result.

LEMMA *Let $w_0, w_1, w_2, \ldots$ be a sequence of real numbers which satisfy*

$$w_{n+1} \leqslant (1+a)\,w_n + B, n = 0, 1, 2, \ldots$$

where a, B are positive constants and $w_0 = 0$. Then

$$w_n \leqslant \left(B\,\frac{e^{na}-1}{a}\right), n = 0, 1, 2, \ldots \tag{2.9}$$

THEOREM 2.2 *With assumptions* (i) *and* (ii) *the error* $\epsilon_n = y_n - y(t_n)$ *of Taylor's series method of order p is bounded by*

$$|\epsilon_n| \leqslant \frac{h^p}{(p+1)!} M_{p+1} \left\{ \frac{\exp(L(t_n - t_0)) - 1}{L} \right\} \tag{2.10}$$

This shows that the error ϵ_n tends to zero at least like h^p as $t_n = t$ is fixed and $h \to 0$; i.e. the error tends to zero as $h \to 0$ like Ch^p for some constant C for $t_n \in [t_0, b]$. We shall now state a result which tells us about how the error ϵ_n tends to zero.

THEOREM 2.3 *If f is sufficiently differentiable,* ϵ_n *will satisfy*

$$\epsilon_n = h^p \, \delta(t_n) + 0(h^{p+1}) \tag{2.11}$$

where $\delta(t)$ *is the solution of the initial value problem*

$$\delta'(t) = f_y(t, y(t))\, \delta(t) - \frac{1}{(p+1)!} y^{(p+1)}(t), \; \delta(t_0) = 0 \tag{2.12}$$

Let us denote $y_n(h)$ the approximate value of $y(t_n)$ calculated from (2.6) with step h. Then (2.11) can be written as

$$y_n(h) = y(t_n) + h^p \, \delta(t_n) + 0(h^{p+1}) \tag{2.13}$$

In conclusion, Taylor's series method has advantages; it is easily derived in any order, and values of $y(t)$ for t not on the grid are easily obtained. However, the method suffers from the time consumed in calculating the higher derivatives.

2.3 RUNGE-KUTTA METHODS

We first explain the principle involved in the Runge-Kutta methods. By the Mean-Value Theorem any solution of

$$y' = f(t, y), \; y(t_0) = y_0, \; t \in [t_0, b]$$

satisfies

$$\begin{aligned} y(t_{n+1}) &= y(t_n) + hy'(\xi_n) \\ &= y(t_n) + hf(\xi_n, y(\xi_n)) \end{aligned}$$

where

$$\xi_n = t_n + \theta_n h, \; 0 < \theta_n < 1$$

We put $\theta_n = 1/2$. By Euler's method with spacing $h/2$, we get

$$y\left(t_n + \frac{h}{2}\right) \cong y_n + \frac{h}{2} f(t_n, y_n)$$

Thus, we have the approximation

$$y_{n+1} = y_n + hf\left(t_n + \frac{h}{2}, \; y_n + \frac{h}{2} f(t_n, y_n)\right) \tag{2.14}$$

Alternatively, again using Euler's method, we proceed as follows:

$$\begin{aligned} y'\left(t_n + \frac{h}{2}\right) &\cong \frac{1}{2}[y'(t_n) + y'(t_{n+1})] \\ &\cong \frac{1}{2}[f(t_n, y_n) + f(t_{n+1}, y_n + hf_n)] \end{aligned}$$

and thus we have the approximation

$$y_{n+1} = y_n + \frac{h}{2}[f(t_n, y_n) + f(t_{n+1}, y_n + hf(t_n, y_n))] \tag{2.15}$$

Either (2.14) or (2.15) can be regarded as

$$y_{n+1} = y_n + h \text{ (average slope)} \tag{2.16}$$

This is the underlying idea of the Runge-Kutta approach. In general, we find the slope at t_n and at several other points: average these slopes, multiply by h, and add the result to y_n. Thus the Runge-Kutta method with v slopes can be written as

$$K_i = hf(t_n + c_i h, y_n + \sum_{j=1}^{i-1} a_{ij} K_j),\ c_1 = 0,\ i = 1, 2, \ldots, v \tag{2.17}$$

or

$$\begin{aligned} K_1 &= hf(t_n, y_n) \\ K_2 &= hf(t_n + c_2 h, y_n + a_{21} K_1) \\ K_3 &= hf(t_n + c_3 h, y_n + a_{31} K_1 + a_{32} K_2) \\ K_4 &= hf(t_n + c_4 h, y_n + a_{41} K_1 + a_{42} K_2 + a_{43} K_3) \\ &\vdots \end{aligned}$$

and

$$y_{n+1} = y_n + \sum_{i=1}^{v} w_i K_i$$

where the parameters $c_2, c_3, \ldots, c_v, a_{2j} \ldots, a_{v(v-1)}$ and w_i are arbitrary.

From (2.16), we may interpret the increment function as the linear combination of the slopes at t_n and at several other points between t_n and t_{n+1}. To obtain specific values for the parameters, we expand y_{n+1} in powers of h such that it agrees with the Taylor series expansion of the solution of the differential equation to a specified number of terms.

Let us study this approach with just two slopes.

2.3.1 Second Order Methods

Define

$$\begin{aligned} K_1 &= hf(t_n, y_n) \\ K_2 &= hf(t_n + c_2 h, y_n + a_{21} K_1) \end{aligned}$$

and

$$y_{n+1} = y_n + w_1 K_1 + w_2 K_2 \tag{2.18}$$

where the parameters c_2, a_{21}, w_1 and w_2 are chosen to make y_{n+1} closer to $y(t_{n+1})$.

Now Taylor's series gives

$$y(t_{n+1}) = y(t_n) + hy'(t_n) + \frac{h^2}{2!} y''(t_n) + \frac{h^3}{3!} y'''(t_n) + \ldots \tag{2.19}$$

where

$$\begin{aligned} y' &= f(t, y) \\ y'' &= f_t + ff_y \\ y''' &= f_{tt} + 2ff_{ty} + f_{yy}f^2 + f_y(f_t + ff_y) \end{aligned}$$

The values of $y'(t_n)$, $y''(t_n)$, ... are obtained by substituting $t = t_n$. We expand K_1 and K_2 about the point (t_n, y_n).

$$\begin{aligned}
K_1 &= hf_n \\
K_2 &= hf(t_n+c_2 h, y_n+a_{21} hf_n) \\
&= h[f(t_n, y_n)+(c_2 hf_t+a_{21} hf_n f_y)+ \\
&\qquad \frac{1}{2!}(c_2^2 h^2 f_{tt}+2c_2 a_{21} h^2 f_n f_{ty}+a_{21}^2 h^2 f_n^2 f_{yy})+\ldots] \\
&= hf_n+h^2(c_2 f_t+a_{21} f_n f_y)+ \\
&\qquad \frac{1}{2} h^3 (c_2^2 f_{tt}+2c_2 a_{21} f_n f_{ty}+a_{21}^2 f_n^2 f_{yy})+\ldots
\end{aligned}$$

Substituting the values of K_1 and K_2 in (2.18), we get

$$\begin{aligned}
y_{n+1} &= y_n+(w_1+w_2)hf_n+h^2(w_2 c_2 f_t+w_2 a_{21} f_n f_y)+ \\
&\qquad \frac{1}{2} h^3 w_2(c_2^2 f_{tt}+2c_2 a_{21} f_n f_{ty}+a_{21}^2 f_n^2 f_{yy})+\ldots \qquad (2.20)
\end{aligned}$$

Comparing (2.19) with (2.20) and matching coefficients of powers of h, we obtain three equations for the parameters

$$\begin{aligned}
w_1+w_2 &= 1 \\
c_2 w_2 &= 1/2 \\
a_{21} w_2 &= 1/2
\end{aligned}$$

From these equations, we see that if c_2 is chosen arbitrarily (nonzero), then

$$a_{21} = c_2,\ w_2 = \frac{1}{2c_2},\ w_1 = 1-\frac{1}{2c_2} \qquad (2.21)$$

Using (2.21) in (2.20), we get

$$y_{n+1} = y_n+hf_n+\frac{h^2}{2}(f_t+f_n f_y)+\frac{c_2 h^3}{4}(f_{tt}+2f_n f_{ty}+f_n^2 f_{yy})+\ldots \qquad (2.22)$$

Subtracting (2.22) from (2.19), we obtain the local truncation error

$$\begin{aligned}
T_n &= y(t_{n+1})-y_{n+1} \\
&= h^3\left[\left(\frac{1}{6}-\frac{c_2}{4}\right)\left(f_{tt}+2f_n f_{ty}+f_n^2 f_{yy}\right)+\frac{1}{6} f_y\left(f_t+f_n f_y\right)\right]+\ldots \\
&= \frac{h^3}{12}[(2-3c_2)\, y''' + 3c_2 f_y y_n''] + \ldots
\end{aligned}$$

We observe that no choice of the parameter c_2 will make the leading term of T_n vanish for all $f(t, y)$. The local truncation error depends not only on derivatives of the solution $y(t)$ but also on the function f. This is typical of all the Runge-Kutta methods; in most other methods the truncation error depends only on certain derivatives of $y(t)$. Generally, c_2 would be chosen between 0 and 1. From the definition of the Runge-Kutta equations, we see that any Runge-Kutta formula must reduce to a quadrature formula of the same order or greater for $f(t, y)$ independent of y, $\{w_i\}$ and $\{c_i\}$ being, the weights and abscissas of such formula. In the present case, $c_2 = 1/2$ and $c_2 = 1$ give the mid-point and the trapezoidal rule of integration for $f(t, y)$ independent of y. An alternative way of choosing the arbitrary parameters is to produce zeros among w_i's, where possible, to simplify the final formula. The choice of $c_2 = 1/2$, for example, makes $w_1 = 0$. Sometimes the free parameters are chosen either to have as large as possible the interval of absolute stability or to minimize the sum of the absolute values of the coefficients in the term T_n. Such a choice is called *optimal*. In the latter case we define

$$\left|\frac{\partial^{i+j} f}{\partial t^i \partial y^j}\right| < \frac{L^{i+j}}{M^{j-1}},\ i, j = 0, 1, 2, \ldots$$

We find

$$\begin{array}{ll} |f| < M, & |f_{ty}| < L^2 \\ |f_t| < LM, & |f_{tt}| < L^2 M \\ |f_y| < L, & |f_{yy}| < \dfrac{L^2}{M} \end{array}$$

and thus $|T_n|$ becomes

$$|T_n| < ML^2h^3\left[4\left|\frac{1}{6}-\frac{c_2}{4}\right|+\frac{1}{3}\right]$$

Obviously the minimum value of $|T_n|$ occurs for $c_2 = 2/3$ in which case $|T_n| < ML^2h^3/3$. We state the Runge-Kutta method by listing the coefficients as follows:

$$\begin{array}{c|c} c_2 & a_{21} \\ \hline & w_1 \; w_2 \end{array}$$

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 0 \;\; 1 \end{array}$$

Improved tangent

$$\begin{array}{c|cc} \frac{2}{3} & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \qquad \begin{array}{c|cc} 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Optimal *Euler-Cauchy*

2.3.2 Third order methods

The above approach gives the second order methods. Using three K's we get a third order method. Here we define

$$\begin{aligned} K_1 &= hf(t_n, y_n) \\ K_2 &= hf(t_n+c_2h, y_n+a_{21}K_1) \\ K_3 &= hf(t_n+c_3h, y_n+a_{31}K_1+a_{32}K_2) \\ y_{n+1} &= y_n+w_1K_1+w_2K_2+w_3K_3 \end{aligned} \tag{2.23}$$

Expanding as before and comparing with (2.19) we get six equations for eight parameters:

$$\begin{aligned} a_{21} &= c_2 & c_2w_2+c_3w_3 &= \frac{1}{2} \\ a_{31}+a_{32} &= c_3 & c_2^2w_2+c_3^2w_3 &= \frac{1}{3} \\ w_1+w_2+w_3 &= 1 & c_2a_{32}w_3 &= \frac{1}{6} \end{aligned} \tag{2.24}$$

Equations (2.24) are typical of all the Runge-Kutta methods; the sum of the a_{ij} in any row equals the corresponding c_i, and the sum of the w_i's equals 1. Equations (2.24) are linear in w_2 and w_3 and have a solution for w_2 and w_3 if and only if

$$\begin{vmatrix} c_2 & c_3 & -\frac{1}{2} \\ c_2^2 & c_3^2 & -\frac{1}{3} \\ 0 & c_2a_{32} & -\frac{1}{6} \end{vmatrix} = 0 \tag{2.25}$$

Simplifying we get

$$c_2(2-3c_2)a_{32}-c_3(c_3-c_2) = 0,\ c_2 \neq 0 \tag{2.26}$$

Thus, we pick c_2, c_3 and a_{32} to satisfy (2.26). We can do this in most cases by picking c_2 and c_3 arbitrarily and setting

$$a_{32} = \frac{c_3(c_3-c_2)}{c_2(2-3c_2)}$$

However, if $c_3 = 0$ or $c_2 = c_3$, then $c_2 = 2/3$ and a_{32} is arbitarily chosen (nonzero). We then calculate w_i's and a_{ij}'s from Equations (2.24). We display the solution in the form

$$\begin{array}{c|ccc} c_2 & a_{21} & & \\ c_3 & a_{31} & a_{32} & \\ \hline & w_1 & w_2 & w_3 \end{array}$$

$$\begin{array}{c|ccc} \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{2}{8} & \frac{3}{8} & \frac{3}{8} \end{array} \qquad \begin{array}{c|ccc} \frac{1}{2} & \frac{1}{2} & & \\ \frac{3}{4} & 0 & \frac{3}{4} & \\ \hline & \frac{2}{9} & \frac{3}{9} & \frac{4}{9} \end{array}$$

Nystrom *Nearly Optimal*

$$\begin{array}{c|ccc} \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \end{array} \qquad \begin{array}{c|ccc} \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

Classical *Heun*

2.3.3 Fourth order methods

The details of the derivation of the fourth order method will be omitted, since they follow the same pattern as above.

In the above notations we can write the fourth order formulas as:

$$\begin{array}{c|cccc} \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array} \qquad \begin{array}{c|cccc} \frac{1}{3} & \frac{1}{3} & & & \\ \frac{2}{3} & -\frac{1}{3} & 1 & & \\ 1 & 1 & -1 & 1 & \\ \hline & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} \end{array}$$

Classical *Kutta*

$$\begin{array}{c|cccc} \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & (\sqrt{2}-1)/2 & (2-\sqrt{2})/2 & & \\ 1 & 0 & -\sqrt{2}/2 & 1+\sqrt{2}/2 & \\ \hline & \frac{1}{6} & (2-\sqrt{2})/6 & (2+\sqrt{2})/6 & \frac{1}{6} \end{array}$$

Gill

$$
\begin{array}{c|ccccc}
\frac{1}{3} & \frac{1}{3} & & & & \\
\frac{1}{3} & \frac{1}{6} & \frac{1}{6} & & & \\
\frac{1}{2} & \frac{1}{8} & 0 & \frac{3}{8} & & \\
1 & \frac{1}{2} & 0 & -\frac{3}{2} & 2 & \\
\hline
 & \frac{1}{6} & 0 & 0 & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Merson

Example 2.3 Solve the initial value problem

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

by classical fourth order Runge-Kutta method with $h = .1$.

For $n = 0$ $\quad t_0 = 0,\ y_0 = 1$

$$K_1 = hf(t_0, y_0) = (.1)\,(0+1) = .1$$

$$K_2 = hf\left(t_0+\frac{h}{2},\ y_0+\frac{K_1}{2}\right)$$

$$= (.1)\left[0+\frac{.1}{2}+\left(1+\frac{.1}{2}\right)\right] = .11$$

$$K_3 = hf\left(t_0+\frac{h}{2},\ y_0+\frac{K_2}{2}\right)$$

$$= (.1)\left[0+\frac{.1}{2}+\left(1+\frac{.11}{2}\right)\right] = .1105$$

$$K_4 = hf(t_0+h,\ y_0+K_3)$$

$$= (.1)\,[(0+.1)+(1+.1105)] = .121$$

$$y_1 = 1+\frac{1}{6}[.1+.22+.2210+.12105]$$

$$= 1.11034167$$

For $n = 1$

$$t_1 = .1,\ y_1 = 1.11034167$$

$$K_1 = hf(t_1, y_1)$$

$$= (.1)\,[.1+1.11034167] = .121034167$$

$$K_2 = hf\left(t_1+\frac{h}{2},\ y_1+\frac{K_1}{2}\right)$$

$$= (.1)\left[\left(.1+\frac{.1}{2}\right)+\left(1.11034167+\frac{1}{2}(.121034167)\right)\right]$$

$$= .132085875$$

$$K_3 = hf\left(t_1+\frac{h}{2}, y_1+\frac{1}{2}K_2\right)$$
$$= (.1)\left[\left(.1+\frac{.1}{2}\right)+\left(1.11034167+\frac{1}{2}(.132085875)\right)\right]$$
$$= .132638461$$
$$K_4 = hf(t_1+h, y_1+K_3)$$
$$= (.1)\,[(.1+.1)+(1.11034167+.132638461)]$$
$$= .144303013$$
$$y_2 = 1.11034167+\frac{1}{6}[.121034167+2(.132085875)$$
$$+2(.132638461)+.144303013]$$
$$= 1.24280514$$

The exact solution is

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

The computed solution is given in Table 2.1.

TABLE 2.1 SOLUTION OF $y' = t+y$, $y(0) = 1$, BY CLASSICAL FOURTH ORDER RUNGE-KUTTA METHOD WITH $h = 0.1$

t_n	y_n	$y(t_n)$
0	1	1
0.1	1.11034167	1.11034184
0.2	1.24280514	1.24280552
0.3	1.39971699	1.39971762
0.4	1.58364848	1.58364940
0.5	1.79744128	1.79744254
0.6	2.04423592	2.04423760
0.7	2.32750325	2.32750542
0.8	2.65107913	2.65108186
0.9	3.01920283	3.01920622
1.0	3.43655949	3.43656366

2.3.4 High order Runge-Kutta methods

We have seen that the values $v = 2$, 3, and 4 in (2.17) give the formulas of order two, three and four, respectively. Surprisingly $v = 5$ gives only fourth order formula. We need $v = 6$ to give a fifth order method, $v = 7$ or 8 to give a sixth order method and $v = k$ to give a $(k-2)$th order method, $k \geqslant 9$. We now list a few high order methods.

Fifth order methods

$$
\begin{array}{c|cccccc}
\frac{1}{3} & \frac{1}{3} & & & & & \\[1ex]
\frac{2}{5} & \frac{4}{25} & \frac{6}{25} & & & & \\[1ex]
1 & \frac{1}{4} & -\frac{12}{4} & \frac{15}{4} & & & \\[1ex]
\frac{2}{3} & \frac{6}{81} & \frac{90}{81} & -\frac{50}{81} & \frac{8}{81} & & \\[1ex]
\frac{4}{5} & \frac{6}{75} & \frac{36}{75} & \frac{10}{75} & \frac{8}{75} & 0 & \\[1ex]
\hline
 & \frac{23}{192} & 0 & \frac{125}{192} & 0 & -\frac{81}{192} & \frac{125}{192}
\end{array}
$$

Nystrom

$$
\begin{array}{c|cccccc}
\frac{1}{2} & \frac{1}{2} & & & & & \\[1ex]
\frac{1}{4} & \frac{3}{16} & \frac{1}{16} & & & & \\[1ex]
\frac{1}{2} & 0 & 0 & \frac{1}{2} & & & \\[1ex]
\frac{3}{4} & 0 & -\frac{3}{16} & \frac{6}{16} & \frac{9}{16} & & \\[1ex]
1 & \frac{1}{7} & \frac{4}{7} & \frac{6}{7} & -\frac{12}{7} & \frac{8}{7} & \\[1ex]
\hline
 & \frac{7}{90} & 0 & \frac{32}{90} & \frac{12}{90} & \frac{32}{90} & \frac{7}{90}
\end{array}
$$

Lawson

Sixth order methods

$$
\begin{array}{c|ccccccc}
\frac{1}{3} & \frac{1}{3} \\[2mm]
\frac{2}{3} & 0 & \frac{2}{3} \\[2mm]
\frac{1}{3} & \frac{1}{12} & \frac{1}{3} & -\frac{1}{12} \\[2mm]
\frac{1}{2} & -\frac{1}{16} & \frac{9}{8} & -\frac{3}{16} & -\frac{3}{8} \\[2mm]
\frac{1}{2} & 0 & \frac{9}{8} & -\frac{3}{8} & -\frac{3}{4} & \frac{1}{2} \\[2mm]
1 & \frac{9}{44} & -\frac{9}{11} & \frac{63}{44} & \frac{18}{11} & 0 & -\frac{16}{11} \\[2mm]
\hline
 & \frac{11}{120} & 0 & \frac{27}{40} & \frac{27}{40} & -\frac{4}{15} & -\frac{4}{15} & \frac{11}{120}
\end{array}
$$

Butcher

$$
\begin{array}{c|cccccccc}
\frac{1}{9} & \frac{1}{9} \\[2mm]
\frac{1}{6} & \frac{1}{24} & \frac{3}{24} \\[2mm]
\frac{1}{3} & \frac{1}{6} & -\frac{3}{6} & \frac{4}{6} \\[2mm]
\frac{1}{2} & -\frac{5}{8} & \frac{27}{8} & -\frac{24}{8} & \frac{6}{8} \\[2mm]
\frac{2}{3} & \frac{221}{9} & -\frac{981}{9} & \frac{867}{9} & -\frac{102}{9} & \frac{1}{9} \\[2mm]
\frac{5}{6} & -\frac{183}{48} & \frac{678}{48} & -\frac{472}{48} & -\frac{66}{48} & \frac{80}{48} & \frac{3}{48} \\[2mm]
1 & \frac{716}{82} & -\frac{2079}{82} & \frac{1002}{82} & \frac{834}{82} & -\frac{454}{82} & -\frac{9}{82} & \frac{72}{82} \\[2mm]
\hline
 & \frac{41}{840} & 0 & \frac{216}{840} & \frac{27}{840} & \frac{272}{840} & \frac{27}{840} & \frac{216}{840} & \frac{41}{840}
\end{array}
$$

Huta

2.3.5 Results from computations for Runge-Kutta methods

We have used various order Runge-Kutta methods to solve the initial value problem

$$\frac{dy}{dt} = -y^2, \; y(0) = 1$$

with analytic solution $y(t) = 1/(1+t)$.
The step sizes $h = 2^{-m}$, $m = 4(1)\,8$ have been used in each case. The error values $\epsilon_n = y_n - y(t_n)$ are tabulated at $t = 5$ in Table 2.2. To avoid round-off errors, we have performed all calculations in double precision floating-point arithmetic throughout. Thus the error values presented in the Table 2.2 are practically pure discretization errors. The graph of the error $(-\log_{10} | y_n - y(t_n) |)$ against $-\log_2 h$ is shown in Figure 2.1. The number attached to each curve indicates the order of the corresponding method.

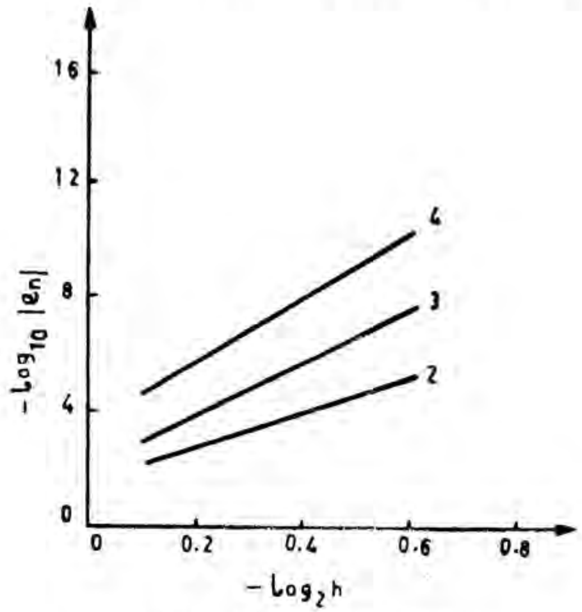


Fig. 2.1 Representation of error

If $\partial f/\partial y = \lambda$, a constant, then the methods of the same order produce identical results. However, if $\partial f/\partial y = -\phi(t, y)$, a function of t and y, then the methods of the same order produce slightly different results, though of the same order of magnitude. Thus, we may conclude that it is immaterial which one of the same order methods is chosen for solving the initial value problems. If we choose a fixed step size to solve an initial value problem over a given interval, we observe from the Table 2.2 and Figure 2.1 that the low-order methods produce less accurate results as compared to high-order methods. The error values decrease as the step size h diminishes or the order of the method increases. If N denotes the number of evaluation of f, then basing our comparison on an equal number of evaluation of f for a given interval of integration, we find that high-order methods are economical to get high accuracy with small step size.

TABLE 2.2 COMPARISON OF ERROR IN RUNGE-KUTTA METHODS,

$y' = -y^2,\ y(0) = 1,\ t = 5$

Second Order Methods

h	Improved tangent	Euler-Cauchy	Optimal	N
2^{-4}	721696−10	637310−10	468629−10	160
2^{-5}	174836−10	154920−10	115093−10	320
2^{-6}	430382−11	381970−11	285149−11	640
2^{-7}	106774−11	948376−12	709647−12	1280
2^{-8}	265919−12	236282−12	177009−12	2560

Third Order Methods

h	Nystrom	Heun	Nearly Optimal	N
2^{-4}	−118873−11	−157779−11	−117753−11	240
2^{-5}	−142853−12	−190086−12	−142199−12	480
2^{-6}	−175095−13	−233239−13	−174700−13	960
2^{-7}	−216736−14	−288848−14	−216493−14	1920
2^{-8}	−269597−15	−359382−15	−269447−15	3840

Fourth Order Methods

h	Classical	Kutta	N
2^{-4}	581973−14	283369−14	320
2^{-5}	366262−15	214773−15	640
2^{-6}	235234−16	150162−16	1280
2^{-7}	207396−17	157031−17	2560
2^{-8}	732941−18	[illegible] 18	5120

2.3.6 Convergence

To discuss the convergence of the Runge-Kutta methods, we shall apply Theorem 2.1 to the third order method. The increment function is given by

$$\phi(t_n, y_n, h) = h^{-1}(w_1K_1 + w_2K_2 + w_3K_3) \tag{2.27}$$

We know from Theorem 1.1, that $f(t, y)$ satisfies a Lipschitz condition. Thus K_1, K_2 and K_3 satisfy

$$
\begin{aligned}
K_1 &= hf(t_n, y_n)\\
|K_1 - K_1^*| &= h\,|f(t_n, y_n) - f(t_n, y_n^*)| \leqslant hL\,|y_n - y_n^*|\\
K_2 &= hf(t_n + c_2h, y_n + a_{21}K_1)\\
|K_2 - K_2^*| &= h\,|f(t_n + c_2h, y_n + a_{21}K_1) - f(t_n + c_2h, y_n^* + a_{21}K_1^*)|\\
&\leqslant hL\,|y_n + a_{21}K_1 - y_n^* - a_{21}K_1^*|\\
&\leqslant hL(1 + hLa_{21})\,|y_n - y_n^*|\\
K_3 &= hf(t_n + c_3h, y_n + a_{31}K_1 + a_{32}K_2)\\
|K_3 - K_3^*| &\leqslant hL\,|y_n + a_{31}K_1 + a_{32}K_2 - y_n^* - a_{31}K_1^* - a_{32}K_2^*|\\
&\leqslant hL(1 + a_{31}hL + a_{32}hL(1 + hLa_{21}))\,|y_n - y_n^*|
\end{aligned}
$$

when we use (2.27), the increment function satisfies

$$
\begin{aligned}
&|\phi(t_n, y_n, h) - \phi(t_n, y_n^*, h)|\\
&\quad = h^{-1}\,|w_1K_1 + w_2K_2 + w_3K_3 - w_1K_1^* - w_2K_2^* - w_3K_3^*|\\
&\quad \leqslant h^{-1}(w_1\,|K_1 - K_1^*| + w_2\,|K_2 - K_2^*| + w_3\,|K_3 - K_3^*|)\\
&\quad \leqslant h^{-1}[w_1hL\,|y_n - y_n^*| + w_2hL(1 + hLa_{21})\,|y_n - y_n^*|\\
&\qquad + w_3hL(1 + a_{31}hL + a_{32}hL(1 + hLa_{21}))\,|y_n - y_n^*|]\\
&\quad \leqslant L[(w_1 + w_2 + w_3) + (w_2a_{21} + w_3(a_{31} + a_{32}))\,hL\\
&\qquad + w_3a_{21}a_{32}(hL)^2]\,|y_n - y_n^*|
\end{aligned}
$$

The use of Equation (2.24) yields

$$
|\phi(t_n, y_n, h) - \phi(t_n, y_n^*, h)| \leqslant L\left(1 + \frac{1}{2}hL + \frac{1}{6}(hL)^2\right)|y_n - y_n^*|
$$

Therefore the increment function ϕ satisfies a Lipschitz condition in y and it is also continuous in h. Thus, we conclude that the third order Runge-Kutta method is convergent.

The Runge-Kutta methods are widely used for solving initial value problems. These methods provide approximations which converge to the true solution as $h \to 0$ and also have the advantage of self starting. The disadvantages of the Runge-Kutta methods are that they involve considerably more computation per step.

2.3.7 Approximation of truncation error

In the numerical solution of differential equations, it is desirable to have estimates of the local discretization (or truncation) errors of the solutions at each step. The estimate may be used not only to provide some idea of the errors, but also to indicate when to adjust the step size. If the magnitude of the estimate is greater than the preassigned upper bound, the step size is reduced to achieve smaller local errors. If the magnitude of the estimate is less than the preassigned lower bound, the step size is increased to save the computing time. For our discussion the rounding error will be ignored. A scheme for estimating the discretization error is called *extrapolation* or, sometimes *Richardson's extrapolation*. It is useful for calculation of the total (not local) truncation error for any method. If the function $f(t, y)$ is sufficiently differentiable and if p is the order of the numerical method, then from Theorem 2.3 we have

$$\epsilon_n = h^p\delta(t_n)+0(h^{p+1}) \tag{2.28}$$

where $\delta(t)$ is called the *magnified error function* and $\epsilon_n = y_n-y(t_n)$. Suppose we calculate $y(t)$ using a certain h and get $y_n(h)$. Then we repeat the calculation using $h/2$, and obtain $y_n(h/2)$. It follows from (2.28) that

$$y_n(h)-y(t_n) = h^p\delta(t_n)+0(h^{p+1})$$

$$y_n\left(\frac{h}{2}\right)-y(t_n) = \left(\frac{h}{2}\right)^p\delta(t_n)+0(h^{p+1}) \tag{2.29}$$

Hence $$y_n(h)-y_n\left(\frac{h}{2}\right) = \left(1-\frac{1}{2^p}\right)h^p\delta(t_n)+0(h^{p+1}) \tag{2.30}$$

From the equations in (2.28) and (2.30) we obtain the equation

$$\epsilon_n = \frac{2^p}{2^p-1}\left[y_n(h)-y_n\left(\frac{h}{2}\right)\right]+0(h^{p+1})$$

Thus, we obtain the *Richardson* extrapolation to the true solution at the mesh point t_n

$$y(t_n) = \frac{2^p y_n\left(\frac{h}{2}\right)-y_n(h)}{2^p-1}+0(h^{p+1})$$

The right sides of the relations of the following

$$\epsilon_n \cong \frac{2^p}{2^p-1}\left(y_n(h)-y_n\left(\frac{h}{2}\right)\right) \tag{2.31}$$

$$y(t_n) \cong \frac{2^p y_n\left(\frac{h}{2}\right)-y_n(h)}{2^p-1} \tag{2.32}$$

help, respectively, to determine the estimate of the accumulated truncation error and the true solution at t_n with an error whose order exceeds the order of the singlestep method by one.

We denote the predicted accumulated error by P_n and the actual error in the extrapolated solution by T_n where

$$P_n = \frac{2^p}{2^p-1}\left(y_n(h)-y_n\left(\frac{h}{2}\right)\right)$$

and $$T_n = \frac{2^p y_n\left(\frac{h}{2}\right)-y_n(h)}{2^p-1}-y(t_n)$$

We have estimated the truncation error at $t=5$ for the differential equation

$$\frac{dy}{dt} = -y^2, \quad y(0) = 1$$

when solved by the various order Runge-Kutta methods **with step sizes** $h = 2^{-m}$, $m = 4\,(1)\,8$.

Using the following methods:

(a) the second order Euler-Cauchy method, $p = 2$,
(b) the nearly optimal third order method, $p = 3$,
(c) the classical fourth order method, $p = 4$,

we have tabulated the error ϵ_n, the predicted error P_n, the extrapolated error T_n and the magnified error function $\delta(t_n)$ in Table 2.3.

TABLE 2.3 ESTIMATION OF THE TRUNCATION ERROR IN $y' = -y^2$, $y(0) = 1$, AT $t = 5$

Second order Euler-Cauchy method

h	ϵ_n	P_n	T_n	$\delta(t_n)$
2^{-4}	468629−10	471382−10	−275291−12	119969−07
2^{-5}	115093−10	115437−10	−344374−13	117855−07
2^{-6}	285149−11	285579−11	−430039−14	116797−07
2^{-7}	709647−12	710184−12	−537111−15	116269−07
2^{-8}	177009−12	177076−12	−671063−16	116005−07

Nearly optimal third order method

h	ϵ_n	P_n	T_n	$\delta(t_n)$
2^{-4}	−117753−11	−118324−11	570577−14	−482317−08
2^{-5}	−142199−12	−142547−12	348358−15	−465957−08
2^{-6}	−174700−13	−174916−13	215137−16	−457967−08
2^{-7}	−216493−14	−216627−14	133650−17	−454019−08
2^{-8}	−269447−15	−269530−15	832775−19	−452057−08

Classical fourth order method

h	ϵ_n	P_n	T_n	$\delta(t_n)$
2^{-4}	581973−14	[illegible]−14	269744−17	381402−09
2^{-5}	366262−15	365588−15	674144−18	384053−09
2^{-6}	235234−16	228794−16	644000−18	394657−09
2^{-7}	207396−17	143042−17	643540−18	556725−09
2^{-8}	732941−18	894086−19	643532−18	314796−08

From the numerical results we can draw the following conclusions:

(a) The predicted error P_n gives good estimate for the error value ϵ_n.
(b) The extrapolated error T_n is smaller than the corresponding predicted error P_n and compares favourably with the predicted error P_n of one order higher method.
(c) The value of the magnified error function $\delta(t_n)$ tends to a constant value as h decreases.

2.4 EXTRAPOLATION METHOD

In Section 2.3 we considered the 'Richardson extrapolation method' or the deferred approach to the limit for estimating the accumulated discretization error and improving the approximate value of $y(t_n)$. It was shown that the order of the improved y_n exceeds the order of the method by one. We shall now discuss a successive repeated application of this procedure so that the approximate value of solution tends to the exact value as $h \to 0$.

Let $y(t)$ be the true solution of differential equation

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

and $y(t, h)$ be the approximate solution obtained by using step length h and a suitable numerical method. The value of $y(t, h)$ will contain error. We assume that $y(t, h)$ admits an asymptotic expansion in h of the following form

$$y(t, h) = y(t) + \tau_1 h^{r_1} + \tau_2 h^{r_2} + \tau_3 h^{r_3} + \ldots + \tau_m h^{r_m} + \tau_{m+1} h^{r_{m+1}} + \ldots \quad (2.33)$$

where $0 < r_1 < r_2 \ldots < r_m$, $\tau_1, \tau_2 \ldots$ are independent of h and are determined by evaluating $y(t, h)$ with step length h_i, $i = 0, 1, 2, \ldots$. In practice, we take either $r_i = ir$ and the step size sequence h_i such that $h_0 > h_1 > h_2 \ldots$, or $h_i = h_0 b^i$, $0 < b < 1$, preferably $b = 1/2$. The case $r_i = ir$ with $h_0 > h_1 > h_2, \ldots, > h_m$ is discussed below in detail. Equation (2.33) becomes

$$y(t, h) = y(t) + \tau_1 h^r + \tau_2 h^{2r} + \tau_3 h^{3r} + \ldots + \tau_m h^{mr} + \tau_{m+1} h^{(m+1)r} + \ldots \quad (2.34)$$

We now attempt to eliminate $\tau_1, \tau_2, \ldots$ by evaluating $y(t, h)$ for $h_0 > h_1 > h_2 \ldots$, we get

$$\begin{aligned}
y(t, h_0) &= y(t) + \tau_1 h_0^r + \tau_2 h_0^{2r} + \tau_3 h_0^{3r} + \ldots + \tau_m h_0^{mr} + \ldots \\
y(t, h_1) &= y(t) + \tau_1 h_1^r + \tau_2 h_1^{2r} + \tau_3 h_1^{3r} + \ldots + \tau_m h_1^{mr} + \ldots \\
y(t, h_2) &= y(t) + \tau_1 h_2^r + \tau_2 h_2^{2r} + \tau_3 h_2^{3r} + \ldots + \tau_m h_2^{mr} + \ldots \\
&\vdots \\
y(t, h_m) &= y(t) + \tau_1 h_m^r + \pi_2 h_m^{4r} + \tau_3 h_m^{3r} + \ldots + \tau_m h_m^{mr} + \ldots \\
&\vdots
\end{aligned} \quad (2.35)$$

Eliminating τ_1 in Equation (2.35) we obtain

$$\begin{aligned}
\frac{h_0^r y(t, h_1) - h_1^r y(t, h_0)}{h_0^r - h_1^r} &= y(t) - h_0^r h_1^r \tau_2 - h_0^r h_1^r (h_0^r + h_1^r)\tau_3 - \ldots \\
\frac{h_1^r y(t, h_2) - h_2^r y(t, h_1)}{h_1^r - h_2^r} &= y(t) - h_1^r h_2^r \tau_2 - h_1^r h_2^r (h_1^r + h_2^r)\tau_3 - \ldots \\
&\vdots \\
\frac{h_{m-1}^r y(t, h_m) - h_m^r y(t, h_{m-1})}{h_{m-1}^r - h_m^r} &= y(t) - h_{m-1}^r h_m^r \tau_2 \\
&\quad - h_{m-1}^r h_m^r (h_{m-1}^r + h_m^r)\tau_3 - \ldots
\end{aligned} \quad (2.36)$$

Let us use the following **notation**

$$Y_m^{(k)} = \frac{h_k^r Y_{m-1}^{(k+1)} - h_{k+m}^r Y_{m-1}^{(k)}}{h_k^r - h_{k+m}^r}$$

where the superscript k stands for $y(t, h_k)$, i.e. the approximation obtained by the numerical method with step length h_k and the subscript m denotes the number of times the linear combination has been applied to eliminate $\tau_1, \tau_2, \ldots, \tau_m$. Thus $Y_0^{(k)} = y(t, h_k)$, and $Y_m^{(k)}$ implies m times linear combination performed to eliminate τ_m. Equation (2.36) can now be written as

$$Y_1^{(0)} = y(t) - h_0^r h_1^r \tau_2 - h_0^r h_1^r (h_0^r + h_1^r)\tau_3 - \ldots$$

$$Y_1^{(1)} = y(t) - h_1^r h_2^r \tau_2 - h_1^r h_2^r (h_1^r + h_2^r)\tau_3 - \ldots$$

$$\vdots$$

$$Y_1^{(m-1)} = y(t) - h_{m-1}^r h_m^r \tau_2 - h_{m-1}^r h_m^r (h_{m-1}^r + h_m^r)\tau_3 - \ldots$$

$$\vdots$$

Eliminating τ_2, we get

$$Y_2^{(0)} = y(t) + h_0^r h_1^r h_2^r \tau_3 + \ldots$$

$$Y_2^{(1)} = y(t) + h_1^r h_2^r h_3^r \tau_3 + \ldots$$

$$\vdots$$

$$Y_2^{(m-2)} = y(t) + h_{m-2}^r h_{m-1}^r h_m^r \tau_3 + \ldots$$

Thus to eliminate τ_m, we need $Y_m^{(k)}$ which is given by

$$Y_m^{(k)} = y\,(t) + (-1)^m h_k^r \quad h_{k+1}^r \cdots h_{k+m}^r \,(\tau_{m+1} + 0\,(h_k^r)) \tag{2.37}$$

The calculation of $Y_m^{(k)}$ can be simplified if we form the triangular array shown as follows:

Y-scheme

$$\begin{array}{lllll}
y\,(t, h_0) = Y_0^{(0)} & & & & \\
 & Y_1^{(0)} & & & \\
y\,(t, h_1) = Y_0^{(1)} & & Y_2^{(0)} & & \\
 & Y_1^{(1)} & & Y_3^{(0)} & \\
y\,(t, h_2) = Y_0^{(2)} & & Y_2^{(1)} & & Y_4^{(0)} \\
 & Y_1^{(2)} & & Y_3^{(1)} & \\
y\,(t, h_3) = Y_0^{(3)} & & Y_2^{(2)} & & \\
 & Y_1^{(3)} & & & \\
y\,(t, h_4) = Y_0^{(4)} & & & &
\end{array}$$

where two values are used to form the next approximation according to the rule

$$Y_m^{(k)} = \frac{h_k^r Y_{m-1}^{(k+1)} - h_{k+m}^r \; Y_{m-1}^{(k)}}{h_k^r - h_{k+m}^r} \tag{2.38}$$

For $h_i = h_0 b^i$ with $0 < b < 1$, (2.38) becomes

$$Y_m^{(k)} = \frac{Y_{m-1}^{(k+1)} - b^{mr}\, Y_{m-1}^{(k)}}{1-b^{mr}} \tag{2.39}$$

Equation (2.39) for $b = 1/2$ simplifies to

$$Y_m^{(k)} = \frac{2^m\, Y_{m-1}^{(k+1)} - Y_{m-1}^{(k)}}{2^m - 1}, \; r = 1 \tag{2.40}$$

and

$$Y_m^{(k)} = \frac{4^m\, Y_{m-1}^{(k+1)} - Y_{m-1}^{(k)}}{4^m - 1}, \; r = 2 \tag{2.41}$$

From Equation (2.38), we notice that each $Y_m^{(k)}$ is a linear combination of $y(t, h_i)$, $i = k, k+1, \ldots, k+m$, which can be written in the form

$$Y_m^{(k)} = \sum_{j=0}^{m} c_{m,\, m-j}\, Y_0^{(k+j)} \tag{2.42}$$

where $c_{m,\, m-j}$ are constant coefficients.

Substituting (2.42) into (2.38) we get the recursion relation in the coefficients as

$$c_{m,\, m-j} = \frac{h_k^r\, c_{m-1,\, m-j} - h_{k+m}^r\, c_{m-1,\, m-1-j}}{h_k^r - h_{k+m}^r} \tag{2.43}$$

$$c_{m-1,\, m} = c_{m-1,\, -1} = 0$$

Using (2.43) and (2.42) we may write

$$\begin{bmatrix} Y_0^{(0)} \\ Y_1^{(0)} \\ \vdots \\ Y_m^{(0)} \end{bmatrix} = \begin{bmatrix} c_{00} & & & \\ c_{11} & c_{10} & & \\ c_{22} & c_{21} & c_{20} & \\ \vdots & & \ddots & \\ c_{mm} & & & c_{m0} \end{bmatrix} \begin{bmatrix} Y_0^{(0)} \\ Y_0^{(1)} \\ \vdots \\ Y_0^{(m)} \end{bmatrix}$$

We know that the numerical methods of interest converge as the step size tends to zero, i.e.

$$\lim_{k \to \infty} y(t, h_k) = Y_0^{(k)} = y(t) \tag{2.44}$$

The convergence of $Y_m^{(0)}$ to $y(t)$ can be seen from Equation (2.37). Whenever $\tau_m \neq 0$, $m = 1, 2, \ldots$, this equation states that each column of the Y-scheme converges to $y(t)$ faster than the preceding one; and, in fact, the principal diagonal converges faster than any column.

We illustrate the extrapolation method as applied to Euler's method.

2.4.1 Euler extrapolation method

The approximate value $y_n(h)$ is obtained from the algorithm

$$y_{n+1} = y_n + h f(t_n, y_n), \; n = 0, 1, 2, \ldots$$

Since $p = 1$ for Euler's method, from (2.28) the approximate value $y_n(h)$ to $y(t_n)$ has the asymptotic expansion of the form

$$y(t_n, h) = y(t_n)+\tau_1(t_n)h+\tau_2(t_n)h^2+\ldots$$

We use step lengths h_0, $h_0/2$, $h_0/2^2$, ..., $h_0/2^k$ and generate $Y_0^{(k)}$. In Euler's method, we know y_n at t_n and advance the computation from t_n to t_{n+1} to find y_{n+1}. We take $t_{n+1}-t_n = h_0$ and start the procedure by computing y_{n+1} with step length h_0 and denote it by $Y_0^{(0)}$, i.e.

$$Y_0^{(0)} = y_n+h_0 f_n$$

Next, we put $h_1 = h_0/2$ and apply Euler's method twice to obtain $y(t_{n+1}, h_1)$ at t_{n+1},

$$Y_0^{(1)} = y(t_{n+1}, h_1)$$

for $h_2 = h_0/2^2$, we apply Euler's method four times. Similarly, for $h_k = h_0/2^k$, we apply Euler's method 2^k times to obtain $Y_0^{(k)}$ The above procedure gets simplified if we consider the initial value problem

$$y' = \lambda y,\ y(t_0) = y_0$$

and we obtain

$$Y_0^{(0)} = (1+\lambda h_0)\,y_n$$

$$Y_0^{(1)} = \left(1+\frac{\lambda h_0}{2}\right)^2 y_n$$

$$\vdots$$

$$Y_0^{(k)} = \left(2+\frac{\lambda h_0}{2^k}\right)^{2k} y_n$$

The convergence of $Y_0^{(k)}$ to the exact value for $h_0 = 1$ and $\lambda = 1$ is shown in Figure 2.2.

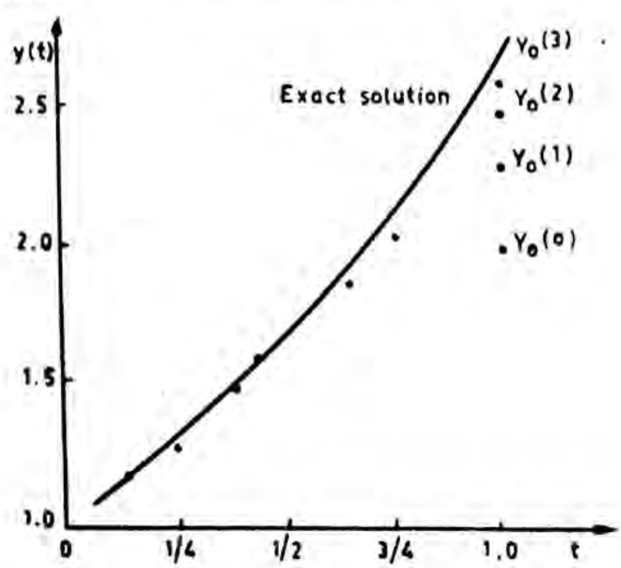


Fig. 2.2 Solution of $y' = y$, $y(0) = 1$ by Euler extrapolation method

After determining the first column $Y_0^{(k)}$ of the Y-scheme, we obtain the other columns with the help of relation (2.40)

$$Y_m^{(k)}=\frac{2^m\, Y_{m-1}^{(k+1)}-Y_{m-1}^{(k)}}{2^m-1},\ m=1,2,3,\ldots$$

The value of m is chosen by comparing the two successive values $Y_{m-1}^{(0)}$ and $Y_m^{(0)}$ and we increase m till this difference is within the prescribed tolerance ϵ.

When the convergence is obtained, $Y_m^{(0)}$ is used as y_{n+1} and the procedure is repeated to obtain y_{n+2}.

2.5 STABILITY ANALYSIS

While numerically solving an initial value problem for ordinary differential equations, an error is introduced at each integration step due to the inaccuracy of the formula. The magnitude of this so called local truncation error is a measure of the accuracy of the integration formula. The magnitude of the total error depends on the magnitude of the local truncation errors and their propagation. Even when the local error at each step is small, the total error may become large due to accumulation and amplification of these local errors. This growth phenomenon is called *numerical instability*. To understand this, consider the simple linear first order differential equation

$$y'=\lambda y,\ y(t_0)=y_0 \tag{2.45}$$

where λ is a constant. It can be seen that, to a first order approximation, the results obtained from a stability analysis on the above linear equation can be extended to a nonlinear case

$$y'=f(t,y),\ y(t_0)=y_0 \tag{2.46}$$

where $\partial f/\partial y$ from Equation (2.46) plays role similar to that of the constant λ in Equation (2.45).

The nonlinear function $f(t, y)$ can be linearized by expansion of the function about the point (t_n, y_n) in the Taylor series truncated after first order terms. The resulting linearized form for Equation (2.46) is given by

$$y'=\lambda y+Bt+C \tag{2.47}$$

where

$$\lambda=\left(\frac{\partial f}{\partial y}\right)_n,$$

$$B=\left(\frac{\partial f}{\partial t}\right)_n,$$

$$C=\left[f_n-y_n\left(\frac{\partial f}{\partial y}\right)_n-t_n\left(\frac{\partial f}{\partial t}\right)_n\right]$$

It can be argued that the stability characteristics of the linear equation (2.47) are very similar to the stability characteristics of the equation of the form given by (2.46). Since the terms Bt and C will give rise to corresponding terms in both numerical and exact solutions which are also linear in $t(\lambda\neq 0)$, we conclude that (2.46) exhibits short-range numerical instability in the neighbourhood of (t_n, y_n), when the corresponding equation (2.45) with $\lambda = f_y(t_n, y_n)$, exhibits numerical instability. Therefore, the stability analysis will be based on the equation

$$y'=f(t, y)\approx\lambda y,\ y(t_0) = y_0 \tag{2.48}$$

where
$$\lambda=\left(\frac{\partial f}{\partial y}\right)_n$$

and it is assumed that $(\partial f/\partial y)$ is relatively invariant in the region of interest. Equation (2.48) has as its solution

$$y(t)=y(t_0)\exp(\lambda(t-t_0))$$

which at $t=t_0+nh$ becomes

$$y(t_n)=y(t_0)\,e^{\lambda nh}=y_0\,(e^{\lambda h})^n$$

A singlestep method when applied to (2.48) will lead to a first order difference equation which has solution of the form

$$y_n=c_1\,(E(\lambda h))^n$$

where c_1 is a constant to be determined from the initial condition and $E(\lambda h)$ is an approximation to $e^{\lambda h}$. We call the singlestep method

$$\text{Absolutely stable if } |E(\lambda h)| \leqslant 1$$
$$\text{Relatively stable if } |E(\lambda h)| \leqslant e^{\lambda h}$$

If $\lambda < 0$, the exact solution decreases as t_n increases and the important condition is the absolute stability, since the numerical solution must also decrease with t_n. If Euler's method is used, we obtain

$$y_{n+1}=y_n+hf_n=E(\lambda h)\,y_n$$

where
$$E(\lambda h)=1+\lambda h.$$

Obviously, Euler's method is absolutely stable if

$$|1+\lambda h| \leqslant 1 \text{ or } -2 \leqslant \lambda h < 0$$

If $\lambda > 0$, the exact solution increases as t_n increases. The numerical solution must also increase with t_n. Thus, we are concerned with the relative accuracy, to a fixed number of significant figures, than with the absolute accuracy, to a fixed number of decimal places. Here, the relative stability is an important condition. This is ensured if the numerical solution does not increase faster than the true solution. For Euler's method we have

$$|1+\lambda h| \leqslant e^{\lambda h},\ \lambda > 0$$

which shows that the method is always relatively stable.

2.5.1 Fourth order Runge-Kutta method

We apply the classical fourth order Runge-Kutta method to Equation (2.45) and get

$$\begin{aligned}
K_1 &= hf(t_n, y_n)\\
&= \lambda h\, y_n\\
K_2 &= hf(t_n+\tfrac{1}{2}h,\ y_n+\tfrac{1}{2}K_1)\\
&= \lambda h\,(y_n+\tfrac{1}{2}\lambda h\, y_n)\\
&= [\lambda h+\tfrac{1}{2}(\lambda h)^2]\, y_n\\
K_3 &= hf(t_n+\tfrac{1}{2}h,\ y_n+\tfrac{1}{2}K_2)\\
&= \lambda h\,(y_n+\tfrac{1}{2}(\lambda h+\tfrac{1}{2}(\lambda h)^2)\, y_n)\\
&= [\lambda h+\tfrac{1}{2}(\lambda h)^2+\tfrac{1}{4}(\lambda h)^3]\, y_n\\
K_4 &= hf(t_n+h,\ y_n+K_3)\\
&= \lambda h\,[y_n+(\lambda h+\tfrac{1}{2}(\lambda h)^2+\tfrac{1}{4}(\lambda h)^3)\, y_n]\\
&= [\lambda h+(\lambda h)^2+\tfrac{1}{2}(\lambda h)^3+\tfrac{1}{4}(\lambda h)^4]\, y_n\\
y_{n+1} &= y_n+\tfrac{1}{6}(K_1+2K_2+2K_3+K_4)\\
&= y_n+\tfrac{1}{6}(\lambda h)\, y_n+\tfrac{2}{6}(\lambda h+\tfrac{1}{2}(\lambda h)^2)\, y_n\\
&\quad +\tfrac{2}{6}(\lambda h+\tfrac{1}{2}(\lambda h)^2+\tfrac{1}{4}(\lambda h)^3)\, y_n\\
&\quad +\tfrac{1}{6}(\lambda h+(\lambda h)^2+\tfrac{1}{2}(\lambda h)^3+\tfrac{1}{4}(\lambda h)^4)\, y_n\\
&= [1+\lambda h+\tfrac{1}{2}(\lambda h)^2+\tfrac{1}{6}(\lambda h)^3+\tfrac{1}{24}(h\lambda)^4]\, y_n
\end{aligned}$$

Thus, the *growth factor* for the fourth order method is

$$E(\lambda h)=1+\lambda h+\frac{(\lambda h)^2}{2!}+\frac{(\lambda h)^3}{3!}+\frac{(\lambda h)^4}{4!}$$

whereas the growth factor of the exact solution is $e^{\lambda h}$. If $\lambda h > 0$, then $e^{\lambda h} \geqslant E(\lambda h)$; so the fourth order Runge-Kutta method is always relatively stable. However, if $\lambda h < 0$, then to find the interval of absolute stability we construct the following table:

λh	0	-1	-2	-2.2	-2.6	-3.0
$E(\lambda h)$	1	0.3750	0.3330	0.4212	0.7547	1.375

The graph of $E(\lambda h)$ and $e^{\lambda h}$ for various order Runge-Kutta methods is shown in Figure 2.3. We notice from this graph that for $\lambda < 0$ the fourth order Runge-Kutta method first fails to be relatively stable, and then to be absolutely stable. The interval of absolute stability is $-2.78 < \lambda h < 0$.

2.5.2 Euler extrapolation method

The first column of the Y-scheme for the Euler extrapolation method for (2.48) is given by

$$Y_0^{(k)}=\left(1+\frac{\lambda h_0}{2^k}\right)^{2^k} y_n$$

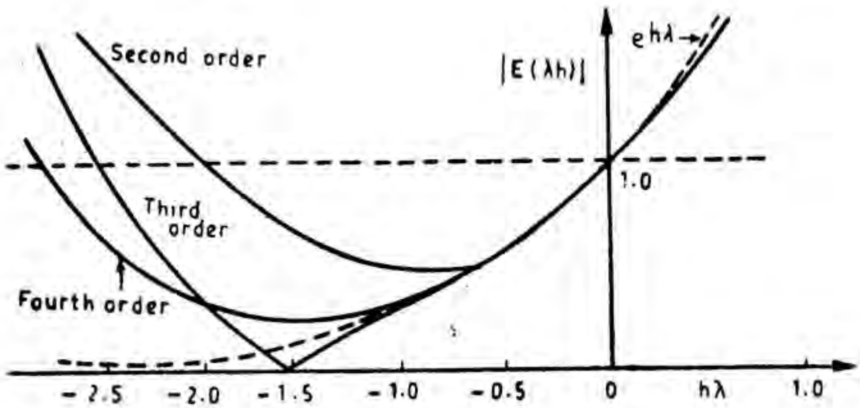


Fig. 2.3 Stability of Runge-Kutta method

and the other columns can be generated from the relation (2.40),

$$Y_m^{(k)} = \frac{2^m Y_{m-1}^{(k+1)} - Y_{m-1}^{(k)}}{2^m - 1} \tag{2.49}$$

$$= \sum_{j=0}^{m} c_{m,\, m-j}\; Y_0^{(k+j)}$$

$$= \left[\sum_{j=0}^{m} c_{m,\, m-j} \left(1 + \frac{\lambda h_0}{2^{k+j}}\right)^{2^{k+j}} \right] y_n$$

where $$c_{m, m-j} = \frac{2^m\, c_{m-1,\, m-j} - c_{m-1,\, m-1-j}}{2^m - 1}$$

$$c_{m-1, m} = c_{m-1,\, -1} = 0$$

If for some $k = K$ and $m = M$, the extrapolated value $Y_M^{(K)}$ is taken as y_{n+1} then we can write (2.49) as

$$y_{n+1} = E(\lambda h_0, K, M)\, y_n$$

where $$E(\lambda h_0, K, M) = \sum_{j=0}^{M} c_{M, M-j} \left(1 + \frac{\lambda h_0}{2^{K+j}}\right)^{2^{k+j}}$$

Thus the Euler extrapolation method is absolutely stable if

$$| E(\lambda h_0, K, M) | \leqslant 1$$

In order to find the interval of absolute stability for various values of K and M, we determine the values of λh_0 corresponding to K and M such that $| E(\lambda h_0, K, M) | = 1$. The principal diagonal of the Y-scheme converges faster than any other diagonal or column and so we determine the interval of absolute stability for $K = 0$ and various values of M. We have for $M = 5$

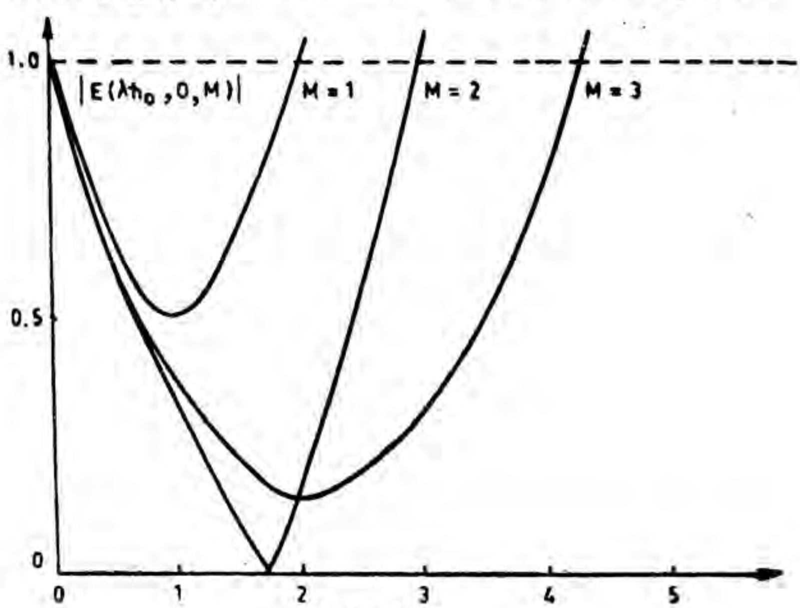
$$\begin{bmatrix} Y_0^{(0)} \\ Y_1^{(0)} \\ Y_2^{(0)} \\ Y_3^{(0)} \\ Y_4^{(0)} \\ Y_5^{(0)} \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ -1 & 2 & & & & \\ \frac{1}{3} & -\frac{6}{3} & \frac{8}{3} & & & \\ -\frac{1}{21} & \frac{14}{21} & -\frac{56}{21} & \frac{64}{21} & & \\ \frac{1}{315} & -\frac{30}{315} & \frac{280}{315} & -\frac{960}{315} & \frac{1024}{315} & \\ -\frac{1}{9765} & \frac{62}{9765} & -\frac{1240}{9765} & \frac{9920}{9765} & -\frac{31744}{9765} & \frac{32768}{9765} \end{bmatrix} \begin{bmatrix} Y_0^{(0)} \\ Y_0^{(1)} \\ Y_0^{(2)} \\ Y_0^{(3)} \\ Y_0^{(4)} \\ Y_0^{(5)} \end{bmatrix}$$

Consider, for example, $M = 2$,

$$\begin{aligned} Y_2^{(0)} &= \frac{1}{3}\,(Y_0^{(0)} - 6Y_0^{(1)} + 8Y_0^{(2)}) \\ &= \left[\frac{1}{3}(1+\lambda h_0) - 2\left(1+\frac{\lambda h_0}{2}\right)^2 + \frac{8}{3}\left(1+\frac{\lambda h_0}{4}\right)^4\right] y_n \\ &= \left[1+\lambda h_0 + \frac{(\lambda h_0)^2}{2} + \frac{(\lambda h_0)^3}{6} + \frac{1}{96}(\lambda h_0)^4\right] y_n \end{aligned}$$

Thus $E(\lambda h_0, 0, 2) = 1+\lambda h_0 + \dfrac{(\lambda h_0)^2}{2} + \dfrac{(\lambda h_0)^3}{6} + \dfrac{(\lambda h_0)^4}{96}$

which gives the stability interval as $-2.785 < \lambda h_0 < 0$. The graph of the function $E(\lambda h_0, 0, M)$ for various values of M is shown in Figure 2.4.



2.6 IMPLICIT RUNGE-KUTTA METHODS

We define an implicit Runge-Kutta method with v slopes by the following equations:

$$K_i = h\,f(t_n+c_i\,h,\ y_n+\sum_{j=1}^{v} a_{ij}\,K_j),\ i = 1, 2,\ldots, v \tag{2.50}$$

and
$$y_{n+1} = y_n+\sum_{i=1}^{v} w_i\,K_i \tag{2.51}$$

where
$$c_i = \sum_{j=1}^{v} a_{ij},\ i = 1, 2, \ldots, v \tag{2.52}$$

and a_{ij}, $1 \leqslant i, j \leqslant v$, $w_1, w_2, \ldots, w_v$ are arbitrary.

The functions K_j are defined by a set of v implicit equations. This makes the derivation of the implicit methods rather complicated. We, therefore, give a brief derivation for the case $v = 2$. Equations (2.50), (2.51) and (2.52) become

$$K_i = hf\,(t_n+c_ih,\ y_n+a_{i1}K_1+a_{i2}K_2),\ i = 1, 2 \tag{2.53}$$

$$y_{n+1} = y_n+w_1K_1+w_2K_2 \tag{2.54}$$

$$c_i = a_{i1}+a_{i2},\ i = 1, 2 \tag{2.55}$$

where a_{11}, a_{12}, a_{21}, a_{22}, w_1, w_2 are six arbitrary parameters. The Taylor series gives

$$y(t_{n+1}) = y\,(t_n)+hy'\,(t_n)+\frac{1}{2}\,h^2y''\,(t_n)+\frac{1}{6}\,h^3y'''\,(t_n)+\frac{1}{24}\,h^4y^{(4)}\,(t_n)+\ldots \tag{2.56}$$

where
$$y'\,(t_n) = f\,(t_n, y\,(t_n))$$

$$y''\,(t_n) = (f_t+ff_y)_n = \left(\frac{\partial}{\partial t}+f_n\,\frac{\partial}{\partial y}\right)f = Df$$

$$y'''\,(t_n) = [(f_{tt}+2ff_{ty}+f^2f_{yy})+f_y(f_t+ff_y)] = D^2f+f_yDf$$

$$\begin{aligned} y^{iv}\,(t_n) &= [(f_{ttt}+3ff_{tty}+3f^2f_{tyy}+f^3f_{yyy})+f_y(f_{tt}+2ff_{ty}+f^2f_{yy}) \\ &\quad +(f_t+ff_y)(3f_{ty}+3ff_{yy}+f_y^2)]_n \\ &= D^3f+f_yD^2f+3Df\,Df_y+f_y^2\,Df \end{aligned}$$

and
$$\begin{aligned} K_i = h\,[f_n&+(c_ihf_t+(a_{i1}K_1+a_{i2}K_2)\,f_y) \\ &+\frac{1}{2}\,(c_i^2\,h^2f_{tt}+2c_ih\,(a_{i1}K_1+a_{i2}K_2)\,f_{ty} \\ &+(a_{i1}K_1+a_{i2}K_2)^2\,f_{yy}) \end{aligned}$$

$$+\frac{1}{6}\,(c_i^3\,h^3 f_{ttt}+3c_i^2\,h^2\,(a_{i1}K_1+a_{i2}K_2)\,f_{tty}$$
$$+3c_i h\,(a_{i1}K_1+a_{i2}K_2)^2\,f_{tyy}$$
$$+(a_{i1}K_1+a_{i2}K_2)^3\,f_{yyy})+\ldots],\ i=1,2 \tag{2.57}$$

Equations (2.57) are implicit and we cannot easily obtain the explicit expressions for K_1 and K_2. In order to determine K_1 and K_2 explicitly, we assume the following form

$$K_i = hA_i+h^2B_i+h^3C_i+h^4D_i+\ldots,\ i=1,2 \tag{2.58}$$

where A_i, B_i, C_i and D_i are unknowns to be determined. Substituting for K_1 and K_2 from (2.58) into (2.57) and on equating powers of h, we obtain

$$A_i = f_n$$
$$B_i = c_i f_t+(a_{i1}\,A_1+a_{i2}\,A_2)\,f_y$$
$$C_i = (a_{i1}\,B_1+a_{i2}\,B_2)\,f_y+\frac{1}{2}\,c_i^2\,f_{tt}+c_i\,(a_{i1}\,A_1+a_{i2}\,A_2)\,f_{ty}$$
$$+\frac{1}{2}\,(a_{i1}\,A_1+a_{i2}\,A_2)^2\,f_{yy}$$
$$D_i = (a_{i1}\,C_1+a_{i2}\,C_2)\,f_y+c_i\,(a_{i1}\,B_1+a_{i2}\,B_2)\,f_{ty}$$
$$+(a_{i1}\,A_1+a_{i2}\,A_2)(a_{i1}\,B_1+a_{i2}\,B_2)\,f_{yy}$$
$$+\frac{1}{6}\,c_i^3\,f_{ttt}+\frac{1}{2}\,c_i^2\,(a_{i1}\,A_1+a_{i2}\,A_2)f_{tty}$$
$$+\frac{1}{2}\,c_i\,(a_{i1}\,A_1+a_{i2}\,A_2)^2\,f_{tyy}$$
$$+\frac{1}{6}\,(a_{i1}\,A_1+a_{i2}\,A_2)^3\,f_{yyy},\quad i=1,2 \tag{2.59}$$

Using (2.55) into (2.59), we get

$$A_i = f_n$$
$$B_i = c_i\,Df$$
$$C_i = (a_{i1}\,c_1+a_{i2}\,c_2)\,f_y\,Df+\frac{1}{2}\,c_i^2\,D^2f$$
$$D_i = [a_{i1}\,(a_{11}\,c_1+a_{12}\,c_2)+a_{i2}\,(a_{21}\,c_1+a_{22}\,c_2)]\,f_y^2\,Df$$
$$+c_i\,(a_{i1}\,c_1+a_{i2}\,c_2)\,Df\,Df_y$$
$$+\frac{1}{2}\,(a_{i1}\,c_1^2+a_{i2}\,c_2^2)\,f_y\,D^2f+\frac{1}{6}\,c_i^3\,D^3f,\ i=1,2 \tag{2.60}$$

Equation (2.54) with the help of (2.58) may be written as

$$y_{n+1} = y_n+h\,(w_1\,A_1+w_2\,A_2)+h^2\,(w_1\,B_1+w_2\,B_2)$$
$$+h^3\,(w_1\,C_1+w_2\,C_2)+h^4\,(w_1\,D_1+w_2\,D_2)+\cdots \tag{2.61}$$

where A_i, B_i, C_i and D_i are given by (2.60). Comparing (2.61) with (2.56) and equating the powers of h, we can obtain implicit Runge-Kutta methods of various orders.

2.6.1 Second order method

Equating the coefficients of h and h^2, we get the following equations

$$w_1+w_2 = 1$$

$$w_1\, c_1+w_2\, c_2 = \frac{1}{2}$$

where $\quad c_1 = a_{11}+a_{12},\ c_2 = a_{21}+a_{22}.$

There are now four arbitrary parameters to be prescribed. If we neglect K_2, i.e. if we choose $a_{21} = a_{22} = a_{12} = 0$, $w_2 = 0$ then on solving the above equations, we find

$$c_1 = \frac{1}{2},\ w_1 = 1$$

The second order implicit Runge-Kutta method with $v = 1$ is obtained

$$K_1 = hf\left(t_n+\frac{1}{2}\,h,\ y_n+\frac{1}{2}\,K_1\right)$$

$$y_{n+1} = y_n+K_1 \tag{2.62}$$

Applying (2.62) to $\quad y' = \lambda y$, we have

$$y_{n+1} = \frac{1+\lambda h/2}{1-\lambda h/2}\, y_n$$

which gives a numerical method based on second order rational approximation to $e^{\lambda h}$ and it has stability interval $(-\infty, 0)$, $\lambda < 0$.

2.6.2 Third order method

Here we have the following system of equations

$$w_1+w_2 = 1$$

$$w_1 c_1+w_2 c_2 = \frac{1}{2}$$

$$w_1\,(a_{11}\, c_1+a_{12}\, c_2)+w_2\,(a_{21}\, c_1+a_{22}\, c_2) = \frac{1}{6}$$

$$w_1\, c_1^2+w_2\, c_2^2 = \frac{1}{3}$$

and $$c_1 = a_{11}+a_{12},\ c_2 = a_{21}+a_{22} \tag{2.63}$$

The two arbitrary parameters can be chosen on the basis that either K_1 is explicit or K_2 is explicit. If we want K_1 to be explicit then we choose

$$a_{11} = a_{12} = 0$$

On solving (2.63), we get

$$c_1 = 0,\quad c_2 = \frac{2}{3},\ a_{21} = a_{22} = \frac{1}{3}$$

$$w_1 = \frac{1}{4},\ w_2 = \frac{3}{4}$$

Thus the third order implicit method which is explicit in K_1 is given by

$$K_1 = hf(t_n, y_n)$$
$$K_2 = hf\left(t_n+\frac{2}{3}h,\ y_n+\frac{1}{3}K_1+\frac{1}{3}K_2\right)$$
$$y_{n+1} = y_n+\frac{1}{4}K_1+\frac{3}{4}K_2 \tag{2.64}$$

In a similar manner, if $a_{12}=a_{22}=0$, a third order implicit method, which is explicit in K_2, is obtained as

$$K_1=hf\left(t_n+\frac{1}{3}h,\ y_n+\frac{1}{3}K_1\right)$$
$$K_2=hf(t_n+h,\ y_n+K_1)$$
$$y_{n+1}=y_n+\frac{3}{4}K_1+\frac{1}{4}K_2 \tag{2.65}$$

2.6.3 Fourth order method

The following equations are obtained

$$w_1+w_2=1$$
$$w_1c_1+w_2c_2=\frac{1}{2}$$
$$w_1(a_{11}c_1+a_{12}c_2)+w_2(a_{21}c_1+a_{22}c_2)=\frac{1}{6}$$
$$w_1c_1^2+w_2c_2^2=\frac{1}{3}$$
$$(w_1a_{11}+w_2a_{21})(a_{11}c_1+a_{12}c_2)+(w_1a_{12}+w_2a_{22})(a_{21}c_1+a_{22}c_2)=\frac{1}{24}$$
$$w_1c_1(a_{11}c_1+a_{12}c_2)+w_2c_2(a_{21}c_1+a_{22}c_2)=\frac{1}{8}$$
$$w_1(a_{11}c_1^2+a_{12}c_2^2)+w_2(a_{21}c_1^2+a_{22}c_2^2)=\frac{1}{12}$$
$$w_1c_1^3+w_2c_2^3=\frac{1}{4}$$

where $\qquad c_1=a_{11}+a_{12},\ c_2=a_{21}+a_{22}.$

Here we have eight equations in six unknowns.

Solving the equations which are independent of a_{11}, a_{12}, a_{21} and a_{22}, we get

$$w_1=w_2=\frac{1}{2},\ c_1=\frac{1}{2}\pm\frac{\sqrt{3}}{6},\ c_2=\frac{1}{2}\mp\frac{\sqrt{3}}{6}$$

On substituting these values in the rest of the equations, we find

$$a_{11}=a_{22}=\frac{1}{4},\ a_{12}=c_1-\frac{1}{4},\ a_{21}=c_2-\frac{1}{4}$$

Thus the fourth order implicit Runge-Kutta method is given by

$$K_1=hf\left(t_n+\left(\frac{1}{2}-\frac{\sqrt{3}}{6}\right)h,\ y_n+\frac{1}{4}K_1+\left(\frac{1}{4}-\frac{\sqrt{3}}{6}\right)K_2\right)$$

$$K_2=hf\left(t_n+\left(\frac{1}{2}+\frac{\sqrt{3}}{6}\right)h,\ y_n+\left(\frac{1}{4}+\frac{\sqrt{3}}{6}\right)K_1+\frac{1}{4}K_2\right)$$

$$y_{n+1}=y_n+\frac{1}{2}(K_1+K_2) \tag{2.66}$$

which in terms of the earlier notations can be written as

$$\begin{array}{c|cc} (3-\sqrt{3})/6 & 1/4 & (3-2\sqrt{3})/12 \\ (3+\sqrt{3})/6 & (3+2\sqrt{3})/12 & 1/4 \\ \hline & 1/2 & 1/2 \end{array}$$

Runge-Kutta-Butcher method

Applying the formula (2.66) to $y'=\lambda y$, we obtain

$$y_{n+1}=\frac{1+\frac{1}{2}\lambda h+\frac{1}{12}(\lambda h)^2}{1-\frac{1}{2}\lambda h+\frac{1}{12}(\lambda h)^2}\ y_n$$

Thus the implicit Runge-Kutta method with $v=2$ has order four and it is absolutely stable in the interval $(-\infty, 0)$.

2.6.4 High order implicit Runge-Kutta methods

If $f(t, y)$ is independent of y, then (2.51) corresponds to a quadrature formula

$$y_{n+1}=y_n+\sum_{i=1}^{v} w_i K_i=y_n+h\sum_{i=1}^{v} w_i f(t_n+c_i h) \tag{2.67}$$

where (t_n+c_ih) and w_i, $i=1, 2,\ldots, v$ are the abscissas and the weights respectively. The quadrature formula (2.67) attains the order $2v$ if c_i and w_i are given by the *Gauss-Legendre quadrature formula*. The abscissas c_i, $i=1, 2, \ldots, v$ are the roots of the modified Legendre polynomial of degree v, i.e. $P_v(2c-1)=0$ and the weights w_i, $i=1, 2,\ldots, v$ are given by the equations

$$\sum_{i=1}^{v} w_i c_i^{k-1}=\frac{1}{k},\ k=1, 2,\ldots, v \tag{2.68}$$

where $c_i\neq 0$.

The parameters a_{ij}, $1\leqslant i, j\leqslant v$ are the solution of the linear system

$$\sum_{j=1}^{v} a_{ij} c_j^{k-1}=\frac{1}{k} c_i^k,\ k=1, 2,\ldots, v \tag{2.69}$$

If in (2.67), we choose $c_1=0$ or $c_v=1$, then (2.67) becomes *Radau's quadrature formula* and the implicit method has order $2v-1$. Using the condition (2.52), we have

(i) $c_1=0$, $a_{11}=a_{12}\cdots=a_{1v}=0$ and $c_2, c_3, \ldots, c_v$ are arbitrary

The arbitrary parameters $c_2, c_3, \cdots, c_v$ are the roots of the polynomial

$$\frac{d^{j-1}}{dc^{j-1}}\left[c^j(1-c)^{j-1}\right]=0,\ j=2, 3, \cdots, v \tag{2.70}$$

(ii) $c_v=1$, $a_{1v}=a_{2v}\ldots=a_{vv}=0$

The parameters $c_1, c_2, \ldots, c_{v-1}$ are arbitrary and can be chosen as the roots of the polynomial

$$\frac{d^{v-1}}{dc^{v-1}}\left[c^{v-1}(1-c)^v\right]=0 \tag{2.71}$$

Similarly, if we take $c_1=0$, $c_v=1$, then (2.67) becomes *Lobatto's quadrature formula* and the implicit method has order $2v-2$. In view of the condition (2.52), we get

$$c_1=0;\ a_{11}=a_{12}\cdots=a_{1v}=0$$
$$c_v=1;\ a_{1v}=a_{2v}\cdots=a_{vv}=0$$

and $c_2, c_3\ldots c_{v-1}$ are given by the roots of the polynomial

$$\frac{d^{v-2}}{dc^{v-2}}\left[c^{v-1}(1-c)^{v-1}\right]=0 \tag{2.72}$$

We now list a few high order methods.

Fifth order methods

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
(6-\sqrt{6})/10 & (9+\sqrt{6})/75 & (24+\sqrt{6})/120 & (168-73\sqrt{6})/600 \\
(6+\sqrt{6})/10 & (9-\sqrt{6})/75 & (168+73\sqrt{6})/600 & (24-\sqrt{6})/120 \\
\hline
 & 1/9 & (16+\sqrt{6})/36 & (16-\sqrt{6})/36
\end{array}$$

Runge-Kutta-Butcher method with Radau nodes

$$\begin{array}{c|ccc}
(4-\sqrt{6})/10 & (24-\sqrt{6})/120 & (24-11\sqrt{6})/120 & 0 \\
(4+\sqrt{6})/10 & (24+11\sqrt{6})/120 & (24+\sqrt{6})/120 & 0 \\
1 & (6-\sqrt{6})/12 & (6+\sqrt{6})/12 & 0 \\
\hline
 & (16-\sqrt{6})/36 & (16+\sqrt{6})/36 & 1/9
\end{array}$$

Runge-Kutta-Butcher method with Radau nodes

Sixth order methods

$(5-\sqrt{15})/10$	$5/36$	$(10-3\sqrt{15})/45$	$(25-6\sqrt{15})/180$
$1/2$	$(10+3\sqrt{15})/72$	$2/9$	$(10-3\sqrt{15})/72$
$(5+\sqrt{15})/10$	$(25+6\sqrt{15})/180$	$(10+3\sqrt{15})/45$	$5/36$
	$5/18$	$8/18$	$5/18$

Runge-Kutta-Butcher method with Gaussian nodes

0	0	0	0	0
$(5-\sqrt{5})/10$	$(5+\sqrt{5})/60$	$1/6$	$(15-7\sqrt{5})/60$	0
$(5+\sqrt{5})/10$	$(5-\sqrt{5})/60$	$(15+7\sqrt{5})/60$	$1/6$	0
1	$1/6$	$(5-\sqrt{5})/12$	$(5+\sqrt{5})/12$	0
	$1/12$	$5/12$	$5/12$	$1/12$

Runge-Kutta-Butcher method with Lobatto nodes

Finally, the implicit Runge-Kutta methods have these advantages: They have large stability interval, and high order for the number of K_i's or the function evaluations. A disadvantage of the methods is that they require a system of linear or nonlinear equations depending on f, to be solved at each step.

2.7 OBRECHKOFF METHODS

The Taylor series method of order p can be obtained easily if it is possible to find the second and higher order derivatives from the given differential equation. The method is explicit and gives a pth degree polynomial approximation to $e^{\lambda h}$ when it is applied to the differential equation $y'=\lambda y$, $y(t_0)=y_0$. The interval of absolute stability is finite.

We shall now develop implicit single step method based on first p derivatives of $y(t)$ at t_n and t_{n+1}. The method has maximum order $2p$ and it is absolutely stable on $(-\infty, 0)$.

The general method is defined by

$$y_{n+1}=y_n+\sum_{i=1}^{q} a_i\, h^i\, y_{n+1}^{(i)}+\sum_{i=1}^{p} b_i\, h^i\, y_n^{(i)} \tag{2.73}$$

where a_i and b_i are arbitrary. The true value $y(t_n)$ will satisfy

$$T_n=y(t_{n+1})-y(t_n)-\sum_{i=1}^{q} a_i\, h^i\, y^{(i)}(t_{n+1})-\sum_{i=1}^{p} b_i\, h^i\, y^{(i)}(t_n) \tag{2.74}$$

where T_n is the local truncation error.

Expanding each term in (2.74) about t_n in the Taylor series and equating the coefficients of the like powers of h, we get $p+q$ equations to determine the arbitrary parameters. The order of the method (2.73) becomes $(p+q)$. The general treatment of (2.73) is difficult, we shall onl give details for $p=q=2$. From (2.73), we get

$$y_{n+1}=y_n+h\,a_1y'_{n+1}+h^2a_2y''_{n+1}+hb_1y'_n+h^2b_2y''_n \tag{2.75}$$

Expanding each term in the Taylor series in (2.74) $(p=q=2)$ and equating the coefficient of the powers of h, we get methods of various orders.

2.7.1 Second order methods

On equating the coefficients of h and h^2, we obtain

$$\begin{aligned} a_1+b_1&=1 \\ a_1+a_2+b_2&=\frac{1}{2} \end{aligned} \tag{2.76}$$

For $a_1=a_2=0$, we get Taylor's series method

$$y_{n+1}=y_n+h\,y'_n+\frac{1}{2}\,h^2y''_n \tag{2.77}$$

which is absolutely stable for $-2<\lambda h<0$.

The values $a_2=b_2=0$ lead to the trapezoidal method

$$y_{n+1}=y_n+\frac{h}{2}\,(y'_{n+1}+y'_n) \tag{2.78}$$

with stability interval $(-\infty, 0)$.

For $b_2=0$, we obtain

$$y_{n+1}=y_n+h\,(1-b_1)\,y'_{n+1}+h^2\left(b_1-\frac{1}{2}\right)y''_{n+1}+h\,b_1\,y'_n \tag{2.79}$$

as one parameter family of second order methods. The parameter b_1 can be determined from the stability consideration.

Applying method (2.79) to the differential equation $y'=\lambda y$, $y(t_0)=y_0$, we get the characteristic equation as

$$\left[1-\lambda h\,(1-b_1)-\lambda^2\,h^2\left(b_1-\frac{1}{2}\right)\right]y_{n+1}-(1+\lambda h\,b_1)\,y_n=0 \tag{2.80}$$

The principal root ξ of (2.80) is given by

$$\xi=\frac{1+\lambda h\,b_1}{1-\lambda h\,(1-b_1)-\lambda^2\,h^2(b_1-\frac{1}{2})} \tag{2.81}$$

The method (2.79) will be absolutely stable if $|\,\xi\,|\leqslant 1$.

The value of ξ given by (2.81) crosses the line $\xi=+1$ when

$$\lambda h=0 \tag{2.82}$$

or
$$\lambda h = 2/(1-2b_1)$$
and the line $\xi = -1$ when
$$\lambda h = 1 \pm [1-4/(1-2b_1)]^{1/2} \tag{2.83}$$

Thus, between $-3/2 \leqslant b_1 < 1/2$ the value of ξ is never less than -1 for any λh, and is above the line 1 only in the range
$$0 < \lambda h < 2/(1-2b_1)$$
Hence, the maximum real stability of the method is achieved when $b_1 = -3/2$, and $|\xi| > 1$ only for $0 < \lambda h < 1/2$. The stability interval for the method (2.79) is shown in Figure 2.5.

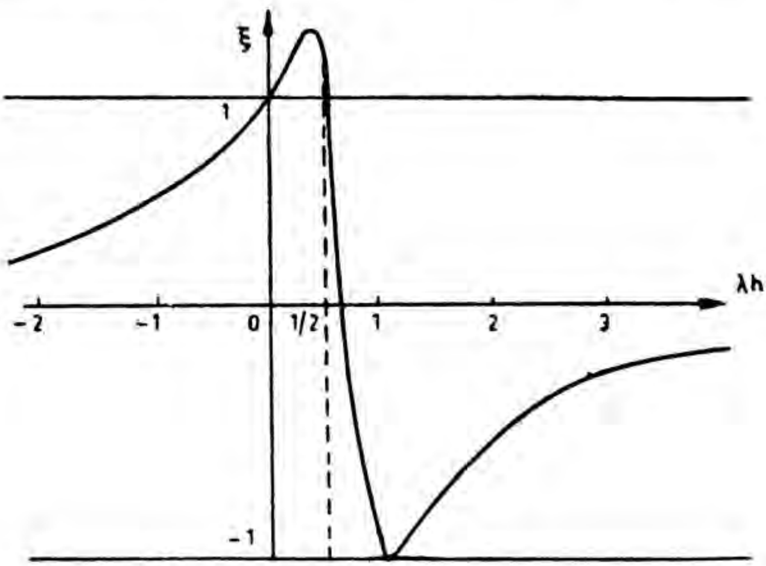


Fig. 2.5 Principal root of the second order method

2.7.2 Third order methods

Here we get the following equations:
$$a_1 + b_1 = 1$$
$$a_1 + a_2 + b_2 = \frac{1}{2}$$
$$\frac{1}{2}a_1 + a_2 = \frac{1}{6} \tag{2.84}$$
If we choose $b_2 = 0$, then we find
$$a_1 = \frac{2}{3},\ b_1 = \frac{1}{3} \text{ and } a_2 = -\frac{1}{6}$$

Thus the method (2.75) becomes

$$y_{n+1} = y_n + \frac{2}{3}hy'_{n+1} - \frac{1}{6}h^2y''_{n+1} + \frac{1}{3}hy'_n \tag{2.85}$$

The principal root of the characteristic equation of method (2.85) is given by

$$\xi = \frac{1+\frac{1}{3}\lambda h}{1-\frac{2}{3}\lambda h+\frac{1}{6}\lambda^2h^2}$$

and it is plotted in Figure 2.6.

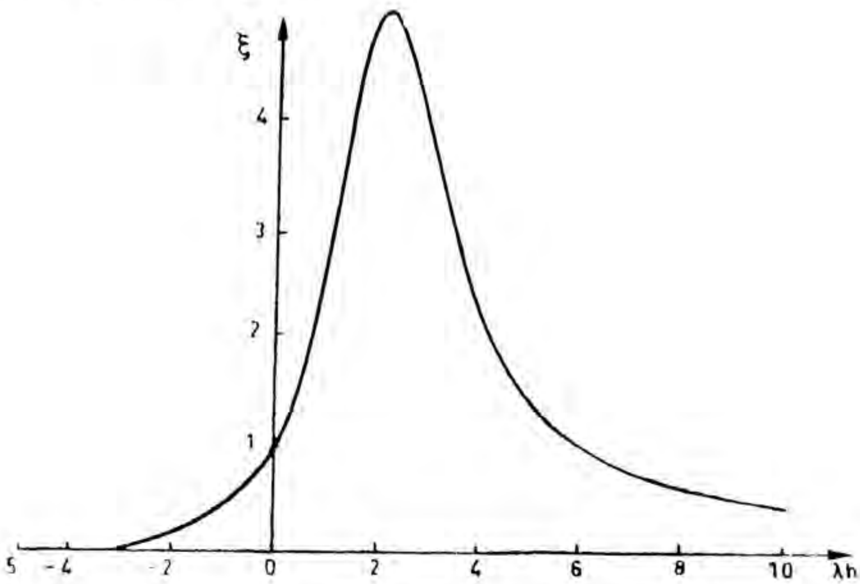


Fig. 2.6 Principal root of the third order method

We find that the method (2.85) is not only absolutely stable in the interval $(-\infty, 0)$ but it is also stable for all positive $\lambda h \geqslant 6$. Keeping a_1 arbitrary, we obtain from (2.84)

$$b_1 = 1-a_1$$
$$a_2 = \frac{1}{6}-\frac{1}{2}a_1$$
$$b_2 = \frac{1}{3}-\frac{1}{2}a_1$$

Substituting in (2.75), we get

$$y_{n+1} = y_n + h\,a_1\,y'_{n+1} + h^2\left(\frac{1}{6}-\frac{1}{2}a_1\right)y''_{n+1} + h(1-a_1)\,y'_n + h^2\left(\frac{1}{3}-\frac{1}{2}a_1\right)y''_n \tag{2.86}$$

a third order method with one arbitrary parameter. The principal root is found to be

$$\xi = \frac{1+\lambda h\,(1-a_1)+\lambda^2 h^2\left(\frac{1}{3}-\frac{1}{2}\,a_1\right)}{1-\lambda h a_1-\lambda^2 h^2\left(\frac{1}{6}-\frac{1}{2}\,a_1\right)}$$

The value $a_1 = 1+\sqrt{3}/3$ gives a third order method which has optimal stability.

2.7.3 Fourth order method

If, in addition to (2.84), we take

$$\frac{1}{6}\,a_1+\frac{1}{2}\,a_2=\frac{1}{24} \tag{2.87}$$

then we obtain a fourth order method as

$$y_{n+1} = y_n+\frac{h}{2}(y'_{n+1}+y'_n)+\frac{h^2}{12}(-y''_{n+1}+y''_n) \tag{2.88}$$

The method (2.88) is absolutely stable on $(-\infty, 0)$.

Alternatively, we may write (2.73) in the form

$$y_{n+1} = P_{p,q}\,(hD)\,y_n \tag{2.89}$$

where

$$P_{p,q}\,(hD) = P_p\,(hD)/Q_q\,(hD)$$

$$P_p\,(hD) = 1+\sum_{i=1}^{p} b_i\,(hD)^i$$

and

$$Q_q\,(hD) = 1-\sum_{i=1}^{q} a_i\,(hD)^i$$

Equation (2.89) represents an approximation to the equation

$$y\,(t_{n+1}) = e^{hD}\,y\,(t_n)$$

The function $P_{p,q}\,(hD)$ is a rational approximation to e^{hD} Table 2.4 contains approximations of e^{hD}. Thus, depending on the values of p and q we obtain the following cases:

(i) $q = 0$, we get $b_i = 1/i!$ and (2.73) becomes the Taylor series method of order p.

(ii) $p = 0$, we obtain $a_i = (-1)^{i+1}\,1/i!$ and (2.73) becomes the backward Taylor series method of order q which is absolutely stable on $(-\infty, 0)$.

(iii) $p = q$, we find that $a_i = (-1)^{i+1}\,b_i$ and $b_i = \dfrac{p!\,(2p-i)!}{(2p)!\,(p-i)!\,i!}$

The method (2.73) becomes

$$y_{n+1} = y_n+\frac{p!}{(2p)!}\sum_{i=1}^{p}\frac{(2p-i)!}{(p-i)!\,i!}\,h^i\,[(-1)^{i-1}\,y^{(i)}_{n+1}+y^{(i)}_n]$$

and it has order $2p$. The interval of absolute stability is $(-\infty, 0)$.

TABLE 2.4 APPROXIMATION TO $\exp(z)$, $z = hD$

$q \backslash p$	0	1	2	3
0	$\frac{1}{1}$	$\frac{1+z}{1}$	$\frac{1+z+\frac{1}{2}z^2}{1}$	$\frac{1+z+\frac{1}{2}z^2+\frac{1}{6}z^3}{1}$
1	$\frac{1}{1-z}$	$\frac{1+\frac{1}{2}z}{1-\frac{1}{2}z}$	$\frac{1+\frac{2}{3}z+\frac{1}{6}z^2}{1-\frac{1}{3}z}$	$\frac{1+\frac{3}{4}z+\frac{1}{4}z^2+\frac{1}{24}z^3}{1-\frac{1}{4}z}$
2	$\frac{1}{1-z+\frac{1}{2}z^2}$	$\frac{1+\frac{1}{3}z}{1-\frac{2}{3}z+\frac{1}{6}z^2}$	$\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	$\frac{1+\frac{3}{5}z+\frac{3}{20}z^2+\frac{1}{60}z^3}{1-\frac{2}{5}z+\frac{1}{20}z^2}$
3	$\frac{1}{1-z+\frac{1}{2}z^2-\frac{1}{6}z^3}$	$\frac{1+\frac{1}{4}z}{1-\frac{3}{4}z+\frac{1}{4}z^2-\frac{1}{24}z^3}$	$\frac{1+\frac{2}{5}z+\frac{1}{20}z^2}{1-\frac{3}{5}z+\frac{3}{20}z^2-\frac{1}{60}z^3}$	$\frac{1+\frac{1}{2}z+\frac{1}{10}z^2+\frac{1}{120}z^3}{1-\frac{1}{2}z+\frac{1}{10}z^2-\frac{1}{120}z^3}$

(iv) $p < q$, we get a method of order $(p+q)$ which is absolutely stable on $(-\infty, 0)$.

(v) $p > q$, we obtain a method order of $(p+q)$ which has a finite stability interval.

2.8 SYSTEMS OF DIFFERENTIAL EQUATIONS

We have already shown that any mth order initial value problem can be replaced by a system of m first order initial value problems. The system of n equations in the vector form may be written as

$$\mathbf{y}' = \frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y}),\ t_0 < t < b \tag{2.90}$$

$$\mathbf{y}(t_0) = \mathbf{y}_0$$

where
$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix},\ \mathbf{f}(t, \mathbf{y}) = \begin{bmatrix} f_1(t, y_1, y_2, \ldots, y_n) \\ f_2(t, y_1, y_2, \ldots, y_n) \\ \vdots \\ f_n(t, y_1, y_2, \ldots, y_n) \end{bmatrix}$$

and
$$\mathbf{y}_0 = \begin{bmatrix} y_{1,0} \\ y_{2,0} \\ \vdots \\ y_{n,0} \end{bmatrix}$$

The singlestep methods developed for a single first order equation can be directly written for the system (2.90). For example, the general singlestep method is given by

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\,\Phi(t_i, \mathbf{y}_i, h) \tag{2.91}$$

where
$$\Phi(t_i, \mathbf{y}_i, h) = \begin{bmatrix} \phi_1(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i}, h) \\ \phi_2(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i}, h) \\ \vdots \\ \phi_n(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i}, h) \end{bmatrix}$$

2.8.1 Taylor series method

We write

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\mathbf{y}_i' + \frac{h^2}{2!}\mathbf{y}_i'' + \ldots + \frac{h^p}{p!}\mathbf{y}_i^{(p)},\ i = 0, 1, 2, \ldots, N-1 \tag{2.92}$$

where
$$\mathbf{y}_i^{(k)} = \begin{bmatrix} y_{1,i}^{(k)} \\ y_{2,i}^{(k)} \\ \vdots \\ y_{n,i}^{(k)} \end{bmatrix} = \begin{bmatrix} \dfrac{d^{k-1}f_1(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i})}{dt^{k-1}} \\ \dfrac{d^{k-1}f_2(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i})}{dt^{k-1}} \\ \vdots \\ \dfrac{d^{k-1}f_n(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i})}{dt^{k-1}} \end{bmatrix}$$

2.8.2 Runge-Kutta methods

The classical fourth order Runge-Kutta formula becomes

$$\mathbf{y}_{i+1} = \mathbf{y}_i + \frac{1}{6}(\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4) \tag{2.93}$$

where $\mathbf{K}_1 = \begin{bmatrix} K_{11} \\ K_{21} \\ \vdots \\ K_{n1} \end{bmatrix}, \mathbf{K}_2 = \begin{bmatrix} K_{12} \\ K_{22} \\ \vdots \\ K_{n2} \end{bmatrix}, \mathbf{K}_3 = \begin{bmatrix} K_{13} \\ K_{23} \\ \vdots \\ K_{n3} \end{bmatrix}, \mathbf{K}_4 = \begin{bmatrix} K_{14} \\ K_{24} \\ \vdots \\ K_{n4} \end{bmatrix}$

and $K_{j1} = hf_j(t_i, y_{1,i}, y_{2,i}, \ldots, y_{n,i})$

$$K_{j2} = hf_j\left(t_i + \frac{1}{2}h, y_{1,i} + \frac{1}{2}K_{11}, y_{2,i} + \frac{1}{2}K_{21}, \ldots, y_{n,i} + \frac{1}{2}K_{n1}\right)$$

$$K_{j3} = hf_j\left(t_i + \frac{1}{2}h, y_{1,i} + \frac{1}{2}K_{12}, y_{2,i} + \frac{1}{2}K_{22}, \ldots, y_{n,i} + \frac{1}{2}K_{n2}\right)$$

$$K_{j4} = hf_j(t_i + h, y_{1,i} + K_{13}, y_{2,i} + K_{23}, \ldots, y_{n,i} + K_{n3}),\ j = 1, 2, \ldots, n$$

In an explicit form (2.93) may be expressed as

$$\begin{bmatrix} y_{1,i+1} \\ y_{2,i+1} \\ \vdots \\ y_{n,i+1} \end{bmatrix} = \begin{bmatrix} y_{1,i} \\ y_{2,i} \\ \vdots \\ y_{n,i} \end{bmatrix} + \frac{1}{6}\left\{\begin{bmatrix} K_{11} \\ K_{21} \\ \vdots \\ K_{n1} \end{bmatrix} + 2\begin{bmatrix} K_{12} \\ K_{22} \\ \vdots \\ K_{n2} \end{bmatrix} + 2\begin{bmatrix} K_{13} \\ K_{23} \\ \vdots \\ K_{n3} \end{bmatrix} + \begin{bmatrix} K_{14} \\ K_{24} \\ \vdots \\ K_{n4} \end{bmatrix}\right\}$$

Example 2.4 Solve the initial value problem

$$x' = y, \quad x(0) = 0$$
$$y' = -x, \ y(0) = 1, \ t \in [0, 1]$$

by second order Runge-Kutta method with $h = 0.1$.

For $n = 0$

$t_0 = 0, x_0 = 0, y_0 = 1$

$K_{11} = hf_1(t_0, x_0, y_0) = .1(1) = .1$

$K_{21} = hf_2(t_0, x_0, y_0) = .1(0) = 0$

$K_{12} = hf_1(t_0 + h, x_0 + K_{11}, y_0 + K_{21}) = .1\ (1+0) = .1$

$K_{22} = hf_2(t_0 + h, x_0 + K_{11}, y_0 + K_{21}) = .1\ (0-.1) = -.01$

$$x_1 = x_0 + \frac{1}{2}(K_{11} + K_{12}) = 0 + \frac{1}{2}(.1 + .1) = .1$$

$$y_1 = y_0 + \frac{1}{2}(K_{21} + K_{22}) = 1 + \frac{1}{2}(0 - .01) = 1 - .005 = .995$$

For $n = 1$

$t_1 = .1, x_1 = .1, y_1 = .995$

$K_{11} = hf_1(t_1, x_1, y_1) = .1\ (.995) = .0995$

$K_{21} = hf_2(t_1, x_1, y_1) = .1\ (-.1) = -.01$

$K_{12} = hf_1(t_1 + h, x_1 + K_{11}, y_1 + K_{21}) = .1\ (.995 - .01)$

$= .0985$

$$K_{22} = h f_2 (t_1+h, x_1+K_{11}, y_1+K_{21}) = .1 [-(.1+.0995)]$$
$$= -.01995$$
$$x_2 = x_1+\frac{1}{2} (K_{11}+K_{12})$$
$$= .1 +\frac{1}{2} (.0995+.0985)$$
$$= .1990$$
$$y_2 = y_1+\frac{1}{2} (K_{21}+K_{22})$$
$$= .995+\frac{1}{2} (-.01-.01995)$$
$$= .980025.$$

The exact solution is given by

$$x(t) = \sin t, y(t) = \cos t$$

The computed solution is listed in Table 2.5.

TABLE 2.5 SOLUTION OF $x' = y, y' = -x, x(0) = 0, y(0) = 1$ BY THE SECOND ORDER RUNGE-KUTTA METHOD WITH $h = 0.1$

t_n	x_n	y_n	$x(t_n)$	$y(t_n)$
0	0	1	0	1
0.1	0.1	0.995	0.099833	0.995005
0.2	0.1990	0.980025	0.198669	0.980067
0.3	0.296008	0.955225	0.295520	0.955336
0.4	0.390050	0.920848	0.389418	0.921061
0.5	0.480185	0.877239	0.479426	0.877583
0.6	0.565507	0.824834	0.564642	0.825336
0.7	0.645163	0.764159	0.644218	0.764842
0.8	0.718353	0.695822	0.717356	0.696707
0.9	0.784344	0.620508	0.783327	0.621610
1.0	0.842473	0.538971	0.841471	0.540302

2.8.3 Stability analysis

The stability of the numerical methods for the system of first order differential equations is discussed by applying the numerical methods to the homogeneous locally linearized form of the equation (2.90). Assuming that the functions f_i have continuous partial derivatives $\frac{\partial f_i}{\partial y_j} = a_{ij}$ and $\mathbf{A}$ denotes the $n \times n$ matrix $[a_{ij}]$, we may to terms of the first order write (2.90) as

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}\mathbf{y} \tag{2.94}$$

The matrix $\mathbf{A}$ is usually a variable depending on the y's and t, but it is possible to forecast the general behaviour of the solution of (2.94) by treating the simple case where $\mathbf{A}$ is constant. Assuming that $\mathbf{A}$ is a constant matrix with distinct eigenvalues. It is easily verified that the analytic solution $\mathbf{y}(t)$ of (2.94) satisfying the initial conditions is given by

$$\mathbf{y}(t) = \exp(\mathbf{A}t)\,\mathbf{y}_0 \tag{2.95}$$

where $\exp(\mathbf{A}t)$ is defined as a matrix function

$$\exp(\mathbf{A}t) = \mathbf{I} + \mathbf{A}t + \frac{(\mathbf{A}t)^2}{2!} + \frac{(\mathbf{A}t)^3}{3!} + \ldots \tag{2.96}$$

and $\mathbf{I}$ is a unit matrix.

From (2.96) it is seen that the transformation $\mathbf{P}$ which diagonalizes $\mathbf{A}$, i.e., $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{D}$, where $\mathbf{D}$ is a diagonal matrix, also diagonalizes $\exp(\mathbf{A}t)$, giving the relation

$$\mathbf{P}^{-1}\exp(\mathbf{A}t)\,\mathbf{P} = \exp(\mathbf{D}t) \tag{2.97}$$

where

$$\mathbf{D} = \begin{bmatrix} \lambda_1 & & & & & & \\ & \lambda_2 & & & & & \\ & & \ddots & & & & \\ & & & \lambda_j & & & \\ & & & & \ddots & & \\ & & & & & & \lambda_n \end{bmatrix}$$

The λ_j, $j = 1, 2, \ldots, n$ are assumed to be distinct or possibly complex eigenvalues with negative real part, of $\mathbf{A}$. The matrix function $\exp(\mathbf{D}t)$ is a diagonal matrix with elements $\exp(\lambda_j t)$, $j = 1, 2, \ldots, n$. The equation (2.94) becomes

$$\frac{d\mathbf{v}}{dt} = \mathbf{D}\mathbf{v} \tag{2.98}$$

where we have put $\mathbf{v} = \mathbf{P}^{-1}\mathbf{y}$.

The analytic solution of (2.98), using (2.97) may be written as

$$\mathbf{v} = \exp(\mathbf{D}t)\,\mathbf{v}_0 \tag{2.99}$$

$$\mathbf{y}_0 = \mathbf{P}\mathbf{v}_0$$

To obtain the numerical values of the function $\mathbf{v}(t)$ at the step points t_i, we get from (2.95) a recurrence relation

$$\mathbf{y}(t_{i+1}) = \exp(\mathbf{A}\,h)\,\mathbf{y}(t_i) \tag{2.100}$$

The equation (2.100) may be used to get the numerical values of the function $\mathbf{y}(t)$ at the step points t_i, but its applicability depends on the computation of $\exp(\mathbf{A}\,h)$ or $\mathbf{P}\exp(\mathbf{D}h)\,\mathbf{P}^{-1}$.

The use of the singlestep method (2.91) to (2.98) will lead to a relation of the form

$$\mathbf{v}_{i+1} = \mathbf{E}(\mathbf{D}h)\,\mathbf{v}_i \tag{2.101}$$

where $\mathbf{E}(\mathbf{D}h)$ represents an approximation to exp $(\mathbf{D}h)$. The matrix $\mathbf{E}(\mathbf{D}h)$ is a diagonal matrix and its each diagonal element $\mathbf{E}_j(\lambda_j h), j = 1, 2, \ldots, n$ is an approximation to the diagonal element exp (λ_j, h), $j = 1, 2, \ldots, n$ respectively, of the matrix exp $(\mathbf{D}\,h)$. We therefore have the important result that the stability analysis of the singlestep method (2.91) as applied to the differential system (2.94) can be discussed by applying the single-step method (2.91) to the scalar equation

$$y' = \lambda_j y \tag{2.102}$$

where λ_j, $j = 1, 2, \ldots, n$ are the eigenvalues of the matrix $\mathbf{A}$. Thus, the single step method (2.91) will be absolutely stable if

$$|\,E_j(\lambda_j h)\,| < 1, \; j = 1, 2, \ldots, \tag{2.103}$$

where $R_e(\lambda_j) < 0$ is the real part of λ_j.

DEFINITION 2.3 The domain on the λh-complex plane is called the stability region in which $|\,y_{i+1}/y_i\,| \leqslant 1$ when the method (2.91) is applied to the differential equation $y' = \lambda y$ where λ is a complex constant with negative real part.

We now use the Taylor series method (2.92) to solve the vector equation (2.94) and obtain, after simplification,

$$\mathbf{y}_{i+1} = \left[\sum_{m=0}^{p} \frac{(\mathbf{A}h)^m}{m!}\right]^i \mathbf{y}_0 \tag{2.104}$$

It is easy to show that the general explicit Runge-Kutta method also gives the solution (2.104), where p is the order of the particular method. For example, $p = 4$ for the fourth order Runge-Kutta method. The eigenvalues of the matrix

$$\sum_{m=0}^{4} \frac{(\mathbf{A}h)^m}{m!} \text{ are given by } \sum_{m=0}^{4} \frac{(h\lambda_j)^m}{m!}$$

where the λ_j's are eigenvalues of $\mathbf{A}$. From the condition (2.103) it can be easily proved that the fourth order Runge-Kutta method is stable, if and only if:

(i) real λ_j; $-2.78 < h\lambda_j < 0$
(ii) pure imaginary λ_j; $0 < |\,h\lambda_j\,| < 2\sqrt{2}$
(iii) complex λ_j; $h\lambda_j$ lie inside the region R, (see Figure 2.7).

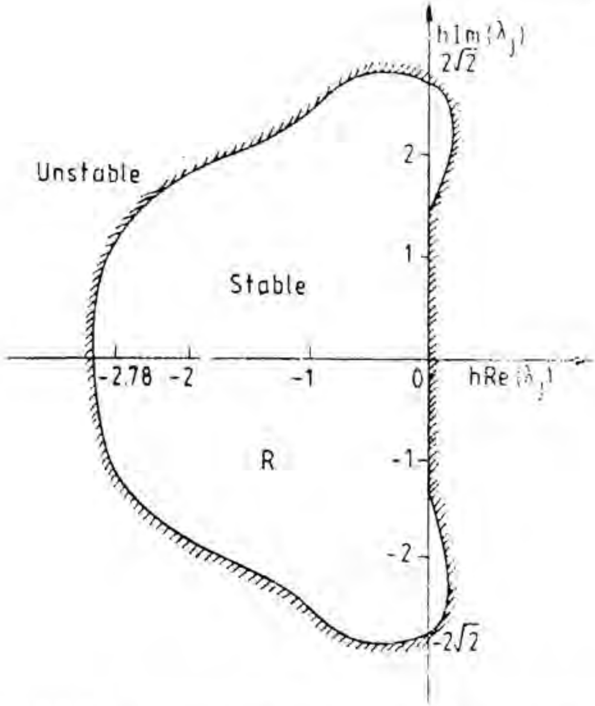


Fig. 2.7 Stability region for the fourth order Runge-Kutta method

2.8.4 Stiff system of differential equations

There are many physical problems which lead to a system of ordinary differential equations with a property given by the following definition.

DEFINITION 2.4 A system of ordinary differential equations (2.90) is said to be stiff if the eigenvalues of the *Jacobian* matrix $\left[\dfrac{\partial \mathbf{f}}{\partial \mathbf{y}}\right]$ at every point of have negative real parts and differ greatly in magnitude.

We now study the main difficulties associated with the numerical solution of the stiff differential equations by applying the fourth order Runge-Kutta method to (2.94) when it is a stiff system, i.e., the eigenvalues λ_j of the matrix $\mathbf{A}$ satisfy the conditions:

(i) Real $\lambda_j < 0, j = 1, 2, \ldots, n$

(ii) $\max\limits_j \mid \text{Real}\,\lambda_j \mid \gg \min\limits_j \mid \text{Real}\,\lambda_j \mid, \quad j = 1, 2, \ldots$

If λ_j is an eigenvalue of $\mathbf{A}$ whose real part is large in magnitude and $\bar{y}_j(t)$ represents, the component of the corresponding numerical solution then using (2.104) with $p = 4$, the following relationship is obtained

$$\bar{y}_j(t_{i+1}) = y_{j,i+1} = \left[1 + h\lambda_j + \frac{(h\lambda_j)^2}{2!} + \frac{(h\lambda_j)^3}{3!} + \frac{(h\lambda_j)^4}{4!}\right] y_{j,i}, \quad i = 0, 1, 2, \ldots \tag{2.105}$$

Initially we require $\bar{y}_i(t)$ to be accurate so we expect to keep $|h\lambda_i|$ small, but when $|\bar{y}_i(t)|$ has become negligible related to $\mathbf{y}(t)$ it is unnecessary to require accuracy and we need only to ensure that $|\bar{y}_i(t)|$ does not grow. It has already been shown that to keep $|y_{j,i+1}| < |y_{j,i}|$ it is necessary that $|h\lambda_i| < 2.78$, approximately. Thus, the main difficulty encountered in solving stiff equations is that even though the component of the true solution corresponding to λ_i, soon becomes negligible, the restriction on step size imposed by the stability requires that $|h\lambda_i|$ remain small throughout the range of integration. Therefore, a numerical method must have very strong stability properties if it is to be efficient.

DEFINITION 2.5 A numerical method of the form (2.91) is called A-stable in the sense of *Dahlquist* if the region of stability associated with the method contains the open left-half-plane.

The fourth order Runge-Kutta method is not A-stable because it has finite region of stability on the left half-plane. The fully implicit Runge-Kutta-Butcher method (2.66) and other similar methods are A-stable. The *Obrechkoff* methods (2.89) are also A-stable. If we use the fourth order Runge-Kutta method to solve the stiff system of differential equations then we must limit the step size to a small value of the order of the reciprocal of the magnitude of the real part of the largest eigenvalue. Alternatively, if an A-stable implicit method is applied to a nonlinear system (2.90) it defines the value $\mathbf{y}(t)$ at t_{n+1} of the numerical solution implicitly by the nonlinear algebraic system

$$\mathbf{y} = \mathbf{g}(\mathbf{y}) \tag{2.106}$$

The stability requirement does no longer restrict the choice of step size. However we must solve the system (2.106) at each step by some iterative method. The convergence requirements for the iterative solution of (2.106) places restrictions on the largest step size that can be used. Thus, to solve the stiff differential system (2.90) we need not only the numerical methods with strong stability condition but also the accurate iterative methods for solving nonlinear algebraic system (2.106).

2.9 HIGHER ORDER DIFFERENTIAL EQUATIONS

The higher order equations can be solved by considering an equivalent system of first order equations. However, it is also possible to develop direct singlestep methods to solve higher order equations.

2.9.1 Runge-Kutta methods

Let us study the Runge-Kutta methods for a general second order equation

$$y'' = f(t, y, y'),\ t \in [t_0, b] \tag{2.107}$$

with the initial conditions

$$y(t_0) = y_0,\ y'(t_0) = y'_0$$

We define

$$K_1 = \frac{h^2}{2!} f(t_n, y_n, y'_n)$$

$$K_2 = \frac{h^2}{2!} f\left(t_n + a_2 h,\ y_n + a_2 h y'_n + a_{21} K_1,\ y'_n + \frac{b_{21}}{h} K_1 \right)$$

$$y_{n+1} = y_n + h y'_n + W_1 K_1 + W_2 K_2$$

$$y'_{n+1} = y'_n + \frac{1}{h}(W'_1 K_1 + W'_2 K_2) \tag{2.108}$$

where a_2, a_{21}, b_{21}, W's and W''s are arbitrary constants to be determined.

The Taylor series expansion gives

$$y_{n+1} = y_n + h\, y'_n + \frac{h^2}{2!} y''_n + \frac{h^3}{3!} y'''_n + \frac{h^4}{4!} y^{iv}_n + \ldots$$

$$y'_{n+1} = y'_n + h y''_n + \frac{h^2}{2!} y'''_n + \frac{h^3}{3!} y^{iv}_n + \ldots \tag{2.109}$$

where

$$y''_n = f(t_n, y(t_n), y'(t_n))$$

$$y'''_n = (f_t + y' f_y + f f_{y'})_n$$

$$y^{iv}_n = [f_{tt} + y'^2 f_{yy} + f^2 f_{y'y'} + 2y' f_{ty} + 2y' f f_{yy'} + 2f f_{ty'} + f_{y'}(f_t + y' f_y + f f_{y'}) + f f_y]_n \tag{2.110}$$

We may write (2.110) as

$$y''_n = f_n$$

$$y'''_n = D f_n$$

$$y^{iv}_n = D^2 f_n + f_{y'} D f_n + f_n f_y$$

where

$$D = \frac{\partial}{\partial t} + y'_n \frac{\partial}{\partial y} + f_n \frac{\partial}{\partial y'}$$

Equation (2.109) becomes

$$y_{n+1} = y_n + h y'_n + \frac{h^2}{2!} f_n + \frac{h^3}{3!} D f_n + \frac{h^4}{4!}(D^2 f_n + f_{y'} D f_n + f_n f_y) + \cdots$$

$$y'_{n+1} = y'_n + h f_n + \frac{h^2}{2!} D f_n + \frac{h^3}{3!}(D^2 f_n + f_{y'} D f_n + f_n f_y) + \cdots \tag{2.111}$$

Simplifying K_2, we get

$$\frac{2}{h^2} K_2 = f_n + h\left(a_2 f_t + a_2 y'_n f_y + \frac{1}{2} b_{21} f_n f_{y'} \right) + \frac{h^2}{2!}\left(a_2^2 f_{tt} + a_2^2 y'^2_n f_{yy} + \frac{1}{4} b_{21}^2 f_n^2 f_{y'y'} \right.$$

$$+2a_2^2 y'_n f_{ty'} + a_2 b_{21} f_n f_{ty'}$$

$$+ a_2 b_{21} f_n y'_n f_{yy'} + a_{21} f_n f_y\Big) + 0(h^3)$$

or
$$K_2 = \frac{h^2}{2} f_n + \frac{h^3}{2} a_2 D f_n + \frac{h^4}{4}(a_2^2 D^2 f_n + a_{21} f_n f_y) + 0(h^5) \quad (2.112)$$

where we have used

$$a_2 = \frac{1}{2} b_{21} \quad (2.113)$$

The substitution of K_1 and K_2 in (2.108) yields

$$y_{n+1} = y_n + h y'_n + \frac{h^2}{2}(W_1 + W_2) f_n + \frac{h^3}{2} a_2 W_2 D f_n$$

$$+ \frac{h^4}{4}(W_2 a_2^2 D^2 f_n + W_2 a_{21} f_n f_y) + 0(h^5) \quad (2.114)$$

$$y'_{n+1} = y'_n + \frac{1}{2} h(W'_1 + W'_2) f_n + \frac{h^2}{2} a_2 W'_2 D f_n$$

$$+ \frac{h^3}{4}(W'_2 a_2^2 D^2 f_n + W'_2 a_{21} f_n f_y) + 0(h^4)$$

On comparing (2.114) with (2.111), we obtain

$$W_1 + W_2 = 1, \quad W'_1 + W'_2 = 2$$

$$a_2 W_2 = \frac{1}{3}, \quad a_2 W'_2 = 1 \quad (2.115)$$

The coefficients of h^4 in y_{n+1} and of h^3 in y'_{n+1} of equation (2.114) will not match with the corresponding coefficients in Equation (2.111) for any choice of a_2, a_{21}, W_2 and W'_2. Thus the local truncation error is $0(h^4)$ in y and $0(h^3)$ in y'. A simple solution of (2.113) and (2.115) may be written as

$$W_1 = W_2 = \frac{1}{2}$$

$$a_2 = a_{21} = \frac{2}{3}, \quad b_{21} = \frac{4}{3}$$

$$W'_1 = \frac{1}{2}$$

$$W'_2 = \frac{3}{2}$$

Thus the Runge-Kutta method (2.108) becomes

$$K_1 = \frac{h^2}{2!} f(t_n, y_n, y'_n)$$

$$K_2 = \frac{h^2}{2!} f\left(t_n + \frac{2}{3} h, y_n + \frac{2}{3} h y'_n + \frac{2}{3} K_1, y'_n + \frac{4}{3h} K_1\right)$$

$$y_{n+1} = y_n + h\, y_n' + \frac{1}{2}(K_1 + K_2)$$

$$y_{n+1}' = y_n' + \frac{1}{2h}(K_1 + 3K_2)$$

The Runge-Kutta method using four K's is given by

$$K_1 = \frac{h^2}{2} f(t_n, y_n, y_n')$$

$$K_2 = \frac{h^2}{2} f\left(t_n + \frac{h}{2}, y_n + \frac{1}{2} h y_n' + \frac{1}{4} K_1, y_n' + \frac{1}{h} K_1\right)$$

$$K_3 = \frac{h^2}{2} f\left(t_n + \frac{h}{2}, y_n + \frac{1}{2} h y_n' + \frac{1}{4} K_1, y_n' + \frac{1}{h} K_2\right)$$

$$K_4 = \frac{h^2}{2} f\left(t_n + h, y_n + h y_n' + K_3, y_n' + \frac{2}{h} K_3\right)$$

$$y_{n+1} = y_n + h y_n' + \frac{1}{3}(K_1 + K_2 + K_3)$$

$$y_{n+1}' = y_n' + \frac{1}{3h}(K_1 + 2K_2 + 2K_3 + K_4) \tag{2.116}$$

If the function f is independent of y', then we can construct a Runge-Kutta method in which the local truncation error in y and y' is $0(h^4)$. Here we get

$$W_1 + W_2 = 1 \qquad W_1' + W_2' = 2$$

$$a_2 W_2 = \frac{1}{3} \qquad W_2' a_2 = 1$$

$$W_2' a_2^2 = \frac{2}{3}$$

$$W_2' a_{21} = \frac{2}{3}$$

which has the solution

$$a_2 = \frac{2}{3}, \qquad a_{21} = \frac{4}{9}$$

$$W_1 = W_2 = \frac{1}{2}, W_2' = \frac{3}{2}, \quad W_1' = \frac{1}{2}$$

Thus the Runge-Kutta method for the second order initial value problem

$$y'' = f(t, y)$$
$$y(t_0) = y_0, \; y'(t_0) = y_0' \tag{2.117}$$

becomes

$$K_1 = \frac{h^2}{2!} f(t_n, y_n)$$

$$K_2 = \frac{h^2}{2!} f\left(t_n + \frac{2}{3} h, y_n + \frac{2}{3} h y_n' + \frac{4}{9} K_1\right) \tag{2.118}$$

$$y_{n+1} = y_n + h\,y'_n + \frac{1}{2}(K_1+K_2)$$

$$y'_{n+1} = y'_n + \frac{1}{2h}(K_1+3K_2) \tag{2.119}$$

The *Runge-Kutta-Nystrom* formula is written as

$$K_1 = \frac{h^2}{2} f(t_n, y_n)$$

$$K_2 = \frac{h^2}{2} f\left(t_n + \frac{2}{5}h, y_n + \frac{2}{5}hy'_n + \frac{4}{25}K_1\right)$$

$$K_3 = \frac{h^2}{2} f\left(t_n + \frac{2}{3}h, y_n + \frac{2}{3}h\,y'_n + \frac{4}{9}K_1\right)$$

$$K_4 = \frac{h^2}{2} f\left(t_n + \frac{4}{5}h, y_n + \frac{4}{5}hy'_n + \frac{8}{25}(K_1+K_2)\right)$$

$$y_{n+1} = y_n + hy'_n + \frac{1}{96}(23K_1+75K_2-27K_3+25K_4)$$

$$y'_{n+1} = y'_n + \frac{1}{96h}(23K_1+125K_2-81K_3+125K_4) \tag{2.120}$$

where the truncation error in y and y' is $0(h^5)$. A formula based on three function evaluations with truncation error $0(h^4)$ is given by

$$K_1 = \frac{h^2}{2} f\left(t_n + \frac{1}{6}h, y_n + \frac{1}{6}h\,y'_n\right)$$

$$K_2 = \frac{h^2}{2} f\left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}h\,y'_n + \frac{1}{3}K_1\right)$$

$$K_3 = \frac{h^2}{2} f\left(t_n + \frac{5}{6}h, y_n + \frac{5}{6}h\,y'_n + \frac{4}{9}K_1 + \frac{2}{9}K_2\right)$$

$$y_{n+1} = y_n + h\,y'_n + \frac{1}{16}(10K_1+4K_2+2K_3)$$

$$h\,y'_{n+1} = h\,y'_n + \frac{1}{16}(12K_1+8K_2+12K_3) \tag{2.121}$$

Example 2.5 Solve the initial value problem

$$y'' = (1+t^2)\,y,\ y(0) = 1,\ y'(0) = 0,\ t \in [0, 1]$$

by the Runge-Kutta method (2.119) with $h = 0.1$.

For $n = 0$

$$t_0 = 0,\ y_0 = 1,\ y'_0 = 0$$

$$K_1 = \frac{h^2}{2} f(t_0, y_0) = \frac{(.1)^2}{2}(1+0)\,1 = .005$$

$$K_2 = \frac{h^2}{2} f\left(t_0 + \frac{2}{3}h, y_0 + \frac{2}{3}h\,y'_0 + \frac{4}{9}K_1\right)$$

$$= \frac{(.1)^2}{2}\left(1+\frac{4}{9}(.1)^2\right)\left(1+\frac{2}{3}(.1)\,0+\frac{4}{9}(.005)\right)$$
$$= .0050333827$$
$$y_1 = y_0+h\,y_0'+\frac{1}{2}(K_1+K_2)$$
$$= 1+0+\frac{1}{2}(.005+.0050333827)$$
$$= 1.0050167$$
$$y_1' = 0+\frac{1}{2\,(.1)}(.005+.0151001481) = 0.10050074$$

The exact solution is given by

$$y(t) = e^{t^2/2}$$

The computed solution is listed in Table 2.6.

TABLE 2.6 SOLUTION OF $y'' = (1+t^2)\,y$, $y(0) = 1$, $y'(0) = 0$ BY THE RUNGE-KUTTA METHOD WITH $h = 0.1$

t_n	y_n	y_n'	$y(t_n)$	$y'(t_n)$
0	1	0	1	0
0.1	1.0050167	0.100501	1.0050125	0.100501
0.2	1.0202098	0.204038	1.0202013	0.204040
0.3	1.0460407	0.313802	1.0460279	0.313808
0.4	1.0833046	0.433303	1.0832871	0.433315
0.5	1.1331710	0.566554	1.1331485	0.566574
0.6	1.1972453	0.718298	1.1972174	0.718330
0.7	1.2776552	0.894286	1.2776213	0.894335
0.8	1.3771681	1.101629	1.3771278	1.101702
0.9	1.4993498	1.349266	1.4993030	1.349372
1.0	1.6487762	1.648568	1.6487213	1.648722

2.9.2 Stability analysis

We can discuss the stability and the error analysis of the Runge-Kutta method (2.119) in a manner similar to that adopted in Section 2.5.

Let us consider the differential equation

$$y'' = \alpha y \tag{2.122}$$

subject to the initial conditions

$$y(t_0) = y_0,\; y'(t_0) = y_0',\; t \in [t_0, b]$$

where α is a real number.

We shall discuss the three cases $\alpha = 0, -k^2, k^2$. Using Equation (2.122) into (2.118), we get

$$K_1 = \frac{h^2}{2}\alpha y_n,\quad K_2 = \left(\frac{h^2\alpha}{2} + \frac{h^4\alpha^2}{9}\right) y_n + \frac{h^3}{3}\alpha y'_n$$

Substituting the expressions for K_1 and K_2 into (2.119), we find

$$\begin{bmatrix} y_{n+1} \\ y'_{n+1} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} y_n \\ y'_n \end{bmatrix} \tag{2.123}$$

where
$$a_{11} = 1 + \frac{h^2\alpha}{2} + \frac{h^4\alpha^2}{18},\quad a_{12} = h + \frac{h^3\alpha}{6}$$

$$a_{21} = \alpha h + \frac{1}{6} h^3 \alpha^2,\quad a_{22} = 1 + \frac{h^2\alpha}{2} \tag{2.124}$$

For $\alpha=0$, we have

$$y_{n+1} = y_n + h\, y'_n$$
$$y'_{n+1} = y'_n \tag{2.125}$$

The solution of (2.125) can be written as

$$y'_n = y'_0$$
$$y_n = y_0 + nh\, y'_0$$

which is an expected result.

We now consider the case $\alpha = -k^2$; the solutions in this case are oscillating. We, therefore, consider the eigenvalues of the matrix in (2.123), which are given by

$$\lambda_1, \lambda_2 = \frac{1}{2}\,[a_{11} + a_{22} \pm [(a_{11} - a_{22})^2 + 4a_{12}\, a_{21}]^{1/2}] \tag{2.126}$$

Substituting $\alpha = -k^2$ into (2.124) and inserting the resulting values into (2.126), we get

$$\lambda_1, \lambda_2 = \frac{1}{2}\left[2 - h^2 k^2 + \frac{h^4 k^4}{18} \pm \left[\left(\frac{hk}{18}\right)^2 (h^6k^6 - 36h^4k^4 + 432h^2k^2 - 1296)\right]^{1/2}\right]$$

$$= \frac{1}{2}\left[2 - h^2 k^2 + \frac{h^4 k^4}{18} \pm \left[\left(\frac{hk}{18}\right)^2 (h^2 k^2 - 4.44044737)(h^4 k^4 - 2\alpha_1 h^2k^2 + \alpha_1^2 + \gamma^2)\right]^{1/2}\right]$$

where $\alpha_1 = 15.779763$ and $\gamma = 6.5467418$.

Computing λ_1 and λ_2 as functions of $h^2 k^2$, we find that the roots have unit modulus for $0 \leqslant h^2 k^2 \leqslant 4.44$. Thus the stability interval of the Runge-Kutta method (2.119) is $0 < h^2k^2 < 4.44$.

It can be shown that the stability interval of the *Runge-Kutta-Nystrom* method (2.120) is (0,8.5).

DEFINITION 2.6 A singlestep method of the form (2.123) is said to have interval of periodicity $(0, h_0)$, if for all $\bar{h} \in (0, h_0)$, $\bar{h}=k^2h^2$, the eigenvalues of the matrix are distinct, complex and of modulii one.

We may verify that the interval of periodicity of the formula (2.121) is (0, 12). The *Runge-Kutta-Nystrom* method does not have interval of periodicity.

For $\alpha=k^2$, the solutions of (2.122) are exponential in nature and can be written in the matrix form as

$$\begin{bmatrix} y(t) \\ y'(t) \end{bmatrix} = \exp((t-t_0)\mathbf{K}) \begin{bmatrix} y_0 \\ y'_0 \end{bmatrix}$$

and

$$\mathbf{K} = \begin{bmatrix} 0 & 1 \\ k^2 & 0 \end{bmatrix}$$

For the point $t=t_0+nh=t_n$, this solution becomes

$$\begin{bmatrix} y(t_n) \\ y'(t_n) \end{bmatrix} = \begin{bmatrix} 1+\frac{h^2k^2}{2}+\frac{h^4k^4}{24}+\ldots & h+\frac{h^3k^3}{6}+\ldots \\ hk^2+\frac{h^3k^4}{6}+\ldots & 1+\frac{h^2k^2}{2}+\frac{h^4k^4}{24}+\ldots \end{bmatrix}^n \begin{bmatrix} y_0 \\ y'_0 \end{bmatrix}$$

and therefore

$$\lim_{h\to 0} \frac{1}{h^4} \left\{ \exp(Kh) - \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \right\} = \begin{bmatrix} -\frac{1}{72}k^4 & 0 \\ 0 & \frac{1}{24}k^4 \end{bmatrix}$$

We now obtain the relative error for the method under discussion in case a large number of integration intervals (large x, small h) are to be considered.

The maximum eigenvalue of the matrix

$$\begin{bmatrix} 1+\frac{h^2k^2}{2}+\frac{h^4k^4}{18} & h+\frac{h^3k^2}{6} \\ hk^2+\frac{h^3k^4}{6} & 1+\frac{h^2k^2}{2} \end{bmatrix}$$

is obtained as

$$\lambda=\frac{1}{2}[a_{11}+a_{22}+[(a_{11}-a_{22})^2+4a_{12}a_{21}]^{1/2}]$$

$$=1+hk+\frac{1}{2}h^2k^2+\frac{1}{6}h^3k^3+\frac{1}{36}h^4k^4+\ldots$$

and therefore the relative error is given by

$$F_\infty \approx \frac{hk - \log \lambda}{h} = \frac{\log (e^{hk}) - \log \lambda}{h} = \frac{1}{h} \log \left[1 + \frac{e^{hk} - \lambda}{\lambda} \right] \approx \frac{1}{72} h^3 k^4$$

Example 2.6 Find $y(t)$ at $t=5$ with the help of the Runge-Kutta method (2.119) for the initial value problem

$$y'' + 100\,[1 - 0.1 \cos (2t)]\,y = 0$$
$$y(0) = 1,\; y'(0) = 0$$

using steplengths 2^{-m}, $m = 1\ (1)\ 9$.

The value of $y(t)$ at $t=5$ correct to seven decimals is obtained as

$$y(t) = 0.9417373$$

The approximate values of $y(t)$ are listed in Table 2.7.

TABLE 2.7 EFFECT OF STABILITY ON THE VALUES OF $y(t)$

h^{-1}	$y(t)$
2	0.22445786+12
4	0.34016505+05
8	0.19377334
16	0.79682350
32	0.92196634
64	0.93921699
128	0.94142020
256	0.94169751
512	0.94173227

2.10 ADAPTIVE NUMERICAL METHODS

The adaptive methods are the numerical methods which contain arbitrary parameters so as to tailor the numerical methods to fit the particular problems. This approach is used to stabilize the numerical methods. The starting point is a homogeneous linear form of the given differential equation and employing the analytic solution of the linear differential equation it is possible to derive a difference equation whose solution is identical to that of the differential equation. Clearly, in this case no possibility of instability can exist. We will now study how the singlestep methods can be stabilized with very little modification.

2.10.1 Runge-Kutta-Treanor method

The first order initial value problem (2.1)

$$y' = f(t, y),\; y(t_0) = y_0$$

can be written in the form

$$y' = -\underbrace{py}_{\text{linear}} + \underbrace{g(t, y)}_{\text{nonlinear}} \tag{2.127}$$

where $g(t, y) = py + f(t, y)$ and $p > 0$ is a parameter to be chosen suitably. To solve the differential equation (2.127), we can approximate $g(t, y)$ by a polynomial of an appropriate degree. Here, we will take a quadratic polynomial for $g(t, y)$ with undetermined coefficients. Equation (2.127) may be written as

$$\frac{dy}{dt} = f(t, y) = -p(y - y_n) + A + B(t - t_n) + \frac{C}{2}(t - t_n)^2 \tag{2.128}$$

where (t_n, y_n) is contained in the region of interest. The four constants A, B, C and p can be obtained by determining the value of $f(t, y)$ at four points in the interval $[t_n, t_n + h]$ and solve the resulting equations. We choose the classical Runge-Kutta nodes t_n, $t_n + \frac{h}{2}$, $t_n + \frac{h}{2}$ and $t_n + h$ and put

$$\begin{aligned}
K_1 &= h\, f(t_n, y_n) \\
K_2 &= h\, f\left(t_n + \frac{h}{2}, \bar{y}_{n+1/2}\right), \quad \bar{y}_{n+1/2} = y_n + \frac{1}{2} K_1 \\
K_3 &= h\, f\left(t_n + \frac{h}{2}, \bar{\bar{y}}_{n+1/2}\right), \quad \bar{\bar{y}}_{n+1/2} = y_n + \frac{1}{2} K_2 \\
K_4 &= h\, f(t_n + h, \bar{y}_{n+1}), \quad \bar{y}_{n+1} = y_n + K_3
\end{aligned} \tag{2.129}$$

The four equations are

$$\begin{aligned}
K_1 &= h\, A \\
K_2 + ph\, \bar{y}_{n+1/2} &= ph\, y_n + Ah + \frac{1}{2} h^2 B + \frac{1}{8} h^3 C \\
K_3 + ph\, \bar{\bar{y}}_{n+1/2} &= ph\, y_n + Ah + \frac{1}{2} h^2 B + \frac{1}{8} h^3 C \\
K_4 + ph\, \bar{y}_{n+1} &= ph\, y_n + Ah + h^2 B + \frac{1}{2} h^3 C
\end{aligned} \tag{2.130}$$

Solving the equations (2.130), we get

$$\begin{aligned}
h\, A &= K_1 \\
h^2 B &= [-3(K_1 + ph\, y_n) + 2(K_2 + ph\, \bar{y}_{n+1/2}) \\
&\quad + 2(K_3 + ph\, \bar{\bar{y}}_{n+1/2}) - (K_4 + ph\, \bar{y}_{n+1})] \\
h^3 C &= 4[(K_1 + ph\, y_n) - (K_2 + ph\, \bar{y}_{n+1/2}) \\
&\quad - (K_3 + ph\, \bar{\bar{y}}_{n+1/2}) + (K_4 + ph\, \bar{y}_{n+1})] \\
ph &= -\left[\frac{K_3 - K_2}{\bar{\bar{y}}_{n+1/2} - \bar{y}_{n+1/2}}\right]
\end{aligned} \tag{2.131}$$

On integrating (2.128) between the limits t_n to t_{n+1}, we obtain

$$y_{n+1} = y_n + h\, AF_1 + h^2\, BF_2 + h^3\, CF_3 \tag{2.132}$$

where

$$F_1=\frac{e^{-ph}-1}{-ph}, \quad F_2=\frac{e^{-ph}+ph-1}{(ph)^2}$$

$$F_3=\frac{e^{-ph}-\frac{1}{2}(ph)^2+ph-1}{(-ph)^3}$$

$$F_{j+1}=\frac{F_j-\frac{1}{j!}}{(-ph)}, \; j=3, 4,... \tag{2.133}$$

Equation (2.132) becomes

$$\begin{aligned} y_{n+1}=y_n+K_1F_1+[&-3(K_1+ph\, y_n)+2(K_2+ph\, \bar{y}_{n+1/2}) \\ &+2(K_3+ph\, \bar{\bar{y}}_{n+1/2})-(K_4+ph\, \bar{y}_{n+1})]F_2+4[(K_1+ph y_n) \\ &-(K_2+ph\, \bar{y}_{n+1/2})-(K_3+ph\, \bar{\bar{y}}_{n+1/2})+(K_4+ph\, \bar{y}_{n+1})]F_3 \end{aligned} \tag{2.134}$$

which is the required *Runge-Kutta-Treanor* method. Substituting the values of $\bar{y}_{n+1/2}$, $\bar{\bar{y}}_{n+1/2}$ and $\bar{y}_{n+1}$ from (2.130), the equation (2.134) can be written as

$$\begin{aligned} y_{n+1}=y_n&+\frac{1}{6}(K_1+2K_2+2K_3+K_4) \\ &-(ph)^2[(K_2-K_3)F_3+(K_1-4K_2+2K_3 \\ &+K_4)F_4-4(K_1-K_2-K_3+K_4)F_5)] \end{aligned} \tag{2.135}$$

The value of p is given by

$$\frac{1}{2}ph=-\left(\frac{K_3-K_2}{K_2-K_1}\right) \tag{2.136}$$

The first part in (2.135) is due to the fourth order Runge-Kutta method and the additional term is fifth order and higher in h. It is seen that when the equation (2.134) or (2.135) is used to integrate over the interval where ph is small, the result will be identical with the Runge-Kutta method. If ph is large, a condition where the Runge-Kutta method is known to be unstable then the equation (2.134) gives a far superior solution.

DEFINITION 2.7 An adaptive numerical method is said to be A-stable in the sense of *Dahlquist* if when the method is applied to the equation $y'=\lambda y$, $y(t_0)=y_0$, $\lambda < 0$ with exact initial condition, it gives the true solution which is identical to that of the differential equation for arbitrary h and $p=\lambda$. Here, $f(t, y)=\lambda y$, then $p=-\lambda$ and the equation (2.134) gives

$$y_{n+1}=e^{\lambda h}y_n \tag{2.137}$$

Since $\lambda < 0$ and therefore $y_n \to 0$ when $n \to \infty$ and for any fixed h.

2.10.2 Runge-Kutta-Liniger-Willoughby method

From the order equations in Subsection 2.6.1, the first order Runge-Kutta method which is explicit in K_1 and implicit in K_2 is written as

$$
\begin{aligned}
K_1 &= h\,f(t_n, y_n) \\
K_2 &= h\,f(t_n+h,\ y_n+\theta K_1+(1-\theta)K_2) \\
y_{n+1} &= y_n+\theta K_1+(1-\theta)K_2
\end{aligned}
\tag{2.138}
$$

where $\theta = w_1$ is an arbitrary parameter to be determined.

DEFINITION 2.8 An adaptive numerical method is said to be exponentially fitted at a value λ_0, if when the method is applied to the equation $y' = \lambda y$, $y(t_0) = y_0$ and λ a complex constant with negative real part, it gives the true solution for an arbitrary h when $\lambda = \lambda_0$.

The parameter θ in (2.138) is determined to achieve exponential fitting. Applying the method (2.138) to the test equation $y' = \lambda y$, we may obtain

$$y_n = \left[\frac{1+\theta\lambda h}{1-(1-\theta)\,\lambda h}\right]^n y_0 \tag{2.139}$$

This coincides with the theoretical value

$$y(t_n) = [\exp\,(\lambda h)]^n y(t_0) \tag{2.140}$$

in the case $\lambda = \lambda_0$ if we choose θ such that

$$\frac{1+\theta\lambda_0 h}{1-(1-\theta)\lambda_0 h} = \exp\,(\lambda_0 h)$$

or

$$\theta = -\frac{1}{\lambda_0 h} - \frac{\exp\,(\lambda_0 h)}{1-\exp\,(\lambda_0 h)} \tag{2.141}$$

Since it is difficult to have some a priori knowledge of λ_0, the value of θ is determined such that

$$\max_{-\infty \leqslant \lambda h < 0} \left| e^{\lambda h} - \frac{1+\theta\,\lambda h}{1-(1-\theta)\,\lambda h} \right| = \min \tag{2.142}$$

We obtain $\theta = 0.122$. The numerical method (2.138) with $\theta = 0.122$ is termed as the *Runge-Kutta-Liniger-Willoughby* method.

2.10.3 Runge-Kutta-Nystrom-Treanor method

Let us consider the stabilization of the *Runge-Kutta-Nystrom* method for the initial value problem (2.117).

We assume that the equation (2.117) can be approximated by

$$y' = f(t, y) = -p(y-y_n) + A + B(t-t_n) + \frac{C}{2}(t-t_n)^2 \tag{2.143}$$

Integrating (2.143), we obtain the following equations

$$y_{n+1}=y_n+hy'_nF_1+h^2AF_2+h^3BF_3+h^4CF_4$$
$$hy'_{n+1}=h\,y'_nF_0+h^2AF_1+h^3BF_2+h^4CF_3 \tag{2.144}$$

where

$$w=\sqrt{p}\,h,$$
$$F_0=\cos w, \quad F_1=\frac{\sin w}{w}$$
$$w^2F_{m+2}=\frac{1}{m!}-F_m, \quad m=0,1,2,\ldots \tag{2.145}$$

Using the *Runge-Kutta-Nystrom* nodes, t_n, $t_n+\frac{2}{5}h$, $t_n+\frac{2}{3}h$, $t_n+\frac{4}{5}h$, we get four equations for the determination of the four unknowns A, B, C and p.

Denoting

$$K_1=\frac{h^2}{2}f(t_n,y_n)$$
$$K_2=\frac{h^2}{2}f\left(t_n+\frac{2}{5}h,\ y_{n+2/5}\right)$$
$$y_{n+2/5}=y_n+\frac{2}{5}h\,y'_n+\frac{4}{25}K_1$$
$$K_3=\frac{h^2}{2}f\left(t_n+\frac{2}{3}h,\ y_{n+2/3}\right)$$
$$y_{n+2/3}=y_n+\frac{2}{3}h\,y'_n+\frac{4}{9}K_1$$
$$K_4=\frac{h^2}{2}f\left(t_n+\frac{4}{5}h,\ y_{n+4/5}\right)$$
$$y_{n+4/5}=y_n+\frac{4}{5}h\,y'_n+\frac{8}{25}(K_1+K_2) \tag{2.146}$$

We obtain the values of A, B, C and p as

$$h^2A=2K_1$$
$$h^3B=-8K_1+\frac{25}{2}K_2-\frac{9}{2}K_3+w^2hy'_n$$
$$h^4C=-\frac{75}{2}K_2+\frac{45}{2}K_3+15K_1+2w^2K_1$$
$$w^2=ph^2=\frac{5}{4}\,\frac{(K_1-5K_2+9K_3-5K_4)}{(K_2-K_1)} \tag{2.147}$$

Substituting the above values in (2.144) and using (2.145) to simplify, we have

$$y_{n+1}=y_n+hy_n'+\frac{1}{48}(14K_1+25K_2+9K_3)-\frac{w^2}{2}[(-16K_1+25K_2$$
$$-9K_3)F_5+(30K_1-75K_2+45K_3)F_6]$$
$$h\,y_{n+1}'=h\,y_n'+\frac{1}{2}(K_1+3K_3)-\frac{w^2}{2}[(-16K_1+15K_2$$
$$-9K_3)F_4+(30K_1-75K_2+45K_3)F_5] \qquad (2.148)$$

The term in w^2 in (2.148) is the modification to the *Runge-Kutta-Nystrom* method.

DEFINITION 2.9 An adaptive numerical method is said to be *P*-stable if, when the method is applied to the equation $y''=-\lambda y$, $\lambda > 0$, $y(t_0)=y_0$, $y'(t_0)=y_0'$ with exact initial conditions it gives rise to the solution which is identical to that of the differential equation for an arbitrary h and the free parameter is chosen as the square of the frequency.

Here, $p=\lambda$ and the equations (2.144) become

$$y_{n+1}=y_n\cos w+h\,y_n'\frac{\sin w}{w}$$
$$hy_{n+1}'=-y_n w\sin w+h\,y_n'\cos w \qquad (2.149)$$

which may be written in the matrix form as

$$\begin{bmatrix} y_{n+1} \\ hy_{n+1}' \end{bmatrix}=\mathbf{E}(w)\begin{bmatrix} y_n \\ hy_n' \end{bmatrix} \qquad (2.150)$$

where

$$\mathbf{E}(w)=\begin{bmatrix} \cos w & \dfrac{\sin w}{w} \\ -w\sin w & \cos w \end{bmatrix}$$

is a 2×2 matrix. The eigenvalues of the matrix $\mathbf{E}(w)$ are complex and of unit modulii.

Bibliographical Note

There are many text books which deal with the singlestep methods for solving initial value problems of ordinary differential equations. Particularly useful are 33, 46, 93, 113, 161 and 163.

An automatic integration programme based on the Taylor series method for solving initial value problems is given in 94. The Runge-Kutta methods of various order are studied in 23, 25, 174, 175, 209 and 222. The stability of the Runge-Kutta formulas is given in 68. We find the methods with minimum truncation error in 118, 156 and 199, the methods with extended region of stability in 165 and 166, and the error bounds of the methods in 34, 137 and 220.

By an m-fold predifferentiation of the differential equations and a simple transformation of the variables, the Runge-Kutta formulas of high accuracy have been discussed in 82, 83, 145 and 146. The extrapolation algorithms for the initial value problems are established in 21 and 100. The implicit Runge-Kutta methods are given in 22, 24, 28, 208 and 252. The two point Runge-Kutta formulas are found in 27. Using higher order derivatives, the obrechkoff methods are obtained in 177 and 188.

The singlestep methods based upon quadratures and interpolations have been studied in 51, 63, 64, 65, 66, 140 and 223. The Runge-Kutta methods for the system and the higher order initial value problems are discussed in 5, 42, 109, 111, 148, 213, 219 and 260. The adaptive numerical methods are given in 136 and 238.

Problems

1. Obtain the Taylor series solution of the initial value problem
$$y' = 1-2ty,\ y(0) = 0$$
and determine:
   (i) t when the error in $y(t)$ obtained from four terms only is to be less than 10^{-6} after rounding.
   (ii) The number of terms in the series to find results correct to 10^{-10} for $0 \leqslant t \leqslant 1$.
2. For the solution of the initial value problem
$$y'=p_1(t)\,y+q_1(t),\ y(t_0)=y_0$$
by Taylor's series method, show that
$$y\,(t+h)=\left(1+h\,p_1+\frac{1}{2}\,h^2\,p_2+\dots\right)y(t)+\left(h\,q_1+\frac{1}{2}\,h^2\,q_2+\dots\right)$$
where
$$p_{r+1}=p_r'+p_1\,p_r$$
$$q_{r+1}=q_r'+q_1\,p_r$$
3. Apply Taylor's series method of order p to the problem
$$y'=y,\ y(0)=1$$
to show that
$$|\,y_n-y(t_n)\,| \leqslant \frac{h^p}{(p+1)!}\,t_n\,e^{t_n}$$
4. The function $y(t)$ is the solution of the initial value problem
$$y'(t)=f(t,y),\quad t \in [t_0,b]$$
$$y(t_0)=y_0$$

and the sequence $\{y_n\}$ is defined by

$$y_{n+1}=y_n+hf(t_n, y_n),\ n=0, 1, \ldots, N-1$$

where $$h=\frac{b-t_0}{N} \text{ and } t_n=t_0+nh,$$

and the function $f(t, y)$ and its first and second partial derivatives are continuous in the region $t \in [t_0, b]$, $|y| < \infty$, and $f_y(t, y)$ is bounded in the region. Show that

(i) $|y_n-y(t_n)| \leqslant Kh$

where K is a constant independent of h.

(ii) $$\epsilon_{n+1}=\epsilon_n+h^2\left\{f_y(t_n, y(t_n))\left(\frac{\epsilon_n}{h}\right)-\frac{1}{2}y''(t_n)\right\}$$
$$+h^3\left\{\frac{1}{2}f_{yy}(t_n, y^*)\left(\frac{\epsilon_n}{h}\right)^2-\frac{1}{3!}y'''(t_n^*)\right\}$$

where $t_n < t_n^* < t_{n+1}$ and y^* lies between $y(t_n)$ and y_n and $\epsilon_n=y_n-y(t_n)$.

(iii) $\dfrac{\epsilon_n}{h}=e(t)+0(h)$

where $e(t)$ is the solution of the initial value problem

$$e'(t)=f_y(t, y(t))e(t)-\frac{1}{2}y''(t)$$

$$e(t_0)=0$$

Calculate $e(t)$ for the equation

$$y'=\frac{2y}{t},\quad t \in [1, 2]$$

$$y(1)=1$$

5. Apply the Euler-Cauchy method with step length h to the problem

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

(a) Determine an explicit expression for y_n.

(b) For which values of h is the sequence $\{y_n\}_0^\infty$ bounded?

(c) Compute $\lim\limits_{h\to 0}\{(y(x, h)-e^{-x})/h^2\}$.

6. Consider the initial value problem

$$y'=f(y),\ y(t_0)=y_0$$

Derive the third order Runge-Kutta method when $c_3=a_{31}+a_{32}$ and $w_2=w_3$. Find also the bounds of the local truncation error.

7 Show that when a third order Runge-Kutta method is applied to $y'=\lambda y$, it gives

$$\frac{y_{n+1}}{y_n}=e^{\lambda h}+0((\lambda h)^4)$$

8. Prove that if $f(t, y)$ is independent of y, the Euler-Cauchy method reduces to the trapezoidal rule for quadrature, classical third and fourth order methods reduce to Simpson's rule for quadrature, and Kutta's fourth order formula reduces to the three-eighth rule for quadrature.

9. Determine y at $t=0.2\,(0.2)\,0.8$ by the fourth order Runge-Kutta method, given that

$$y'=\frac{1}{t+y},\ y(0)=2$$

10. The local truncation error of the fourth order Runge-Kutta method for the problem $y'=f(t, y)$, $y(t_0)=y_0$ is given by

$$\begin{aligned}T_n=\frac{h^5}{120}\{&[1-5\,(w_2c_2^4+w_3c_3^4+w_4c_4^4)]\,D^4 f\\&+[6-60(w_3c_2c_3^2a_{32}+w_4c_4^2(c_2a_{42}+c_3a_{43}))]\,D^2 f_y\, Df\\&+[4-60(w_3a_{32}c_2^2c_3+w_4c_4(a_{42}c_2^2+a_{41}c_3^2))]\,Df_y\, D^2 f\\&+[1-60w_4a_{43}a_{32}c_2^2]\,f_y^2\, D^2 f\\&+[3-60(w_3a_{32}^2c_2^2+w_4(a_{43}c_3+a_{42}c_2)^2)]\,f_{yy}D^2 f\\&+[1-20(w_3a_{32}c_2^3+w_4(a_{43}c_3^3+a_{42}c_2^3))]\,f_y\, D^3 f\\&+[7-120w_4a_{43}a_{32}c_2(c_3+c_4)]\,f_y\, Df_y\, Df+f_y^3\, Df]\}+0(h^6)\end{aligned}$$

Show that in the fourth order classical Runge-Kutta method it is bounded by

$$|\,T_n\,| \leqslant (73/720)\, ML^4h^5$$

where
$$|\,f(t, y)\,| < M \text{ and } \left|\frac{\partial^{i+j} f}{\partial t^i\, \partial y^j}\right| < \frac{L^{i+j}}{M^{j-1}}$$
$$0 \leqslant i+j \leqslant 4,\ 0 \leqslant j \leqslant 4$$

11. Prove that the error $\epsilon_i=y_i-y(t_i)$ in the solution y_i obtained by the classical fourth order Runge-Kutta method of the initial value problem $y'=f(t, y)$, $y(t_0)=y_0$ is $0\,(h^4)$ for all i if $f(t, y)$ satisfies a Lipschitz condition.

12. Let $g(t, y)=f'(t, y)=f_t+f_yf$, $y'=f(t, y)$. Prove that the method

$$y_{n+1}=y_n+h\left[f(t_n, y_n)+\frac{1}{2}hg\left(t_n+\frac{1}{3}h,\ y_n+\frac{1}{3}hf_n\right)\right]$$

is of the order 3. Find the interval of absolute stability.

13. Show that the asymptotic expansion of the approximate value y_n obtained from the fourth order classical Runge-Kutta method for the equation $y'=\lambda y$, $y(0)=1$ has the form

$$y_n=y\ (t_n)+\tau_4\,(t_n)\, h^4+\tau_5\,(t_n)\, h^5+\dots$$

and find the expression to the approximate value of $y\,(t_n)$ which is $0\,(h^6)$.

14. Solve the differential equation

$$\frac{dy}{dt}=\frac{t}{y},\ y(0)=1$$

by the Euler method with $h=0.1$ to get $y(0.2)$. Then repeat with $h=0.2$ to get another estimate of $y(0.2)$. Extrapolate these results assuming that errors are proportional to step-size, and compare the derived result to the analytical result.

15. In a computation with Euler's method, the following results are obtained with various step sizes:

$h=2^{-2}$	$h=2^{-3}$	$h=2^{-4}$
2.44141	2.56578	2.63793

Compute a better value by extrapolation.

16. Obtain the Runge-Kutta method of the form

$$K_1=h[1-h\,af_y(y_n)]^{-1}f(y_n)$$
$$y_{n+1}=y_n+W_1K_1$$

for the differential equation $y'=f(y)$, and determine the interval of absolute stability for the equation

$$y'=\lambda y,\ \lambda<0$$

17. Find the Runge-Kutta method of the form

(i)
$$K_1=hf(y_n+a_{11}K_1)$$
$$y_{n+1}=y_n+W_1K_1$$

(ii)
$$K_1=hf(y_n)$$
$$K_2=hf(y_n+a(K_1+K_2))$$
$$y_{n+1}=y_n+W_1K_1+W_2K_2$$

for the initial value problem

$$y'=f(y)$$
$$y(t_0)=y_0$$

and obtain the interval of absolute stability for

$$y'=\lambda y,\ \lambda<0$$

18. Find the order of the implicit Runge-Kutta method

$$y_{n+1}=y_n+\frac{1}{6}h[4f(t_n,y_n)+2f(t_{n+1},y_{n+1})+hf'(t_n,y_n)]$$

and determine its interval of absolute stability.

19. The use of the fourth order implicit Runge-Kutta method (2.66) requires the solution of the nonlinear equations at each step. They can be solved by an iteration method. Find the condition for the convergence of the iteration method.

20. The implicit Runge-Kutta method (2.62) is applied to the problem

$$y'=\lambda y,\ y(t_0)=y_0$$

(a) Determine an explicit expression for $Y_0^{(k)}$.

(b) Find the propagating factor

$$E(\lambda h,\ K,\ M) \text{ for } K=0,\ M=1$$

21. Use $|\,\partial^{i+j} f/\partial t^i\, \partial y^j\,| \leqslant L^{i+j}/M^{i-1}$ to determine the bounds of the local truncation error of the implicit Runge-Kutta methods (2.64) and (2.65).

22. Apply the fifth order Runge-Kutta-Lawson method to the problem

$$y'=\lambda y,\ y(t_0)=y_0,\ \lambda < 0$$

to determine the propagating factor of the approximate solution.

23. Find the order of the method

$$y_{n+1}=y_n+\frac{1}{2}\,h[f(y_n)+f(y_{n+1})]+\frac{1}{12}\,h^2[f'(y_n)-f'(y_{n+1})]$$

where $y'=f(y)$

24. Find the principal part of the local truncation error of the method

$$y_{n+1}=y_n+\frac{h}{2}\,(y'_{n+1}+y'_n)-\frac{h^2}{10}\,(y''_{n+1}-y''_n)+\frac{h^3}{120}\,(y'''_{n+1}+y'''_n)$$

What is the interval of absolute stability?

25. Use Taylor series method of order four for the step by step integration of the differential equations

$$y'=tz+1, \qquad y(0)=0$$
$$z'=-ty, \qquad z(0)=1$$

with $h=.1$ and $0 \leqslant t \leqslant 0.2$

26. The system

$$y'=z, \qquad y(t_0)=y_0$$
$$z'=-by-az, \qquad z(t_0)=z_0$$

where $0 < a < 2\sqrt{b},\ b > 0$, is to be integrated by Euler's method. What is the largest step length h for which all solutions of the corresponding difference equations are bounded? (BIT7 (1967),247)

27. The classical Runge-Kutta method is used for solving the system

$$y'=-kz, \qquad y(t_0)=y_0$$
$$z'=ky, \qquad z(t_0)=z_0,$$

where $k > 0$ and t, t_0, y, y_0, z and z_0 are real and h is the step length. Prove that

$$\begin{bmatrix} y_{n+1} \\ z_{n+1} \end{bmatrix}=\mathbf{A}\begin{bmatrix} y_n \\ z_n \end{bmatrix}$$

where **A** is a real 2×2 matrix. Find under what conditions the solutions do not grow exponentially for increasing values of n. (BIT 6(1966), 359)

28. Write the initial value problem

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

as a set of two simultaneous first order differential equations. Compute the solution at $t=0.2$ using the following methods:

(a) Improved tangent method, $h=0.1$;
(b) Runge-Kutta fourth order method, $h=0.2$;
(c) Taylor series expansion up to and including the t^4-term;
(d) The Runge-Kutta method (2.119).

29. Discuss the stability of the numerical solution of the equation

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

using the Runge-Kutta method (2.119).

30. The function $y(x)$ satisfies the initial value problem

$$y'''=f(y)$$
$$y(t_0)=y_0,\ y'(t_0)=y_0',\ y''(t_0)=y_0''$$

Find the maximum order Runge-Kutta method of the form

$$K_1=\frac{h^3}{6}f(y_n)$$

$$K_2=\frac{h^3}{6}f\left(y_n+\alpha h\, y_n'+\alpha^2\frac{h^2}{2}y_n''+\alpha^3 K_1\right)$$

$$y_{n+1}=y_n+h\,y_n'+\frac{h^2}{2}y_n''+W_1K_1+W_2K_2$$

$$y_{n+1}'=y_n'+h\,y_n''+W_1'\frac{K_1}{h}+W_2'\frac{K_2}{h}$$

$$y_{n+1}''=y_n''+W_1''\frac{K_1}{h^2}+W_2''\frac{K_2}{h^2}$$

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

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

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

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

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

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

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 $y_1, y_2, \cdots, y_{k-1}$ 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 $t_n, t_{n-1}, \cdots, t_{n-k+1}$. 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

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

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

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

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

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.

From the definition of the backward difference operator ∇, we find

$$\nabla^m f_n = \sum_{p=0}^{m} (-1)^p \binom{m}{p} f_{n-p} \tag{3.12}$$

Substituting in (3.11) and regrouping, we obtain

$$y_{n+1} = y_{n-j} + h \sum_{m=0}^{k-1} \gamma_m^{*(j)} f_{n-m} \tag{3.13}$$

It is obvious from (3.9) that with k computed values, we obtain explicit multistep methods of order k, since the truncation error is of the form $C\,h^{k+1}$, where C is independent of h. A number of interesting formulas can be obtained for various integer values of j.

3.2.1 Adams-Bashforth formulas (j = 0)

On replacing the coefficients $\gamma_m^{(0)}$ by their values in (3.11), we get

$$y_{n+1} = y_n + h\left[f_n + \frac{1}{2}\nabla f_n + \frac{5}{12}\nabla^2 f_n + \frac{3}{8}\nabla^3 f_n + \frac{251}{720}\nabla^4 f_n + \frac{475}{1440}\nabla^5 f_n + \dots\right]$$

The coefficients $\gamma_m^{*(0)}$ for formula (3.13) are given in Table 3.1.

TABLE 3.1 COEFFICIENTS FOR THE FORMULA

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

k	$\gamma_0^{*(0)}$	$\gamma_1^{*(0)}$	$\gamma_2^{*(0)}$	$\gamma_3^{*(0)}$	$\gamma_4^{*(0)}$	$\gamma_5^{*(0)}$
1	1					
2	$\frac{3}{2}$	$-\frac{1}{2}$				
3	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$			
4	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$		
5	$\frac{1901}{720}$	$-\frac{2774}{720}$	$\frac{2616}{720}$	$-\frac{1274}{720}$	$\frac{251}{720}$	
6	$\frac{4277}{1440}$	$-\frac{7923}{1440}$	$\frac{9982}{1440}$	$-\frac{7298}{1440}$	$\frac{2877}{1440}$	$-\frac{475}{1440}$

The error term associated with truncation after $(k-1)$th ∇ is

$$T_k^{(0)} = h^{k+1}\int_0^1 \frac{u\,(u+1)\dots(u+k-1)}{k\,!}\,f^{(k)}(\xi)\,du$$

Since the coefficient of $f^{(k)}(\xi)$ does not change sign in (0, 1), it is possible to write

$$T_k^{(0)} = \gamma_k^{(0)} h^{k+1} f^{(k)}(\xi)$$

Example 3.1 Solve the initial value problem

$$y' = -y^2,\ y(0) = 1,\ t \in [0, 1]$$

Use the third order Adams-Bashforth method with $h = .1$.

The third order Adams-Bashforth method is given by

$$y_{n+1} = y_n + \frac{h}{12}(23f_n - 16f_{n-1} + 5f_{n-2}),\ n \geqslant 2$$

We require the values of y_0, y_1 and y_2 to start the computation. The values y_1 and y_2 are determined using the singlestep method of order three.
The Taylor series method of order three becomes

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2} y_n'' + \frac{h^3}{6} y_n'''$$

where

$$y_n' = -y_n^2$$
$$y_n'' = -2y_n y_n' = 2y_n^3$$
$$y_n''' = 6y_n^2 y_n' = -6y_n^4$$

we have

$$y_{n+1} = y_n - hy_n^2 + h^2 y_n^3 - h^3 y_n^4,\quad n = 0, 1$$

Thus, the starting values are given be

$$y_1 = .909,\ y_1' = -.826281$$
$$y_2 = .8332001,\ y_2' = -.6942224$$

Using starting values, we obtain,

for $n = 2$;

$$y_3 = y_2 + \frac{h}{12}(23f_2 - 16f_1 + 5f_0)$$

$$y_3 = .8332001 + \frac{.1}{12}[23(-.6942224)$$
$$-16(-.826281) + 5(-1)]$$

$$y_3 = .768645$$

$$\vdots$$

for $n = 9$;

$$y_{10} = y_9 + \frac{h}{12}(23y_9' - 16y_8' + 5y_7')$$

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

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

$$y_{10} = .4992074$$

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 $y' = t+y$, $y(0) = 1$, $0 \leqslant t \leqslant 1$ 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

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

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) $y' = -y$, $\quad y(0) = 1$,

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

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

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.

TABLE 3.5 Comparison of Errors in Adams-Bashforth Methods

$y' = -y,\ y(0) = 1,\ t = 5$

h	Second order	Third order	Fourth order	Fifth order
2^{-5}	138850−10	−393711−12	115388−13	−344260−15
2^{-6}	344884−11	−487010−13	710535−15	−105524−16
2^{-7}	859472−12	−605583−14	440792−16	−326583−18
2^{-8}	214530−12	−754999−15	274471−17	−101563−19

$y' = -y^2,\ y(0) = 1,\ t = 5$

h	Second order	Third order	Fourth order	Fifth order
2^{-5}	568533−10	−365723−11	345730−12	−427887−13
2^{-6}	141718−10	−460309−12	222750−13	−143096−14
2^{-7}	353759−11	−577419−13	141392−14	−462985−16
2^{-8}	883718−12	−723062−14	890643−16	−147251−17

$y' = -t\,(y+y^2),\ y(0) = 1,\ t = 5$

h	Second order	Third order	Fourth order	Fifth order
2^{-5}	100382−12	−946960−14	900407−15	−795755−16
2^{-6}	240987−13	−112385−14	524529−16	−228893−17
2^{-7}	591872−14	−136871−15	316472−17	−685903−19
2^{-8}	146752−14	−168876−16	194334−18	−208970−20

TABLE 3.6 Comparison of Errors in Nystrom Methods

$y' = -y,\ y(0) = 1,\ t = 5$

h	Second order	Third order	Fourth order	Fifth order
2^{-5}	370653−09	245941−09	188803−08	353071−06
2^{-6}	477957−10	177666−10	116657−09	245409−06
2^{-7}	619175−11	118679−11	121595−10	182088−05
2^{-8}	817258−12	844988−13	235654−11	−180580−05

$y' = -y^2,\ y(0) = 1,\ t = 5$

h	Second order	Third order	Fourth order	Fifth order
2^{-5}	519885−09	489842−09	327484−08	246166−06
2^{-6}	710399−10	376276−10	198742−09	291459−07
2^{-7}	978744−11	260210−11	884250−11	205047−08
2^{-8}	141185−11	170325−12	128293−12	−628150−09

$y' = -t(y+y^2),\ y(0) = 1,\ t = 5$

h	Second order	Third order	Fourth order	Fifth order
2^{-5}	−788635−06	−603084+69	−122600+50	−562878+69
2^{-6}	−483239−07	−154901−05	−766248+49	−502570+69
2^{-7}	−299164−08	−960616−06	−301542+69	−392004+69
2^{-8}	−182068−09	233003−06	−328154−05	−409594+69

3.3 IMPLICIT MULTISTEP METHODS

In the preceding section we have expressed y_{n+1} in terms of previously calculated ordinates and slopes. A formula similar to (3.11) or (3.13), which involves the unknown slope y'_{n+1} on the right hand side, can be obtained if we replace $f(t, y)$ in (3.6) by a polynomial which interpolates $f(t, y)$ at t_{n+1}, $t_n, \ldots, t_{n-k+1}$ for an integer $k > 0$. Let us assume that $f(t, y)$ has $k+1$ continuous derivatives. The Newton backward difference formula which interpolates at these $k+1$ points in terms of $u = (t-t_n)/h$ is given by

$$\begin{aligned} P_k(t_n+hu) &= f_{n+1}+(u-1)\nabla f_{n+1}+\frac{(u-1)u}{2!}\nabla^2 f_{n+1} \\ &\quad + \ldots + \frac{(u-1)u(u+1)\ldots(u+k-2)}{k!}\nabla^k f_{n+1} \\ &\quad + \frac{(u-1)u(u+1)\ldots(u+k-1)}{(k+1)!}h^{k+1}f^{(k+1)}(\xi) \\ &= \sum_{m=0}^{k}(-1)^m\binom{1-u}{m}\nabla^m f_{n+1}+(-1)^{k+1}\binom{1-u}{k+1}h^{k+1}f^{(k+1)}(\xi) \end{aligned} \tag{3.14}$$

Substituting (3.14) into (3.6), we get

$$\begin{aligned} y(t_{n+1}) = y(t_{n-j})+h\int_{-j}^{1}\Bigg[&\sum_{m=0}^{k}(-1)^m\binom{1-u}{m}\nabla^m f_{n+1} \\ &+(-1)^{k+1}\binom{1-u}{k+1}h^{k+1}f^{(k+1)}(\xi)\Bigg]du \end{aligned}$$

or

$$y(t_{n+1}) = y(t_{n-j})+h\sum_{m=0}^{k}\delta_m^{(j)}\nabla^m f_{n+1}+T_{k+1}^{*(j)} \tag{3.15}$$

where

$$T_{k+1}^{*(j)} = h^{k+2}\int_{-j}^{1}(-1)^{k+1}\binom{1-u}{k+1}f^{(k+1)}(\xi)\,du$$

$$\delta_m^{(j)} = \int_{-j}^{1}(-1)^m\binom{1-u}{m}du \tag{3.16}$$

Neglecting $T_{k+1}^{*(j)}$ in (3.15), we get

$$y_{n+1} = y_{n-j}+h\sum_{m=0}^{k}\delta_m^{(j)}\nabla^m f_{n+1} \tag{3.17}$$

where

$$\delta_0^{(j)} = 1+j$$

$$\delta_1^{(j)} = -\frac{1}{2}(1+j)^2$$

$$\delta_2^{(j)} = -\frac{1}{12}(1+j)^2(1-2j)$$

$$\delta_3^{(j)} = -\frac{1}{24}(1+j)^2(1-j)^2$$

$$\delta_4^{(j)} = -\frac{1}{720}(1+j)^2(19-38j+27j^2-6j^3)$$

$$\delta_5^{(j)} = -\frac{1}{1440}(1+j)^2(27-54j+45j^2-16j^3+2j^4)$$

If we replace the difference operator $\nabla^m f_{n+1}$ in terms of the function values, we obtain

$$y_{n+1} = y_{n-j}+h\sum_{m=0}^{k} \delta_m^{*(j)} f_{n-m+1} \tag{3.18}$$

From (3.17) or (3.18) we can obtain a number of multistep formulas for various values of j. It is obvious from (3.15) that the implicit multistep methods are of one order higher than the corresponding explicit multistep methods with the same number of previously calculated ordinates and slopes.

3.3.1 Adams-Moulton formulas ($j = 0$)

Substituting $j = 0$ in (3.17), we get

$$y_{n+1} = y_n+h\left[f_{n+1}-\frac{1}{2}\nabla f_{n+1}-\frac{1}{12}\nabla^2 f_{n+1}-\frac{1}{24}\nabla^3 f_{n+1} -\frac{19}{720}\nabla^4 f_{n+1}-\frac{27}{1440}\nabla^5 f_{n+1}\cdots\right]$$

The error term associated with truncation after kth ∇ is

$$T_{k+1}^{*(0)} = h^{k+2}\int_0^1 (-1)^{k+1}\frac{(u-1)\,u\,(u+1)\ldots(u+k-1)}{(k+1)!} f^{(k+1)}(\xi)\,du \tag{3.19}$$

Since the coefficient of $f^{(k+1)}(\xi)$ does not change sign in (0, 1), it is possible to write (3.19) as

$$T_{k+1}^{*(0)} = h^{k+2}\,\delta_{k+1}^{(0)} f^{(k+1)}(\xi)$$

The coefficients $\delta_m^{*(0)}$ in the formula

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

are given in Table 3.7.

3.3.2 Milne-Simpson formulas ($j = 1$)

These formulas can be obtained by substituting $j = 1$ in (3.17) and we find

$$y_{n+1} = y_{n-1}+h\left(2f_{n+1}-2\nabla f_{n+1}+\frac{1}{3}\nabla^2 f_{n+1}+0\nabla^3 f_{n+1} -\frac{1}{90}\nabla^4 f_{n+1}-\frac{1}{90}\nabla^5 f_{n+1}-\cdots\right) \tag{3.20}$$

The coefficients $\delta_m^{*(1)}$ of formula (3.18) are listed in Table 3.8.

TABLE 3.7 COEFFICIENTS FOR THE FORMULA

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

k	$\delta_0^{*(0)}$	$\delta_1^{*(0)}$	$\delta_2^{*(0)}$	$\delta_3^{*(0)}$	$\delta_4^{*(0)}$	$\delta_5^{*(0)}$
0	1					
1	$\frac{1}{2}$	$\frac{1}{2}$				
2	$\frac{5}{12}$	$\frac{8}{12}$	$-\frac{1}{12}$			
3	$\frac{9}{24}$	$\frac{19}{24}$	$-\frac{5}{24}$	$\frac{1}{24}$		
4	$\frac{251}{720}$	$\frac{646}{720}$	$-\frac{264}{720}$	$\frac{106}{720}$	$-\frac{19}{720}$	
5	$\frac{475}{1440}$	$\frac{1427}{1440}$	$-\frac{798}{1440}$	$\frac{482}{1440}$	$-\frac{173}{1440}$	$\frac{27}{1440}$

With $k = 2$ in (3.20), the formula

$$y_{n+1} = y_{n-1} + \frac{h}{3}(f_{n+1} + 4f_n + f_{n-1})$$

$$T_3^{*(1)} = -\frac{h^5}{90} f^{(4)}(\xi)$$

is of special interest since in this case the coefficient of the third difference is zero and the use of second or third difference gives the same accuracy. This formula also reduces to Simpson's rule of integration when $f(t, y)$ is independent of y.

TABLE 3.8 COEFFICIENTS FOR THE FORMULA

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

k	$\delta_0^{*(1)}$	$\delta_1^{*(1)}$	$\delta_2^{*(1)}$	$\delta_3^{*(1)}$	$\delta_4^{*(1)}$	$\delta_5^{*(1)}$
0	2					
1	0	2				
2	$\frac{1}{3}$	$\frac{4}{3}$	$\frac{1}{3}$			
3	$\frac{1}{3}$	$\frac{4}{3}$	$\frac{1}{3}$	0		
4	$\frac{29}{90}$	$\frac{124}{90}$	$\frac{24}{90}$	$\frac{4}{90}$	$-\frac{1}{90}$	
5	$\frac{28}{90}$	$\frac{129}{90}$	$\frac{14}{90}$	$\frac{14}{90}$	$-\frac{6}{90}$	$\frac{1}{90}$

3.4 MULTISTEP METHODS BASED ON DIFFERENTIATION

We have so far discussed implicit multistep methods which required the replacement of $f(t, y)$ under the integral sign by an interpolation polynomial which takes values $f_{n+1}, f_n, \ldots, f_{n-k+1}$ at $t_{n+1}, t_n, \ldots, t_{n-k+1}$. We shall now develop methods which are based on the replacement of the function $y(t)$ on the left hand side of

$$y'(t) = f(t, y(t)) \tag{3.21}$$

by an interpolation polynomial and differentiating it. We write (3.21) at t_{n+1} as

$$hDy(t_{n+1}) = hf(t_{n+1}, y(t_{n+1})) \tag{3.22}$$

Using operator relation

$$h\,D = -\log(1-\nabla),$$

we may express (3.22) as

$$-\log(1-\nabla)\,y(t_{n+1}) = hf(t_{n+1}, y(t_{n+1}))$$

or

$$\left[\sum_{\nu=0}^{\infty} \frac{\nabla^{\nu}}{\nu}\right] y(_{n+1}) = hf(t_{n+1}, y(t_{n+1})) \tag{3.23}$$

If we truncate the series on the left hand side of (3.23) after kth difference, we get

$$\left[\sum_{\nu=1}^{k} \frac{\nabla^{\nu}}{\nu}\right] y_{n+1} = h f_{n+1} \tag{3.24}$$

The above expression (3.24) in terms of function values y_m becomes

$$\sum_{m=0}^{k} \gamma_m y_{n-m+1} = hf_{n+1} \tag{3.25}$$

where γ_m for $1 \leqslant k \leqslant 6$ are given in Table 3.9.

TABLE 3.9 Coefficients for the Formula

$$\sum_{m=0}^{k} \gamma_m y_{n-m+1} = hf_{n+1}$$

k	γ_0	γ_1	γ_2	γ_3	γ_4	γ_5	γ_6
1	1	-1					
2	$\frac{3}{2}$	-2	$\frac{1}{2}$				
3	$\frac{11}{6}$	-3	$\frac{3}{2}$	$-\frac{1}{3}$			
4	$\frac{25}{12}$	-4	3	$-\frac{4}{3}$	$\frac{1}{4}$		
5	$\frac{137}{60}$	-5	5	$-\frac{10}{3}$	$\frac{5}{4}$	$-\frac{1}{5}$	
6	$\frac{147}{60}$	-6	$\frac{15}{2}$	$-\frac{20}{3}$	$\frac{15}{4}$	$-\frac{6}{5}$	$\frac{1}{6}$

3.5 GENERAL LINEAR MULTISTEP METHODS

Let us consider the general linear multistep methods of the form

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + \dots + a_k y_{n-k+1} + h(b_0 y'_{n+1} + b_1 y'_n + \dots + b_k y'_{n-k+1}) \tag{3.26}$$

or

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

Symbolically, we can write (3.26) as

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

where ρ and σ are polynomials defined by

$$\rho(\xi) = \xi^k - a_1 \xi^{k-1} - a_2 \xi^{k-2} - \dots - a_k$$

$$\sigma(\xi) = b_0 \xi^k + b_1 \xi^{k-1} + \dots + b_k$$

The above formula (3.26) can only be used if we know the values of the solution $y(t)$ and $y'(t)$ at k successive points. These k values will be assumed to be given. Further, if $b_0 = 0$, the resulting equation is called an explicit or predictor formula because y_{n+1} occurs only on the left hand side of the formula. In other words, y_{n+1} can be calculated directly from the right hand side values. If $b_0 \neq 0$, the equation is referred to as an implicit or corrector formula since y_{n+1} occurs in both sides of the equation. In other words the unknown y_{n+1} cannot be calculated directly since it is contained within y'_{n+1}. We can also assume that the polynomials $\rho(\xi)$ and $\sigma(\xi)$ have no common factors since, otherwise, (3.26) can be reduced to an equation of lower order. In order that the difference equation (3.26) should be useful for numerical integration, it is necessary that (3.26) be satisfied with good accuracy by the solution of the differential equation $y' = f(t, y)$, when h is small for an arbitrary function $f(t, y)$. This imposes restrictions on the coefficients a_i and b_i.

With the difference equation (3.26), we associate the difference operator L defined by

$$L[y(t), h] = y(t_{n+1}) - \sum_{i=1}^{k} a_i y\,(t_{n-i+1}) - h \sum_{i=0}^{k} b_i y'(t_{n-i+1}) \tag{3.27}$$

We assume that the function $y(t)$ has continuous derivatives of sufficiently high order. Expanding $y(t_{n-i+1})$ and $y'(t_{n-i+1})$ in Taylor's series, we have

$$y(t_{n-i+1}) = y(t_n) + (1-i)hy'(t_n) + \frac{(1-i)^2}{2!}\, h^2 y''(t_n) + \dots + \frac{(1-i)^p}{p!}\, h^p y^{(p)}(t_n) + \frac{1}{p!} \int_{t_n}^{t_{n-i+1}} (t_{n-i+1} - s)^p y^{(p+1)}(s)\, ds$$

$$y'(t_{n-i+1}) = y'(t_n)+(1-i)hy''(t_n)+ \frac{(1-i)^2}{2!} h^2y'''(t_n) + \dots + \frac{(1-i)^{p-1}}{(p-1)!} h^{p-1}y^{(p)}(t_n) + \frac{1}{(p-1)!} \int_{t_n}^{t_{n-i+1}} (t_{n-i+1}-s)^{p-1}y^{(p+1)}(s)\, ds$$

Substituting in (3.27), we get

$$L[y(t), h] = C_0y(t_n)+C_1hy'(t_n)+C_2h^2y''(t_n)+\cdots + C_ph^py^{(p)}(t_n)+T_n \tag{3.28}$$

where
$$C_0 = 1-\sum_{i=1}^{k} a_i$$

$$C_q = \frac{1}{q!}[1-\sum_{i=1}^{k} a_i(1-i)^q]-\frac{1}{(q-1)!}\sum_{i=0}^{k} b_i(1-i)^{q-1}, \quad q = 1, 2,\dots, p$$

$$T_n = \frac{1}{p!}\left[\int_{t_n}^{t_{n+1}} (t_{n+1}-s)^py^{(p+1)}(s)\, ds - \sum_{i=1}^{k} a_i \int_{t_n}^{t_{n-i+1}} (t_{n-i+1}-s)^py^{(p+1)}(s)\, ds - hp \int_{t_n}^{t_{n+1}} b_0(t_{n+1}-s)^{p-1}y^{(p+1)}(s)\, ds - hp \sum_{i=1}^{k} b_i \int_{t_n}^{t_{n-i+1}} (t_{n-i+1}-s)^{p-1}y^{(p+1)}_{(s)}ds \right] \tag{3.29}$$

DEFINITION 3.1 The difference operator (3.27) and the associated linear multistep method (3.26) are said to be of order p if, in (3.28)

$$C_0 = C_1 = C_2 = \dots = C_p = 0 \text{ and } C_{p+1} \neq 0 \tag{3.30}$$

Thus for any function $y(t) \in C^{(p+2)}$ and for some nonzero constant C_{p+1}, we have

$$L[y(t), h] = -C_{p+1}h^{p+1}y^{(p+1)}_{(t_n)} + 0(h^{p+2}) \tag{3.31}$$

where $C_{p+1}/\sigma(1)$ is called the *error constant*.

In particular, $L[y(t), h]$ vanishes identically when $y(t)$ is a polynomial whose degree is less than or equal to p. We now introduce the following definitions.

DEFINITION 3.2 The linear multistep method (3.26) is said to be consistent if it has order $p \geqslant 1$.

DEFINITION 3.3 The linear multistep method (3.26) is said to satisfy the *root condition* if the roots of the equation $\rho(\xi) = 0$ be inside the unit circle in the complex plane, and are simple if they lie on the circle.

We shall now use the definitions of order, consistency, and root condition to determine the parameters a_i and b_i in the linear multistep method (3.26).

3.5.1 Determination of a_i and b_i

Equation (3.31) holds good for any function $y(t) \in C^{(p+2)}$. The constants C_i and p are independent of $y(t)$. These can thus be determined by a particular case $y(t) = e^t$, and substituting it in (3.31) we obtain

$$\begin{aligned} L[(e^t, h] &= e^{t_{n+1}} - a_1 e^{t_n} - \ldots - a_k e^{t_{n-k+1}} \\ &\qquad - h(b_0 e^{t_{n+1}} + b_1 e^{t_n} + \ldots + b_k e^{t_{n-k+1}}) \\ &= -C_{p+1} h^{p+1} e^{t_n} + 0(h^{p+2}) \end{aligned}$$

Simplifying we get

$$\begin{aligned} L[e^t, h] &= [(e^{kh} - a_1 e^{(k-1)h} - \ldots - a_k) - h(b_0 e^{kh} + b_1 e^{(k-1)h} + \ldots + b_k)]\, e^{t_{n-k+1}} \\ &= -C_{p+1} h^{p+1} e^{t_n} + 0\,(h^{p+2}) \end{aligned}$$

or
$$\rho(e^h) - h\sigma(e^h) \simeq -C_{p+1} h^{p+1} + 0\,(h^{p+2})$$

Putting $e^h = \xi$, as $h \to 0$, $\xi \to 1$, the above equation becomes

$$\rho(\xi) - (\log \xi)\sigma(\xi) = -C_{p+1}(\xi - 1)^{p+1} + 0((\xi - 1)^{p+2}) \tag{3.32}$$

or
$$\frac{\rho(\xi)}{\log \xi} - \sigma(\xi) = -C_{p+1}(\xi - 1)^p + 0((\xi - 1)^{p+1}) \tag{3.33}$$

Equations (3.32) and (3.33) provide us with the methods for determining $\rho(\xi)$ or $\sigma(\xi)$ for maximum order if $\sigma(\xi)$ or $\rho(\xi)$ is given.

If $\sigma(\xi)$ is specified, (3.32) can be used to determine a $\rho(\xi)$ of degree k such that the order is at least k. The $(\log \xi)\ \sigma(\xi)$ can be expanded as a power series in $(\xi - 1)$ and the terms up to $(\xi - 1)^k$ can be used to find $\rho(\xi)$. If, on the other hand, we are given $\rho(\xi)$ we can use (3.33) to determine $\sigma(\xi)$ of degree $\leqslant k$ such that the order is at least $k+1$. The $\rho(\xi)/\log \xi$ is expanded as a power series in $(\xi - 1)$, and terms up to $(\xi - 1)^k$ are used to get $\sigma(\xi)$. For example, a few choices of the polynomial $\rho(\xi)$ and the resulting polynomials $\sigma(\xi)$ which give the well-known methods are as follows:

Adams-Bashforth Methods

$$\rho(\xi) = \xi^{k-1}(\xi - 1) \text{ and } \sigma(\xi) \text{ of degree } k-1$$

$$\sigma(\xi) = \xi^{k-1} \sum_{m=0}^{k-1} \gamma_m (1 - \xi^{-1})^m$$

where $$\gamma_m+\frac{1}{2}\gamma_{m-1}+\ldots+\frac{1}{m+1}\gamma_0 = 1,\ m = 0, 1, 2, \ldots$$

Nystrom Methods

$$\rho(\xi) = \xi^{k-2}(\xi^2-1) \text{ and } \sigma(\xi) \text{ of degree } k-1$$

$$\sigma(\xi) = \xi^{k-1}\sum_{m=0}^{k-1}\gamma_m(1-\xi^{-1})^m$$

where $$\gamma_m+\frac{1}{2}\gamma_{m-1}+\ldots+\frac{1}{m+1}\gamma_0 = \begin{cases} 2, & m = 0 \\ 1, & m = 1, 2, \ldots \end{cases}$$

Adams-Moulton Methods

$$\rho(\xi) = \xi^{k-1}(\xi-1) \text{ and } \sigma(\xi) \text{ of degree } k$$

$$\sigma(\xi) = \xi^{k}\sum_{m=0}^{k}\gamma_m(1-\xi^{-1})^m$$

where $$\gamma_m+\frac{1}{2}\gamma_{m-1}+\ldots+\frac{1}{m+1}\gamma_0 = \begin{cases} 1, & m = 0 \\ 0, & m = 1, 2, \ldots \end{cases}$$

Milne-Simpson Methods

$$\rho(\xi) = \xi^{k-2}(\xi^2-1) \text{ and } \sigma(\xi) \text{ of degree } k$$

$$\sigma(\xi) = \xi^{k}\sum_{m=0}^{k}\gamma_m(1-\xi^{-1})^m$$

where $$\gamma_m+\frac{1}{2}\gamma_{m-1}+\ldots+\frac{1}{m+1}\gamma_0 = \begin{cases} 2, & m = 0 \\ -1, & m = 1 \\ 0, & m = 2, 3, \ldots \end{cases}$$

As the number of coefficients in (3.26) is equal to $2k+1$ we may expect that they can be chosen so that $2k+1$ relations of the type (3.30) are satisfied, in which p is equal to $2k$. However, the root condition to be satisfied by the method considerably restricts this order.

We now state the fundamental theorem which specifies the maximum order of a linear k-step method.

THEOREM 3.1 *For any positive integer k although there exists a consistent method of order $p = 2k$, the order of a k-step method satisfying the root condition cannot exceed $k+2$. If k is odd it cannot exceed $k+1$.*

Example 3.3 Let $\rho(\xi) = (\xi-1)(\xi-\lambda)$ where λ is real and $-1 \leqslant \lambda < 1$, find $\sigma(\xi)$.

We have

$$\frac{\rho(\xi)}{\log \xi} = \frac{(\xi-1)[(1-\lambda)+(\xi-1)]}{\log(1+(\xi-1))}$$

$$C(\xi-1)^{p+1} + \sigma(\xi) = 1-\lambda+\frac{3-\lambda}{2}(\xi-1)+\frac{5+\lambda}{12}(\xi-1)^2$$
$$-\frac{1+\lambda}{24}(\xi-1)^3+0((\xi-1)^4)$$

Note that for $\lambda \neq -1$, the order is 3 and for $\lambda = -1$, the order is 4.

3.5.2 Estimate of truncation error

We can write (3.29) as

$$T_n = \frac{1}{p!}\int_{t_{n-k+1}}^{t_{n+1}} \{\overline{(t_{n+1}-s)^p} - ph\, b_0\overline{(t_{n+1}-s)}^{p-1}$$
$$+\sum_{i=1}^{k} a_i\overline{(t_{n-i+1}-s)}^p + ph\, b_i\overline{(t_{n-i+1}-s)}^{p-1}\}\, y^{(p+1)}(s)\, ds$$
$$= \frac{1}{p!}\int_{t_{n-k+1}}^{t_{n+1}} G(s) y^{(p+1)}(s)\, ds$$

where
$$\overline{(t_{n-i+1}-s)} = \begin{cases} t_{n-i+1}-s & \begin{cases} t_{n-i+1} \leqslant s \leqslant t_n & i \neq 0 \\ t_n \leqslant s & i = 0 \end{cases} \\ 0 & \text{otherwise} \end{cases}$$

Substituting $u = (s-t_n)/h$, we get

$$T_n = \frac{h^{p+1}}{p!}\int_{-k+1}^{1} \{\overline{(1-u)^p} - p\, b_0\overline{(1-u)}^{p-1}$$
$$+\sum_{i=1}^{k} [a_i\overline{(1-i-u)}^p + p\, b_i\overline{(1-i-u)}^{p-1}]\}\, y^{(p+1)}(t_n+hu)\, du$$
$$= \frac{h^{p+1}}{p!}\int_{-k+1}^{1} G(u)\, y^{(p+1)}(t_n+hu)\, du \tag{3.34}$$

The function $G(u)$ is called the *influence function*. If $G(u)$ does not change sign over the interval of integration $[-k+1, 1]$, then we may write (3.34) in the form

$$T_n = \frac{h^{p+1}}{p!}\, y^{(p+1)}(\eta)\int_{-k+1}^{1} G(u)\, du \tag{3.35}$$

where $-k+1 < \eta < 1$. But if the influence function $G(u)$ does change sign over $[-k+1, 1]$, then the error cannot be expressed in the form (3.35), although we may bound the error as

$$| T_n | \leqslant \frac{h^{p+1}}{p\,!} \, | \, y^{(p+1)}(\eta) \, | \int_{-k+1}^{1} | \, G(u) \, | \, du$$

Example 3.4 Obtain a fifth order formula of the form

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + a_3 y_{n-2} + a_4 y_{n-3} + h\,(b_0 y'_{n+1} + b_1 y'_n + b_2 y'_{n-1})$$

Express each coefficient in terms of a_2. Calculate the explicit form of the error term.

Expanding each term about t_n in the Taylor series and equating the cofficients of h^0 through h^5 to zero, we get

$$\begin{aligned}
1 &= a_1 + a_2 + a_3 + a_4 \\
1 &= -a_2 - 2a_3 - 3a_4 + b_0 + b_1 + b_2 \\
\frac{1}{2} &= \frac{1}{2}(a_2 + 4a_3 + 9a_4) + b_0 - b_2 \\
\frac{1}{6} &= \frac{1}{6}(-a_2 - 8a_3 - 27a_4) + \frac{1}{2}(b_0 + b_2) \\
\frac{1}{24} &= \frac{1}{24}(a_2 + 16a_3 + 81a_4) + \frac{1}{6}(b_0 - b_2) \\
\frac{1}{120} &= \frac{1}{120}(-a_2 - 32a_3 - 243a_3) + \frac{1}{24}(b_0 + b_2)
\end{aligned}$$

The truncation error is given by

$$T_n = -\frac{h^6}{5!} \int_{-3}^{1} G(u)\, y^{(6)}(t_n + hu)\, du$$

where
$$G(u) = \begin{cases}
(u-1)^5 + 5b_0\,(u-1)^4, & 0 \leqslant u \leqslant 1 \\
a_2\,(u+1)^5 - 5b_2\,(u+1)^4 + \\
a_3\,(u+2)^5 + a_4\,(u+3)^5, & -1 \leqslant u \leqslant 0 \\
a_2\,(u+2)^5 + a_4\,(u+3)^5, & -2 \leqslant u \leqslant -1 \\
a_4\,(u+3)^5, & -3 \leqslant u \leqslant -2
\end{cases}$$

The coefficients a_i and b_i may be obtained as

$$\begin{aligned}
306a_1 &= -413a_2 + 468, & 34a_3 &= 13a_2 - 20 \\
153a_4 &= -5a_2 + 9, & 34b_0 &= -a_2 + 12 \\
51b_1 &= 31a_2 + 36, & 34b_2 &= 37a_2 - 36
\end{aligned}$$

The value of T_n is given by

$$T_n = \frac{h^6}{5! \times 17} \left(-216 + 86a_2\right) y^{(6)} (\eta)$$

where $-3 < \eta < 1$.

3.5.3 Stability and convergence

If we use the linear multistep method (3.26) to find the difference solution exactly, then we are faced with the phenomenon of round-off errors. We obtain only an approximation to y_n, which we denote by $\bar{y}_n$ and which satisfies

$$\rho (E)\, \bar{y}_{n-k+1} = h\sigma (E)\, \bar{y}'_{n-k+1} + \bar{R}_n$$

The value of the local error $\bar{R}_n$ will depend on the details of the rounding procedures and, in the implicit case, on how the iterations are started, and terminated.

Carrying more decimal places, changing rounding procedures, and so on, will yield a new approximation $\bar{\bar{y}}_n$ which satisfies

$$\rho (E)\, \bar{\bar{y}}_{n-k+1} = h\sigma (E)\, y'_{n-k+1} + \bar{R}_n$$

We now define the stability of the method (3.26).

DEFINITION 3.4 The linear multistep method (3.26) is said to be stable, relative to a class of functions, if for each member of the class and for any $\epsilon > 0$ there exist $\delta = \delta (\epsilon) > 0$, h_0, b such that

$$| \bar{y}_{n+1} - \bar{\bar{y}}_{n+1} | < \epsilon$$

whenever

$$\sum_{i=0}^{n+1} | \bar{R}_i - \bar{\bar{R}}_i | < \delta$$

the result being required to hold uniformly for $h \in (0, h_0)$ and for all n such that $0 \leqslant t_n \leqslant b$.

For the class of functions $f(t, y)$ which are continuous and which satisfy a Lipschitz condition of the form

$$| f(t, \bar{y}) - f(t, \bar{\bar{y}}) | \leqslant L \, | \bar{y} - \bar{\bar{y}} |$$

in a region of the t-y plane which contains all the points being considered, we have the result.

THEOREM 3.2 *The linear multistep method (3.26) is said to be stable, relative to the given class of functions, if and only if it satisfies the root condition.*

For a stable method, we may expect that the starting errors will not be amplified as they propagate through the sequence $\{\bar{y}_n\}$ regardless of how large n becomes as $h \to 0$. This suggests a close relationship between stability and convergence. We now state the definition of convergence for the method (3.26).

DEFINITION 3.5 The linear multistep method (3.26) is said to be convergent, if, for all initial value problems (3.1) subject to hypotheses of theorem 1.1, we have

$$\lim_{\substack{h \to 0 \\ nh = t_n - t_0}} y_n = y(t_n)$$

holds for all $t \in [t_0, b]$, and for all solutions $\{y_n\}$ of the difference equation (3.26) satisfying starting conditions $y_\nu = y_\nu(h)$ for which

$$\lim_{h \to 0} y_\nu(h) = y_0, \quad \nu = 0(1)\, k-1$$

We now state the following results.

THEOREM 3.3 *If the linear multistep method (3.26) is convergent, then it must satisfy the root condition.*

THEOREM 3.4 *If the linear multistep method (3.26) is convergent, then it must be consistent.*

THEOREM 3.5 *Consistency and stability are together necessary and sufficient conditions for convergence.*

In order to illustrate the effect of the root condition on the stability and convergence we use the method

$$y_{n+1} - 4y_n + 3y_{n-1} = -2h\, f_{n-1} \tag{3.36}$$

to solve the initial value problem

$$y' = \lambda y, \; y(0) = 1$$

which has the solution $y(t) = e^{\lambda t}$.

Here, we obtain the polynomial equation

$$\rho(\xi) = \xi^2 - 4\xi + 3 = 0$$

which has roots $\xi_1 = 1$ and $\xi_2 = 3$. Hence, the method (3.36) does not satisfy the root condition. The truncation error is given by

$$T_n = \frac{2}{3} h^3 y'''(t_n) + 0(h^4)$$

Therefore, the method is consistent and has order two. Applying the method (3.36) to $y' = \lambda y$, we get the difference equation

$$y_{n+1} - 4y_n + (3 + 2\bar{h}) y_{n-1} = 0 \tag{3.37}$$

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

This is a linear difference equation of order two with constant coefficients Its characteristic polynomial is

$$\xi^2-4\xi+(3+2\bar{h}) = 0$$

which has roots

$$\xi_{1h} = 2-\sqrt{(1-2\bar{h})}$$

and

$$\xi_{2h} = 2+\sqrt{(1-2\bar{h})}$$

The general solution of (3.37) may be written as

$$y_n = C_1\, \xi_{1h}^n+C_2\, \xi_{2h}^n \tag{3.38}$$

where C_1 and C_2 are two arbitrary constants. Choosing the conditions

$$y_0 = 1, \quad y_1 = z_1$$

where z_1 is still unspecified, we obtain

$$C_1 = (\xi_{2h}-z_1)/(\xi_{2h}-\xi_{1h}),\ C_2 = (z_1-\xi_{1h})/(\xi_{2h}-\xi_{1h})$$

We now study the asymptotic behaviour of y_n as $h \to 0$ and $n \to \infty$ while $nh = t$ remains fixed. Let us choose $y_1 = e^{\bar{h}}$, which is the value of the exact solution at $t = h$, satisfying $\lim\limits_{h\to 0} y_1 = 1$. Now we get

$$\begin{aligned}
\xi_{1h} &= 1+\bar{h}+\frac{1}{2}\,\bar{h}^2+0\,(\bar{h}^3)\\
\xi_{2h} &= 3-\bar{h}+0\,(\bar{h}^2)\\
\xi_{2h}-\xi_{1h} &= 2\sqrt{(2-\bar{h})}\\
z_1-\xi_{1h} &= e^{\bar{h}}-\xi_{1h} = -\frac{1}{3}\,\bar{h}^3+0\,(\bar{h}^4)\\
\xi_{2h}-z_1 &= \xi_{2h}-e^{\bar{h}} = 2+0\,(\bar{h})\\
\xi_{1h}^n &= e^{\lambda t}+0\,(\bar{h})\\
\xi_{2h}^n &= 3^n\,(\exp\left(-\frac{1}{3}\,\lambda t\right)+0\,(\bar{h}))
\end{aligned}$$

where $nh = t$, fixed.

Therefore, the solution (3.38) may be written as

$$y_n = \frac{1}{2\sqrt{1-2\bar{h}}}\,(\exp\,(\lambda t)+0\,(\bar{h}))\,(2+0\,(\bar{h}))$$
$$+\frac{1}{2\sqrt{1-2\bar{h}}}\,3^n\,(\exp\left(-\frac{1}{3}\,\lambda t\right)+0\,(\bar{h}))\left(-\frac{1}{3}\,\bar{h}^3+0\,(\bar{h}^4)\right)$$

As $h \to 0$, we see that the first term converges to the exact solution $\exp\,(\lambda t)$. The second term behaves asymptotically like

$$-\frac{1}{6}\,\lambda^3\, t^3 \exp\left(-\frac{1}{3}\,\lambda t\right)(3^n/n^3) \text{ as } n \to \infty$$

Hence $y_n \to -\infty$. The method (3.36) is not convergent for the initial value problem $y' = \lambda y$, $y(0) = 1$. Next, we assume $y_1 = e^{\bar{h}}+h^2$ and obtain a numerical solution $\bar{y}_n$ of (3.37) which behaves asymptotically like $\frac{1}{2}t^2$

$\exp(-\lambda t)(3^n/n^2)$ as $n \to \infty$, $nh = t$ fixed. We find $y_n - \bar{y}_n \to -\infty$ as $h \to 0$ while the perturbation h^2 in y_n also approaches zero. Therefore, Definition 3.4 cannot be satisfied for any h_0.

3.5.4 Other stability results

In order to discuss the stability in a quantitative way, we must define a differential equation as well as the numerical method used in the approximate solution. The equation studied in this connection is the simple linear first order differential equation

$$y' = \lambda y, \quad y(t_0) = y_0$$

where λ may be a complex number. The exact solution for this equation at $t = t_n$ is given by

$$y(t_n) = y(t_0)\, e^{\lambda nh} = y(t_0)\,(e^{\lambda h})^n \tag{3.39}$$

Ignoring the round-off errors, the computed solution satisfies

$$y_{n+1} = \sum_{i=1}^{k} a_i\, y_{n-i+1} + h\lambda \sum_{i=0}^{k} b_i\, y_{n-i+1} \tag{3.40}$$

The true solution satisfies

$$y(t_{n+1}) = \sum_{i=1}^{k} a_i\, y(t_{n-i+1}) + h\lambda \sum_{i=0}^{k} b_i\, y(t_{n-i+1}) + T_n \tag{3.41}$$

where T_n is the local truncation error.

Subtracting (3.41) from (3.40) and substituting $\epsilon_n = y_n - y(t_n)$, we get

$$\epsilon_{n+1} = \sum_{i=1}^{k} a_i\, \epsilon_{n-i+1} + h\lambda \sum_{i=0}^{k} b_i\, \epsilon_{n-i+1} - T_n \tag{3.42}$$

or

$$(\rho(E) - h\lambda\sigma(E))\, \epsilon_{n-k+1} + T_n = 0 \tag{3.43}$$

This is a kth order, linear, nonhomogeneous, difference equation with constant coefficients. If the estimates of $\epsilon_0, \epsilon_1, \ldots, \epsilon_{k-1}$ are available and T_n is known, the difference equation can be solved for all n. Let as assume that T_n is constant and is equal to T. The solution of (3.43) will consist of a particular solution plus a linear combination of the independent solution of the homogeneous equation with $T = 0$. The homogeneous equation is

$$(\rho(E) - h\lambda\sigma(E))\, \epsilon_{n-k+1} = 0 \tag{3.44}$$

We seek the solution of (3.44) in the form

$$\epsilon_n = A\xi^n \tag{3.45}$$

where ξ is to be determined and A is a constant. Substituting (3.45) in (3.44), we get

$$A(\rho(\xi) - h\lambda\sigma(\xi))\, \xi^{n-k+1} = 0$$

or

$$\rho(\xi) - h\lambda\sigma(\xi) = 0 \tag{3.46}$$

The general solution of the difference equation (3.43) for distinct roots can be written as

$$\epsilon_n = A_1\xi_{1h}^n + A_2\xi_{2h}^n + \cdots + A_k\xi_{kh}^n + \frac{T}{h\lambda\,\rho'(1)} \tag{3.47}$$

where $A_1, A_2, \ldots, A_k$ are constants to be determined from the initial errors $\epsilon_0, \epsilon_1, \ldots, \epsilon_{k-1}$, and $\xi_{1h}, \xi_{2h}, \ldots, \xi_{kh}$ are the distinct roots of the characteristic equation (3.46), and $T/h\lambda\,\rho'(1)$ is the particular solution of the difference equation (3.43). If the roots are not distinct, the form of solution (3.43) gets modified. For example, if $\xi_{1h} = \xi_{2h} = \ldots = \xi_{mh} = \eta_h$, the combination $A_1\xi_{1h}^n + A_2\xi_{2h}^n + \ldots A_m\xi_{mh}^n$ is replaced by $(A_1 + nA_2 + \ldots + n^{m-1}A_m)\eta_h^n$. In what follows we shall restrict ourselves to the distinct roots.

Let us consider the solution of the difference equation (3.40). The characteristic equation of (3.40) is the same as (3.46). Thus the solution of the homogeneous equation (3.40) can be written as

$$y_n = B_1\xi_{1h}^n + B_2\xi_{2h}^n + \ldots + B_k\xi_{kh}^n \tag{3.48}$$

where $B_1, B_2, \ldots, B_k$ are constants to be determined from the knowledge of $y_0, y_1, \ldots y_{k-1}$ usually computed by a singlestep method.

On comparing (3.48) with (3.39), we find that one of the roots of the characteristic equation (3.46), say ξ_{1h}, approximates $e^{\lambda h}$ to give meaningful results. This root is called the *principal root* and the other $k-1$ roots are called *extraneous roots* which arise because a first order differential equation is replaced by a kth order difference equation. For $h \to 0$, the roots of the characteristic equation (3.46) approach the roots of the equation $\rho(\xi) = 0$. This is called the reduced characteristic equation. Let $\xi_1, \xi_2, \ldots, \xi_k$ be the roots of $\rho(\xi) = 0$, then for sufficiently small λh we may write

$$\xi_{jh} = \xi_j(1 + \lambda h\, k_j + 0(|\lambda h|^2)),\ j = 1, 2, \ldots, k \tag{3.49}$$

where k_j is called the *growth parameter*.

Substituting (3.49) in (3.46) and simplifying, we obtain

$$k_j = \frac{\sigma(\xi_j)}{\xi_j\rho'(\xi_j)} \tag{3.50}$$

From (3.49), we get

$$\xi_{jh}^n = \xi_j^n(1 + \lambda h\, k_j + 0(|\lambda h|^2))^n$$

or

$$\xi_{jh}^n = \xi_j^n\, e^{k_j\lambda nh},\ j = 1, 2, \ldots, k \tag{3.51}$$

If the linear multistep method (3.26) is consistent then we have, $C_0 = 0$ and $C_1 = 0$ i.e., $\rho(1) = 0$, and $\rho'(1) = \sigma(1)$. We get $\xi_1 = 1$. The growth parameter, from (3.50) becomes $k_1 = 1$. Using (3.49), we obtain

$$\xi_{1h} = 1 + \lambda h + 0(|\lambda h|^2)$$

We now introduce the following definition.

DEFINITION 3.6 The linear multistep method (3.26), is said to be

strongly stable if $|\xi_j| < 1$ for $j \neq 1$,

strongly unstable if $|\xi_j| > 1$ for some j or if there is a double root of $\rho(\xi) = 0$ of modulus unity

Conditionally stable if it is not strongly unstable and if some $j \neq 1$ we have $|\xi_j| = 1$.

The particular solution in (3.47) is constant, and hence the homogeneous solution affects the growth of the error ϵ_n. If $|\xi_{jh}| > 1$, the error ϵ_n in (3.47) will grow without bound as n becomes large. A similar effect is also evident if a root of (3.46) of multiplicity greater than one, has modulus one.

The behaviour of the principal root ξ_{1h} depends on λ, or at least on the sign of λ.

DEFINITION 3.7 The linear multistep method (3.26) is said to be *absolutely stable* if

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

The region of absolute stability is defined to be a set of points in λh-plane for which the method is absolutely stable. The largest modulus of the roots ξ_{jh} of the characteristic equation (3.46) for the Adams-Bashforth methods and the Adams-Moulton methods is shown in Figure 3.1.

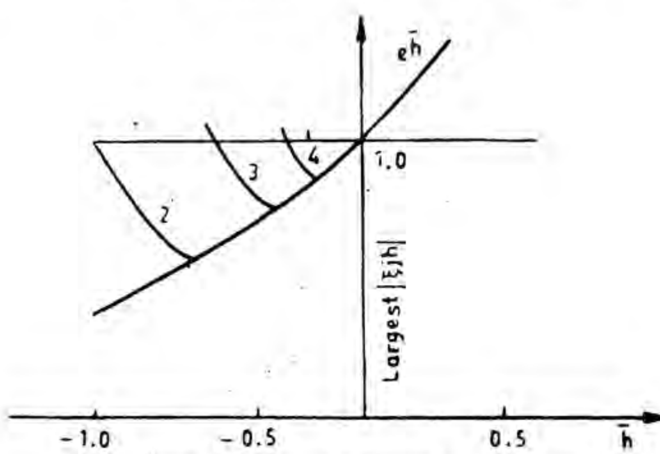


Fig. 3.1 (a) Dominant root in Adams-Bashforth methods

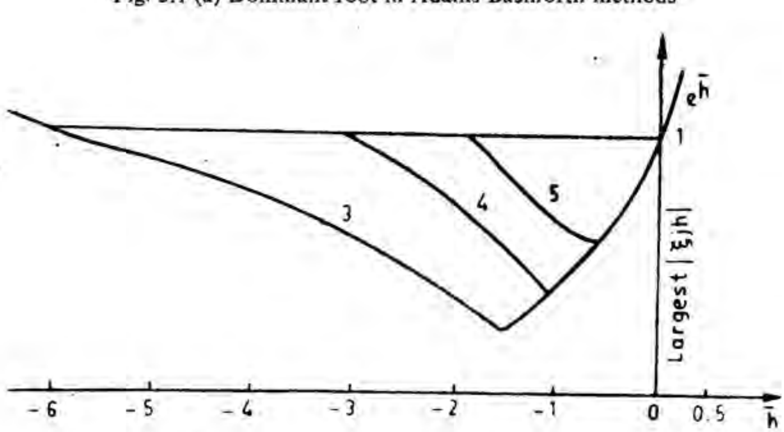


Fig. 3.1 (b) Dominant root in Adams-Moulton methods

The interval of absolute stability is listed in Table 3.10.

TABLE 3.10 INTERVAL OF ABSOLUTE STABILITY ON REAL LINE

k	1	2	3	4	5
		Adams-Bashforth methods			
$(\beta, 0)$	-2	-1.33	-0.55	-0.3	-0.2
		Adams-Moluton methods			
$(\beta, 0)$	$-\infty$	$-\infty$	-6	-3.0	-1.8

The linear multistep methods having the interval of absolute stability $(-\infty, 0)$ are called *A-stable* methods. Here, we have $|\xi_{jh}| < 1, j = 1(1)k$.

DEFINITION 3.8 A linear multistep method when applied to the differential equation of the form $y' = \lambda y$ and λ is a (complex) constant with negative real part is called *A-stable* if all solutions of (3.26) tend to zero, as $n \to \infty$.

The region of stability is shown in Figure 3.2.

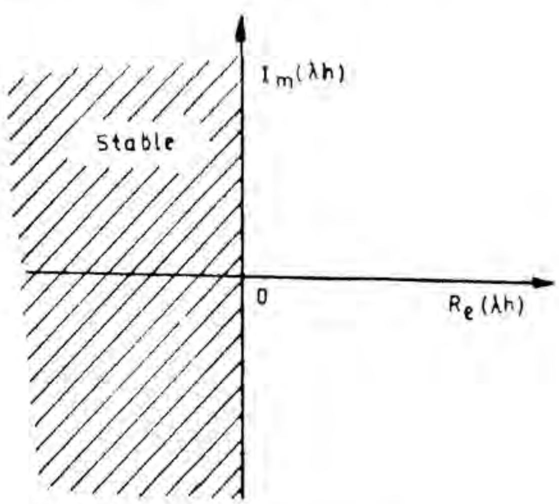


Fig. 3.2 Stability region

We now state the main result about A-stable linear multistep methods.

THEOREM 3.6 *The order p, of an A-stable linear multistep method cannot exceed 2 and the method must be implicit.*

If we use the trapezoidal formula or the second order Adams-Moulton method

$$y_{n+1} = y_n + \frac{h}{2}\,(y'_{n+1} + y'_n) \tag{3.52}$$

to approximate $y' = \lambda y$, then Equation (3.52) becomes

$$(2-\bar{h})\,y_{n+1} - (2+\bar{h})\,y_n = 0 \tag{3.53}$$

The characteristic Equation of (3.53) is given by

$$(2-\bar{h})\,\xi - (2+\bar{h}) = 0$$

The solution of the difference Equation (3.53) can be written as

$$y_n = \bar{c}_1 \left(\frac{2+\bar{h}}{2-\bar{h}}\right)^n$$

The root ξ_{1h} is shown in Figure 3.3.

From Figure 3.3, it is obvious that the trapezoidal formula is stable for all values of $\bar{h}$. Similarly, we can show that the backward Euler method

$$y_{n+1} = y_n + h\,y'_{n+1}$$

is also stable for all values of $\bar{h}$.

Thus, the trapezoidal and backward Euler methods are A-stable.

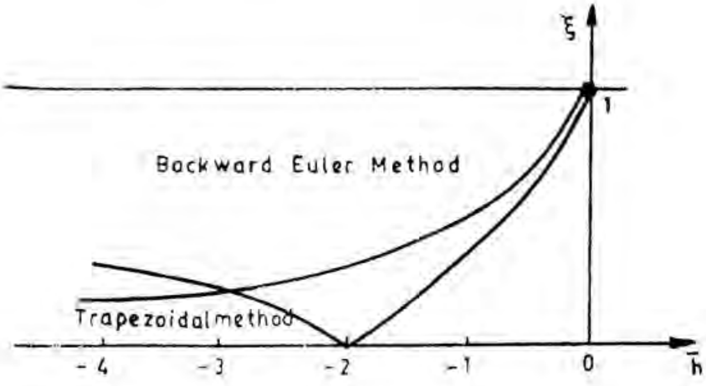


Fig. 3.3 Roots of trapezoidal and backward Euler methods

The A-stable linear multistep methods are very useful for integrating stiff systems of ordinary differential equations. Unfortunately, the class of A-stable linear multistep methods is rather small. A natural weakening of the stability requirement is to demand that the absolute stability condition

$|\xi_{jh}| < 1, j = 1(1)k$ holds whenever $\lambda h \in R$ where R is some domain of the complex λh-plane. Typically, we consider domain which do not contain all of the left-half λh-plane.

DEFINITION 3.9 The multistep method (3.26) is said to be *stiffly stable* if in the region R_1 it is absolutely stable, and in R_2 it is accurate and stable, when applied to the initial value problem $y' = \lambda y$, $y(t_0) = y_0$, λ a complex constant with $Re\,\lambda < 0$ where

$$R_1 = \{\lambda h \mid Re\,\lambda h \leqslant D\}$$
$$R_2 = \{\lambda h \mid D < Re\,\lambda h < \alpha, \mid Im\,(\lambda h) \mid < \theta\}$$

and D, θ and α are parameters.

The regions R_1 and R_2 are shown in Figure 3.4. The underlying idea of the definition is as follows. The solution to the stiff equations contain the stiff and non-stiff components. The stiff solution components which represent rapidly decaying terms will correspond to the values of λh in R_1; the step-size h may be chosen so that the negligible stiff solution components are approximated stably with $\lambda h \in R_1$. The non-stiff solution components vary slowly in comparison to the stiff solution components; the stepsize h may be so chosen that $\lambda h \in R_2$ will ensure an accurate and stable approximation to the non-stiff solution components. Thus we notice that inside the region bounded by the rectangle, the multistep method (3.26) is stable as $h \to 0$ and outside the rectangle in the negative half plane the multistep method is stable for all values of h. The characteristic equation is given by (3.46) as

$$\rho(\xi) - \lambda h \sigma(\xi) = 0$$

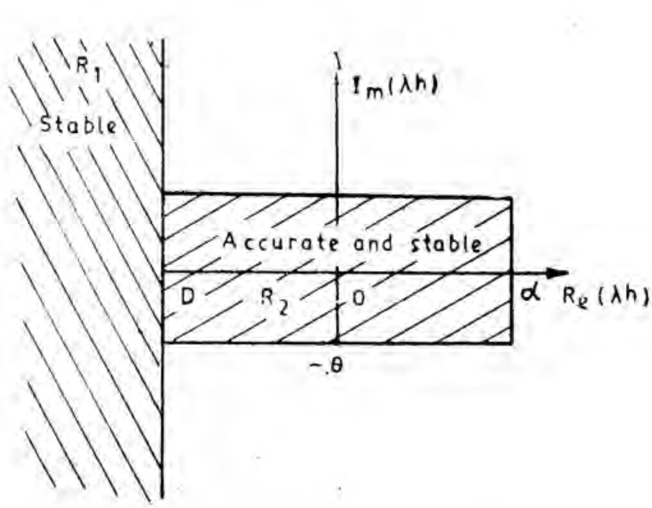


Fig. 3.4 Stability and accuracy region

We want λh values such that the characteristic equation has roots inside the unit circle or on the unit circle and simple. This region is bounded by the locus of $\rho(\xi)/\sigma(\xi)$ in the λh-plane for $\xi = \exp(i\theta)$, $\theta \in [0, 2\pi]$. If $\sigma(\xi)$ is stable, the method will be stable at $\lambda h =$ infinity, so by continuity arguments any region connected to $\lambda h =$ infinity will be stable. In order to obtain values for plotting this locus, we put

$$\lambda h = \frac{\rho(\xi)}{\sigma(\xi)} \text{ with } \xi = \exp(i\theta)$$

and calculate λh for $\theta = 0(\pi/M)\pi$ where M is chosen to provide a small enough increment to obtain a suitable number of points. We find

$$\lambda h = \frac{\rho(\xi)}{\sigma(\xi)}$$

$$= \frac{e^{ki\theta} - a_1 e^{(k-1)i\theta} - \ldots - a_k}{b_0 e^{ki\theta} + b_1 e^{(k-1)i\theta} + \ldots + b_k}$$

Substituting

$$R = \cos k\theta - a_1 \cos(k-1)\theta - \ldots - a_k$$

$$S = \sin k\theta - a_1 \sin(k-1)\theta - \ldots - a_{k-1} \sin\theta$$

$$A = b_0 \cos k\theta + b_1 \cos(k-1)\theta + \ldots + b_k$$

$$B = b_0 \sin k\theta + b_1 \sin(k-1)\theta + \ldots + b_{k-1} \sin\theta$$

we get

$$\lambda h = \frac{R + iS}{A + iB}$$

$$= \frac{(RA + SB) + i(SA - RB)}{A^2 + B^2} = x + iy$$

where

$$x = \frac{RA + SB}{A^2 + B^2} \text{ and } y = \frac{SA - RB}{A^2 + B^2}$$

The desired locus is obtained by plotting the curve passing through the x, y values calculated for θ varying over the range 0 to π, giving the upper half, and then rotating this curve 180° to obtain the lower half, since the locus is symmetric about the real axis. The stiffly stable methods are obtained for $\sigma(\xi) = \xi^k$, $k = 1(1)6$. These methods are given in Table 3.9. Figure 3.5 shows a sample plot for $\sigma(\xi) = \xi^k$ with $k = 6$. The value $k = 7$ gives an unstable method. However, if we choose

$$\sigma(\xi) = \xi^{k-r}(\xi - c)^r, \; r = 0, 1, 2, \ldots, k$$

where $-1 \leqslant c < 1$, we find

r	0	1	2	3	4	6
order of stable method	$k \leqslant 6$	$k \leqslant 7$	$k \leqslant 8$	$k \leqslant 9$	$k \leqslant 10$	$k \leqslant 11$

The value $r = 5$ does not give eleventh order method. There are no twelfth order and higher order stiffly stable multistep methods of this type.

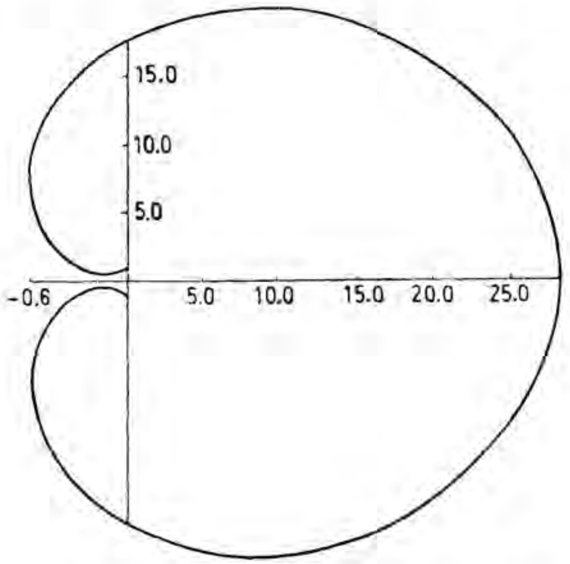


Fig. 3.5 Locus of $\rho(\xi)/\sigma(\xi)$, $\xi = \exp(i\theta)$, $\theta \in [0, 2\pi]$

DEFINITION 3.10 The linear multistep method (3.26) is said to be relatively stable if

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

The region of relative stability is defined to be a set of points in the λh-plane for which the method is relatively stable.

It may be pointed out here that absolute stability does not mean relative stability, because we may have

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

To illustrate the difference between absolute and relative stabilities, let us apply the third order Adams-Moulton method

$$y_{n+1} = y_n + \frac{h}{12}(5y'_{n+1} + 8y'_n - y'_{n-1}) \tag{3.54}$$

to the initial value problem $y' = \lambda y$, $y(t_0) = y_0$. Equation (3.54) becomes

$$\left(1 - \frac{5}{12}\bar{h}\right)y_{n+1} - \left(1 + \frac{2}{3}\bar{h}\right)y_n + \frac{\bar{h}}{12}y_{n-1} = 0 \tag{3.55}$$

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

Equation (3.55) is a second order difference equation which will give one extraneous solution. We are concerned with the rate of growth of this extraneous solution as n gets large. The solution of the Equation (3.55) is of the form

$$y_n = \bar{c}_1 \xi_{1h}^n + \bar{c}_2 \xi_{2h}^n$$

where
$$\xi_{jh} = \frac{12+8\bar{h} \pm \sqrt{144+144\bar{h}+84\bar{h}^2}}{2(12-5\bar{h})}, j = 1, 2 \quad (3.56)$$

The roots are shown in Figure 3.6, where ξ_{1h} is the principal root and ξ_{2h} is an extraneous root. At $\bar{h} = -6.0$, $|\xi_{2h}|$ is greater than one: the term ξ_{2h}^n in Equation (3.56) will overwhelm the true solution as n gets large. Thus the method is unstable for $\bar{h} < -6$. The region to the right of the point $\bar{h} = -1.5$ in Figure 3.6 is the region of relative stability, and the region to the right of the point $\bar{h} = -6.0$ is of absolute stability. The common region is both absolutely and relatively stable, that is, the asymptotic behaviour of the approximate solution will behave like that of the true solution.

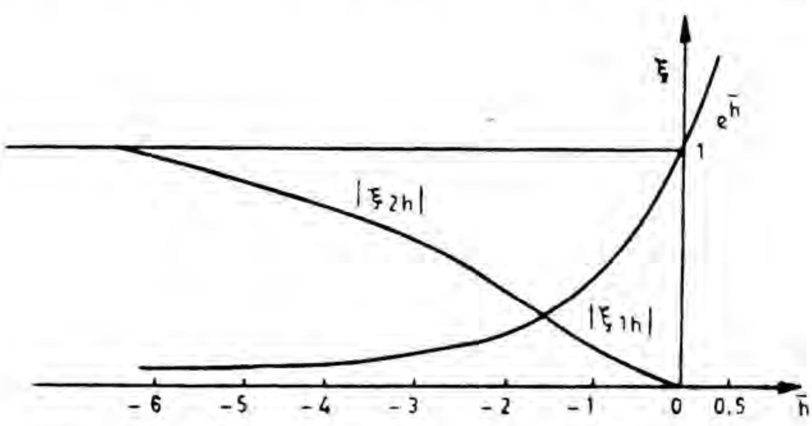


Fig. 3.6 Roots of third order Adam-Moulton corrector as function of $\bar{h}$

DEFINITION 3.11 The multistep method (3.26) is said to be *weakly stable* if there is more than one simple root of the polynomial equation $\rho(\xi) = 0$ on the unit circle (and strongly stable if not).

For the roots on the unit circle, Equation (3.51) becomes

$$|\xi_{jh}| = |e^{k_j \lambda nh}|$$

For $j = 1$, we get $k_1 = 1$ from (3.50). When $\lambda < 0$, the roots on the unit circle for which $k_j < 0$ give exponentially increasing components of the numerical solution, which soon invalidate the true solution.

Let us consider the stability of Milne's method

$$y_{n+1} = y_{n-1} + \frac{h}{3}(y'_{n+1} + 4y'_n + y'_{n-1}) \quad (3.57)$$

The substitution $y' = \lambda y$ in (3.57) yields a second order difference equation

$$\left(1-\frac{\bar{h}}{3}\right)y_{n+1}-4\,\frac{\bar{h}}{3}y_n-\left(1+\frac{\bar{h}}{3}\right)y_{n-1}=0 \tag{3.58}$$

The characteristic equation is given by

$$\left(1-\frac{\bar{h}}{3}\right)\xi^2-4\,\frac{\bar{h}}{3}\,\xi-\left(1+\frac{\bar{h}}{3}\right)=0 \tag{3.59}$$

This is a quadratic equation and has two roots

$$\xi_{1h}=\left[\frac{2}{3}\,\bar{h}+\left(1+\frac{\bar{h}^2}{3}\right)^{1/2}\right]\left(1-\frac{\bar{h}}{3}\right)^{-1}$$

$$\xi_{2h}=\left[\frac{2}{3}\,\bar{h}-\left(1+\frac{\bar{h}^2}{3}\right)^{1/2}\right]\left(1-\frac{\bar{h}}{3}\right)^{-1} \tag{3.60}$$

The graph of the roots as function of $\bar{h}$ is shown in Figure 3.7.

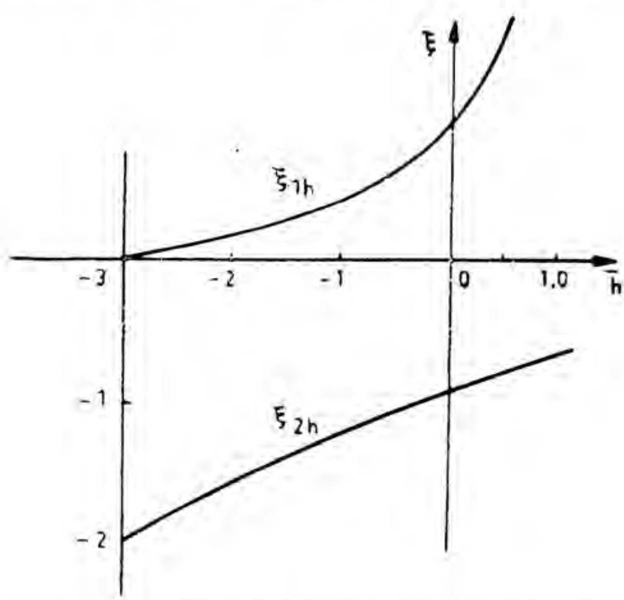


Fig. 3.7 Roots of Milne corrector as function of $\bar{h}$

Substituting $\bar{h} = 0$ in (3.57), we get the reduced characteristic equation

$$\xi^2-1=0$$

It gives $\xi = \pm 1$ and so Milne's method is stable according to Definition 3.6.

The growth parameters are found from the equation (3.50) as $\xi = 1$, $k_1 = 1$ and $\xi = -1$, $k_2 = -1/3$.

Equation (3.60) can be rewritten in the form

$$\xi_{1h} \approx e^{\lambda h}$$

$$\xi_{2h} \approx -e^{(-1/3)\lambda h}$$

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 $A_1, A_2, \ldots, A_k$ in (3.47) are chosen so that the initial conditions are satisfied; thus

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

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

The principal root ξ_{1h} of the characteristic equation for sufficiently small λh is approximately equal to $e^{\lambda h}$. The other roots $\xi_{2h}, \xi_{3h}, \ldots, \xi_{kh}$ 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 $A_2, \ldots, A_k$. To find A_1, we use *Cramer's rule* and obtain

$$A_1 = \frac{\begin{vmatrix} E_0 & 1 & \ldots & 1 \\ E_1 & \xi_{2h} & \ldots & \xi_{kh} \\ \vdots & & & \\ E_{k-1} & \xi_{2h}^{k-1} & \ldots & \xi_{kh}^{k-1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \ldots & 1 \\ \xi_{1h} & \xi_{2h} & \ldots & \xi_{kh} \\ \vdots & & & \\ \xi_{1h}^{k-1} & \xi_{2h}^{k-1} & \ldots & \xi_{kh}^{k-1} \end{vmatrix}} \tag{3.61}$$

Substituting

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

in Equation (3.61), we can write

$$A_1 = \frac{c_{k-1}\,E_{k-1} + c_{k-2}\,E_{k-2} + \ldots + c_0E_0}{C(\xi_{1h})}$$

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

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

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 $\lambda \to 0$. 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 $y^{(0)}_{n+1}$ for y_{n+1}

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

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

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

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

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

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

$\vdots$

The sequence of operations

PECECE...

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

$$y^{(0)}_{n+1},\ y^{(1)}_{n+1},\ y^{(2)}_{n+1},\ \ldots \tag{3.63}$$

Let us examine the convergence of this sequence.

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

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

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

For the Adams-Moulton methods, we have

$$| hL | < 2 = 2.0 \text{ for second order method,}$$

$$| hL | < \frac{12}{5} = 2.4 \text{ for third order method,}$$

$$| hL | < \frac{8}{3} = 2.67 \text{ for fourth order method,}$$

$$| hL | < \frac{720}{251} = 2.87 \text{ for fifth order method.}$$

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 $y^{(0)}_{n+1}$ requires the procedure Predict-Estimate-Correct-... (PECECE...) which converges to y_{n+1} if $| hLb_0 | < 1$.

A simple way to find $y^{(0)}_{n+1}$ 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

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

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

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

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

where $\qquad f^{(\mu)}_{n+1} = f(t_{n+1}, y^{(\mu)}_{n+1})$

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

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

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

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

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

$$E: y'^{(1)}_{n+1} = \lambda y^{(1)}_{n+1}$$

$$C: y^{(2)}_{n+1} = \sum_{i=1}^{k} (a_i + h\lambda b_i)\, y_{n-i+1} + h\,\lambda b_0\, y^{(1)}_{n+1}$$

Simplifying, we get

$$C: y^{(2)}_{n+1} = (1+h\lambda b_0) \sum_{i=1}^{k} (a_i + h\,\lambda b_i)\, y_{n-i+1}$$

$$+ (h\,\lambda b_0)^2 \sum_{i=1}^{k} (a_i^{(0)} + h\lambda b_i^{(0)})\, y_{n-i+1}$$

$$E: y'^{(2)}_{n+1} = \lambda y^{(2)}_{n+1}$$

Hence we can write

$$y^{(m)}_{n+1} = (1+h\,\lambda b_0 + \ldots + (h\lambda b_0)^{m-1}) \sum_{i=1}^{k} (a_i + h\lambda b_i)\, y_{n-i+1}$$

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

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

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

Substitute $y^{(m)}_{n+1} = y_{n+1}$, we get for $P(EC)^m E$ scheme

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

$$+ (h\lambda b_0)^m \sum_{l=1}^{k} (a_i^{(0)} + h\lambda b_i^{(0)})\, y_{n-l+1} \tag{3.68}$$

The characteristic equation can be obtained if we put $y_n = A\xi^n$ and simplify (3.68). Using

$$\begin{aligned}
\rho(\xi) &= \xi^k - a_1\xi^{k-1} - \ldots - a_k \\
\sigma(\xi) &= b_0\xi^{k} + b_1\xi^{k-1} + \ldots + b_k \\
\rho^{(0)}(\xi) &= \xi^k - a_1^{(0)}\,\xi^{k-1} - \ldots - a_k^{(0)} \\
\sigma^{(0)}(\xi) &= b_1^{(0)}\,\xi^{k-1} + b_2^{(0)}\,\xi^{k-2} + \ldots + b_k^{(0)}
\end{aligned} \tag{3.69}$$

in (3.68), we get the characteristic equation as

$$\frac{1-(h\lambda b_0)^m}{1-h\lambda b_0} (\rho(\xi) - h\lambda\sigma(\xi)) + (h\lambda b_0)^m (\rho^{(0)}(\xi) - h\lambda\sigma^{(0)}(\xi)) = 0 \tag{3.70}$$

Let ξ_{jh} be the roots of (3.70). The moduli of these ξ_{jh} determine the growth behaviour of the error $\epsilon_n = y_n - y(t_n)$. The $P-C$ scheme is called ***absolutely stable*** if

$$|\,\xi_{jh}\,| \leqslant 1,\ j = 1, 2, \ldots, k$$

and is called *relatively stable* if

$$| \xi_{jh} | \leqslant | \xi_{1h} | , \; j = 2, 3, \ldots,$$

where ξ_{1h} is the principal root.

The largest modulus of the root of the characteristic equation (3.70) for the Adams-predictor-corrector methods of order three and four is shown in Figure 3.8.

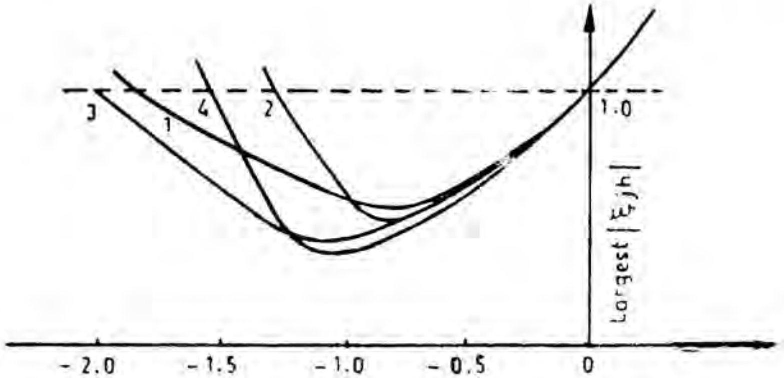


Fig. 3.8 (a) Dominant root of $P(EC)^m E$ for third order Adams-Bashforth-Moulton method $m = 1\,(1)\,4$

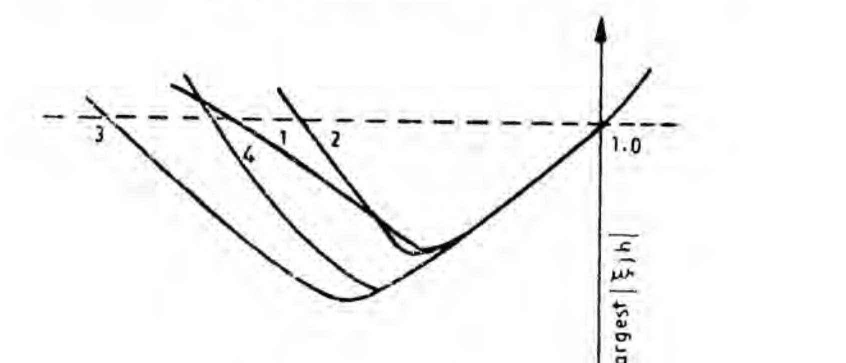


Fig. 3.8 (b) Dominant root of $P(EC)^m E$ for fourth order Adams-Bashforth-Moulton method $m = 1\,(1)\,4$

Next we study the truncation error of the predictor-corrector methods. Let us consider the $P-C$ set

$$P : y_{n+1} = y_n + hf_n$$

$$C : y_{n+1} = y_n + \frac{h}{2}(f_{n+1} + f_n) \tag{3.71}$$

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

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

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

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

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

Therefore,
$$
y_{n+1} = \left(\frac{1+\dfrac{\lambda h}{2}-2\left(\dfrac{\lambda h}{2}\right)^{m+2}}{1-\dfrac{\lambda h}{2}}\right) y_n \tag{3.73}
$$

If the corrector is iterated to converge, i.e. $m \to \infty$, 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

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

$$+\left(\frac{1+\frac{\lambda h}{2}-2\left(\frac{\lambda h}{2}\right)^{m+2}}{1-\frac{\lambda h}{2}}\right)\epsilon_n \qquad (3.74)$$

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

$$-\frac{1}{2}(\lambda h)^2+0\,(\,|\,\lambda h\,|^3) \text{ for } \mathbf{0} \text{ corrector}$$

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

$$\frac{1}{12}(\lambda h)^3+0\,(\,|\,\lambda h\,|^4) \text{ for } \mathbf{2} \text{ corrector}$$

$$\frac{1}{12}(\lambda h)^3+0\,(\,|\,\lambda h\,|^4) \text{ for 3 corrector}$$

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

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

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

have been solved with the help of the Adams P-C set of various orders with $P(EC)^m E$, $m = 1\ (1)\ 5$. We denote the order of the predictor and corrector used by an ordered pair (p, q). The computation has been performed in double precision with step size $h = 2^{-4}$ and the error values $\epsilon_n = y_n^{(m)} - y(t_n)$ at $t = 5$ are listed in Table 3.11. We have examined the three possibilities $p > q$, $p = q$ and $p < q$. From Table 3.11, we find that the effect of the predictor formula after three or four iterations is negligible.

TABLE 3.11 COMPARISON OF ERRORS IN ADAMS-BASHFORTH PREDICTOR AND ADAMS-MOULTON CORRECTOR, $P(EC)^m E$

$y' = -y,\ y(0) = 1,\ t = 5,\ h = 2^{-4}$

m	(3, 2)	(3, 3)	(3, 4)	(4, 3)	(4, 4)	(4, 5)
1	−11169−09	56994−11	19130−11	34699−11	−26785−12	−11518−12
2	−10675−09	33584−11	−18824−12	33730−11	−13408−12	89731−14
3	−10691−09	34209−11	−13784−12	33756−11	−13729−12	62092−14
4	−10690−09	34193−11	−13902−12	33755−11	−13721−12	62694−14
5	−10690−09	34193−11	−13899−12	33755−11	−13721−12	62680−14

$y' = -y^2,\ y(0) = 1,\ t = 5,\ h = 2^{-4}$

m	(3, 2)	(3, 3)	(3, 4)	(4, 3)	(4, 4)	(4, 5)
1	−39539−09	52925−10	18766−10	22259−10	−78314−11	−36091−11
2	−39198−09	26893−10	−45802−11	24846−10	−30840−11	79417−12
3	−39200−09	27830−10	−38274−11	24747−10	−32382−11	66148−12
4	−39200−09	27795−10	−38521−11	24751−10	−32332−11	66549−12
5	−39200−09	27795−10	−38513−11	24751−10	−32334−11	66537−12

$y' = -t(y+y^2),\ y(0) = 1,\ t = 5,\ h = 2^{-4}$

m	(3, 2)	(3, 3)	(3, 4)	(4, 3)	(4, 4)	(4, 5)
1	−69798−12	35994−12	23964−11	17339−11	69797−11	32172−11
2	−74566−12	44979−13	−40044−13	85001−13	−44197−14	70790−14
3	−73650−12	85597−13	−79129−14	80872−13	−11619−13	95071−15
4	−73791−12	80909−13	−11259−13	81368−13	−10853−13	15573−14
5	−73769−12	81464−13	−10903−13	81307−13	−10936−13	14964−14

3.6.4 Modified predictor-corrector methods

Here the values of the dependent variables obtained from one application of the corrector formula are regarded as the final values. The predicted and corrected values are compared to obtain an estimate of the truncation error associated with the integration step. The corrected values are accepted if this error estimate does not exceed a specified maximum value. Otherwise, the corrected values are rejected and the interval of integration is reduced starting from the last accepted point. Likewise, if the error estimate becomes unnecessarily small, the interval of integration may be increased. In this procedure, only two derivative evaluations are required per integration step. Furthermore, we can use the estimates of the truncation error to modify the predicted and corrected values.

Let us consider the k-step $P-C$ set

$$\text{Predictor :} \quad y_{n+1}^{(P)} = \sum_{i=1}^{k} (a_i^{(0)} y_{n-i+1} + h\, b_i^{(0)} y'_{n-i+1}) \tag{3.75}$$

$$\text{Corrector :} \quad y_{n+1}^{(C)} = \sum_{i=1}^{k-1} (a_i y_{n-i+1} + h\, b_i y'_{n-i+1}) + h\, b_0 y'_{n+1} \tag{3.76}$$

where the local truncation error term of predictor and corrector are

$$C^*_{p+1} h^{p+1} y^{(p+1)}(t_n) + 0(h^{p+2}) \text{ and } C_{p+1} h^{p+1} y^{(p+1)}(t_n) + 0(h^{p+2})$$

To obtain the estimate of the truncation error associated with each step, we examine the error equation. The exact value of $y(t)$ satisfies the following equations

$$y(t_{n+1}) = \sum_{i=1}^{k} (a_i^{(0)} y(t_{n-i+1}) + h\, b_i^{(0)} y'(t_{n-i+1}))$$
$$+ C^*_{p+1} h^{p+1} y^{(p+1)}(t_n) + 0(h^{p+2}) \tag{3.77}$$

$$y(t_{n+1}) = \sum_{i=1}^{k-1} (a_i\, y(t_{n-i+1}) + h\, b_i\, y'(t_{n-i+1}))$$
$$+ h\, b_0\, y'(t_{n+1}) + C_{p+1} h^{(p+1)} y^{p+1}(t_n) + 0(h^{p+2}) \tag{3.78}$$

Substituting $y_n = y(t_n) + \epsilon_n$ in (3.75) and (3.76), we get

$$y_{n+1}^{(P)} = \sum_{i=1}^{k} (a_i^{(0)} y(t_{n-i+1}) + h\, b_i^{(0)} y'(t_{n-i+1}))$$
$$+ \sum_{i=1}^{k} (a_i^{(0)} \epsilon_{n-i+1} + h\, b_i^{(0)} \epsilon'_{n-i+1})$$

$$y_{n+1}^{(C)} = \sum_{i=1}^{k-1} (a_i\, y(t_{n-i+1}) + h\, b_i\, y'(t_{n-i+1})) + h\, b_0\, y'(t_{n+1})$$
$$+ \sum_{i=1}^{k-1} (a_i \epsilon_{n-i+1} + h\, b_i \epsilon'_{n-i+1}) + h\, b_0 \epsilon'_{n+1}$$

Using (3.77) and (3.78), we obtain

$$y_{n+1}^{(P)} = y(t_{n+1}) - C^*_{p+1} h^{p+1} y^{(p+1)}(t_n) + 0(h^{p+2})$$
$$+ \sum_{i=1}^{k} (a_i^{(0)} \epsilon_{n-i+1} + h\, b_i^{(0)} \epsilon'_{n-i+1}) \tag{3.79}$$

$$y_{n+1}^{(C)} = y(t_{n+1}) - C_{p+1} h^{p+1} y^{(p+1)}(t_n) + 0(h^{p+2})$$
$$+ \sum_{i=1}^{k-1} (a_i \epsilon_{n-i+1} + h\, b_i \epsilon'_{n-i+1}) + h\, b_0 \epsilon'_{n+1} \tag{3.80}$$

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

$$y_{n+1}^{(P)} - y_{n+1}^{(C)} = (C_{p+1} - C_{p+1}^{*})\, h^{p+1}\, y^{(p+1)}(t_n) + 0\,(h^{p+2}) \tag{3.81}$$

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

$$C_{p+1}^{*}\, h^{p+1}\, y^{(p+1)}(t_n) + 0\,(h^{p+2})$$
$$= C_{p+1}^{*}\,(C_{p+1} - C_{p+1}^{*})^{-1}\,(y_{n+1}^{(P)} - y_{n+1}^{(C)})$$

and
$$C_{p+1}\, h^{p+1}\, y^{(p+1)}(t_n) + 0\,(h^{p+2})$$
$$= C_{p+1}\,(C_{p+1} - C_{p+1}^{*})^{-1}(y_{n+1}^{(P)} - y_{n+1}^{(C)})$$

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 :

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

The Runge-Kutta method may be used to calculate the starting values, i.e. $y_1, y_2, \ldots, y_n$. 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

$$\begin{vmatrix} \xi^{k'} & -\xi^{k'}+(\rho^{(0)}(\xi) - h\lambda\sigma^{(0)}(\xi)) & 0 & 0 \\ \xi+\dfrac{C^*_{p+1}}{C_{p+1}-C^*_{p+1}} & 0 & -\xi & -\dfrac{C^*_{p+1}}{C_{p+1}-C^*_{p+1}} \\ 0 & \xi^k-(\rho(\xi)-h\lambda\sigma(\xi)) - h\lambda b_0\xi^k & h\lambda b_0\xi^k & -\xi^k \\ \dfrac{C_{p+1}}{C_{p+1}-C^*_{p+1}} & -1 & 0 & -\dfrac{C^*_{p+1}}{C_{p+1}-C^*_{p+1}} \end{vmatrix} = 0 \tag{3.83}$$

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

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

and

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

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 $y' = \lambda y$, $y(0) = 1$, $\bar{h} \leqslant 0$. 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 stable as $\theta \to -0$. We, therefore, wish to find the value θ^M of θ in $(-1, 0)$, if any, at which the method violates absolute stability : $(\theta^M, 0)$ is then the range of absolute stability.

Using the transformation $\xi = (1+z)/(1-z)$ in (3.85), we get

$$\sum_{i=0}^{k+2} v_i z^{k+2-i} = 0 \tag{3.87}$$

where

$$\begin{aligned} v_0 &= c_0 - c_1 + c_2 \cdots + (-1)^{k+2} c_{k+2}, \\ v_1 &= [k+2]\, c_0 + [1-(k+1)]\, c_1 + (-2+k)\, c_2 + \\ &\vdots \qquad\qquad \cdots + (-1)^{k+1} (k+2)\, c_{k+2} \\ v_{k+2} &= c_0 + c_1 + \cdots + c_{k+2}. \end{aligned}$$

Substituting the values of $c_0, c_1, \cdots, c_{k+2}$ from (3.86), we get

$$v_0 = 2(1-R) + 4\theta + \frac{\theta}{b_0}[-\tau + (2\theta - R)\,\tau^*]$$

$$v_{k+2} = \frac{\theta}{b_0}(R-1)$$

where

$$\begin{aligned} \tau &= b_0 - b_1 + b_2 - \ldots + (-1)^k b_k \\ \tau^* &= b_1^{(0)} - b_2^{(0)} + b_3^{(0)} - \ldots + (-1)^k b_{k+1}^{(0)} \end{aligned}$$

The roots of the polynomial equation (3.87) for a stable method will lie in the left half-plane. For (3.87) to have all its roots in the left half-plane or on the imaginary axis, it is necessary that the *Routh-Hurwitz* criterion is satisfied.

Here, we find that v_0 and v_{k+2} are always positive in $-1 < \theta \leqslant 0$ and one or more of the remaining v_i may not satisfy this condition. In such cases we find θ^M by satisfying Theorem 1.2. Then $(\theta^M, 0)$ is the required interval of absolute stability for modified predictor-corrector methods.

For example, for $k = 1$, the $P-C$ set is given by

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

$$\text{C}: y_{n+1} = y_n + \frac{h}{2}(y'_{n+1} + y'_n)$$

The modified predictor-corrector scheme becomes

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

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

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

$$y_{n+1} = c_{n+1} + \frac{1}{6}(p_{n+1} - c_{n+1})$$

The characteristic equation (3.85) simplifies to

$$\frac{6}{5}\xi^3-\frac{1}{5}(6+18\theta+15\theta^2)\xi^2+\left(\frac{6}{5}\theta+4\theta^2\right)\xi-\theta^2=0$$

The coefficients of the transformed equation (3.87) become

$$v_0=\frac{4}{5}(3+6\theta+10\theta^2)$$

$$v_1=\frac{4}{5}(6+3\theta-5\theta^2)$$

$$v_2=\frac{4}{5}(3-6\theta-5\theta^2)$$

$$v_3=-\frac{12}{5}\theta$$

The Routh-Hurwitz criterion gives

$$u(\theta)=v_1v_2-v_0v_3>0$$

Substituting the values of v_i and equating $u(\theta)$ to zero, we get

$$\theta^M=-0.6884$$

It is obvious that for $\theta=-0.6884$ we have

$$v_i>0,\ i=0(1)3$$

Thus the second order modified Adams predictor-corrector method is absolutely stable in the interval $(-0.6884, 0)$. The value of θ^M in the interval $(-1, 0)$ for other methods is given below :

k	1	2	3	4
θ^M	-0.6884	-0.4337	-0.3005	-0.2145

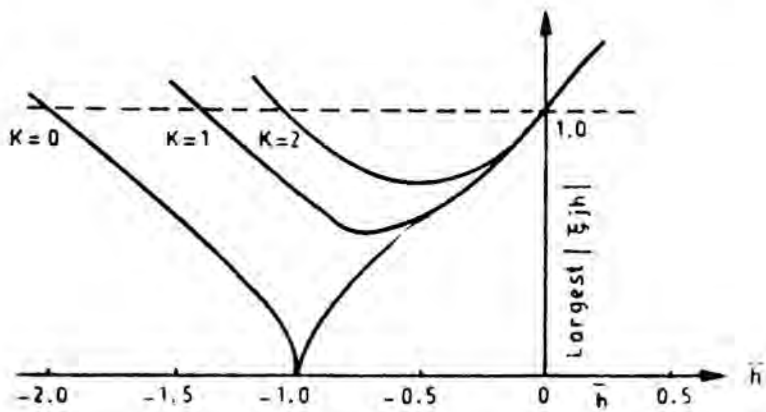


Fig. 3.9 Dominant root in modified Adams predictor-corrector methods

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

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

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

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

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

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

The exact values are

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

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

For $n = 1$

$$p_2 = y_1+\frac{h}{2}(3y'_1-y'_0)$$

$$= 1.11034184+\frac{.1}{2}(3\times 1.21034184-1)$$

$$= 1.241893116$$

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

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

$$m_2 = p_2 = 1.241893116$$

$$m'_2 = t_2+m_2 = .2+1.241893116$$

$$= 1.441893116$$

$$c_2 = y_1+\frac{h}{2}(m'_2+y'_1)$$

$$= 1.11034184+\frac{.1}{2}(1.441893116+1.21034184)$$

$$= 1.2429535878$$

$$p_2 - c_2 = 1.241893116 - 1.2429535878$$

$$= -0.0010604718$$

$$y_2 = c_2 + \frac{1}{6}(p_2 - c_2)$$

$$= 1.2429535878 - \frac{1}{6}(0.0010604718)$$

$$= 1.2427768425$$

For $n=2$

$$p_3 = y_2 + \frac{h}{2}(3y_2' - y_1')$$

$$= 1.2427768425 + \frac{.1}{2}(4.3283305275 - 1.21034184)$$

$$= 1.398676276875$$

$$m_3 = p_3 - \frac{5}{6}(p_2 - c_2)$$

$$= 1.398676276875 - \frac{5}{6}(-0.0010604718)$$

$$= 1.399560003375$$

$$m_3' = t_3 + m_3$$

$$= .3 + 1.399560003375$$

$$= 1.699560003375$$

$$c_3 = y_2 + \frac{h}{2}(m_3' + y_2')$$

$$= 1.2427768425 + \frac{.1}{2}(1.699560003375 + 1.4427768425)$$

$$= 1.39989368479375$$

$$p_3 - c_3 = 1.398676276875 - 1.39989368479375$$

$$= -0.00121740791875$$

$$y_3 = c_3 + \frac{1}{6}(p_3 - c_3)$$

$$= 1.39989368479375 + \frac{1}{6}(-0.0012740791875)$$

$$= 1.39969078347396$$

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 $k \leqslant 6$. 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

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

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

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

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

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

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

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

$$y(t_{n+1}) - \sum_{j=1}^{k} a_j\, y(t_{n-j+1}) - h \sum_{j=0}^{k} b_j\, f(t_{n-j+1}, y(t_{n-j+1}))$$

$$- h \sum_{j=1}^{v} c_j\, f(t_{n-\theta j+1}, y(t_{n-\theta j+1}))$$

$$= \frac{1}{(p+1)!}\, C_{p+1}\, h^{p+1}\, y^{(p+1)}_{(t_n)} + 0\,(h^{p+2}) \tag{3.90}$$

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

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

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

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

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:

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

The principal term of the truncation error is given by

$$\frac{1}{4!}\, C_4 h^4 y^{(4)}_{(t_n)} + 0\,(h^5)$$

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

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

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

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

and C_4 is given by

$$C_4 = -\frac{(1-6b_1)}{9\,(1-2b_1)} = C$$

To find the suitable values of b_1, we plot C as a function of b_1 in Figure 3.10.

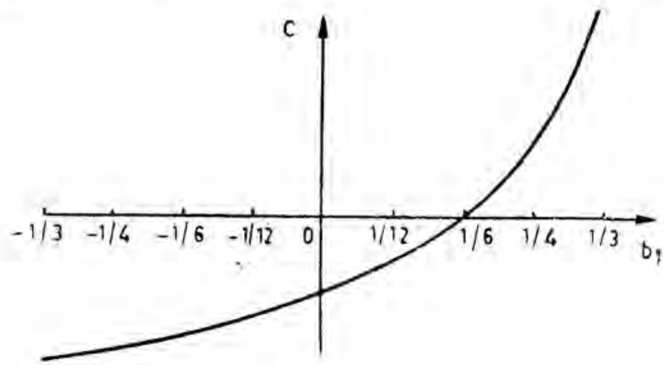


Fig. 3.10 Truncation error coefficient versus arbitrary parameter

We consider the following cases:

(i) $b_1 = 0;\ a_1 = 1,\ b_0 = \frac{1}{4},\ c_1 = \frac{3}{4},\ \theta_1 = \frac{2}{3},\ C_4 = -\frac{1}{9}$

$$y_{n+1} = y_n + \frac{h}{4}\,(f_{n+1} + 3f_{n+1/3})$$

(ii) $b_1 = \frac{1}{4};\ a_1 = 1,\ b_0 = 0,\ c_1 = \frac{3}{4},\ \theta_1 = \frac{1}{3},\ C_4 = \frac{1}{9}$

$$y_{n+1} = y_n + \frac{h}{4}\,(f_n + 3f_{n+2/3})$$

(iii) $b_1 = \frac{1}{6};\ a_1 = 1,\ b_0 = \frac{1}{6},\ c_1 = \frac{2}{3},\ \theta_1 = \frac{1}{2},\ C_4 = 0$

$$y_{n+1} = y_n + \frac{h}{6}\,(f_{n+1} + 4f_{n+1/2} + f_n)$$

This is an implicit one step hybrid method of order 4 and in fact it is Milne-Simpson's method compressed to one step.

3.7.2 Two step hybrid methods

Using $k = 2$ into (3.91), we obtain

$$y_{n+1} = a_1 y_n + a_2 y_{n-1} + h\,(b_0 f_{n+1} + b_1 f_n + b_2 f_{n-1}) + hc_1 f_{n-\theta_1+1} \qquad (3.94)$$

where a_1, a_2 b_0, b_1, b_2, c_1 and θ_1 are seven arbitrary parameters and $0 < \theta_1 < 1$.

Thus we hope to get a two step hybrid method of order six. Expanding as before we have the following equations :

$$
\begin{aligned}
a_1+a_2 &= 1\\
-a_2+b_0+b_1+b_2+c_1 &= 1\\
a_2+2b_0-2b_2+2\,(1-\theta_1)\,c_1 &= 1\\
-a_2+3b_0+3b_2+3\,(1-\theta_1)^2\,c_1 &= 1\\
a_2+4b_0-4b_2+4\,(1-\theta_1)^3\,c_1 &= 1\\
-a_2+5b_0+5b_2+5\,(1-\theta_1)^4\,c_1 &= 1\\
a_2+6b_0-6b_2+6\,(1-\theta_1)^5\,c_1 &= 1
\end{aligned}
\tag{3.95}
$$

The principal term of the truncation error is given by

$$
(1+a_2-7b_0-7b_2-7\,(1-\theta_1)^6\,c_1)\,\frac{h^7}{7!}\,y^{(7)}_{(t_n)}+0\,(h^8) \tag{3.96}
$$

Putting $b_1 = b_2 = 0$ and solving the first five equations in (3.95) and choosing the value of θ_1 in (0, 1), we get

$$
a_1 = \frac{-12+44\sqrt{17}}{63+25\sqrt{17}} \qquad a_2 = \frac{75-19\sqrt{17}}{63+25\sqrt{17}}
$$

$$
b_0 = \frac{10+6\sqrt{17}}{63+25\sqrt{17}} \qquad c_1 = \frac{128}{63+12\sqrt{17}}
$$

$$
\theta_1 = \frac{9-\sqrt{17}}{8}
$$

and the method so obtained is of fourth order.

For $a_2 = b_2 = 0$, we have a fourth order method which is Milne-Simpson's method compressed to one step.

The values $b_0 = a_2 = 0$ give the following explicit hybrid method of order 4

$$
y_{n+1} = y_n + \frac{h}{714}\,(221\,f_n - 7\,f_{n-1} + 500\,f_{n+7/10})
$$

In order to get the meth of order 5, we solve the first six equations in (3.95) in terms of one arbitrary parameter say $\theta_1 \neq 0$, 1 or 2 and obtain

$$
a_1 = \frac{16}{23-15\,\theta_1},\; a_2 = \frac{7-15\,\theta_1}{23-15\,\theta_1},\; b_0 = \frac{9\,\theta_1-5\,\theta_1^2-2}{\theta_1\,(23-15\,\theta_1)}
$$

$$
b_1 = \frac{20\,\theta_1^2-40\theta_1+16}{(1-\theta_1)(23-15\,\theta_1)},\; b_2 = \frac{4-11\,\theta_1+5\,\theta_1^2}{(2-\theta_1)(23-15\,\theta_1)}
$$

$$
c_1 = \frac{4}{\theta_1(1-\theta_1)\,(2-\theta_1)\,(23-15\,\theta_1)},\; \theta_1 \neq \frac{23}{15} \tag{3.97}
$$

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

$$\frac{h^6}{6!}\frac{(16-48\,\theta_1+24\,\theta_1^2)}{(23-15\,\theta_1)}\,y^{(6)}_{(t_n)}+0\,(h^7) \tag{3.98}$$

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:

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

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

$$-8\sqrt{3}/[9(8+5\sqrt{3})]\frac{h^7}{7!}\,y^{(7)}_{(t_n)}+0\,(h^8)$$

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

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

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 $P^{(\theta)}$ 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}.

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

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

$$P^{(H)} : y_{n+1} = \sum_{j=1}^{k} a_j\, y_{n-j+1} + h \sum_{j=1}^{k} b_j\, f_{n-j+1} + h\, c_1\, f_{n-\theta_1+1}$$

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

The above sequence of operations may be called $P^{(\theta)}\, E\, P^{(H)}\, E$ mode. If we use the implicit hybrid method (3.100) to find y_{n+1}, then in addition to the predictor $P^{(\theta)}$, 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) $$P^{(\theta)}\, E\, P^{(k)}\, E\, C^{(H)}\, E \tag{3.102}$$

(ii) $$P^{(\theta)}\, E\, P^{(H)}\, E\, C^{(H)}\, E \tag{3.103}$$

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 $P^{(\theta)} - P^{(H)}$ schemes

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

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

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

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

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

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

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

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

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

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

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

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

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

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

to $y = \lambda y$ and obtain for $P^{(\theta)}\ E\ P^{(H)}\ E\ C^{(H)}\ E$ mode the following characteristic equation

$$y_{n+1} = \left(1+\lambda h+ \frac{(\lambda h)^2}{2}+\frac{(\lambda h)^3}{6}\right) y_n \tag{3.107}$$

Thus $P^{(\theta)}\ E\ P^{(H)}\ E\ C^{(H)}\ E$ is of order three and it is stable for

$$-2.5 < \lambda h < 0$$

Finally, we discuss the stability and accuracy of the following scheme:

$$\begin{aligned} P^{(\theta)} &: y_{n+1/2} = -\frac{45}{64}y_n+\frac{25}{16}y_{n-1}+\frac{9}{64}y_{n-2} \\ &\qquad + h\left(\frac{90}{64}f_n+\frac{15}{16}f_{n-1}\right) \\ P^{(k)} &: \bar{y}_{n+1} = -9y_n+9y_{n-1}+y_{n-2}+h\,(6f_n+6f_{n-1}) \\ C^{(H)} &: y_{n+1} = y_n+\frac{h}{6}\,(\bar{f}_{n+1}+4f_{n+1/2}+f_n) \end{aligned} \tag{3.108}$$

Applying (3.108) to $y' = \lambda y$, we obtain the characteristic equation for $P^{(\theta)}\ E\ P^{(k)}\ E\ C^{(H)}\ E$ mode as

$$\begin{aligned} &96\xi^3-(96-173\lambda h+186\lambda^2h^2)\xi^2 \\ &\quad -(244\lambda h+156\lambda^2h^2)\,\xi-25\lambda h = 0 \end{aligned} \tag{3.109}$$

Substituting $\xi = (1+z)/(1-z)$ and simplifying, we get

$$\begin{aligned} &(192-392\lambda h+30\lambda^2h^2)z^3+(384-4\lambda h+342\lambda^2h^2)z^2 \\ &\quad +(192+492\lambda h-30\lambda^2h^2)z-\lambda h(96+342\lambda h) = 0 \end{aligned} \tag{3.110}$$

The Routh-Hurwitz criterion is satisfied if $-.28 < \lambda h < 0$. Thus the stability interval for $P^{(\theta)}\ E\ P^{(k)}\ E\ C^{(H)}\ E$ is given by $-.28 < \lambda h < 0$.

In order to find the odrer of the scheme (3.108), we determine the truncation error. Let us denote the local truncation errors of $P^{(\theta)}$, $P^{(k)}$ and $C^{(H)}$ by $T^{(\theta)}$, $T^{(k)}$ and $T^{(H)}$, repectively.

The exact value $y(t)$ will satisfy

$$\begin{aligned} y\,(t_{n+1/2}) &= -\frac{45}{64}\,y\,(t_n)+\frac{25}{16}\,y\,(t_{n-1})+\frac{9}{64}\,y\,(t_{n-2}) \\ &\quad + h\left(\frac{90}{64}\,y\,(t_n,\,y\,(t_n))+\frac{15}{16}\,f\,(t_{n-1},\,y\,(t_{n-1}))\right)+T^{(\theta)} \\ \bar{y}\,(t_{n+1}) &= -\,9y\,(t_n)+9y\,(t_{n-1})+y\,(t_{n-2}) \\ &\quad +h\,(6f\,(t_n,\,y\,(t_n))+6f\,(t_{n-1},\,y\,(t_{n-1})))+T^{(k)} \end{aligned}$$

and
$$\begin{aligned} y\,(t_{n+1}) &= y\,(t_n)+\frac{h}{6}\,(\bar{f}\,(t_{n+1},\,\bar{y}\,(t_{n+1})) \\ &\quad +4f\,(t_{n+1/2},\,y\,(t_{n+1/2}))+f\,(t_n,\,y\,(t_n)))+T^{(H)} \end{aligned} \tag{3.111}$$

Assuming the values $y(t_{n-j}) = y_{n-j}$, $j = 0, 1, 2$, and subtracting the equations of (3.108) from the corresponding equations of (3.111) we obtain the following errors :

$$y(t_{n+1/2}) - y_{n+1/2} = T^{(\theta)}$$
$$\bar{y}(t_{n+1}) - \bar{y}_{n+1} = T^{(k)}$$

and $y(t_{n+1}) - y_{n+1} = \frac{h}{6}[\bar{f}(t_{n+1}, \bar{y}(t_{n+1})) - \bar{f}(t_{n+1}, \bar{y}_{n+1}) + 4f(t_{n+1/2}, y(t_{n+1/2}))$

$$-4f(t_{n+1/2}, y_{n+1/2})] + T^{(H)} \tag{3.112}$$

To simplify the last equation in (3.112), we use the mean value theorem and obtain

$$y(t_{n+1}) - y_{n+1} = T^{(H)} + \frac{h}{6}\left[T^{(k)}\frac{\partial f(t_{n+1}, \eta_1)}{\partial y} + 4T^{(\theta)}\frac{\partial f(t_{n+1/2}, \eta_2)}{\partial y}\right] \tag{3.113}$$

where η_1 and η_2 lie between $\bar{y}(t_{n+1})$ and y_{n+1} and $y(t_{n+1/2})$ and $y_{n+1/2}$ respectively.

We now assume that $\partial f(t,y)/\partial y$ does not vary widely in the neighbourhood of (t_{n+1}, η_1) and $(t_{n+1/2}, \eta_2)$, and we approximate it with a constant λ. Then (3.113) is approximated by the formula

$$y(t_{n+1}) - y_{n+1} = T^{(H)} + \frac{\lambda h}{6}(T^{(k)} + 4T^{(\theta)}) \tag{3.114}$$

The values of the local truncation errors are given by

$$T^{(\theta)} = \frac{3}{256}\, h^5\, y^{(5)}(t_n) + 0\,(h^6)$$

$$T^{(k)} = -\frac{1}{20}\, h^5\, y^{(5)}(t_n) + 0\,(h^6)$$

$$T^{(H)} = -\frac{1}{2880}\, h^5\, y^{(5)}(t_n) + 0\,(h^6) \tag{3.115}$$

Substituting from (3.115) into (3.114) we obtain the local truncation error of the formula (3.108) as

$$y(t_{n+1}) - y_{n+1} = -\frac{1}{5760}(2 + 3\lambda h)\, h^5\, y^{(5)}(t_n) + 0(h^6) \tag{3.116}$$

which shows that the mode $P^{(\theta)}\, E\, P^{(k)}\, E\, C^{(H)}\, E$ is of order 5. Furthermore, we also observe that the local truncation error of the predictors will not influence the truncation error of the hybrid corrector as $|\lambda h| < 2/3$ always in this case for reasons of stability.

3.8 HIGHER ORDER DIFFERENTIAL EQUATIONS

The multistep methods discussed previously for the first order initial value problem can easily be applied to obtain the numerical solution of an mth order initial value problem if we replace the mth order equation by an 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

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

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

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

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

Symbolically, we can write (3.118) in the form

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

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

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

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

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

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

$$\rho(1) = 0, \; \rho'(1) = 0, \; \rho''(1) = 2\sigma(1) \tag{3.122}$$

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

$$\rho(\xi)-(\log \xi)^2\sigma(\xi) = C_{p+2}(\xi-1)^{p+2}+0((\xi-1)^{p+3}) \tag{3.123}$$

$$\frac{\rho(\xi)}{(\log \xi)^2}-\sigma(\xi) = C_{p+2}(\xi-1)^{p}+0((\xi-1)^{p+1}) \tag{3.124}$$

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 $\leqslant k$, 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

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

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 $-1 < \lambda \leqslant 1$, find $\sigma(\xi)$.
From equation (3.124), we get

$$\frac{\rho(\xi)}{(\log \xi)^2} = \frac{(\xi-1)^2[(\xi-1)^2+2(\xi-1)+1+\lambda]}{[\log(1+(\xi-1))]^2}$$

$$\begin{aligned}\sigma(\xi) = {} & 1+\lambda+(3+\lambda)(\xi-1)+(4+\lambda)(\xi-1)^2 \\ & + \frac{7}{6}(\xi-1)^3+\frac{1}{240}(19-\lambda)^2(\xi-1)^4 \\ & + \frac{1}{240}(-1+\lambda)(\xi-1)^5+0((\xi-1)^6)\end{aligned}$$

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	$\frac{180}{812}$	$\frac{3132}{812}$	$-\frac{5265}{812}$	$\frac{5080}{812}$	$-\frac{2970}{812}$	$\frac{972}{812}$	$-\frac{137}{812}$

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

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

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

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

and it is called relatively stable if

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

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

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

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

$$a_1 = 2, a_2 = -1, b_2 = 1 - b_0 - b_1 \tag{3.130}$$

second order when, in addition,

$$b_0 - b_2 = 0 \tag{3.131}$$

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

$$b_0 + b_2 = \frac{1}{6} \tag{3.132}$$

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

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

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

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

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

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

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 $b_1 = \dfrac{1}{2}$, 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 $b_1 = \dfrac{2}{3}$ 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 $b_1 = \dfrac{5}{6}$, 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

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

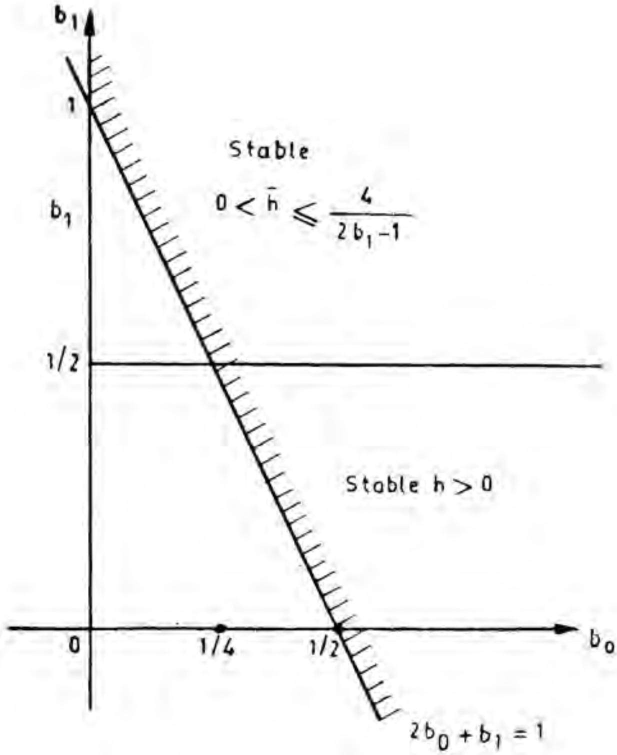


Fig. 3.11 Stability boundaries in the (b_0, b_1) plane

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

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

For $h = .2$, we get

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

We obtain,

for $n = 1$;

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

$$y_2 = 1.9973334-1+\frac{(.2)^2}{12}(-.4y_2-1.9973334)$$

$$y_2 = .9893564$$

for $n = 2$;

$$y_3 = 2y_2-y_1+\frac{h^2}{12}(y_3''+10y_2''+y_1'')$$

$$y_3 = 1.9787128-.9986667$$

$$+\frac{(.2)^2}{12}(-.6y_3-9.893564-.1997333)$$

$$y_3 = .9642605$$

3.8.1 Hybrid methods

A general two-step hybrid method with one off-step point for the numerical solution of (3.117) may be written as

$$y_{n+1}-2y_n+y_{n-1} = h^2\Big[\frac{25r^2-3}{30r^2}y_n'' + \frac{2-5r^2}{60(1-3r^2)}(y_{n+1}''+y_{n-1}'') + \frac{1}{20r^2(1-r^2)}(y_{n-r}''+y_{n+r}'')\Big] \tag{3.140}$$

with truncation error

$$T_n = \frac{42r^2-13}{302400}h^8 y^{(8)}_{(\xi)}, \xi\in(t_{n-1}, t_{n+1}) \tag{3.141}$$

where r is a parameter which fixes the position of the off-step point. The method (3.140) has order six for arbitrary r. We may choose r to minimize the function evaluations in the method (3.140). We have

$$y_{n+1}-2y_n+y_{n-1} = h^2\Big[\frac{7}{12}y_n''+\frac{5}{24}(y_{n-r}''+y_{n+r}'')\Big], r^2=\frac{2}{5} \tag{3.142}$$

and

$$y_{n+1}-2y_n+y_{n-1} = h^2\Big[\frac{7}{264}(y_{n+1}''+y_{n-1}'') + \frac{125}{264}(y_{n-r}''+y_{n+r}'')\Big], r^2=\frac{3}{25} \tag{3.143}$$

The hybrid methods will be of computational value, if the value of $y(t)$ at the off-step points can be determined. If we use the approximation of $0(h^4)$ to $y(t)$ at the off-step points, then we obtain

$$\begin{aligned} y_{n-r} &= \frac{1}{2}(1-\alpha+r)y_{n+1}+\alpha y_n+\frac{1}{2}(1-\alpha-r)y_{n-1} \\ &\quad +\frac{h^2}{12}[(3\alpha-3-r+3r^2+r^3)y''_{n+1} \\ &\quad +(3\alpha-3+r+3r^2-r^3)y''_{n-1}] \\ y_{n-r} &= \frac{1}{2}(1-\alpha-r)y_{n+1}+\alpha y_n+\frac{1}{2}(1-\alpha+r)y_{n-1} \\ &\quad +\frac{h^2}{12}[(3\alpha-3+r+3r^2-r^3)y''_{n+1} \\ &\quad +(3\alpha-3-r+3r^2+r^3)y''_{n-1}] \end{aligned} \tag{3.144}$$

where α is an arbitrary parameter. In order to determine α we examine the stability of the method (3.142). Applying the method to the test equation $y'' = -\lambda y, \lambda>0$ and using (3.144) to simplify the resulting equation we get

$$Ay_{n+1}-2By_n+Ay_{n-1} = 0 \tag{3.145}$$

where

$$\begin{aligned} A &= 1+\frac{5\bar{h}}{24}(1-\alpha)+\frac{\bar{h}^2}{240}(3-5\alpha) \\ B &= 1-\frac{\bar{h}}{24}(7+5\alpha) \\ \bar{h} &= \lambda h^2 \end{aligned}$$

We find that the roots of (3.145) are complex and of unit modulus if and only if $\alpha \leqslant -\frac{1}{5}$. Thus, the method (3.142) with (3.144) is P-stable for $\alpha \leqslant -\frac{1}{5}$. Similarly, it can be shown that the method (3.143) is P-stable for $\alpha \leqslant 0$.

3.8.2 Obrechkoff methods

We discuss two-step fourth order Obrechkoff method of the form

$$\begin{aligned} y_{n+1}-2y_n+y_{n-1} &= h^2[\beta_1(y''_{n+1}+y''_{n-1})+(1-2\beta_1)y''_n] \\ &\quad +h^4\left[\frac{1}{2}\left(\frac{1}{12}-\beta_1-\beta_2\right)(y^{(iv)}_{n+1}+y^{(iv)}_{n-1})+\beta_2 y^{(iv)}_n\right] \end{aligned} \tag{3.146}$$

with the truncation error

$$T_n = \frac{1}{360}(150\beta_1+180\beta_2-14)\,h^6 y^{(vi)}_{(\xi_1)},\ \xi_1\in(t_{n-1}, t_{n+1}) \tag{3.147}$$

where β_1 and β_2 are arbitrary parameters.

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

$$A = 1 + \beta_1 \bar{h} - \frac{1}{2}\left(\frac{1}{12} - \beta_1 - \beta_2\right)\bar{h}^2$$

$$B = 1 - \left(\frac{1}{2} - \beta_1\right)\bar{h} + \frac{1}{2}\beta_2\, \bar{h}^2 \tag{3.149}$$

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

$$\text{(i) } \beta_2 + \frac{3}{4}\beta_1 - \frac{1}{2}\beta_1^2 - \frac{7}{96} \geqslant 0$$

$$\text{(ii) } \beta_1 \geqslant \frac{1}{12} \tag{3.151}$$

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

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

with the minimum truncation error

$$T_n = \frac{1}{360} h^6 y^{(iv)}_{(t_1)}$$

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

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

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

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

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 $y(t) = e^{iwt}$, $w = \dfrac{2\sigma}{h}$, 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:

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

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

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

is the exact solution.

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

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

$$y''+y+y^3 = B\cos \Omega\, t \tag{3.163}$$

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

$$\begin{aligned} y(t) = {} & A_1 \cos\ \Omega t+A_3 \cos 3\,\Omega t+A_5 \cos 5\,\Omega t \\ & +A_7 \cos 7\,\Omega t+A_9 \cos 9\,\Omega t \end{aligned}$$

where

$$\begin{aligned} A_1 &= 0.200179477536 \\ A_3 &= 0.000246946143 \\ A_5 &= 0.000000304014 \\ A_7 &= 0.000000000374 \\ A_9 &= 0.000000000000 \end{aligned}$$

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 step-lengths, 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

3.9 NON-UNIFORM STEP METHODS

The numerical methods with variable or non-uniform steps are useful fo solving differential equations related to the stiff system. Here, the step sizes are adjusted suitably to compute the numerical solution economically. We now give numerical methods with variable steps which for uniform steps reduce to the methods already obtained in Sections 3.2-3.3.

Let $\{h_j\}$, $h_j = x_j - x_{j-1}$, be a sequence of step sizes such that

$$\sum_{j=1}^{N} h_j = b - t_0 \text{ and } h^* = \max\{h_j\} \text{ with } h^*N = \sigma^*.$$

The notation $\{h_j\} \to 0$ signifies that each element of the sequence goes to zero so that quotient of successive step sizes h_{j+1}/h_j still has upper and lower limits, i.e. $\alpha < h_{j+1}/h_j < \beta$, $j = 1, 2, \ldots, N-1$ and $\lim\limits_{N\to\infty} (h^*N) = \sigma^*$, a constant.

3.9.1 Adams-Bashforth methods

Integrating the differential equation $y' = f(t, y)$ between the limits t_n and t_{n+1}, we obtain

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t, y)\, dt \tag{3.164}$$

To get the explicit methods as in Section 3.2, we replace $f(t, y)$ by a polynomial which interpolates $f(t, y)$ at k points $t_n, t_{n-1}, \ldots, t_{n-k+1}$. Since the nodal points are nonuniformly spaced, we use either the Newton divided-difference or the Lagrange interpolation polynomial of degree $(k-1)$ for this purpose. We have

$$\begin{aligned} P_{k-1}(t) &= f_n + (t-t_n) f[t_n, t_{n-1}] \\ &\quad + (t-t_n)(t-t_{n-1}) f[t_n, t_{n-1}, t_{n-2}] + \cdots \\ &\quad + (t-t_n)(t-t_{n-1}) \ldots (t-t_{n-k+2}) f[t_n, t_{n-1}, \ldots, t_{n-k+1}] \end{aligned} \tag{3.165}$$

where

$$\begin{aligned} &f[t_n, t_{n-1}, \ldots, t_{n-k+1}] \\ &= \frac{1}{(t_n - t_{n-k+1})} (f[t_n, t_{n-1}, \ldots, t_{n-k+2}] - f[t_{n-1}, \ldots, t_{n-k+1}]) \end{aligned}$$

Substituting (3.165) in (3.164) and simplifying we get the linear k-step method. For $k = 2$, we obtain

$$y_{n+1} = y_n + h_{n+1} \left[\left(1 + \frac{1}{2} \frac{h_{n+1}}{h_n} \right) f_n - \frac{1}{2} \frac{h_{n+1}}{h_n} f_{n-1} \right] \tag{3.166}$$

For $k = 3$, we have

$$y_{n+1} = y_n + h_{n+1}\left[\left(1 + \frac{h_{n+1}(2h_{n+1}+6h_n+3h_{n-1})}{6h_n(h_n+h_{n-1})}\right) f_n - \frac{h_{n+1}(2h_{n+1}+3h_n+3h_{n-1})}{6h_nh_{n-1}} f_{n-1} + \frac{h_{n+1}(2h_{n+1}+3h_n)}{6h_{n-1}(h_n+h_{n-1})} f_{n-2}\right] \tag{3.167}$$

Similarly, we may obtain the explicit multistep methods for other values of k.

3.9.2 Adams-Moulton methods

In order to find the implicit multistep methods, we replace $f(t, y)$ by a polynomial of degree k which interpolates $f(t, y)$ at $(k+1)$ points $t_{n+1}, t_n, \dots, t_{n-k+1}$. We use the Newton divided-difference interpolation and write as

$$\begin{aligned} P_k(t) &= f_{n+1} + (t-t_{n+1}) f[t_{n+1}, t_n] + (t-t_{n+1})(t-t_n) f[t_{n+1}, t_n, t_{n-1}] \\ &\quad + (t-t_{n+1})(t-t_n)(t-t_{n-1}) f[t_{n+1}, t_n, t_{n-1}, t_{n-2}] \\ &\quad + \dots + (t-t_{n+1})(t-t_n)\dots(t-t_{n-k+2}) f[t_{n+1}, t_n, \dots, t_{n-k+1}] \end{aligned} \tag{3.168}$$

Substituting (3.168) in (3.164) and simplifying, we obtain the implicit methods. For $k = 1$, we have

$$y_{n+1} = y_n + \frac{h_{n+1}}{2}(f_{n+1} + f_n) \tag{3.169}$$

For $k = 2$, we obtain

$$y_{n+1} = y_n + h_{n+1}\left[\left(\frac{1}{2} - \frac{h_{n+1}}{6(h_{n+1}+h_n)}\right) f_{n+1} + \left(\frac{1}{2} + \frac{h_{n+1}}{6h_n}\right) f_n - \frac{h_{n+1}^2}{6h_n(h_{n+1}+h_n)} f_{n-1}\right] \tag{3.170}$$

For $k = 3$, we get

$$\begin{aligned} y_{n+1} = y_n + h_{n+1}\Bigg[&\left(\frac{1}{2} - \frac{h_{n+1}(3h_{n+1}+4h_n+2h_{n-1})}{12(h_{n+1}+h_n)(h_{n+1}+h_n+h_{n-1})}\right) f_{n+1} \\ &+ \left(\frac{1}{2} + \frac{h_{n+1}(h_{n+1}+4h_n+2h_{n-1})}{12h_n(h_n+h_{n-1})}\right) f_n \\ &- \frac{h_{n+1}^2(h_{n+1}+2h_n+2h_{n-1})}{12h_nh_{n-1}(h_{n+1}+h_n)} f_{n-1} \\ &+ \frac{h_{n+1}^2(h_{n+1}+2h_n)}{12h_{n-1}(h_n+h_{n-1})(h_{n+1}+h_n+h_{n-1})} f_{n-2}\Bigg] \end{aligned} \tag{3.171}$$

Similarly, we may write the implicit multistep methods for other values of k.

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

$$u(t) = -1.499875 \exp(-0.5t)$$
$$\qquad +0.499875 \exp(-2000.5t) + 1$$

$$v(t) = -2.99975 \exp(-0.5t)$$
$$\qquad -0.00025 \exp(-2000.5t) + 1$$

From (3.172), we write as

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

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

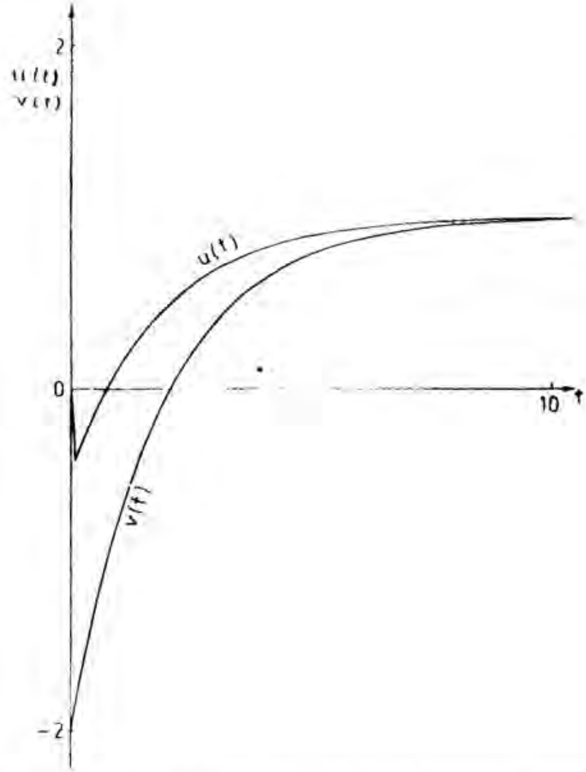


Fig. 3.12 Solution of a stiff problem using trapezoidal method with variable steps

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

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

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

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

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

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

is A-stable.

Determine also the error constant.

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

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

(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

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

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.

24. Consider the following predictor-corrector set:

$$P_v\colon y_{n+1/2}+\frac{9}{16}\,y_n-\frac{25}{16}\,y_{n-1}=\frac{h}{64}(87y'_n+48y'_{n-1}-3y'_{n-2})$$

$$P_k\colon y_{n+1}+8y_n-9y_{n-1}=\frac{h}{3}(17y'_n+14y'_{n-1}-y'_{n-2})$$

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

Show that the local truncation error of the predictor will dominate in the algorithm $P_v\, E\, P_k\, E\, C_H\, E$ unless λh is of the order 0.01, where $y'=\lambda y$.

25. Show that the linear explicit and implicit methods given in the text for the initial value problem $y''=f(t, y)$, $y(t_0)=y_0$, $y'(t_0)=y'_0$ are respectively, in terms of operators

$$(1-\nabla)\,[\log(1-\nabla)]^2\,y_{n+1}=hy''_n$$
$$[\log(1-\nabla)]^2\,y_{n+1}=hy''_{n+1}$$

and hence obtain the expansions given.

26. Find values of the constants such that the predictor formula

$$y_{n+1}+y_{n-3}+\alpha(y_n+y_{n-2})+2\alpha_1 y_{n-1}$$
$$=h^2[\gamma(y''_n+y''_{n-2})+2\delta y''_{n-1}]$$

is of order h^6. (BIT 9 (1969), 87)

Show that the use of the predictor is unstable for all values of h for solving the equation $y''=\lambda y$.

27. Solve the initial value problem

$$y''=-y,\ y(0)=0,\ y'(0)=1,\ 0\leqslant t\leqslant 1$$

with step length $h=0.2$. Use Numerov's method.

28. Find the hybrid linear multistep formula

$$y_{n+1}=a_1y_n+a_2y_{n-1}+h^2\,(b_0y''_{n+1}+b_1y''_n+b_2y''_{n-1})$$
$$+h^2c_0y''_{n-\theta+1},\ 0<\theta<1$$

for the cases (i) $b_0=0$, (ii) $b_0\neq 0$, of maximal order.

29. Find the stability polynomial of the $P\,(EC)^m\,E$ mode for the $P-C$ set

$$P\colon y_{n+1}=2y_n-y_{n-1}+h^2y''_n$$
$$C\colon y_{n+1}=2y_n-y_{n-1}+h^2y''_{n+1}$$

where $y''=\lambda y$.

30. Obtain the $P-M_p-C-M_c$ algorithm for the $P-C$ set:

$$P\colon y_{n+1}=2y_{n-1}-y_{n-3}+\frac{4}{3}\,h^2(y''_n+y''_{n-1}+y''_{n-2})$$

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

where $y'' = \lambda y$.

31. Which of the following difference methods are applicable for solving the initial value problem

$$y' + ky = 0, \quad y(0) = 1, \quad k > 0$$

For what values of k are the methods stable?

(a) $y_{n+1} = \dfrac{1}{2}y_n - \dfrac{1}{4}y_{n-1} + \dfrac{h}{3}(2y'_n + y'_{n-1})$

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

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

with complete iterations of the corrector.

(c) same as (b) but using the corrector just once. (BIT 6 (1966), 83)

32. The difference equation

$$\frac{1}{(1+a)}(y_{n+1} - y_n) + \frac{a}{1+a}(y_n - y_{n-1}) = -h\,y_n,\ h > 0,\ a > 0$$

which approximates the differential equation $y' = -y$, is called strongly stable if, for sufficiently small values of h, $\lim\limits_{n\to\infty} y_n = 0$ for all solutions y_n. Find the values of a for which strong stability holds.

(BIT 8 (1968), 138).

33. To integrate a system of differential equations

$$\mathbf{y}' = \mathbf{f}\,(x, \mathbf{y}),\ \mathbf{y}_0 \text{ is given,}$$

one can use Euler's method as predictor and apply the trapezoidal rule once as corrector, i.e.,

$$\mathbf{y}^*_{n+1} = \mathbf{y}_n + h\,\mathbf{f}\,(x_n, \mathbf{y}_n)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{2}(\,\mathbf{f}\,(x_n, \mathbf{y}_n) + \mathbf{f}\,(x_{n+1}, \mathbf{y}^*_{n+1}))$$

(a) If this method is used on $\mathbf{y}' = \mathbf{A}\mathbf{y}$, where $\mathbf{A}$ is a constant matrix, then

$$\mathbf{y}_{n+1} = \mathbf{B}\,(h)\,\mathbf{y}_n$$

Find the matrix $\mathbf{B}\,(h)$.

(b) Assume that $\mathbf{A}$ has real eigenvalues λ_i satisfying

$$\lambda_i \in [a, b],\ a < b < 0.$$

For what values of h is it true that $\lim\limits_{n\to\infty} \mathbf{y}_n = 0$

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

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

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

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

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

The boundary conditions of the second kind are:

(ii) $y'(a) = \gamma_1, y'(b) = \gamma_2$

The boundary conditions of the third kind, sometimes called *Sturm's boundary conditions*, are:

(iii) $a_0 y'(a) - a_1 y(a) = \gamma_1,\ b_0 y'(b) + b_1 y(b) = \gamma_2$

where a_0, b_0, a_1 and b_1 are all positive constants.

In (4.1) if $r(x) = 0$, the differential equation is called homogeneous; otherwise it is inhomogeneous. Similarly, the boundary conditions are called homogeneous when γ_μ are zero; otherwise inhomogeneous. The boundary value problem is called homogeneous if the differential equation and the boundary conditions are homogeneous. A homogeneous boundary value problem ($r(x) = 0$, $\gamma_\mu = 0$) possesses only a trivial solution $y(x) = 0$. We, therefore, consider those boundary value problems in which a parameter λ occurs either in the differential equation or in the boundary conditions, and we determine values of λ, called *eigenvalues*, for which the boundary value problem has a nontrivial solution. Such a solution is called *eigen-function* and the entire problem is called an *eigenvalue* or *characteristic value problem.*

In the boundary value problems, the arbitrary constants in the solution are determined from the conditions given at more than one point. Therefore, it is possible for more than one solution to exist or no solution may exist. In general, a boundary value problem does not always have a unique solution. However, the existence and uniqueness of the solution for a special class of boundary value problems, called *class M*, can be established.

DEFINITION 4.1 A boundary value problem will be called of class M if it is of the form

$$\begin{gathered} y'' = f(x, y) \\ y(a) = \gamma_1,\ y(b) = \gamma_2 \end{gathered} \tag{4.4}$$

and, (i) the initial value problem

$$\begin{aligned} y'' &= f(x, y) \\ y(a) &= \gamma_1,\ y'(a) = A \end{aligned}$$

with A arbitrary, has a unique solution, and $f(x, y)$ is such that

(ii) $\quad f_y(x, y)$ is continuous and bounded

$\quad f_y(x, y) \geqslant 0$ for $x \in [a, b]$, $y \in (-\infty, \infty)$

In what follows, we shall assume that the boundary value problem has a solution and we shall attempt to determine it.

4.2 APPROXIMATE METHODS

There are many methods for approximating the solution of the boundary value problems. Generally speaking, they fall into two classes: those in which the solution is approximated numerically at a number of discrete points, called "grid, nodal, net or mesh points", and those in which the solution is approximated by a finite number of terms of an infinite expansions in terms of a sequence of functions. The former are usually called *difference* methods and the latter the *weighted residual* or *series* methods.

The difference methods are applicable to a wide class of problems and usually the most convenient for a computer solution. The other methods are more efficient for restricted classes of problems, and usually require more human intervention in obtaining the solution. However, the weighted residual or the variational method with piecewise polynomials as approximate function is called the *finite element method* and is very suitable for automatic computation. The numerical methods are of the following two types.

4.2.1 Shooting methods

These are initial value problem methods. Here, we add sufficient number of conditions at one end and adjust these conditions until the required conditions are satisfied at the other end.

For example, to solve (4.4) by the shooting method we assume $y'(a) = \gamma$ and solve the initial value problem

$$y'' = f(x, y)$$
$$y(a) = \gamma_1, y'(a) = \gamma$$

We calculate $y^{(\gamma)}(b)$ and evaluate

$$g(\gamma) = y^{(\gamma)}(b) - \gamma_2$$

If $g(\gamma) = 0$ then the choice of γ is correct and the numerical solution of the boundary value problem (4.4) is obtained. Otherwise, we choose other values of γ and the process is repeated until the second boundary condition is satisfied. In practice this method is quite slow.

4.2.2 Difference methods

These are difference equations obtained from a given differential equation. The system of equations is then solved by direct or indirect methods.

Let us consider a linear second order boundary value problem of the form

$$-y'' + f(x)\, y = r(x),\ x \in [a, b],$$
$$y(a) = \gamma_1, y(b) = \gamma_2 \tag{4.5}$$

We assume $f(x) \geqslant 0$ for $x \in [a, b]$ to ensure the existence and uniqueness of the solution. In order to compute a numerical approximation to the solution $y(x)$, we first divide the interval $[a, b]$ into $N+1$ subintervals of length $h = (b-a)/(N+1)$, and at each point $x_n = a+nh$, $n = 1, 2, \ldots, N$, approximate $y''(x_n)$ by the second central difference quotient

$$y''(x_n) = \frac{1}{h^2}(y(x_{n+1}) - 2y(x_n) + y(x_{n-1})) + 0(h^2),\ n = 1(1)N \tag{4.6}$$

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

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

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

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

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

The boundary conditions become

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

If

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

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

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

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

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

$$L[y] = y''+\lambda y = 0.$$
$$y(a) = y\,(b) = 0 \tag{4.9}$$

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),

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

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)

The analytic solution of (4.13) is given by

$$y(x) = A_1 + B_1\, e^{-\mu x} \tag{4.15}$$

where A_1 and B_1 are arbitrary constants to be determined with the help of the boundary conditions. Each of the three representations (4.14i)–(4.14iii) has A_1 as a solution so we examine how close are the non-constants components of their solutions to $e^{-\mu x}$. The very least that we expect of the finite difference solutions is that they behave monotonically as $e^{-\mu x}$ for $\mu > 0$ and $\mu < 0$. The equation (4.14i) has the solution

$$y_n = A_1 + B_1 \left(\frac{2-\mu h}{2+\mu h}\right)^n$$

If the behaviour of the exponential term is analysed, it is seen that it only displays the correct monotonic behaviour for $\mu > 0$ and $\mu < 0$ if the condition $h < \left|\frac{2}{\mu}\right|$ is satisfied. This is the condition for stability of the difference equation (4.14i). For μ very large, the stability condition will make a central difference scheme computationally infeasible. Next, we write the solution of (4.14ii) as

$$y_n = A_1 + B_1(1-\mu h)^n$$

The analysis of the exponential term gives that if $\mu > 0$ then $h < 1/\mu$ for stability, and that if $\mu < 0$ there is no condition on h and the difference scheme (4.14ii) is unconditionally stable. If μ becomes very large and positive, then a backward difference scheme becomes infeasible. Finally we write the solution of (4.14iii) in the form

$$y_n = A_1 + B_1 \left(\frac{1}{1+\mu h}\right)^n$$

Again, if $\mu < 0$ then $h < -\dfrac{1}{\mu}$ is the condition for stability, and that if $\mu > 0$, there is no condition on h and proper behaviour is guaranteed for all h. Thus, if μ becomes very large and negative then a forward difference scheme becomes infeasible. Hence, for stability it is necessary that different difference quotient for the first order term must be used depending on the sign of μ.

4.2.3 Difference approximation to derivatives

From (1.13) and Table 1.1, we get

$$hD = \log E = \left|\begin{aligned} &\log(1+\Delta) = \Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \ldots \\ &-\log(1-\nabla) = \nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \ldots \\ &2\sinh^{-1}(\delta/2) = \delta - \frac{1^2}{2^2\,3!}\delta^3 + \ldots \end{aligned}\right. \tag{4.16}$$

The relation (4.16) serves to express the derivative at a point x_n in terms of forward, backward and central differences of $y(x_n)$. However, in the central difference expansion, the right-hand member involves odd central differences, which are generally considered as not so useful for solving differential equations because these require evaluations between the nodal points. To obtain useful expressions, we use mean-odd central differences. On multiplying the right-hand side expansion by μ and dividing it by its equivalent $(1+\delta^2/4)^{1/2}$ we get

$$hD = \frac{\mu}{\sqrt{\left(1+\frac{1}{4}\delta^2\right)}} 2\sinh^{-1}(\delta/2)$$
$$= \mu\left(\delta - \frac{1^2}{3!}\delta^3 + \frac{1^2 \cdot 2^2}{5!}\delta^5 - \dots\right)$$

Thus the first derivative of $y(x)$ at $x = x_n$ in terms of differences can be written in the form

$$hy'_n = \left| \begin{array}{l} \Delta y_n - \frac{1}{2}\Delta^2 y_n + \frac{1}{3}\Delta^3 y_n - \dots \\ \nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \dots \\ \mu\delta y_n - \frac{1^2}{3!}\mu\delta^3 y_n + \dots \end{array} \right.$$

The rth order derivatives of $y(x)$ can be obtained by finding the expansion of $h^r D^r$. We get

$$h^r D^r = \left| \begin{array}{l} \Delta^r - \frac{r}{2}\Delta^{r+1} + \frac{r(3r+5)}{24}\Delta^{r+2} - \dots \\ \nabla^r + \frac{r}{2}\nabla^{r+1} + \frac{r(3r+5)}{24}\nabla^{r+2} + \dots \\ \mu\delta^r - \frac{r+3}{24}\mu\delta^{r+2} + \frac{5r^2+52r+135}{5760}\mu\delta^{r+4} - \dots,\ r \text{ odd} \\ \delta^r - \frac{r}{24}\delta^{r+2} + \frac{r(5r+22)}{5760}\delta^{r+4} - \dots,\ r \text{ even} \end{array} \right.$$

In particular, the difference formulas for $r = 2$ and 4 are given by

$$h^2 y''_n = \left| \begin{array}{l} \Delta^2 y_n - \Delta^3 y_n + \frac{11}{12}\Delta^4 y_n - \frac{5}{6}\Delta^5 y_n + \dots \\ \nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \dots \\ \delta^2 y_n - \frac{1}{12}\delta^4 y_n + \frac{1}{90}\delta^6 y_n - \dots \end{array} \right.$$

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

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 $f_y(x, y) \geqslant 0$, $x \in [a, b]$, 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

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

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, $1 \leqslant n \leqslant N$, which in matrix form can be written as

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

where

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

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

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

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

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,

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

and finally

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

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

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

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

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

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

If we use the transformation

$$t = x_n + \frac{h}{2}(1+u),$$

in (4.20), we obtain

$$\delta^2 y(x_n) = \frac{h^2}{4}\int_{-1}^{1}(1-u)\left[y''\left(x_n - \frac{h}{2}(1+u)\right)\right.$$

$$\left. + y''\left(x_n + \frac{h}{2}(1+u)\right)\right] du \qquad (4.21)$$

Let us replace the integral in (4.21) by the trapezoidal rule and we get the second order difference scheme

$$\delta^2 y_n = h^2 y_n'' \qquad (4.22)$$

If we apply Simpson's rule to the integral in (4.21) and use the relation

$$y''\left(x_n - \frac{h}{2}\right) + y''\left(x_n + \frac{h}{2}\right) = \frac{3}{2}\, y_n'' + \frac{1}{4}\,(y_{n-1}'' + y_{n+1}'') + 0(h^4),$$

we obtain the fourth order Numerov method

$$\delta^2 y_n = \frac{h^2}{12}(y_{n-1}'' + 10y_n'' + y_{n+1}'') \qquad (4.23)$$

On replacing the integral in (4.21) by the four point Lobatto rule, the sixth order hybrid difference scheme based on two off-step points is given by

$$\delta^2 y_n = h^2\left[\frac{1}{6}\, y_n'' + \frac{10}{24} s(y_{n-r}'' + y_{n+r}'') + \frac{10}{24}\, r(y_{n-s}'' + y_{n+s}'')\right] \qquad (4.24)$$

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

We can also use the Gauss three point rule to evaluate the integral in (4.21) to have the sixth order hybrid difference scheme based on three off-step points. In general, by applying suitable quadrature rules, the integral on the right side of (4.21) can be evaluated as

$$W_0 y_n'' + W_1(y_{n-1}'' + y_{n+1}'') + \sum_{j=2}^{v} W_j(y_{n-\theta_j}'' + y_{n+\theta_j}'') + E \qquad (4.25)$$

where $0 < \theta_j < 1$, W_0, W_1, W_j are the weights and E is the error term of the quadrature rule. Neglecting E, the difference scheme based on v off-step points is given by

$$\delta^2 y_n = h^2\left[W_0 y_n'' + W_1(y_{n-1}'' + y_{n+1}'') + \sum_{j=2}^{v} W_j(y_{n-\theta_j}'' + y_{n+\theta_j}'')\right] \qquad (4.26)$$

The truncation error T_n^* associated with the difference scheme (4.26) can be written as

$$T_n^* = \delta^2 y(x_n) - h^2\Big[W_0 y''(x_n) + W_1(y''(x_{n-1}) + y''(x_{n+1}))$$

$$+ \sum_{j=2}^{v} W_j(y''(x_{n-\theta_j}) + y''(x_{n+\theta_j}))\Big] \tag{4.27}$$

To determine the unknown weights and the abscissas, we expand the terms on the right-hand side of (4.27) in a Taylor's series about $x = x_n$ and equate the coefficients of the various powers of h to zero to get the required order. From the system of linear equations thus obtained, the W_i's can be solved in terms of the θ_j's which can then be chosen as the nodes of a known quadrature rule or as parameters which increase the order of the method.

We now derive difference schemes of order six, depending on one and two off-step points. For $v = 2$, the difference scheme (4.26) becomes

$$\delta^2 y_n = h^2\,[W_0 y''_n + W_1(y''_{n-1} + y''_{n+1}) + W_2(y''_{n-r} + y''_{n+r})] \tag{4.28}$$

where $\theta_2 = r$. It is easy to verify that

$$\delta^2 y_n = h^2\Big[\frac{25r^2-3}{30r^2}y''_n + \frac{2-5r^2}{60(1-r^2)}(y''_{n-1} + y''_{n+1})$$

$$+ \frac{1}{20r^2(1-r^2)}(y''_{n-r} + y''_{n+r})\Big] \tag{4.29}$$

gives one parameter family of sixth order hybrid difference scheme. The truncation error is given by

$$\frac{42r^2-13}{302400}h^8 y^{(8)}(\xi_5),\ x_{n-1} < \xi_5 < x_{n+1} \tag{4.30}$$

The two difference methods corresponding to $r^2 = 2/5$ and $r^2 = 3/25$ are of special interest since they involve the minimum number of function values. The methods are

$$\delta^2 y_n = h^2\Big[\frac{7}{12}y''_n + \frac{5}{24}(y''_{n-r} + y''_{n+r})\Big],\ r^2 = \frac{2}{5} \tag{4.31}$$

with the truncation error

$$T_n^* = \frac{19}{1512000}h^8 y^{(8)}(\xi_6),\ x_{n-1} < \xi_6 < x_{n+1}$$

and $$\delta^2 y_n = h^2\Big[\frac{7}{264}(y''_{n-1} + y''_{n+1}) + \frac{125}{264}(y''_{n-r} + y''_{n+r})\Big],\ r^2 = \frac{3}{25} \tag{4.32}$$

with the truncation error

$$T_n^* = -\frac{199}{7560000}h^8 y^{(8)}(\xi_7),\ x_{n-1} < \xi_7 < x_{n+1}$$

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

$$\begin{aligned}\delta^2 y_n = h^2 [&W_0 y_n'' + W_1 (y_{n-1}'' + y_{n+1}'') \\ &+ W_2 (y_{n-r}'' + y_{n+r}'') + W_3 (y_{n-s}'' + y_{n+s}'')]\end{aligned} \tag{4.34}$$

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

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

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

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

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

Approximation II

$$y_{n+q} = (1-q)\,y_n + q\,y_{n+1} + \frac{q\,(q-1)}{24}\,h^2[(q^2-q-1)\,y''_{n-1}$$
$$-2(q^2+q-5)\,y''_n + (q^2+3q+3)y''_{n+1}] \tag{4.43}$$

$$y_{n-q} = (1-q)\,y_n + q\,y_{n-1} + \frac{q(q-1)}{24}\,h^2[(q^2+3q+3)\,y''_{n-1}$$
$$-2\,(q^2+q-5)\,y''_n + (q^2-q-1)\,y''_{n+1}] \tag{4.44}$$

where $q = \theta_j$. The truncation error in (4.43) and (4.44) are respectively

$$T_n^{(2)} = R_5^* h^5 y^{(5)}(x_n) + R_6^* h^6 y^{(6)}(\xi_1^*)$$
$$T_n^{*(2)} = -R_5^* h^5 y^{(5)}(x_n) + R_6^* h^6 y^{(6)}(\xi_2^*)$$
$$R_5^* = \frac{1}{360}\,(3q^5 - 10q^3 + 7q)$$
$$R_6^* = \frac{1}{1440}\,(2q^6 - 5q^4 + 3q),\ x_{n-1} < \xi_1^*,\ \xi_2^* < x_{n+1} \tag{4.45}$$

4.3.2 Second order linear boundary value problems

We shall consider now the numerical solution of the differential equation

$$y''(x) = f(x)\,y(x) + g(x) \tag{4.46}$$

subject to the boundary conditions

$$y(a) = A,\ y(b) = B \tag{4.47}$$

where (i) $-\infty < a < b < \infty$;

(ii) A, B are arbitrary finite constants;

(iii) the functions $f(x)$ and $g(x)$ are assumed to be sufficiently differentiable.

This boundary value problem has a unique solution provided $f(x) \geqslant 0$ in $x \in [a, b]$.

We denote the approximate value of $y(x)$ at $x = x_n$ by y_n. From (4.46) we substitute $y''(x)$ into (4.18), and obtain

$$(-1+A_n)\,y_{n-1} + (2+B_n)\,y_n + (-1+C_n)\,y_{n+1} = D_n,\ 1 \leqslant n \leqslant N \tag{4.48}$$

where $\quad A_n = h^2\beta_0 f(x_{n-1}),\ B_n = h^2\beta_1 f(x_n)$

$\quad C_n = h^2\beta_2 f(x_{n+1})$

and $\quad D_n = -h^2\,(\beta_0\,g(x_{n-1}) + \beta_1\,g(x_n) + \beta_2\,g(x_{n+1}))$

The difference scheme (4.18) is of order two for arbitrary values of β_i's and it considerably simplifies if

$$\beta_0 = \beta_2 = 0,\ \beta_1 = 1 \tag{4.49}$$

and the order of (4.18) becomes four if

$$\beta_0 = \beta_2 = \frac{1}{12}, \beta_1 = \frac{10}{12} \tag{4.50}$$

For sixth order difference scheme (4.24) with Approximation I, the values of A_n, B_n, C_n and D_n in (4.48) are given by

$$
\begin{aligned}
A_n &= \frac{h^2}{720} [(60-(1+\sqrt{5})\, h^2 f_{n-1})\, P_{n-r} + (60-(1-\sqrt{5})\, h^2 f_{n-1})\, P_{n-s}] \\
B_n &= \frac{h^2}{720} [120 f_n + (P_{n+r}+P_{n-r})\, (30(3+\sqrt{5}) \\
&\quad + (1+\sqrt{5})\, h^2 f_n) + (P_{n+s}+P_{n-s})\, (30(3-\sqrt{5}) \\
&\quad + (1-\sqrt{5})\, h^2 f_n)] \\
C_n &= \frac{h^2}{720} [(60-(1+\sqrt{5})\, h^2 f_{n+1}) P_{n+r} + (60-(1-\sqrt{5})\, h^2 f_{n+1}) P_{n+s}] \\
D_n &= -\frac{h^2}{720} [120\, g_n + 30\, ((5+\sqrt{5})\, (g_{n+r}+g_{n-r}) \\
&\quad + (5-\sqrt{5})\, (g_{n+s}+g_{n-s})) \\
&\quad + h^2(g_n-g_{n+1})\, ((1+\sqrt{5})\, P_{n+r} + (1-\sqrt{5})\, P_{n+s}) \\
&\quad + h^2(g_n-g_{n-1})\, ((1+\sqrt{5})\, P_{n-r} + (1-\sqrt{5})\, P_{n-s}) \\
&\quad - 3h^2((5+\sqrt{5})\, P_{n+r}\, g_{n+r} + (5-\sqrt{5})\, P_{n+s}\, g_{n+s}) \\
&\quad - 3h^2((5+\sqrt{5})\, P_{n-r}\, g_{n-r} + (5-\sqrt{5})\, P_{n-s}\, g_{n-s})]
\end{aligned} \tag{4.51}
$$

in which

$$P_{n+q} = \frac{f_{n+q}}{1+\frac{h^2}{10} f_{n+q}}, \quad q = \pm r, \pm s,$$

$$f(x_n) = f_n \quad \text{and} \quad g(x_n) = g_n$$

The system of linear equations (4.48) can be written in matrix form as follows:

$$\mathbf{M}\mathbf{y} = (\mathbf{J}+\mathbf{Q})\, \mathbf{y} = \mathbf{R} \tag{4.52}$$

where $\mathbf{M}$ is an $N \times N$ tridiagonal matrix which may be written as the sum of two $N \times N$ tridiagonal marices $\mathbf{J}+\mathbf{Q}$ whose nonzero elements are

$$
\begin{aligned}
j_{i,i} &= 2,\ j_{i,\ i+1} = j_{i+1,i} = -1 \\
q_{ii} &= B_i,\ q_{i+1,i} = A_i,\ q_{i,i+1} = C_i
\end{aligned} \tag{4.53}
$$

and $\mathbf{R} = (r_i)$ is an N-dimensional column vector such that

$$
\begin{aligned}
r_1 &= D_1 - (-1+A_1)A \\
r_i &= D_i,\ 2 \leqslant i \leqslant N-1 \\
r_N &= D_N - (-1+C_N)B
\end{aligned}
$$

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

$$\begin{aligned}
w_1 &= \frac{c_1}{a_1}, & g_1 &= \frac{d_1+b_1A}{a_1}\\
w_2 &= \frac{c_2}{a_2-b_2w_1}, & g_2 &= \frac{d_2+b_2g_1}{a_2-b_2w_1}\\
&\vdots & &\vdots\\
w_N &= \frac{c_N}{a_N-b_N\, w_{N-1}}, & g_N &= \frac{d_N+b_N\, g_{N-1}}{a_N-b_N\, w_{N-1}}
\end{aligned}$$

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

$$\begin{aligned} y'(a) - cy(a) &= A \\ y'(b) + dy(b) &= B \end{aligned} \tag{4.58}$$

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

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

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

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

$$\begin{aligned} y(x_1) = y(x_0) + h\, y'(x_0) &+ \frac{h^2}{24}[2y''(x_0) + (5+\sqrt{5})\, y''(x_0+rh) \\ &+ (5-\sqrt{5})\, y''(x_0+sh)] + \frac{h^7}{25\,2000} y^{(6)}(\xi) \end{aligned}$$

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

$$(1+B_0)\, y_0 + (-1+C_0)\, y_1 = D_0 \tag{4.61}$$

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

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

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

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

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

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

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

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

$$\begin{aligned} P &= (E-1-hD)\,(hD)^{-2} \\ &= (\Delta-\log(1+\Delta))\left(\Delta-\frac{1}{2}\,\Delta^2+\frac{1}{3}\,\Delta^3-\dots\right)^{-2} \\ &= \frac{1}{2}\left(1+\frac{1}{3}\Delta-\frac{1}{12}\,\Delta^2+\frac{2}{45}\,\Delta^3-\frac{7}{240}\,\Delta^3+\dots\right) \end{aligned}$$

Thus, we have

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

Similarly, we get for the second boundary condition

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

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

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

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

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

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

Suppose N is replaced by $N+1$ in (4.68), and so we have

$$y_n^{(N+1)} = w_n y_{n+1}^{(N+1)} + l_n \tag{4.70}$$
$$y_0^{(N+1)} = A,\ y_{N+2}^{(N+1)} = 0$$

where w_n and l_n are given by (4.69).

Substracting (4.70) from (4.68), we get

$$y_n^{(N+1)} - y_n^{(N)} = w_n(y_{n+1}^{(N+1)} - y_{n+1}^{(N)}),\ 1 \leqslant n \leqslant N \tag{4.71}$$

Therefore

$$y_n^{(N+1)} - y_n^{(N)} = w_n\, w_{n+1} \dots w_{N-1}\, w_N\, (y_{N+1}^{(N+1)} - y_{N+1}^{(N)}),\ 1 \leqslant n \leqslant N+1,$$

where $$y_{N+1}^{(N)} = 0 \text{ and } y_{N+1}^{(N+1)} = l_{N+1}$$

Thus to apply the criterion

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

a first test is simply to examine

$$y_{N+1}^{(N+1)} = l_{N+1}$$

If this is not small enough, set N to $N+1$ and continue. Then, when this is met we further require that

$$\max_{1 \leqslant n \leqslant N} \ |\, w_n\, w_{n+1} \dots w_N\, l_{N+1} \,| < \epsilon$$

Thus for the starting value of h, we are able to test that our finite replacement for infinity is resonable before computing the solution of the finite-difference approximation.

Example 4.3 Obtain the finite difference solution of the boundary value problem

$$-y'' - 2y' + 2y = e^{-2x}$$
$$y(0) = 1,\ y(\infty) = 0$$

It can be easily verified that the analytical solution of the boundary value problem is

$$y(x) = \frac{1}{2}\,(e^{-(1+\sqrt{3})x} + e^{-2x})$$

The finite difference approximation to the differential equation at the nodal point $x = x_n$ is given by

$$-\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} - 2\,\frac{y_{n+1} - y_{n-1}}{2h} + 2y_n = e^{-2x_n}$$

The boundary conditions become

$$y_0 = 1,\ y_{N+1} = 0$$

For $h = 1/2$, the difference equation becomes

$$-y_{n-1}+5y_n-3y_{n+1} = \frac{1}{2}\, e^{-n}$$

The values of y_1 for a series of values of n are given in Table 4.3. Furthermore, with $\epsilon = 10^{-8}$, we obtain $N = 16$ so that $b^{(N)} = 8.5$.

TABLE 4.3 SOLUTION OF $-y''-2y'+2y = e^{-2x}$, $y(0) = 1$, $y(\infty) = 0$ FROM FINITE BOUNDARY CONDITIONS, $h = 1/2$

y_N	$y_N = 0$	Differences
$y_2 = \frac{5}{3}\left(y_1-\frac{1}{5}-\frac{1}{10}\,e^{-1}\right)$	$y_1 = 0.2367879$	
		0.415165−01
$y_3 = \frac{22}{9}\left(y_1-\frac{5}{22}-\frac{5}{44}\,e^{-1}-\frac{3}{44}e^{-2}\right)$	$y_1 = 0.2783046$	
		0.891351−02
$y_4 = \frac{95}{27}\left(y_1-\frac{22}{95}-\frac{22}{190}e^{-1}-\frac{3}{38}e^{-2}-\frac{9}{190}\,e^{-3}\right)$	$y_1 = 0.2872182$	
		0.204293−02
$y_5 = \frac{409}{81}\left(y_1-\frac{95}{409}-\frac{95}{818}e^{-1}-\frac{33}{409}\,e^{-2}-\frac{45}{818}e^{-3}-\frac{27}{818}e^{-4}\right)$	$y_1 = 0.2892611$	

4.3.6 High order methods

The sixth order difference scheme (4.24) when applied to the boundary value problem consisting of (4.4) and (4.47) gives rise to the nonlinear system of equations

$$\delta^2 y_n = \frac{h^2}{12}[2f(x_n, y_n)+5s\,(f(x_{n-r}, y_{n-r})+f(x_{n+r}, y_{n+r})) + 5r(f(x_{n-s}, y_{n-s})+f(x_{n+s}, y(_{n+s}))],\ 1 \leqslant n \leqslant N \tag{4.72}$$

We cannot use *Approximation I* to determine the values of y at the off-step points $x_{n\pm r}$ and $x_{n\pm s}$. *Approximation II* can be used to find the values of y at the off-step points. The resulting system of nonlinear equations will be of the form (4.19). The truncation error is found as

$$T_n^* = \left[\frac{1}{302400}\, y^{(8)}(x_n)-\frac{1}{8640} f_y\, y^{(6)}(x_n) - \frac{1}{720}\,(f_{xy}+f_{yy}\,y')\,y^{(5)}(x_n)\right]h^8+0\,(h^{10}),\ 1 \leqslant n \leqslant N \tag{4.73}$$

An alternative sixth order difference scheme which does not use off-step points can be obtained if we write

$$\delta^2 y_n = h^2\left[\frac{\delta}{2\sinh^{-1}(\delta/2)}\right]^2 y''(x_n) = h^2\left[1+\frac{1}{12}\,\delta^2-\frac{1}{240}\,\delta^4+\dots\right]y''(x_n) \tag{4.74}$$

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

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

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

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

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

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:

$$(1+hc)\,y_0 - y_1 + h^2\left(\frac{1}{3} f_0 + \frac{1}{6} f_1\right) + hA = 0,$$

$$-y_{n-1} + 2y_n - y_{n+1} + h^2(\beta_0 f_{n-1} + \beta_1 f_n + \beta_2 f_{n+1}) = 0,\ 1 \leqslant n \leqslant N,$$

$$-y_N + (1+hd)\,y_{N+1} + h^2\left(\frac{1}{6} f_N + \frac{1}{3} f_{N+1}\right) - hB = 0 \quad (4.78)$$

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

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

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

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

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

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

$$\begin{aligned} y_0^{(p+1)} &= y_0^{(p)} + \Delta y_0^{(p)} \\ y_1^{(p+1)} &= y_1^{(p)} + \Delta y_1^{(p)} \\ y_2^{(p+1)} &= y_2^{(p)} + \Delta y_2^{(p)} \end{aligned}$$

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 $\left|\frac{\partial f}{\partial z}\right| \le W$, for some positive W.

These conditions assure us that the boundary value problem (4.87) has a unique solution. The grid points are given by $x_n = a+nh$, $n = 0(1)N+1$, $h = (b-a)/(N+1)$. A simple difference scheme for (4.87) is written as

$$y_{n-1}-2y_n+y_{n+1} = h^2 f(x_n, y_n, y'_n) \tag{4.88}$$

where the first derivative y_n may be replaced by one of the expressions

$$y'_n = \begin{cases} \text{(i) } (y_{n+1}-y_{n-1})/2h \\ \text{(ii) } (y_n-y_{n-1})/h \\ \text{(iii) } (y_{n+1}-y_n)/h \end{cases} \tag{4.89}$$

The backward and forward differences are accurate to order h. Therefore the difference scheme (4.88) is of $0(h)$. The central difference is accurate to order h^2 and the difference scheme (4.88) will be of $0(h^2)$.

4.4.1 Difference schemes

We now list two difference schemes for the differential Equation (4.87).

Fourth order method

$$\bar{y}'_n = (y_{n+1}-y_{n-1})/2h$$

$$\bar{y}'_{n+1} = (3y_{n+1}-4y_n+y_{n-1})/2h$$

$$\bar{y}'_{n-1} = (-y_{n+1}+4y_n-3y_{n-1})/2h$$

$$\bar{\bar{y}}'_n = \bar{y}'_n - \frac{h}{20}(\bar{f}_{n+1}-\bar{f}_{n-1})$$

$$y_{n-1}-2y_n+y_{n+1} = \frac{h^2}{12}(\bar{f}_{n+1}+10\bar{\bar{f}}_n+\bar{f}_{n-1}) \tag{4.90}$$

where $\bar{\bar{f}}_n = f(x_n,\ y_n,\ \bar{\bar{y}}'_n)$

and $\bar{f}_{n\pm1} = f(x_{n\pm1}, y_{n\pm1}, \bar{y}'_{n\pm1})$

Sixth order method

$$\bar{y}'_n = (y_{n+1}-y_{n-1})/2h$$

$$\bar{y}'_{n+1} = (3y_{n+1}-4y_n+y_{n-1})/2h$$

$$\bar{y}'_{n-1} = (-y_{n+1}+4y_n-3y_{n-1})/2h$$

$$\bar{\bar{y}}'_{n+1} = \bar{y}'_n + \frac{h}{3}(2\bar{f}_n+\bar{f}_{n+1})$$

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

$$\bar{y}_{n+1/2} = \frac{1}{32}(15y_{n+1}+18y_n-y_{n-1})-\frac{h^2}{64}(3\bar{f}_{n+1}+4\bar{f}_n-\bar{f}_{n-1})$$

$$\bar{y}_{n-1/2} = \frac{1}{32}(-y_{n+1}+18y_n+15y_{n-1})-\frac{h^2}{64}(-\bar{f}_{n+1}+4\bar{f}_n+3\bar{f}_{n-1})$$

$$\bar{\bar{y}}'_{n+1/2} = \frac{1}{4h}(5y_{n+1}-6y_n+y_{n-1})-\frac{h}{48}(3\bar{f}_{n+1}+8\bar{f}_n+\bar{f}_{n-1})$$

$$\bar{\bar{y}}'_{n-1/2} = \frac{1}{4h}(-y_{n+1}+6y_n-5y_{n-1})+\frac{h}{48}(\bar{f}_{n+1}+8\bar{f}_n+3\bar{f}_{n-1})$$

$$\hat{y}'_n = \bar{y}'_n+h\left[\frac{1}{78}(\bar{f}_{n+1}-\bar{f}_{n-1})-\frac{1}{52}(\bar{\bar{f}}_{n+1}-\bar{\bar{f}}_{n-1}) -\frac{2}{13}(\bar{\bar{f}}_{n+1/2}-\bar{\bar{f}}_{n-1/2})\right]$$

$$y_{n-1}-2y_n+y_{n+1} = \frac{h^2}{60}[26\hat{f}_n+\bar{\bar{f}}_{n+1}+\bar{\bar{f}}_{n-1}+16(\bar{\bar{f}}_{n+1/2}+\bar{\bar{f}}_{n-1/2})] \tag{4.91}$$

where

$$f_n = f(x_n, y_n, \bar{y}'_n),\ \bar{f}_{n\pm1} = f(x_{n\pm1}, y_{n\pm1}, \bar{y}'_{n\pm1})$$
$$\bar{\bar{f}}_{n\pm1} = f(x_{n\pm1}, y_{n\pm1}\ \bar{\bar{y}}'_{n\pm1})$$
$$\bar{\bar{f}}_{n\pm1/2} = f(x_{n\pm1/2}, \bar{y}_{n\pm1/2}, \bar{\bar{y}}'_{n\pm1/2})$$
$$\hat{f}_n = f(x_n, y_n, \hat{y}'_n)$$

4.4.2 Compact implicit difference schemes

These are the implicit relations between the derivatives and the function values at the adjacent nodal points. We use either a Taylor series analysis or a Hermite polynomial interpolation to obtain the relations. We write the difference scheme in the following form

$$\sum_{\nu=-m}^{m}(a_\nu y_{n+\nu}+A_\nu y^{(k)}_{n+\nu}) = 0 \tag{4.92}$$

where $y^{(k)}_{n+\nu}$ represents the kth order derivative of $y(x)$ at $x_{n+\nu}$. The weighting factor a_ν and A_ν are determined by requiring that the method (4.92) satisfies certain accuracy conditions.

We associate with (4.92) the difference operator $L[y(x), h]$ and write

$$L[y(x_n), h] = \sum_{\nu=-m}^{m}[a_\nu y(x_{n+\nu})+A_\nu y^{(k)}(x_{n+\nu})] \tag{4.93}$$

The largest value of p for which the relation

$$L[y(x), h] = 0(h^{k+p}) \tag{4.94}$$

holds for all sufficiently differentiable functions $y(x)$, is the order of the operator. For example, (4.92) and (4.93), for $k = 2$, $m = 1$, become

$$a_{-1}y_{n-1}+a_0y_n+a_1y_{n+1}+(A_{-1}y''_{n-1}+A_0y''_n+A_1y''_{n+1}) = 0 \tag{4.95}$$

$$\begin{aligned} L[y(x), h] = {} & a_{-1}y(x_{n-1})+a_0y(x_n)+a_1y(x_{n+1}) \\ & +A_{-1}y''(x_{n-1})+A_0y''(x_n)+A_1y''(x_{n+1}) \end{aligned} \tag{4.96}$$

Expanding each term on the right-hand side of (4.96) in the Taylor series about x_n and equating the coefficients of $h^\nu y^{(\nu)}_n/\nu!$, $\nu = 0(1)\,5$ to zero, we get

$$a_{-1}+a_0+a_1 = 0$$
$$-a_{-1}+a_1 = 0$$

$$a_{-1}+a_1+\frac{2}{h^2}(A_{-1}+A_0+A_1)=0$$

$$-a_{-1}+a_1+\frac{6}{h^2}(-A_{-1}+A_1)=0$$

$$a_{-1}+a_1+\frac{12}{h^2}(A_{-1}+A_1)=0$$

$$-a_{-1}+a_1+\frac{20}{h^2}(-A_{-1}+A_1)=0 \tag{4.97}$$

and

$$L[y(x),h]=\frac{1}{5!}\Bigg[a_{-1}\int_{x_n}^{x_{n-1}}(x_{n-1}-s)^5\,y^{(6)}(s)\,ds+a_1\int_{x_n}^{x_{n+1}}(x_{n+1}-s)^5\,y^{(6)}(s)\,ds$$

$$+20\left(A_{-1}\int_{x_n}^{x_{n-1}}(x_{n-1}-s)^3\,y^{(6)}(s)\,ds+A_1\int_{x_n}^{x_{n+1}}(x_{n+1}-s)^3\,y^{(6)}(s)\,ds\right)\Bigg] \tag{4.98}$$

The last equation in (4.97) is automatically satisfied in view of the second and fourth equations. We are thus left with five equations in six unknowns. We can choose one of the unknowns arbitrary, say $a_1=1$, and determine the remaining unknowns. We find

$$a_{-1}=1,\ a_0=-2,\ A_{-1}=A_1=-\frac{1}{12}h^2,\ A_0=-\frac{10}{12}h^2 \tag{4.99}$$

Substituting (4.99) into (4.98) and simplifying we obtain

$$L[y(x),h]=\frac{h^6}{360}\int_{-1}^{1}(1-|u|)^3(3u^2-6|u|-2)y^{(6)}(x_n+hu)\,du$$

$$=-\frac{h^6}{240}y^{(6)}(\xi)$$

where $x_n+hu=s$ and $|\xi|<1$. Equation (4.96) becomes

$$y(x_{n-1})-2y(x_n)+y(x_{n+1})-\frac{h^2}{12}(y''(x_{n-1})+10y''(x_n)+y''(x_{n+1}))=-\frac{h^6}{240}y^{(6)}(\xi)$$

Neglecting the remainder (truncation) term, we get the Numerov method

$$y_{n-1}-2y_n+y_{n+1}=\frac{h^2}{12}(y''_{n-1}+10y''_n+y''_{n+1}) \tag{4.100}$$

which holds good at each nodal point with an error

$$\frac{1}{240}h^6M_6$$

where $M_6=\max\limits_{|\xi|<1}|y^{(6)}(\xi)|$.

From (4.94), we find that the difference equation (4.100) is of order four.

Similarly, for the first order derivative the compact implicit scheme is given by the Milne method

$$y_{n+1}-y_{n-1}=\frac{h}{3}\,(y'_{n+1}+4y'_n+y'_{n-1}) \tag{4.101}$$

For certain type of differential equations, it is useful to replace the derivative term $y^{(k)}$ by the linear differential operator $L[y]$ when constructing the compact implicit difference scheme. We have

$$\sum_{\nu=-m}^{m}(a_\nu\, y_{n+\nu}+A_\nu\,(L[y])_{n+\nu})=0 \tag{4.102}$$

For the linear differential operator

$$L[y]=p(x)y''+q(x)y' \tag{4.103}$$

and $m=1$, we obtain the compact implicit difference scheme

$$\begin{aligned}q_n^{+}(L[y])_{n+1}&+q_n^{0}(L[y])_n+q_n^{-}(L[y])_{n-1}\\&=\frac{1}{h^2}\,(r_n^{+}\,y_{n+1}+r_n^{0}\,y_n+r_n^{-}\,y_{n-1})\end{aligned} \tag{4.104}$$

where

$$\begin{aligned}
q_n^{+}&=6p_n\,p_{n-1}+h(5p_{n-1}\,q_n-2p_n\,q_{n-1})-h^2\,q_n\,q_{n-1}\\
q_n^{0}&=4[15\,p_{n+1}\,p_{n-1}-4h(p_{n+1}\,q_{n-1}-q_{n+1}\,p_{n-1})-h^2\,q_{n+1}\,q_{n-1}]\\
q_n^{-}&=6p_n\,p_{n+1}-h(5p_{n+1}\,q_n-2p_n\,q_{n+1})-h^2\,q_n\,q_{n+1}\\
r_n^{+}&=\frac{1}{2}\,[q_n^{+}(2p_{n+1}+3h\,q_{n+1})+q_n^{0}(2p_n+hq_n)+q_n^{-}(2p_{n-1}-hq_{n-1})]\\
r_n^{-}&=\frac{1}{2}\,[q_n^{+}(2p_{n+1}+hq_{n+1})+q_n^{0}(2p_n-hq_n)+q_n^{-}(2p_{n-1}-3hq_{n-1})]\\
r_n^{0}&=-(r_n^{+}+r_n^{-})\\
p_n&=p(x_n)\text{ and }q_n=q(x_n).
\end{aligned}$$

However, if we apply the fourth order difference scheme (4.90) to (4.103), we get the difference scheme

$$\begin{aligned}&\gamma_{n+1}\,y_{n+1}+\gamma_n\,y_n+\gamma_{n-1}\,y_{n-1}\\&=h^2[l_{n+1}\,r_{n+1}+l_n\,r_n+l_{n-1}\,r_{n-1}]\end{aligned} \tag{4.105}$$

where

$$\begin{aligned}\gamma_{n+1}=p_n\,p_{n-1}\,p_{n+1}&+\frac{h}{24}\,(3q_{n+1}\,p_n\,p_{n-1}+10q_n\,p_{n+1}\,p_{n-1}-q_{n-1}\,p_n\,p_{n+1})\\&+\frac{h^2}{48}\,(3q_n\,q_{n+1}\,p_{n-1}+q_n\,q_{n-1}\,p_{n+1})\end{aligned}$$

$$\gamma_{n-1} = p_n p_{n-1} p_{n+1} + \frac{h}{24}(q_{n+1} p_n p_{n-1} - 10 q_n p_{n+1} p_{n-1} - 3 q_{n-1} p_n p_{n+1})$$
$$+ \frac{h^2}{48}(q_n q_{n+1} p_{n-1} + 3 q_n q_{n-1} p_{n+1})$$

$$\gamma_n = -2[p_n p_{n-1} p_{n+1} + \frac{h}{12}(q_{n+1} p_n p_{n-1} - q_{n-1} p_n p_{n+1})$$
$$+ \frac{h^2}{24}(q_n q_{n+1} p_{n-1} + q_n q_{n-1} p_{n+1})]$$
$$= -(\gamma_{n+1} + \gamma_{n-1})$$

$$l_{n+1} = \frac{1}{12}\left(p_n p_{n-1} + \frac{h}{2} q_n p_{n-1}\right)$$

$$l_{n-1} = \frac{1}{12}\left(p_n p_{n+1} - \frac{h}{2} q_n p_{n+1}\right)$$

$$l_n = \frac{10}{12} p_{n-1} p_{n+1}$$

$$p_n = p(x_n), \qquad q_n = q(x_n) \quad \text{and} \quad r_n = (L[y])_n$$

4.4.3 Difference schemes based on cubic spline function

We shall derive the cubic spline relations which are relevant for constructing the difference schemes for the second order differential equations.

DEFINITION 4.2 A spline function of degree m with nodes at the points $x_n = 0(1)N+1$, is a function $S_\Delta(x)$ with the properties:

(i) On each interval $[x_{n-1}, x_n]$, $n = 1(1)N+1$, $S_\Delta(x)$ is a polynomial of degree m.

(ii) $S_\Delta(x)$ and its first $(m-1)$ derivatives are continuous on $[a, b]$.

If the function $S_\Delta(x)$ has only $(m-k)$ continuous derivatives then k is defined as the deficiency and is usually denoted by $S_\Delta(m, k)$. The cubic spline is a cubic polynomial of deficiency one, i.e. $S_\Delta(3, 1)$. We now use the definition 4.2 to find the cubic spline function approximation for the function $y(x)$, $x \in [a, b]$. We have

$$S_\Delta''(x) = \frac{(x_n - x)}{h} M_{n-1} + \frac{(x - x_{n-1})}{h} M_n \tag{4.106}$$

where primes denote differentiation with respect to x and $S_\Delta''(x_n) = M_n$. Integrating (4.106) and satisfying the interpolating conditions, $S_\Delta(x_{n-1}) = y_{n-1}$ and $S_\Delta(x_n) = y_n$ we obtain the cubic spline approximation function

$$S_\Delta(x) = \frac{(x_n - x)^3}{6h} M_{n-1} + \frac{(x - x_{n-1})^3}{6h} M_n + (y_{n-1} - \frac{h^2}{6} M_{n-1}) \frac{(x_n - x)}{h}$$
$$+ (y_n - \frac{h^2}{6} M_n) \frac{(x - x_{n-1})}{h} \tag{4.107}$$

The function $S_\Delta(x)$ on the interval $[x_n, x_{n+1}]$ is obtained with $n+1$ replacing n in (4.107). The continuity of the first derivative of $S_\Delta(x)$ at $x = x_n$ requires $S'_\Delta(x_n-) = S'_\Delta(x_n+)$. We have

$$\text{(i)}\ S'_\Delta(x_n-) = \frac{h}{3}M_n+\frac{h}{6}M_{n-1}+\frac{y_n-y_{n-1}}{h},\ n = 1(1)N+1$$

$$\text{(ii)}\ S'_\Delta(x_n+) = -\frac{h}{3}M_n-\frac{h}{6}M_{n+1}+\frac{y_{n+1}-y_n}{h},\ n = 0(1)N \tag{4.108}$$

and so that the continuity of the first derivatives implies

$$\frac{h}{6}M_{n-1}+\frac{2h}{3}M_n+\frac{h}{6}M_{n+1} = \frac{1}{h}(y_{n+1}-2y_n+y_{n-1}),\ n = 1(1)N \tag{4.109}$$

Additional spline relations that are deduciable from (4.107) are listed as follows:

$$\text{(i)}\ m_n = -\frac{h}{6}(M_{n+1}+2M_n)+\frac{y_{n+1}-y_n}{h}$$

$$\text{(ii)}\ m_{n+1} = \frac{h}{6}(M_n+2M_{n+1})+\frac{y_{n+1}-y_n}{h}$$

$$\text{(iii)}\ m_{n+1}-m_n = \frac{h}{2}(M_{n+1}+M_n)$$

$$\text{(iv)}\ m_{n+1}+m_n = \frac{h}{6}(M_{n+1}-M_n)+\frac{2(y_{n+1}-y_n)}{h} \tag{4.110}$$

The truncation error of the spline functions is obtained by putting $E = e^{hD}$ and expanding in powers of hD. We get the following results.

$$\text{(i)}\ S'_\Delta(x_n) = m_n = y'(x_n)-\frac{1}{180}h^4y^{(4)}_{(x_n)}+0(h^6)$$

$$\text{(ii)}\ S''_\Delta(x_n) = M_n = y''(x_n)-\frac{1}{12}h^2y^{(4)}_{(x_n)}+\frac{1}{360}h^4y^{(6)}_{(x_n)}+0(h^6)$$

$$\text{(iii)}\ S'''_\Delta(x_n) = y'''(x_n)+\frac{1}{2}hy^{(4)}_{(x_n)}+\frac{1}{12}h^2y^{(5)}_{(x_n)}$$

$$-\frac{1}{360}h^4y^{(7)}_{(x_n)}-\frac{1}{1440}h^5y^{(8)}_{(x_n)}+0(h^6) \tag{4.111}$$

From (4.111 iii) we may have

$$\frac{1}{2}(S'''_\Delta(x_n+)+S'''_\Delta(x_n-)) = y'''(x_n)+\frac{1}{12}h^2y^{(5)}_{(x_n)}+0(h^3)$$

$$S'''_\Delta(x_n+)-S'''_\Delta(x_n-) = hy^{(4)}_{(x_n)}-\frac{1}{720}h^5y^{(8)}_{(x_n)}+0(h^7) \tag{4.112}$$

The error $\epsilon(x) = y(x) - S_\Delta(x)$ at any off-nodal point is obtained by substituting (4.111) in the Taylor series expansion of $\epsilon(x_n+\theta h)$, $0 \leqslant \theta \leqslant 1$. We obtain

$$\epsilon(x_n+\theta h) = \frac{\theta^2(\theta-1)^2}{24} h^4 y^{(4)}_{(x_n)} + \frac{\theta(\theta^2-1)(3\theta^2-2)}{360} h^5 y^{(5)}_{(x_n)} + 0(h^6) \quad (4.113)$$

The error is zero for $\theta = 0$ and 1 and also if $y(x)$ is a cubic polynomial so that its fourth and higher derivatives vanish. From (4.113) we get

$$|\ \epsilon(x_n+\theta h)\ | \leqslant \max_{0<\theta<1} \left\{ \frac{\theta^2(\theta-1)^2}{24} h^4 \ |\ y^{(4)}_{(x_n)}\ | \ \right\} = \frac{h^4}{384}\ |\ y^{(4)}_{(x_n)}\ | \quad (4.114)$$

Using (4.112) we may write from (4.113) an estimate of the maximum error in $x_n \leqslant x \leqslant x_{n+1}$ as

$$|\ \epsilon_n\ | \leqslant \frac{h^3}{384} \max\{\ |\ d_n\ |,\ |\ d_{n+1}\ |\ \},\ n = 1(1)N-1 \quad (4.115)$$

where

$$y^{(4)}_{(x_n)} = (S'''_\Delta(x_n+) - S'''_\Delta(x_n-))/h + 0(h^4) = \frac{1}{4} d_n + 0(h^4)$$

Now we use the spline function approximation (4.107) to determine difference scheme for the differential equation (4.87). Differentiating $S_\Delta(x)$ in $[x_{n-1}, x_n]$, we get

$$S'_\Delta(x) = M_n \left[\frac{(x-x_{n-1})^2}{2h} - \frac{h}{6}\right] + M_{n-1}\left[-\frac{(x_n-x)^2}{2h} + \frac{h}{6}\right] + \frac{y_n - y_{n-1}}{h} \quad (4.116)$$

Putting $x = x_{n-\lambda} = x_n - \lambda h$ in $S_\Delta(x)$ and (4.116), we have

$$\text{(i)}\ \ S(x_{n-\lambda}) = M_{n-1}\frac{h^2}{6}\lambda(\lambda^2-1) + M_n\frac{h^2}{6}(1-\lambda)((1-\lambda)^2-1) + \lambda y_{n-1} + (1-\lambda)y_n$$

$$\text{(ii)}\ S'(x_{n-\lambda}) = \frac{y_n-y_{n-1}}{h} - M_{n-1}\frac{h}{2}\left(\lambda^2 - \frac{1}{3}\right) - M_n\frac{h}{2}\left(\frac{1}{3} - (1-\lambda)^2\right) \quad (4.117)$$

where $0 < \lambda \leqslant 1$.

By considering $S_\Delta(x)$ and $S'_\Delta(x)$ in $[x_n, x_{n+1}]$ and putting $x = x_{n+\lambda} = x_n + \lambda h$ we obtain

$$\text{(i)}\ \ S_\Delta(x_{n+\lambda}) = M_{n+1}\frac{h^2}{6}\lambda(\lambda^2-1) + M_n\frac{h^2}{6}(1-\lambda)((1-\lambda)^2-1) + \lambda y_{n+1} + (1-\lambda)y_n$$

$$\text{(ii)}\ S'_\Delta(x_{n+\lambda}) = \frac{y_{n+1}-y_n}{h} + M_{n+1}\frac{h}{2}\left(\lambda^2 - \frac{1}{3}\right) + M_n\frac{h}{2}\left(\frac{1}{3} - (1-\lambda)^2\right) \quad (4.118)$$

We define

$$\text{(i)} \quad h\bar{m}_n = \frac{1}{2}(y_{n+1}-y_{n-1}) - \frac{\alpha_1}{2}\delta^2 y_n$$

$$\text{(ii)} \quad h\bar{m}_{n\pm1} = \frac{1}{2}(y_{n+1}-y_{n-1}) \mp \frac{\beta_1}{2}\delta^2 y_n$$

$$\text{(iii)} \quad \bar{f}_j = f_j(x_j, y_j, \bar{m}_j) \qquad j = n, n\pm1 \tag{4.119}$$

where α_1 and β_1 are arbitrary constants.
Using the cubic spline relations (4.117) and (4.118), we write as

$$\text{(i)} \quad \bar{\bar{y}}_{n\pm\lambda} = \lambda y_{n\pm1} + (1-\lambda)y_n + h^2(a_1\bar{f}_{n\pm1} + a_2\bar{f}_n)$$

$$\text{(ii)} \quad \bar{\bar{m}}_{n\pm\lambda} = \pm(y_{n\pm1}-y_n)/h \pm h(a_1'\bar{f}_{n\pm1} + a_2'\bar{f}_n)$$

$$\text{(iii)} \quad \bar{\bar{f}}_{n\pm\lambda} = f(x_{n\pm\lambda}, \bar{\bar{y}}_{n\pm\lambda}, \bar{\bar{m}}_{n\pm\lambda}) \tag{4.120}$$

where $a_1 = a_1(\lambda) = \frac{\lambda}{6}(\lambda^2-1)$, $a_2 = a_1((1-\lambda))$ and a_1', a_2' are the derivatives of a_1 and a_2 with respect to λ.

Next we define

$$\text{(i)} \quad \hat{m}_n = \bar{m}_n + \frac{\alpha_1 h}{2}(\bar{f}_{n+1}+\bar{f}_{n-1}) - \frac{h}{12}(\bar{f}_{n+1}-\bar{f}_{n-1})$$

$$\text{(ii)} \quad \hat{f}_n = f(x_n, y_n, \hat{m}_n) \tag{4.121}$$

The difference equation for the differential equation (4.87) may be written as

$$-y_{n-1}+2y_n-y_{n+1}+h^2(\theta\bar{\bar{f}}_{n+\lambda}+(1-2\theta)\hat{f}_n+\theta\bar{\bar{f}}_{n-\lambda}) = 0 \tag{4.122}$$

where θ is a parameter.
The truncation error of the method (4.122) is given by

$$T_n = -h^4\left[\left(\theta\lambda^2-\frac{1}{12}\right)y^{(4)}_{(x_n)} + \left(1+\frac{\beta_1}{2}\right)y''_{(x_n)}F^2_{1,n}\left(\frac{1}{6}(1-2\theta)-2a_1'\theta\right)\right]$$
$$+0(\alpha_1 h^5) + 0(h^6) \tag{4.123}$$

where $F_{r,n} = \left(\frac{\partial rf}{\partial y'^r}\right)_n$.

It is clear from (4.123) that for arbitrary α_1, β_1, λ and θ the difference scheme (4.122) is of order two. However, if we choose $\beta_1 = -2$ and $\theta = \frac{1}{12\lambda^2}$ then the coefficient of h^4 is zero and $\alpha_1 \neq 0$ the scheme is of third order. If in addition we choose $\alpha_1 = 0$ then the scheme (4.122) becomes a fourth order scheme.

4.4.4 Second order linear differential equation with significant first derivative

In order to examine the applicability of the difference schemes given in Sections 4.4.1-4.4.3 we apply these schemes to the boundary value problem

$$y''-Ky'=0$$

$$y(0)=1,\quad y(1)=0 \tag{4.124}$$

where K is a positive constant and $K \gg 1$. The theoretical solution of (4.124) at the nodal point x_n is given by

$$y(x_n)=A_1+B_1\,(e^{2R})^n \tag{4.125}$$

where $R=\dfrac{Kh}{2}$ and A_1 and B_1 are arbitrary constants to be determined with the help of the boundary conditions.

Difference schemes

Putting (4.124) into (4.90), we obtain

$$\left(1-R+\frac{R^2}{3}\right)y_{n+1}-2\left(1+\frac{R^2}{3}\right)y_n+\left(1+R+\frac{R^2}{3}\right)y_{n-1}=0 \tag{4.126}$$

The solution of the difference scheme may be written as

$$y_n=A_2+B_2\xi^n \tag{4.127}$$

where

$$\xi=\frac{1+R+\dfrac{R^2}{3}}{1-R+\dfrac{R^2}{3}} \tag{4.128}$$

The root ξ is (2, 2) Padé approximation to e^{2R} (see Table 2.4). The difference scheme has order four. The root ξ remains finite and positive which ensures an oscillation free solution for (4.126). The graph of ξ against R, shown in Fig. 4.1, rises till $R=\sqrt{3}$ and then falls off and becomes asymptotic with $R=1$. If we apply the difference scheme (4.91) to (4.124) then we get

$$\left(1-R+\frac{2}{5}R^2-\frac{1}{15}R^3\right)y_{n+1}-2\left(1+\frac{2}{5}R^2\right)y_n$$

$$+\left(1+R+\frac{2}{5}R^2+\frac{1}{15}R^3\right)y_{n-1}=0 \tag{4.129}$$

which has the root

$$\xi=\frac{\left(1+R+\dfrac{2}{5}R^2+\dfrac{1}{15}R^3\right)}{\left(1-R+\dfrac{2}{5}R^2-\dfrac{1}{15}R^3\right)}$$

This root is (3, 3) Padé approximation to e^{2R} (see Table 2.4). The graph of ξ, given in Fig. 4.1, has an infinite discontinuity at $R = 2.322\ldots$, which is real positive zero of the denominator $\left(1 - R + \frac{2}{5}R^2 - \frac{1}{15}R^3\right)$. Beyond this point, ξ is negative and consequently the difference solution is expected to have oscillations when $R \geqslant 2.5$.

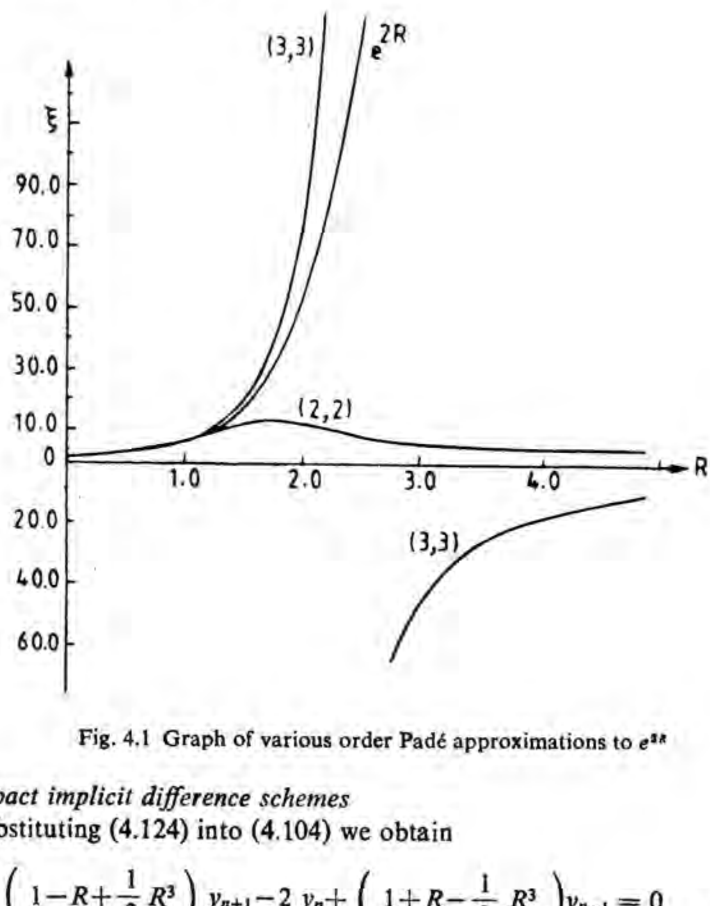


Fig. 4.1 Graph of various order Padé approximations to e^{2R}

Compact implicit difference schemes

Substituting (4.124) into (4.104) we obtain

$$\left(1 - R + \frac{1}{3}R^3\right) y_{n+1} - 2\, y_n + \left(1 + R - \frac{1}{3}R^3\right) y_{n-1} = 0 \tag{4.130}$$

The root ξ is given by

$$\xi = \frac{3 + R(3 - R^2)}{3 - R(3 - R^2)} \tag{4.131}$$

Three cases are possible for general R:

(i) $R < \sqrt{3}$, $\xi > 1$. The difference solution (4.127) with (4.131) is monotone increasing, concave up, and properly approximates the true solution (4.125).

(ii) $\sqrt{3} < R < 2.1038$ (R value where numerator of ξ vanishes), $0 < \xi < 1$. The difference solution (4.127) is monotone increasing but concave down and completely wrong.

(iii) $R > 2.1038$, $-1 > \xi < 0$. The difference solution is oscillatory.

Compact implicit-block methods

In order to solve the boundary value problem (4.124) with the help of the implicit compact schemes (4.100) and (4.101) we develop the following 3×3 block tridiagonal system of equations

$$\text{(i)}\quad \frac{y_{n+1}-y_{n-1}}{2h}-\frac{m_{n+1}+4m_n+m_{n-1}}{6}=0$$

$$\text{(ii)}\quad \frac{y_{n+1}-2\,y_n+y_{n-1}}{h^2}-\frac{M_{n+1}+10M_n+M_{n-1}}{12}=0$$

$$\text{(iii)}\quad M_n-K\,m_n=0 \tag{4.132}$$

where $m_n \approx (y')_n$ and $M_n \approx (y'')_n$.

The above equations hold for $n = 1\,(1)N$. Alternatively, eliminating M_n and using only y_n, m_n, a block tridiagonal system results from using (4.132i) and

$$\frac{y_{n+1}-2\,y_n+y_{n-1}}{h^2}-\frac{K}{12}\,(m_{n+1}+10m_n+m_{n-1})=0 \tag{4.133}$$

The boundary values ($n = 0, N+1$) are required for m_n in (4.133) and for m_n and M_n in (4.132). These are obtained by the methods discussed in Chapter 3. To find the solution of 2×2 system, we write

$$\begin{bmatrix} y_n \\ m_n \end{bmatrix} = \xi^n \begin{bmatrix} c_1 \\ c_2 \end{bmatrix},\; n = 0(1)\,N+1 \tag{4.134}$$

Substituting (4.134) into (4.132 i) and (4.133), we obtain two homogeneous equations in c_1 and c_2. A nontrivial solution results if the determinental equation

$$(\xi-1)\,[(2-R)\xi^3+(6-11R)\xi^2-(6+11R)\xi-(2+R)]=0 \tag{4.135}$$

holds. For $R < 2$, there are always three real roots of (4.135), ξ_+, ξ_-, ξ_0 such that

$$\xi_+ > 1,\; \xi_- < -1,\; -1 < \xi_0 < 0$$

A proper analysis of the difference solution will require consideration of the particular schemes used to approximate the required derivatives at the boundaries. However, in the range of R values ($0 < R < 2/(15)^{1/2}$) where $\xi_+ \leqslant |\,\xi_-\,|$ no dominant oscillations occur.

Difference schemes based on cubic spline

We now apply the difference scheme (4.122) to (4.124) and obtain

$$y_{n+1}[1-(1-\alpha_1+2\alpha_1\theta)R-(1-2\theta)\left(\alpha_1+\frac{\beta_1}{3}\right)R^2+4\beta_1\theta a_1' R^2]$$

$$-2y_n\left[1+\alpha_1 R(1-2\theta)+\beta_1 R^2\left(4\theta a_1'-\frac{1}{3}(1-2\theta)\right)\right]$$

$$+y_{n-1}[1+(1+\alpha_1-2\alpha_1\theta)R+(1-2\theta)\left(\alpha_1-\frac{\beta_1}{3}\right)R^2+4\beta_1\theta a_1' R^2]=0 \quad (4.136$$

We now discuss some special cases of (4.136).

(i) $\lambda = \dfrac{1}{\sqrt{3}}$, $\theta = \dfrac{1}{2}$, α_1 and β_1 arbitrary.

The difference scheme (4.136) becomes

$$(1-R)y_{n+1}-2y_n+(1+R)y_{n-1}=0$$

which is of second order and has oscillations in the difference solution for $R > 1$. The difference scheme (4.122) for the values $\alpha_1 = 0$, $\beta_1 = 0$, becomes

$$\delta^2 y_n = \frac{h^2}{2}\left[\bar{\bar{f}}_{n+\frac{1}{\sqrt{3}}}+\bar{\bar{f}}_{n-\frac{1}{\sqrt{3}}}\right] \quad (4.137)$$

(ii) $\alpha_1 = 0$, $\beta_1 = -2$, $\theta = \dfrac{1}{12\lambda^2}$, λ arbitrary.

The difference scheme (4.136) reduces to the fourth order scheme (4.126). Choosing $\lambda = \dfrac{1}{\sqrt{6}}$ in (4.122) we obtain a fourth order method

$$\delta^2 y_n = \frac{h^2}{2}\left[\bar{\bar{f}}_{n+\frac{1}{\sqrt{6}}}+\bar{\bar{f}}_{n-\frac{1}{\sqrt{6}}}\right] \quad (4.138$$

(iii) $\lambda = \dfrac{1}{\sqrt{3}}$, $\beta_1 = -3\alpha_1$, $\theta = \dfrac{\alpha_1-1}{2\alpha_1}$, $\alpha_1 \geqslant 1$.

The difference scheme (4.136) becomes

$$y_{n+1}-2(1+R+R^2)y_n+(1+2R+2R^2)y_{n-1}=0$$

which is of second order and oscillation free for all R. The parameter α can be suitably chosen. The difference scheme (4.122) becomes

$$\delta^2 y_n = \frac{h^2}{2\alpha_1}\left[(\alpha_1-1)\bar{\bar{f}}_{n+\frac{1}{\sqrt{3}}}+2\hat{f}_n+(\alpha_1-1)\bar{\bar{f}}_{n-\frac{1}{\sqrt{3}}}\right] \quad (4.139)$$

For $\alpha_1 = 1$, we get

$$\delta^2 y_n = h^2 \hat{f}_n$$

(iv) $\theta = \frac{1}{2}, \alpha_1 = 0, \beta_1 = -2, \lambda = \left(\frac{1}{3} - \frac{L}{2R}\right)^{1/2}, L < 2R/3.$

In this case the difference scheme (4.136) assumes the form

$$(1-R+LR)y_{n+1} - 2(1+LR)y_n + (1+R+LR)y_{n-1} = 0.$$

The solution (4.127) becomes

$$y_n = A_2 + B_2 \left(\frac{1+R(1+L)}{1-R(1-L)}\right)^n \tag{4.140}$$

The circumstances under which there are no oscillations follow directly from (4.140):

(i) $R = 0$ all L

(ii) $R > 0$ $L > 1 - \frac{1}{R}$ (4.141)

In particular, if $0 < R < 1$, $L = 0$ leads to no oscillations. As $R \to \infty$, (4.141) requires that $L \to 1$, which results in backward difference approximation. If the off-step point is determined by

$$L = \coth R - \frac{1}{R} \tag{4.142}$$

then we get the theoretical solution (4.125). Furthermore, the fourth order accuracy in y_n can be achieved if we take

$$L = \frac{R}{3}, 0 \leqslant R \leqslant 3 \tag{4.143}$$

This is obtained by expanding coth R in (4.142) and dropping higher order terms in R. The values of L determined by (4.141), (4.142) and (4.143) are referred to as the critical value, optimal value, and high order value, respectively. As can be clearly seen from Figure 4.2, the higher-order value is a good approximation to the optimal value for small R, whereas the critical value closely approximates the optimal value for large R. The difference scheme (4.122) becomes

$$\delta^2 y_n = \frac{h^2}{2}\left[\bar{\bar{f}}_{n+\lambda} + \bar{\bar{f}}_{n-\lambda}\right]. \tag{4.144}$$

4.5 CONVERGENCE OF DIFFERENCE SCHEMES

We shall discuss some properties of the matrices which are relevant for establishing the convergence of the difference schemes for the numerical solution of the boundary value problems.

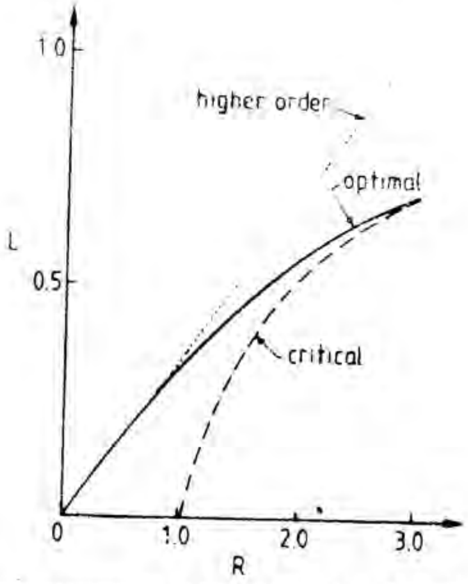


Fig. 4.2 Representation of higher order $L = R/3$, optimal $L = (\coth R - \frac{1}{R})$ and critical $L > 1 - \frac{1}{R}$ values

DEFINITION 4.3 A matrix **A** is said to be reducible if and only if it is similar to a block matrix of the form

$$\mathbf{P}^T\mathbf{A}\mathbf{P} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{0} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

where $\mathbf{A}_{11}$, $\mathbf{A}_{22}$ are square and $\mathbf{P}$ is a permutation matrix. In particular, a tridiagonal matrix $\mathbf{A} = (a_{i,j})$ is irreducible if and only if

$$a_{i,i-1} \neq 0 \quad 2 \leqslant i \leqslant n$$

and

$$a_{i,i+1} \neq 0 \quad 1 \leqslant i \leqslant n-1 \tag{4.145}$$

DEFINITION 4.4 A matrix $\mathbf{A} = (a_{i,j})$ is called diagonally dominant if

$$\sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{i,j}| \leqslant |a_{i,i}|,\ 1 \leqslant i \leqslant n \tag{4.146}$$

and strictly diagonally dominant if strict inequality holds in (4.146) for all i; the matrix is irreducibly diagonally dominant if **A** is irreducible, diagonally dominant, and strict inequality holds in (4.146) for at least one i. If by the notation $\mathbf{v} > \mathbf{0}$ (either for vectors or matrices) we mean that all the elements are nonnegative, then we can define: *a matrix* **A** *is monotone if*

$\mathbf{Az} \geqslant 0$ *implies* $\mathbf{z} \geqslant \mathbf{0}$. A direct consequence of the definition is that every monotone matrix is non singular. A fundamental result of the theory is:

THEOREM 4.1 *A matrix* $\mathbf{A}$ *is monotone if and only if* $\mathbf{A}^{-1} \geqslant \mathbf{0}$.

Another important result is the following:

THEOREM 4.2 *If a matrix* $\mathbf{A}$ *is irreducibly diagonally dominant and has nonpositive off-diagonal elements then* $\mathbf{A}$ *is monotone.*

Finally we quote for further use:

THEOREM 4.3 *If the matrices* $\mathbf{A}$ *and* $\mathbf{B}$ *are monotone and* $B \leqslant A$ *then*

$$\mathbf{A}^{-1} \leqslant \mathbf{B}^{-1}$$

We recall the concept of a norm of a vector, $\| \mathbf{x} \|$. The nonnegative quantity $\| \mathbf{x} \|$ is a measure of the size or length of a vector satisfying;

(i) $\| \mathbf{x} \| > 0$, for $\mathbf{x} \neq \mathbf{0}$ and $\| \mathbf{0} \| = 0$

(ii) $\| c\, \mathbf{x} \| = | c | \; \| \mathbf{x} \|$, for an arbitrary complex number c

(iii) $\| \mathbf{x}+\mathbf{y} \| \leqslant \| \mathbf{x} \| + \| \mathbf{y} \|$ (4.147)

We shall in most cases use the maximum norm

$$\| \mathbf{x} \| = \max_{1 \leqslant i \leqslant n} | x_i | \tag{4.148}$$

At this point we must also recall the concept of a matrix norm. In addition to properties analogous to (4.147) the matrix norm must be consistent with the vector norm that we are using for any vector $\mathbf{x}$ and matrix $\mathbf{A}$

$$\| \mathbf{A}\, \mathbf{x} \| \leqslant \| \mathbf{A} \| \; \| \mathbf{x} \|$$

It is easy to verify that the norm

$$\| \mathbf{A} \| = \max_{1 \leqslant i \leqslant n} \sum_{j=1}^{n} | a_{i,\,j} | \quad \text{(max-row sum)} \tag{4.149}$$

is consistent with max norm $\| \mathbf{x} \|$.

The exact solution $y(x)$ of (4.48) satisfies

$$\begin{aligned}(-1+A_n)y(x_{n-1})+(2+B_n)\, y(x_n)+(-1+C_n)\, y(x_{n+1})& \\ = D_n - T_n,\ 1 \leqslant n \leqslant N&\end{aligned} \tag{4.150}$$

where the truncation error T_n is given by

$$T_n = \frac{1}{12} h^4\, y^{(4)}\,(\xi_1),\ x_{n-1} < \xi_1 < x_{n+1},\ 1 \leqslant n \leqslant N \tag{4.151}$$

for $\quad \beta_0 = \beta_2 = 0,\ \beta_1 = 1$

and $\quad T_n = -\dfrac{1}{240}\, h^6\, y^{(6)}(\xi_2),\ x_{n-1} \leqslant \xi_2 \leqslant x_{n+1},\ 1 \leqslant n \leqslant N \qquad (4.152)$

for $\quad \beta_0 = \beta_2 = \frac{1}{12}, \beta_1 = \frac{10}{12}$

Subtracting Equations (4.150) from (4.48) and substituting $y_n - y(x_n) = \epsilon_n$, we derive the error equation in matrix form as

$$\mathbf{M}\,\mathbf{E} = (\mathbf{J}+\mathbf{Q})\,\mathbf{E} = \mathbf{T} \tag{4.153}$$

where $\mathbf{E} = (\epsilon_i)$ and $\mathbf{T} = (T_i)$ are N-dimensional column vectors.

Thus we note from Equation (4.153) that the convergence of the difference schemes depends on the properties of the matrix **M**. We now show that the matrix $\mathbf{M} = \mathbf{J}+\mathbf{Q}$ is an irreducible, monotone matrix such that $\mathbf{M} \geqslant \mathbf{J}$ and $\mathbf{Q} \geqslant 0$. To prove that the tridiagonal matrix **Q** is nonnegative, we consider A_n, B_n and C_n given in Equation (4.153). Since $\beta_\nu > 0$, $\nu = 0, 1, 2$, we find that A_n's, B_n's and C_n's are positive as $f(x) > 0$, $x \in [a, b]$. Consequently $\mathrm{Q} > \mathbf{0}$, and hence

$$\mathbf{M} = \mathbf{J}+\mathbf{Q} > \mathbf{J}$$

Now from the theory of monotone matrices, it follows that each of the matrices **M** and **J** is irreducible and monotone for sufficiently small values of h. Hence, we have $\mathbf{0} < \mathbf{M}^{-1} < \mathbf{J}^{-1}$.. We now return to the error equation (4.153) and write it in the form

$$\| \mathbf{E} \| \leqslant \| \mathbf{M}^{-1} \| \, \| \mathbf{T} \| \leqslant \| \mathbf{J}^{-1} \| \, \| \mathbf{T} \| \tag{4.154}$$

In order to simplify (4.154) further, we determine $\mathbf{J}^{-1} = (j_{i,j})$ explicitly. On multiplying the rows of **J** by the jth column of $\mathbf{J}^{-1}$, we have the following difference equations:

$$
\begin{aligned}
&\text{(i)}\ \ 2j_{1,j} - j_{2,j} = 0 \\
&\text{(ii)}\ \ -j_{i-1,j} + 2j_{i,j} - j_{i+1,j} = 0, 2 \leqslant i \leqslant j-1 \\
&\text{(iii)}\ \ -j_{j-1,j} + 2j_{j,j} - j_{j+1,j} = 1 \\
&\text{(iv)}\ \ -j_{i-1,j} + 2j_{i,j} - j_{i+1,j} = 0, j+1 \leqslant i \leqslant N-1 \\
&\text{(v)}\ \ -j_{N-1,j} + 2j_{N,j} = 0
\end{aligned} \tag{4.155}
$$

The solution of (4.155 ii) with condition (4.155 (i)) is

$$j_{i,j} = c_2\, i \tag{4.156}$$

where c_2 is independent of i, but may depend on j. Similarly, the solution of (4.155 iv) with condition (4.155 v) is

$$j_{i,j} = c_1 \left(1 - \frac{i}{N+1} \right) \tag{4.157}$$

The constant c_1 depends only on j. On equating the expression for $j_{i,j}$ obtained from (4.156) and (4.157), it is found that

$$c_2 j = c_1 \left(1 - \frac{j}{N+1} \right) \tag{4.158}$$

Also, on substituting the values of $j_{i,j}$ $(i = j-1, j+1)$ obtained from (4.156) and (4.157) in (4.155 iii), we have

$$c_2 + \frac{c_1}{N+1} = 1 \tag{4.159}$$

Finally from Equations (4.159) and (4.158), we get

$$c_1 = j,\ c_2 = \frac{N-j+1}{N+1} \tag{4.160}$$

On substituting the values of c_1 and c_2, the result is

$$j_{i,\,j} = \begin{cases} i\,(N-j+1)/(N+1),\ i \leqslant j \\ j\,(N-i+1)/(N+1),\ i \geqslant j \end{cases} \tag{4.161}$$

From (4.161) we see that $\mathbf{J}^{-1}$ is symmetric. Thus to find $\| \mathbf{J}^{-1} \|$, we calculate the row sum as

$$\begin{aligned} \sum_{j=1}^{N} j_{i,\,j} &= \frac{i\,(N-j+1)}{2} \\ &= \frac{(x_i-a)\,(b-x_i)}{2h^2} \end{aligned} \tag{4.162}$$

Hence we obtain

$$\| \mathbf{J}^{-1} \| = \max_{1 \leqslant i \leqslant N} \sum_{j=1}^{N} | j_{i,j} | \leqslant \frac{(b-a)^2}{8h^2} \tag{4.163}$$

In view of Equation (4.163), Equation (4.154) becomes

$$\| \mathbf{E} \| \leqslant \frac{(b-a)^2}{8h^2} \| \mathbf{T} \| \tag{4.164}$$

Substituting for $\| \mathbf{T} \|$ from Equations (4.151) and (4.152), we get

$$\| \mathbf{E} \| \leqslant \frac{1}{96}\,(b-a)^2\, h^2\, M_4 = 0\,(h^2) \tag{4.165}$$

and
$$\| \mathbf{E} \| \leqslant \frac{1}{1920}(b-a)^2\, h^4\, M_6 = 0\,(h^4) \tag{4.166}$$

where
$$M_i = \max_{a \leqslant x \leqslant b} | y^{(i)}\,(x) |$$

From Equations (4.165) and (4.166) it follows that $\| \mathbf{E} \| \to 0$ or $y_n \to y(x_n)$ as $h \to 0$. This establishes the convergence of second and fourth order methods.

The truncation error for (4.51) is given by

$$T_n = \left[\frac{1}{302400}\ M_8 + \frac{1}{21600}\ M_6 f_M + \frac{1}{3600}\, f'_M\ M_5 \right] h^8 + 0\,(h^{10}),$$
$$1 \leqslant n \leqslant N \tag{4.167}$$

where $$f'_M = \max_{a \leqslant x \leqslant b} |f'(x)|$$

Substituting the value of $\| \mathbf{T} \|$ in Equation (4.164) from Equation (4.167), we establish the convergence of the sixth order method. In a similar manner, we may prove the convergence of the difference scheme based on the four-point Lobatto quadrature formula as applied to the mixed boundary value problem in Section 4.3.4.

4.6 NONLINEAR BOUNDARY VALUE PROBLEM $y^{(iv)} = f(x, y)$

We consider two-point boundary value problems involving the fourth order differential equation

$$y^{(iv)} = f(x, y) \tag{4.168}$$

With the boundary conditions prescribing either

$$\begin{aligned} y(a) &= A_0, & y(b) &= B_0 \\ y'(a) &= A_1, & y'(b) &= B_1 \end{aligned} \tag{4.169}$$

or

$$\begin{aligned} y(a) &= A_0, & y(b) &= B_0 \\ y''(a) &= A_2, & y''(b) &= B_2 \end{aligned} \tag{4.170}$$

Here, $-\infty < a \leqslant x \leqslant b < \infty$, $A_0, B_0, A_1, B_1, A_2, B_2$ are finite constants. In the following we shall assume that $y(x)$ is sufficiently differentiable and that a unique solution of (4.168) subject to either (4.169) or (4.170) exists.

4.6.1 Difference schemes

Consider the identity

$$\delta^4 y(x_n) = \frac{1}{6}\left\{ \int_{x_n}^{x_{n+2}} (x_{n+2}-t)^3 \left[y^{iv}(t) + y^{iv}(2x_n - t) \right] dt \right.$$
$$\left. - 4 \int_{x_n}^{x_{n+1}} (x_{n+1}-t)^3 \left[y^{iv}(t) + y^{iv}(2x_n - t) \right] dt \right\} \tag{4.171}$$

If we use the transformations $t = x_n + h(1+u)$ in the first integral on the right-hand side and $t = x_n + h(1+u)/2$ in the second integral, (4.171) changes into

$$\delta^4 y(x_n) = \frac{h^4}{6}\int_{-1}^{1} (1-u)^3 \left\{ y^{iv}(x_n - h(1+u)) + y^{iv}(x_n + h(1+u)) \right.$$
$$\left. - \frac{1}{4} y^{iv}\left(x_n - \frac{h}{2}(1+u) \right) - \frac{1}{4} y^{iv}\left(x_n + \frac{h}{2}(1+u) \right) \right\} du \tag{4.172}$$

As in Section 4.3.1, we replace the integral in (4.172) with the aid of a suitable quadrature rule and obtain the difference scheme of the form

$$\delta^4 y_n = h^4 \left\{ W_0 y_n^{iv} + W_1(y_{n-1}^{iv} + y_{n+1}^{iv}) + W_2(y_{n-2}^{iv} + y_{n+2}^{iv}) + \sum_{j=3}^{v} W_j[(y_{n-\theta_j}^{iv} + y_{n+\theta_j}^{iv}) - \frac{1}{4}(y_{n-1/2\theta_j}^{iv} + y_{n+1/2\theta_j}^{iv})] \right\} \quad (4.173)$$

The values $W_0 = 1$, $W_1 = W_2 = W_j = 0$ give a difference scheme

$$\delta^4 y_n = h^4 y_n^{iv} \quad (4.174)$$

which is of the order two with local truncation error $(1/6)\ h^6\ y^{(6)}\ (\xi)$, $x_{n-2} < \xi < x_{n+2}$. If we take $W_2 = 0$, $W_j = 0$, $j = 3, 4 \ldots$, we find that the values $W_0 = 2/3$, $W_1 = 1/6$ give fourth order difference scheme

$$\delta^4 y_n = \frac{h^4}{6}[y_{n-1}^{iv} + 4y_n^{iv} + y_{n+1}^{iv}] \quad (4.175)$$

with the local truncation error

$$T_n^* = -\frac{I}{720}\ h^8\ y^{(8)}\ (x_n) + \ldots \quad (4.176)$$

In Equation (4.173) if $W_j = 0$, $j = 3, 4 \ldots$, we can determine W_0, W_1, and W_2 uniquely so that (4.173) has order six. Thus, the sixth order scheme is

$$\delta^4 y_n = \frac{h^4}{720}[474\ y_n^{iv} + 124(y_{n-1}^{iv} + y_{n+1}^{iv}) - (y_{n-2}^{iv} + y_{n+2}^{iv})] \quad (4.177)$$

with local truncation error

$$T_n^* = \frac{1}{3024}\ h^{10}\ y^{(10)}(x_n) + \ldots \quad (4.178)$$

We also require the difference expressions for the derivatives $y'(x)$ and $y''(x)$ at the boundary points x_0 and x_{N+1}. We define

$$\text{(i)} \quad \sum_{k=0}^{3} b_k y_k + ch^{1+\alpha} y_0^{(1+\alpha)} + h^4 \sum_{k=0}^{3} d_k f_k = 0$$

$$\text{(ii)} \quad \sum_{k=0}^{3} b_k y_{N+1-k} + c(-h)^{1+\alpha} y_{N+1}^{(1+\alpha)} + h^4 \sum_{k=0}^{3} d_k f_{N+1-k} = 0 \quad (4.179)$$

where $\alpha \in \{0, 1\}$ and b_k, c and d_k, are arbitrary parameters to be determined. Here, we require that the local truncation error in (4.179) to be of the form $0\ (h^{7+\alpha})$; for then the difference expressions of the boundary conditions (4.169) and (4.170) together with the difference equation (4.177) give $0(h^6)$ difference method. Now so that each difference equation (4.179i) and (4.179ii) is consistent we obtain a system of four equations for the determination of five parameters b_0, b_1, b_2, b_3 and c. If we put $b_3 = 1$, then, for $\alpha = 0$,

(i) $b_0 = -\frac{11}{2}$, $b_1 = 9$, $b_2 = -\frac{9}{2}$, $b_3 = 1$, $c = -3$ and, for $\alpha = 1$,

(ii) $b_0 = -2$, $b_1 = 5$, $b_2 = -4$, $b_3 = 1$, $c = 1$ (4.180)

For $\alpha = 0$, we obtain d_0, d_1, d_2 in terms of d_3 as a free parameter. For simplicity, we set $d_3 = 0$, and then

(i) $d_0 = -\frac{1}{40}$, $d_1 = -\frac{22}{40}$, $d_2 = -\frac{7}{40}$, $d_3 = 0$

For $\alpha = 1$ all the d_k are uniquely determined given by

(ii) $d_0 = \frac{28}{360}$, $d_1 = \frac{245}{360}$, $d_2 = \frac{56}{360}$, $d_3 = \frac{1}{360}$ (4.181)

The truncation error is given by

(i) $T_1^{(\alpha)} = C_\alpha h^{7+\alpha} y^{(7+\alpha)}_{(\xi_1)}$

(ii) $T_N^{(\alpha)} = C_\alpha(-h)^{7+\alpha} y^{(7+\alpha)}_{(\xi_N)}$ (4.182)

where

$$\xi_1 \in (x_0, x_3),\ \xi_N \in (x_{N-2}, x_{N+1}) \text{ and}$$

$$C_\alpha = \begin{vmatrix} -\frac{1}{280}, & \alpha = 0 \\ \frac{241}{60480}, & \alpha = 1 \end{vmatrix}$$

With the parameter values in (4.180) and (4.181), the difference equation: (4.179) become

(i) $-\frac{11}{2} y_0 + 9y_1 - \frac{9}{2} y_2 + y_3 - 3h\, y'_0 - \frac{h^4}{40}(f_0 + 22f_1 + 7f_2) = 0$

(ii) $-\frac{11}{2} y_{N+1} + 9y_N - \frac{9}{2} y_{N-1} + y_{N-2} + 3h\, y'_{N+1}$

$- \frac{h^4}{40}(f_{N+1} + 22f_N + 7f_{N-1}) = 0$ (4.183

and

(i) $-2y_0 + 5y_1 - 4y_2 + y_3 + h^2 y''_0 + \frac{h^4}{360}(28f_0 + 245f_1 + 56f_2 + f_3) = 0$

(ii) $-2y_{N+1} + 5y_N - 4y_{N-1} + y_{N-2} + h^2 y''_{N+1}$

$+ \frac{h^4}{360}(28f_{N+1} + 245f_N + 56f_{N-1} + f_{N-2}) = 0$ (4.184)

4.6.2 Fourth order linear boundary value problem

Let us solve numerically the differential equation

$$y^{(iv)} + f(x)\, y = g(x),\ f(x) \geqslant 0,\ x \in [a, b] \tag{4.185}$$

subject to the boundary conditions

$$\begin{aligned} y(a) &= \alpha_1,\ y''(a) = \beta_1 \\ y(b) &= \alpha_2,\ y''(b) = \beta_2 \end{aligned} \tag{4.186}$$

Replacing the differential equation by the difference equation at the nodal points $x_n = a+nh$, $1 \leqslant n \leqslant N$, we get

$$y_{n-2}-4y_{n-1}+6y_n-4y_{n+1}+y_{n+2}+h^4 f_n y_n = h^4 g_n,\ 1 \leqslant n \leqslant N \tag{4.187}$$

where $\qquad f(x_n) = f_n,\ g(x_n) = g_n$ and $h = (b-a)/(N+1)$

The boundary conditions become

$$y_0 = \alpha_1,\ y_{-1}-2\alpha_1+y_1 = h^2\beta_1+\frac{h^4}{12}(-f_0\alpha_1+g_0)$$

$$y_{N+1} = \alpha_2\ \ y_{N+2}-2\alpha_2+y_N = h^2\beta_2+\frac{h^4}{12}(-f_{N+1}\alpha_2+g_{N+1}) \tag{4.188}$$

Substituting from (4.188) for y_{-1} and y_{N+2} in the first $(n = 1)$ and the last $(n = N)$ equations in (4.187), we obtain

$$\begin{aligned} &(5+h^4 f_1)\,y_1-4y_2+y_3 = c_1 \\ &-4y_1+(6+h^4 f_2)\,y_2-4y_3+y_4 = c_2 \\ &y_{n-2}-4y_{n-1}+(6+h^4 f_n)\,y_n-4y_{n+1}+y_{n+2} = c_n,\ 3 \leqslant n \leqslant N-2 \\ &y_{N-3}-4y_{N-2}+(6+h^4 f_{N-1})\,y_{N-1}-4y_N = c_{N-1} \\ &y_{N-2}-4y_{N-1}+(5+h^4 f_N)\,y_N = c_N \end{aligned} \tag{4.189}$$

where

$$\begin{aligned} c_1 &= h^4 g_1+2\alpha_1-h^2\beta_1+\frac{h^4}{12}(f_0\alpha_1-g_0) \\ c_2 &= h^4 g_2-\alpha_1 \\ c_n &= h^4 g_n,\ 3 \leqslant n \leqslant N-2 \\ c_{N-1} &= h^4 g_{N-1}-\alpha_2 \\ c_N &= h^4 g_N+2\alpha_2-h^2\beta_2+\frac{h^4}{12}(f_{N+1}\alpha_2-g_{N+1}) \end{aligned} \tag{4.190}$$

Equations (4.189) in matrix form become

$$\mathbf{A}\,\mathbf{y} = \mathbf{c} \tag{4.191}$$

where $\mathbf{A}$ is a matrix of order N,

$$\mathbf{A} = \begin{bmatrix} 5+h^4 f_1 & -4 & 1 & & & & \\ -4 & 6+h^4 f_2 & -4 & 1 & & & \\ 1 & -4 & 6+h^4 f_3 & -4 & 1 & & \\ & \cdot & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot & \\ & & & 1 & -4 & 6+h^4 f_{N-1} & -4 \\ & & & & 1 & -4 & 5+h^4 f_N \end{bmatrix} \tag{4.192}$$

and $\mathbf{c} = (c_i)$ is the N-dimensional column vector defined by (4.190). The truncation errors associated with equations in (4.189) can be obtained as

$$T_1 = \frac{59}{360} h^6 M_6 \tag{4.193}$$

$$T_n = \frac{1}{6} h^6 M_6,\ 2 \leqslant n \leqslant N-1 \tag{4.194}$$

$$T_N = \frac{59}{360} h^6 M_6 \tag{4.195}$$

where $M_6 = \max\limits_{a \leqslant x \leqslant b} | y^{(6)}(x) |$

We now use the fourth order difference scheme (4.175) to solve the fourth order boundary value problem. We note that the scheme (4.175)

$$\delta^4 y_n = \frac{h^4}{6} (y_{n-1}^{iv} + 4y_n^{iv} + y_{n+1}^{iv}),\ 2 \leqslant n \leqslant N-1 \tag{4.196}$$

gives us $N-2$ relations in the N unknowns y_i, $1 \leqslant i \leqslant N$. If we make use of the boundary conditions (4.186), we get two more relations

$$5y_1 - 4y_2 + y_3 = 2\alpha_1 - h^2\beta_1 + \frac{h^4}{360} (28y_0^{iv} + 245y_1^{iv} + 56y_2^{iv} + y_3^{iv}) \tag{4.197}$$

and

$$\begin{aligned} y_{N-2} - 4y_{N-1} + 5y_N &= 2\alpha_2 - h^2\beta_2 \\ &\quad + \frac{h^4}{360} (y_{N-2}^{iv} + 56y_{N-1}^{iv} + 245y_N^{iv} + 28y_{N+1}^{iv}) \end{aligned} \tag{4.198}$$

Substituting the values of y_n^{iv}, $0 \leqslant n \leqslant N+1$ in the relations (4.196), (4.197) and (4.198) the system of equations can be replaced by a single matrix equation of the form (4.191),

$$A\mathbf{y} = \mathbf{c}$$

where

$$\mathbf{A} = \begin{bmatrix} 5+\frac{49}{72}h^4f_1 & -4+\frac{7}{45}h^4f_2 & 1+\frac{1}{360}h^4f_3 & & & \\ -4+\frac{1}{6}h^4f_1 & 6+\frac{2}{3}h^4f_2 & -4+\frac{1}{6}h^4f_3 & 1 & & \\ 1 & -4+\frac{1}{6}h^4f_2 & 6+\frac{2}{3}h^4f_3 & -4+\frac{1}{6}h^4f_4 & 1 & \\ & \cdot & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot & \cdot \\ & & 1 & -4+\frac{1}{6}h^4f_{N-2} & 6+\frac{2}{3}h^2f_{N-1} & 4+\frac{1}{6}h^4f_N \\ & & & 1+\frac{1}{360}h^4f_{N-2} & -4+\frac{7}{45}h^4f_{N-1} & 5+\frac{49}{72}h^4f_N \end{bmatrix}$$

and
$$\mathbf{c} = \begin{bmatrix} \left(2-\frac{7}{90}h^4 f_0\right)\alpha_1 - h^2\beta_1 + \frac{h^4}{360}(28g_0+245g_1+56g_2+g_3) \\ -\alpha_1 \qquad + \frac{h^4}{6}(g_1+4g_2+g_3) \\ \vdots \\ -\alpha_2 \qquad + \frac{h^4}{6}(g_{N-2}+4g_{N-1}+g_N) \\ \left(2-\frac{7}{20}h^4 f_N\right)\alpha_1 - h^2\beta_2 + \frac{h^4}{360}(g_{N-2}+56g_{N-1}+245g_N+28g_{N+1}) \end{bmatrix}$$

The truncation error of the difference equations is given by

$$|T_n| \leqslant \frac{241}{60480}h^8 M_8,\ n = 1, N$$

$$|T_n| \leqslant 0.002183h^8 M_8,\ 2 \leqslant n \leqslant N-1$$

where
$$M_n = \max_{a\leqslant x\leqslant b} |y^{(n)}(x)|$$

The matrix **A** is a five-band matrix, the nonzero elements appearing only along the principal diagonals. We can easily extend the method of solution of a tridiagonal system to a five-band system.

4.6.3 Solution of five-band system

The above system of equations can be written as

$$\begin{bmatrix} C_1 & D_1 & E_1 & & & & \\ B_2 & C_2 & D_2 & E_2 & & & \\ A_3 & B_3 & C_3 & D_3 & E_3 & & \\ & & \cdots\cdots & & & & \\ & & A_{N-1} & B_{N-1} & C_{N-1} & D_{N-1} & \\ & & & A_N & B_N & C_N & \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{bmatrix} = \begin{bmatrix} \alpha_1^* \\ \alpha_2^* \\ \vdots \\ \alpha_{N-1}^* \\ \alpha_N^* \end{bmatrix} \tag{4.199}$$

where A_i B_i, C_i, D_i, E_i and α_i^* are the known quantities. As in Section 4.3.3, we assume the following recurrence relations

$$y_n = h_n - \omega_n y_{n+1} - \gamma_n y_{n+2},\ 0 \leqslant n \leqslant N \tag{4.200}$$

We use (4.200) to find y_{n-1} and y_{n-2} and substitute them in the equation

$$A_n y_{n-2} + B_n y_{n-1} + C_n y_n + D_n y_{n+1} + E_n y_{n+2} = \alpha_n^*,\ 2 \leqslant n \leqslant N-2 \tag{4.201}$$

and by comparing it with (4.200), we get

$$h_n = (\alpha_n^* - A_n h_{n-2} - \delta_n h_{n-1})/\omega_n^*$$
$$\omega_n = (D_n - \delta_n \gamma_{n-1})/\omega_n^*$$
$$\gamma_n = E_n/\omega_n^*$$

$$\omega_n^* = C_n - \gamma_{n-2}A_n - \omega_{n-1}\delta_n \tag{4.202}$$

where $\delta_n = B_n - A_n\omega_{n-2}$.

In view of the first boundary conditions in (4.186) we have

$$h_0 = y_0,\ \omega_0 = 0,\ \gamma_0 = 0 \tag{4.203}$$

Equation (4.200) will be identical with the first equation in (4.199) if

$$h_1 = \alpha_1^*/\omega_1^*,\ \omega_1 = D_1/\omega_1^*,\ \gamma_1 = E_1/\omega_1^* \tag{4.204}$$

where $\omega_1^* = c_1$.

The second condition in (4.186) will be fulfilled if

$$\gamma_N = 0$$

The relation (4.202) together with (4.203) and (4.204) will hold for $0 \leqslant n \leqslant N$ if

$$\gamma_{N-1} = 0$$

and hence

$$y_N = h_N - \omega_N y_{N+1}$$

The values $y_{N-1}, y_{N-2}, \ldots, y_2, y_1$ can be obtained by backward substitution in the equation

$$y_n = h_n - \omega_n y_{n+1} - \gamma_n y_{n+2},\ n = N-1, \ldots, 2, 1$$

Example 4.5 Use a second order difference scheme to solve the boundary value problem

$$y^{(iv)} + 4y = 1$$
$$y(\pm 1) = 0,\ y''(\pm 1) = 0$$

with $h = \dfrac{1}{2}$ and $\dfrac{1}{128}$.

The theoretical solution is given by

$$y(x) = \frac{1}{4}[1 - 2(\sin 1 \sinh 1 \sin x \sinh x$$
$$+ \cos 1 \cosh 1 \cos x \cosh x)/(\cos 2 + \cosh 2)$$

We define the nodal points $x_{\pm i}$

$$x_{\pm i} = \pm ih,\ h = 1/(N+1),\ i = 0, 1, 2, \ldots, N+1$$

In view of the symmetry, we need to replace the differential equation by the difference equation at nodal points $x_0, x_1, \ldots, x_N$.

Equations in (4.188) become

$$y_{N+1} = 0,\ y_{N+2} = -y_N + \frac{h^4}{12}$$

The necessary equations are given by

$$\begin{aligned} (6+4h^4)\, y_0 - 8y_1 + 2y_2 &= h^4, & n &= 0 \\ -4y_0 + (7+4h^4)\, y_1 - 4y_2 + y_3 &= h^4, & n &= 1 \end{aligned}$$

$$y_{n-2}-4y_{n-1}+(6+4h^4)\,y_n-4y_{n+1}+y_{n+2} = h^4,\ 2 \leqslant n \leqslant N-2$$
$$y_{N-3}-4y_{N-2}+(6+4h^4)\,y_{N-1}-4y_N = h^4,\ n = N-1$$
$$y_{N-2}-4y_{N-1}+(5+4h^4)\,y_N = \frac{11}{12}h^4, \qquad n = N$$

Using the boundary conditions, the above equations for $h = \frac{1}{2}$ become

$$100\,y_0-128y_1 = 1$$
$$-64\,y_0+100\,y_1 = \frac{11}{12}$$

Solving we obtain

$$y_0 = 0.1202,\ y_1 = 0.0861$$

For $h = 1/128$, we have listed the values of y_l and $\epsilon_l = y(x_l)-y_l$ at intervals of 1/4 in Table 4.5.

TABLE 4.5 SOLUTION OF $y^{(iv)}+4y = 1,\ y(\pm 1) = 0,\ y''(\pm 1) = 0,\ h = 1/128$

$\pm x_l$	y_l	ϵ_l
1.0	0.0	0.0
0.75	0.049150	1.929−06
0.50	0.089793	3.557−06
0.25	0.116257	4.640−06
0.0	0.125411	5.018−06

4.7 LINEAR EIGENVALUE PROBLEMS

Let us consider the numerical solution of the linear homogeneous second order differential equation

$$y''+\Lambda\,y = 0,\ \Lambda \text{ a constant} \tag{4.205}$$

subject to the homogeneous boundary conditions

$$y(a) = 0,\ y(b) = 0 \tag{4.206}$$

Applying (4.18) at nodal points $x_n = x_0+nh,\ 1 \leqslant n \leqslant N$, and substituting $y''_n = -\Lambda\,y_n$ and $y_0 = 0,\ y_{N+1} = 0$, we get the following system of homogeneous equations

$$-y_{n-1}+2y_n-y_{n+1}-\lambda\,(\beta_0 y_{n-1}+\beta_1 y_n+\beta_2\,y_{n+1}) = 0,\ 1 \leqslant n \leqslant N \tag{4.207}$$

where $\lambda = h^2\Lambda$.

This in matrix notation can be put in the form

$$(\mathbf{J}-\lambda\mathbf{B})\,\mathbf{y} = \mathbf{0} \tag{4.208}$$

where the matrices **J** and **B** are defined in (4.19). However, in general the forms of the matrices **J** and **B** depend on the difference scheme used in approximating (4.205). An interesting special case of (4.208) is given by

$$(\mathbf{A}-\lambda\mathbf{I})\,y = \mathbf{0} \tag{4.209}$$

In fact, (4.208) can be reduced to (4.209) if we assume $\mathbf{B}$ is nonsingular and $\mathbf{A} = \mathbf{B}^{-1}\mathbf{J}$. Thus, we have reduced (4.205) and (4.206) to the eigenvalue problem (4.209). The eigenvalues and eigenvectors of $\mathbf{A}$ determined from (4.209) will give approximations to the nontrivial solution of (4.205). We now briefly give some elementary properties of the eigenvalues and eigenvectors of the matrices.

4.7.1 Eigenvalues and eigenvectors

The equations represented by (4.209) are a set of N homogeneous linear equations in N unknowns and such a system of equations will be consistent if and only if

$$\det [\mathbf{A}-\lambda\mathbf{I}] = 0 \tag{4.210}$$

The expansion of this determinant will lead to a polynomial equation of degree $\leqslant N$ in λ. The roots of this are called *eigenvalues* of matrix $\mathbf{A}$, and the equation is called the *characteristic equation* of the matrix. The eigenvalues may be distinct or repeated, real or complex. If all the eigenvalues are distinct, there is a nontrivial solution $\mathbf{y}_r$ (eigenvector) corresponding to each eigenvalue λ_r such that

$$\mathbf{A}\ \mathbf{y}_r = \lambda_r\ \mathbf{y}_r \tag{4.211}$$

The eigenvector $\mathbf{y}_r$ is arbitrary to the extent of an indeterminate multiplier. We usually scale the eigenvectors so that they have unit length. This is called *normalizing* the eigenvector. If we premultiply (4.211) by the transpose $\mathbf{y}_r^T$ of $\mathbf{y}_r$, we get

$$\lambda_r = \frac{\mathbf{y}_r^T\mathbf{A}\mathbf{y}_r}{\mathbf{y}_r^T\ \mathbf{y}_r} \tag{4.212}$$

which gives an expression for the eigenvalues in terms of the eigenvectors. For an arbitrary vector $\mathbf{y}$, (4.212) is called the *Rayleigh quotient*

$$\lambda_R = \frac{\mathbf{y}^T\ \mathbf{A}\ \mathbf{y}}{\mathbf{y}^T\ \mathbf{y}} \tag{4.213}$$

Let us denote by $\mathbf{A}^T$ the transpose of matrix $\mathbf{A}$. Then $(\mathbf{A}^T-\lambda\mathbf{I})$ is the transpose of $(\mathbf{A}-\lambda\mathbf{I})$ and therefore has the same determinant as (4.210). It follows that the characteristic equation and the set of eigenvalues of $\mathbf{A}^T$ are the same as those of $\mathbf{A}$. However, the eigenvectors are generally different unless $\mathbf{A}$ is a symmetric matrix. We can easily prove that

(i) the eigenvalues of a real symmetric matrix are real,

(ii) the eigenvectors of a real symmetric matrix associated with different eigenvalues are orthogonal.

In physical problems we rarely need to determine the whole set of eigenvalues of (4.209). We are generally interested in the *largest* or *smallest* eigenvalue. We assume that the eigenvalues of $\mathbf{A}$ are real and distinct and we can arrange these as

$$|\lambda_1| > |\lambda_2| \cdots > |\lambda_N| \tag{4.214}$$

Furthermore, let us denote the complete set of eigenvectors of $\mathbf{A}$ by $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N$. We can easily determine the largest or smallest eigenvalue and the corresponding eigenvector.

4.7.2 The iteration method

We take an arbitrary initial vector $\mathbf{y}^{(0)}$ which we express as a linear combination of the eigenvectors

$$\mathbf{y}^{(0)} = c_1\mathbf{y}_1 + c_2\mathbf{y}_2 + \cdots + c_N\mathbf{y}_N \tag{4.215}$$

Repeated applications of $\mathbf{A}$ give

$$\begin{aligned}\mathbf{y}^{(k)} &= \mathbf{A}\,\mathbf{y}^{(k-1)} = A^k\ \mathbf{y}^{(0)} \\ &= \lambda_1^k\left[c_1\,\mathbf{y}_1 + \sum_{r=2}^{N} c_r\left(\frac{\lambda_r}{\lambda_1}\right)^k \mathbf{y}_r\right]\end{aligned} \tag{4.216}$$

In view of (4.214) and for sufficiently large values of k, the vector

$$c_1\,\mathbf{y}_1 + \sum_{r=2}^{N} c_r\left(\frac{\lambda_r}{\lambda_1}\right)^k \mathbf{y}_r$$

converges to $c_1\mathbf{y}_1$, which is the eigenvector corresponding to the eigenvalue λ_1. The ratio of $\mathbf{y}^{(k+1)}$ to $\mathbf{y}^{(k)}$ will tend to λ_1, that is to say, the ratio of the corresponding elements of $\mathbf{y}^{(k+1)}$ and $\mathbf{y}^{(k)}$ will tend to λ_1. This algorithm is called the *power-method*. From (4.216) the convergence is given by the factor $(\lambda_2/\lambda_1)^k$. In principle this enables us to determine λ_1 and the associated $\mathbf{y}_1$ to any desired accuracy. Unless λ_2/λ_1 is much less than unity, this method is not very efficient. In the case of symmetric matrices, we can obtain better estimates for λ_1 if we use (4.216) to construct the *Rayleigh* quotient (4.213). We obtain

$$\lambda_R = \frac{(\mathbf{y}^{(k)})^T\,(\mathbf{y}^{(k)})}{(\mathbf{y}^{(k)})^T\,(\mathbf{y}^{(k-1)})}$$

For real symmetric matrices, the eigenvectors are orthogonal. Thus we have

$$(\mathbf{y}^{(k)})^T\,(\mathbf{y}^{(k)}) = \sum_{r=1}^{N} c_r^2\lambda_r^{2k} = \lambda_1^{2k}\sum_{r=1}^{N} c_r^2\left(\frac{\lambda_r}{\lambda_1}\right)^{2k}$$

$$(\mathbf{y}^{(k)})^T\,(\mathbf{y}^{(k-1)}) = \sum_{r=1}^{N} c_r^2\lambda_1^{2k-1} = \lambda_1^{2k-1}\sum_{r=1}^{N} c_r^2\left(\frac{\lambda_r}{\lambda_1}\right)^{2k-1}$$

and hence

$$\lambda_R \approx \lambda_1\left[\frac{c_1^2 + \sum_{r=1}^{N} c_r^2\left(\frac{\lambda_r}{\lambda_1}\right)^{2k}}{c_1^2 + \sum_{r=1}^{N} c_r^2\left(\frac{\lambda_r}{\lambda_1}\right)^{2k-1}}\right]$$

The convergence to λ_1 is given by a factor $(\lambda_2/\lambda_1)^{2k}$ which is twice as fast as given by (4.216).

For computation the procedure just described can be formulated in the following way. We use the formula

$$\mathbf{y}^{(k+1)} = \mathbf{A}\mathbf{y}^{(k)}\quad k = 0, 1, 2, \cdots \tag{4.217}$$

to compute the sequence of iterated vectors from the initial approximation $\mathbf{y}^{(0)}$. The initial approximation may be taken as $[0\ 0\ \dots\ 1]^T$ or $[1\ 1\ \dots\ 1]^T$. We define the scalar α_0 as

$$[(\mathbf{y}^{(0)})^T\,(\mathbf{y}^{(0)})]^{1/2} = \alpha_0$$

We now determine $\mathbf{y}^{(1)}$ from (4.217) and calculate the scalar α_1 as

$$\alpha_1 = [(\mathbf{y}^{(1)})^T\,(\mathbf{y}^{(1)})]^{1/2}$$

We now demand that $\mathbf{y}^{(1)}$ be scaled as $\widetilde{\mathbf{y}}^{(1)}$ such that

$$[(\widetilde{\mathbf{y}}^{(1)})^T\,(\widetilde{\mathbf{y}}^{(1)})]^{1/2} = \alpha_0$$

Thus we multiply $\mathbf{y}^{(1)}$ by the factor $\sqrt{(\alpha_0/\alpha_1)}$.

We repeat in this manner and generate the successive trial vectors and scale the results by a factor $\sqrt{(\alpha_1/\alpha_k)}$. The factors α_k approach an asymptotic value λ_1 and at a rate dependent on $(\lambda_2/\lambda_1)^{2k}$. Thus we can find λ_1 by calculating the quantity α_i.

If the *smallest* eigenvalue of λ is required, we may first transform (4.209) to the equation

$$\mathbf{y} = \lambda \mathbf{A}^{-1}\,\mathbf{y}$$

which we may write as

$$\mathbf{M}\mathbf{y} = \mu \mathbf{y} \tag{4.218}$$

where $$\mathbf{M} = \mathbf{A}^{-1},\ \mu = \frac{1}{\lambda}$$

The largest eigenvalue of μ for (4.218) can then be determined by the iteration method and its reciprocal is the smallest eigenvalue of (4.209).

We now state two results which give us the criterion for localizing eigenvalues of the square matrix $A = (a_{ij})$.

THEOREM (*Gerschgorin*) 4.4 *The modulus of the largest eigenvalue of* **A** *cannot exceed the largest sum of the moduli of the terms along any row or any column.*

THEOREM (*Brauer*) 4.5 *Let P_s be the sum of the moduli of the terms along the* sth *row excluding the diagonal elements a_{ss}. Then every eigenvalue of* **A** *lies inside or on the boundary of at least one of the circles* $|\lambda - a_{ss}| = P_s$.

4.7.3 Convergence analysis

We consider the eigenvalue problem

$$y'' + (\lambda q(x) - r(x))\,y = 0$$
$$y(a) = 0,\ y(b) = 0 \tag{4.219}$$

where $q(x)$, $r(x)$ are continuous on $[a, b]$ and $q(x) > 0$, $r(x) \geqslant 0$ on $[a, b]$. The equation (4.219) is a special case of the *Sturm-Liouville* problem. The nodal points are given by $x_n = a+nh$, $n = 0(1)N$, $h = (b-a)/N$. The problem (4.219) has an infinite sequence of real and positive eigenvalues $0 < \lambda_1 < \lambda_2 < \lambda_3 \ldots$ Applying the Numerov method (4.23) to (4.219), we get the $N-1$ linear system of equations

$$(\mathbf{J}+h^2\mathbf{B}\,\mathbf{R})\mathbf{y}-h^2\mathbf{B}\Lambda\mathbf{Q}\mathbf{y} = \mathbf{0} \tag{4.220}$$

where Λ is an approximation to λ and

$$\mathbf{J} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}, \quad \mathbf{B} = \frac{1}{12}\begin{bmatrix} 10 & 1 & & & \\ 1 & 10 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 10 & 1 \\ & & & 1 & 10 \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} r_1 & & & \\ & r_2 & & \\ & & \ddots & \\ & & & r_{N-1} \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} q_1 & & & \\ & q_2 & & \\ & & \ddots & \\ & & & q_{N-1} \end{bmatrix}$$

$$\mathbf{y} = [y_1 y_2 \cdots y_{N-1}]^T, \; r_n = r(x_n), \; q_n = q(x_n).$$

We now show that the equation (4.220) provides real, positive and $0(h^4)$-convergent approximations for λ. We observe that the matrix $\mathbf{J}$ is symmetric, the matrix $\mathbf{B}(\mathbf{R}-\Lambda\mathbf{Q})$ is not symmetric and therefore to express (4.220) in terms of the symmetric matrices we rewrite (4.220) as

$$(\mathbf{B}^{-1}\mathbf{J}+h^2\mathbf{R})\mathbf{y}-h^2\Lambda\mathbf{Q}\mathbf{y} = \mathbf{0} \tag{4.221}$$

The matrices $\mathbf{B}^{-1}\mathbf{J}+h^2\mathbf{R}$ and $\mathbf{Q}$ are symmetric. The eigenvalues $h^2\Lambda$ will be real and positive if the matrices $\mathbf{Q}$ and $(\mathbf{B}^{-1}\mathbf{J}+h^2\mathbf{R})$ are symmetric and positive definite. Using the arguments given in (4.155)-(4.161) we determine

$$\mathbf{B}^{-1} = (\bar{b}_{ij}) \tag{4.222}$$

where

$$\bar{b}_{ij} = \begin{cases} \dfrac{3(s^i-r^i)(r^j-ps^j)}{\sqrt{6}(1-p)}, & i \leqslant j \\[2ex] \dfrac{3(s^j-r^j)(r^i-ps^i)}{\sqrt{6}(1-p)}, & i \geqslant j \end{cases} \tag{4.223}$$

$$r = -5+2\sqrt{6}, \quad s = -5-2\sqrt{6}, \quad p = r^{2N}$$

Since $rs = 1$ and $|\,r\,| < 1$, from (4.223), we find that

$$\bar{b}_{jj} = \frac{3(1-r^{2j})(1-r^{2(N-j)})}{\sqrt{6}(1-r^{2N})} > 0 \tag{4.224}$$

Thus, the diagonal elements of $\mathbf{B}^{-1}$ are positive. We now determine the following two sums:

$$\text{(i)} \sum_{m=1}^{j-1} | \bar{b}_{jm} | = \frac{3}{\sqrt{6}} \frac{| r^j - ps^j |}{(1-p)} \sum_{m=1}^{j-1} | s^m - r^m |$$

$$\text{(ii)} \sum_{m=j+1}^{N-1} | \bar{b}_{jm} | = \frac{3}{\sqrt{6}} \frac{| s^j - r^j |}{(1-p)} \sum_{m=j+1}^{N-1} | r^m - ps^m | \tag{4.225}$$

Putting $r = -\alpha$ and $s = -\beta$, we obtain

$$\text{(i)} \sum_{m=1}^{j-1} | s^m - r^m | = \frac{1}{8}(\beta^j - \alpha^j) - \frac{1}{8} [(\beta^{j-1} - \alpha^{j-1}) + (\beta - \alpha)]$$

and

$$\text{(ii)} \sum_{m=j+1}^{N-1} | r^m - ps^m | = \frac{1}{8}(\alpha^j - \alpha^{2N} \beta^j) - \frac{1}{8}[\alpha^{j+1}(1 - \alpha^{2(N-j-1)}) + \alpha^{N-1}(1 - \alpha^2)] \tag{4.226}$$

Since the expressions in square brackets in (4.226) are positive, we may write (4.226) as

$$\sum_{m=1}^{j-1} | s^m - r^m | < \frac{1}{8} | s^j - r^j | , \ j = 2(1)N-1$$

and

$$\sum_{m=j+1}^{N-1} | r^m - ps^m | < \frac{1}{8} | r^j - ps^j | , \ j = 1(1)N-2 \tag{4.227}$$

Substituting from (4.227) into (4.225) and with $\bar{b}_{jj}$ as given by (4.224), we obtain

$$\text{(i)} \sum_{m=1}^{j-1} | \bar{b}_{jm} | < \frac{1}{8} \bar{b}_{jj}, \ \ j = 2(1)N-1$$

and

$$\text{(ii)} \sum_{m=j+1}^{N-1} | \bar{b}_{jm} | < \frac{1}{8} \bar{b}_{jj}, \ \ j = 1(1)N-2 \tag{4.228}$$

From (4.228), we have

$$\sum_{\substack{m=1 \\ m \neq j}}^{N-1} | \bar{b}_{jm} | < \frac{1}{4} \bar{b}_{jj}, \ \ j = 1(1)N-1$$

which shows that the matrix $\mathbf{B}^{-1}$ is strictly diagonally dominant. We know that the product of two positive definite matrices is a positive definite matrix if and only if the matrices commute. Now, $\mathbf{B}$ is positive definite, the matrix $\mathbf{B}^{-1}$ is positive definite, and it is easily verified that $\mathbf{B}^{-1}$ and $\mathbf{J}$ commute. Thus, the matrix $\mathbf{B}^{-1}\mathbf{J}$ is positive definite. Further, $r(x) \geqslant 0$ on $[a, b]$, therefore $\mathbf{R} \geqslant 0$ and hence the matrix $\mathbf{B}^{-1}\mathbf{J} + h^2\mathbf{R}$ is symmetric and positive definite. Thus, the Numerov method gives real and positive approximations for an eigenvalue λ of (4.219). The eigenvalue λ, using the Numerov method is given by

$$(\mathbf{B}^{-1}\mathbf{J} + h^2 \mathbf{R})\mathbf{Y} - h^2\lambda\mathbf{Q}\mathbf{Y} = \mathbf{B}^{-1}\mathbf{T} \tag{4.229}$$

where

$$\mathbf{Y} = [y(x_1)y(x_2) \dots y(x_{N-1})]^T,$$
$$\mathbf{T} = [T_1 T_2 \dots T_{N-1}]^T$$
$$T_n = \frac{h^6}{240} y^{(6)}_{(x_n)} + 0(h^8), \quad n = 1(1)N-1 \tag{4.230}$$

We now state the following result.

THEOREM (Keller) 4.6 For each eigenvalue λ of (4.219) and corresponding normalized eigenvector $\mathbf{Y}(x)$, there exists an eigenvalue $h^2\Lambda$ of $\mathbf{Q}^{-1}(\mathbf{B}^{-1}\mathbf{J} + h^2\mathbf{R})$ such that

$$|\Lambda - \lambda| \leqslant \| Q^{-1} \| \; \| \mathbf{B}^{-1} \| \frac{\| \boldsymbol{\tau}(\mathbf{Y}) \|}{\| \mathbf{Y} \|} \tag{4.231}$$

where $h^2 \boldsymbol{\tau} = \mathbf{T}$.

From this result we obtain the error estimates in the maximum norm $\| \boldsymbol{\tau}(\mathbf{Y}) \|_\infty$. We use the normalization

$$\int_a^b q(x) y^2(x)\, dx = 1$$

We have

$$\text{(i)} \quad h \| \mathbf{Y} \|^2 = \left[\sum_{j=1}^{N-1} h y^2(x_j) + \frac{h}{2} (y^2(x_0) + y^2(x_N)) - \int_a^b y^2(x)\, dx + \int_a^b y^2(x)\, dx \right]$$
$$= \int_a^b y^2(x)\, dx + \frac{h^2}{12} y''(c),\ c \in [a, b]$$
$$\geqslant \frac{1}{q^*} + \frac{h^2}{12} y''(c)$$

where $q^* = \max\limits_{a \leq x \leqslant b} q(x)$.

(ii) $h \| \boldsymbol{\tau} \|^2 = h \sum\limits_{j=1}^{N-1} \tau_j^2 \leqslant (b-a) \| \boldsymbol{\tau} \|_\infty^2$

(iii) $\| \boldsymbol{\tau} \| = 0(h^4)$

(iv) $\| \mathbf{B}^{-1} \| = \dfrac{3}{2}$

(v) $| \mathbf{Q}^{-1} \| = \dfrac{1}{q_*}$

where

$$q_* = \min_{a \leqslant x \leqslant b} q(x) \tag{4.232}$$

Substituting from (4.232) we may write (4.231) as

$$|\Lambda - \lambda| \leqslant 0(h)^4 \tag{4.233}$$

Thus, we obtain that as $h \to 0$ any fixed eigenvalue λ of (4.219) is approximated by some eigenvalue of the difference equation (4.220) with an error of $0(h^4)$.

4.8 RESULTS FROM COMPUTATION

In addition to Examples 4.1-4.4, the nonlinear differential equation

$$y'' = \frac{3}{2} y^2$$

subject to the boundary conditions

$$y(0) = 4,\ y(1) = 1$$

and

$$y'(0) - y(0) = -12$$
$$y'(1) + y(1) = 0$$

with exact solution

$$y(x) = \frac{4}{(1+x)^2}$$

has been solved by difference methods using different mesh sizes. The values $E = \max_{0 \leqslant n \leqslant N} | y_n - y(x_n) |$, are tabulated in Tables 4.6, 4.7 and 4.8.

We have solved Example 4.1 with the different order methods over [2, 3] with $h = 2^{-m}$, $2 \leqslant m \leqslant 7$ and the value E determined for each case. The results are given in Table 4.6. We observe that if we solve a first boundary value problem with a fixed step size over a given interval, the low-order methods produce less accurate results as compared to high-order methods. The error values decrease as the step size h diminishes or the order of the method increases. The sixth order method based on the three-point *Gauss* quadrature with *Approximation* I gives most accurate results and in this case it requires the minimum number of equations for solution.

From Table 4.6, we find that if E is to be less than or equal to 0.5×10^{-10}, the number of equations to be solved is 63 in the *Numerov* method, 7 in the *Lobatto* four-point and *Gauss* three-point methods with *Approximation* I and 22 in the h^4-extrapolation of the *Numerov* scheme, while in the case of Usmani's method as also *Lobatto* four-point and *Gauss* three-point methods with *Approximation* II, it is 15. From the function evaluation viewpoint, the *Gauss* three-point method with *Approximation* I is most expensive whereas the h^4-extrapolation *Numerov* method and the *Lobatto* four points with *Approximation* II require almost about the same number.

We have again used the methods of various orders to solve the problem in Example 4.2 with $h = 2^{-m}$, $2 \leqslant m \leqslant 8$, over the interval [0, 1] and the results are listed in Table 4.7. We find as in Example 4.1 that the high order methods and the smaller values of h yield higher accuracy results.

The finite points to represent infinity in the second boundary conditions in Example 4.3 have been determined. With

$$\epsilon = 10^{-8}$$

and

$$h = 1,\ 0.5,\ 0.25$$

we get

$$x = 10,\ 9.5,\ 8.75$$

TABLE 4.6 COMPARISON OF ERROR IN NUMERICAL METHODS FOR THE LINEAR BOUNDARY VALUE PROBLEM
$y''-2x^{-2}y+x^{-1}=0,\ y(2)=y(3)=0$ WITH $h=2^{-m}$

m	Second order method	Numerov fourth order method	*Approximation* I Lobatto method	*Approximation* I Gauss method	Numerov h^4-extrapolation method	Usmani method	*Approximation* II Lobatto method	*Approximation* II Gauss method
2	0.159−03	0.260−05	0.257−08	0.277−09	0.323−08	0.377−07	0.163−07	0.142−07
3	0.412−04	0.174−06	0.445−10	0.485−11	0.567−10	0.647−09	0.279−09	0.244−09
4	0.104−04	0.109−07	0.702−12	0.767−13	0.878−12	0.102−10	0.439−11	0.383−11
5	0.261−05	0.685−09	0.110−13	0.120−14	0.138−13	0.159−12	0.689−13	0.603−13
6	0.652−06	0.429−10	0.169−15	0.171−16	0.216−15	0.229−14	0.107−14	0.941−15
7	0.163−06	0.268−11	0.119−17	0.109−17	0.573−17	0.172−13	0.155−16	0.138−16

TABLE 4.7 COMPARISON OF ERRORS IN NUMERICAL METHODS FOR THE MIXED BOUNDARY VALUE PROBLEM
$y''-y+4xe^x = 0,\ y'(0)-y(0) = 1,\ y'(1)+y(1) = -e$ WITH $h = 2^{-m}$

m	Second order method	Fourth order method	*Approximation* I Lobatto method	*Approximation* I Gauss method	*Approximation* II Lobatto method	*Approximation* II Gauss method
2	0.807−01	0.364−03	0.379−06	0.309−06	0.174−05	0.174−05
3	0.203−01	0.232−04	0.600−08	0.482−08	0.304−07	0.304−07
4	0.509−02	0.146−05	0.941−10	0.756−10	0.502−09	0.501−09
5	0.127−02	0.913−07	0.147−11	0.118−11	0.806−11	0.806−11
6	0.319−03	0.571−08	0.238−13	0.183−13	0.127−12	0.128−12
7	0.797−04	0.357−09	0.567−15	0.243−15	0.177−14	0·196−14
8	0.199−04	0.212−10	0.795−16	0.103−16	0.455−16	0.247−16

TABLE 4.8 COMPARISON OF ERROR IN SIXTH ORDER METHOD FOR THE NONLINEAR BOUNDARY VALUE PROBLEMS WITH AND WITHOUT MIXED BOUNDARY CONDITIONS WITH $h = 2^{-m}$

m	$y'' = \frac{1}{2}(1+x+y)^3$; $y(0) = y(1) = 0$	$y'' = \frac{1}{2}(1+x+y)^3$; $y'(0)-y(0) = -\frac{1}{2}$, $y'(1)+y(1) = 1$	$y'' = \frac{3}{2}y^2$; $y(0) = 4$, $y(1) = 1$	$y'' = \frac{3}{2}y^2$; $y'(0)-y(0) = -12$, $y'(1)+y(1) = 0$
3	0.270−06	0.629−06	0.488−05	0.930−05
4	0.435−08	0.125−07	0.797−07	0.187−06
5	0.718−10	0.290−09	0.126−08	0.339−08
6	0.432−11	0.651−10	0.204−10	0.628−10

These results are quite reasonable since in this case $y(x) < 10^{-8}$ for $x > 9$. Thus, we find that the position of the finite points depends on ϵ and to some extent on h also.

The nonlinear differential equations with or without mixed boundary conditions have been solved with $h = 2^{-m}$, $3 \leqslant m \leqslant 6$. The results obtained with the four-point *Lobatto* quadrature with *Approximation* II are listed in Table 4.8. We find that the sixth order methods with *Approximation* II are particularly useful for nonlinear differential equations with or without mixed boundary conditions since we need to solve a fewer number of nonlinear equations to get higher accurate results.

Finally, we arrive at the following conclusions:

(i) The sixth order methods with *Approximation* II are applicable to linear and nonlinear differential equations with or without mixed boundary conditions.

(ii) The numerical results show that the sixth order method based on four-point *Lobatto* quadrature and *Approximation* II is highly desirable for both linear and nonlinear boundary value problems.

4.9 NONUNIFORM GRID METHODS FOR THE SECOND ORDER BOUNDARY VALUE PROBLEMS

Let $a = x_0 < x_1 < x_2, \ldots, x_{N-1} < x_N = b$ be a subdivision of an interval $[a, b]$, where $h_j = x_j - x_{j-1}$, $j = 1\,(1)\,N$. We now obtain the difference schemes for the second order differential equations which when used to solve the two point boundary value problem will lead to a tridiagonal system.

4.9.1 Nonlinear boundary value problems $y'' = f(x, y)$

Let us approximate the differential equation $y'' = f(x, y)$ by the difference scheme of the form

$$2y_n - C_{1n}y_{n-1} - C_{2n}y_{n+1} + h_{n+1}^2\,(B_{0n}f_{n-1} + B_{1n}f_n + B_{2n}f_{n+1}) = 0 \qquad (4.234)$$

where f_n and y_n represent the approximate values of $f(x_n, y(x_n))$ and $y(x_n)$, respectively. The C's and B's are unknowns to be determined. We now write the difference operator $L[y(x), h_n]$ associated with the equation (4.234) as

$$L[y(x), h_n] = 2y(x_n) - C_{1n}y(x_n - h_n) - C_{2n}y(x_n + h_{n+1}) + h_{n+1}^2\,[B_{0n}y''(x_n - h_n) + B_{1n}y''(x_n) + B_{2n}y''(x_n + h_{n+1})] \qquad (4.235)$$

We expand the various y's on the right-hand side of (4.235) in the Taylor series about x_n and equate the coefficients of $h_n^{\nu} y^{(\nu)}_{(x_n)}$, $(\nu = 0\,(1)\,4)$ to zero. We have

$$\begin{aligned}
2 - C_{1n} - C_{2n} &= 0\\
C_{1n} - \sigma C_{2n} &= 0\\
-\frac{1}{2}C_{1n} - \frac{\sigma^2}{2}C_{2n} + \sigma^2\,(B_{0n} + B_{1n} + B_{2n}) &= 0\\
\frac{1}{6}\,(C_{1n} - \sigma^3\,C_{2n}) - \sigma^2\,B_{0n} + \sigma^3\,B_{2n} &= 0\\
-\frac{1}{24}\,(C_{1n} + \sigma^4\,C_{2n}) + \frac{1}{2}\,(\sigma^2 B_{0n} + \sigma^4\,B_{2n}) &= 0
\end{aligned} \qquad (4.236)$$

and

$$L\,[y(x), h_n] = \left[\frac{1}{5\,!}\,(C_{1n} - \sigma^5\,C_{2n}) + \frac{1}{3\,!}\,(\sigma^2\,B_{0n} + \sigma^6\,B_{2n})\right] h_n^5 y^{(v)}_{(x_n)} + \cdots \qquad (4.237)$$

where $h_{n+1} = \sigma\,h_n$.

Solving (4.236) for C's and B's we obtain

$$C_{1n} = \frac{2\sigma}{(1+\sigma)}, \qquad C_{2n} = \frac{2}{(1+\sigma)}$$

$$B_{0n} = \frac{1+\sigma-\sigma^2}{6\sigma(1+\sigma)}, \qquad B_{1n} = \frac{\sigma^3+4\sigma^2+4\sigma+1}{6\sigma^2\,(1+\sigma)}$$

$$B_{2n} = \frac{\sigma^2+\sigma-1}{6\sigma^2\,(1+\sigma)} \qquad (4.238)$$

Substituting (4.238) into (4.237) and simplifying, we get

$$L\,[y(x),\,h_n] = \frac{1}{180}\,\sigma\,(\sigma-1)\,(2\,\sigma+1)\,(\sigma+2)\,h_n^5 y^{(v)}_{(x_n)} + \cdots \tag{4.239}$$

Equation (4.235) becomes

$$\begin{aligned}(1+\sigma)\,y\,(x_n) - \sigma y\,(x_n - h_n) - y\,(x_n+h_{n+1}) + \frac{h_{n+1}^2}{12}\Bigg[\frac{1+\sigma-\sigma^2}{\sigma}\,y''\,(x_n-h_n) \\ + \frac{\sigma^3+4\,\sigma^2+4\,\sigma+1}{\sigma^2}\,y''\,(x_n) + \frac{\sigma^2+\sigma-1}{\sigma^2}\,y''\,(x_n+h_{n+1})\Bigg] \\ = \frac{1}{360}\,\sigma\,(\sigma^2-1)\,(2\,\sigma+1)\,(\sigma+2)\,h_n^5 y^{(v)}_{(x_n)} + \cdots\end{aligned} \tag{4.240}$$

Neglecting the truncation term in (4.240), we have the difference scheme

$$\begin{aligned}(1+\sigma)y_n - \sigma y_{n-1} - y_{n+1} + \frac{h_{n+1}^2}{12}\left(\frac{1+\sigma-\sigma^2}{\sigma}\,f_{n-1} + \frac{\sigma^3+4\,\sigma^2+\,4\,\sigma+1}{\sigma^2}\,f_n \right. \\ \left. + \frac{\sigma^2+\sigma-1}{\sigma^2}\,f_{n+1}\right) = 0\end{aligned} \tag{4.241}$$

Since $\sigma > 0$, the convergence of the difference scheme (4.241) when applied to solve (4.4) is ensured if B's are positive, i.e.

$$1+\sigma-\sigma^2 > 0 \quad \text{and} \quad \sigma^2+\sigma-1 > 0$$

which implies

$$\sigma < \frac{1}{2} + \frac{\sqrt{5}}{2} \cong 1.618$$

and

$$\sigma > \frac{\sqrt{5}}{2} - \frac{1}{2} \cong .618$$

Thus, we obtain

$$.618 < \sigma < 1.618 \tag{4.242}$$

4.9.2 Nonlinear boundary value problems $y'' = f(x, y, y')$

The three-point difference scheme similar to (4.241) may be written as

$$\begin{aligned}(1+\sigma)y_n - \sigma y_{n-1} - y_{n+1} + \frac{h_{n+1}^2}{12}\left(\frac{1}{\sigma}(1+\sigma-\sigma^2)\,f_{n-1} + \frac{1}{\sigma^2}\,(\sigma^3+4\sigma^2+4\sigma+1)f_n \right. \\ \left. + \frac{1}{\sigma^2}(\sigma^2+\sigma-1)f_{n+1}\right) = 0\end{aligned} \tag{4.243}$$

where

$$\begin{aligned} f_{n-1} &= f(x_{n-1},\, y_{n-1},\, y'_{n-1}) \\ f_n &= f(x_n,\, y_n,\, y'_n) \\ f_{n+1} &= f(x_{n+1},\, y_{n+1},\, y'_{n+1}) \end{aligned}$$

$$h_n y'_{n-1} = -\frac{1}{\sigma(1+\sigma)} y_{n+1} + \frac{(1+\sigma)}{\sigma} y_n - \frac{2+\sigma}{(1+\sigma)} y_{n-1}$$

$$h_{n+1} y'_{n+1} = \frac{2\sigma+1}{\sigma+1} y_{n+1} - (1+\sigma) y_n + \frac{\sigma^2}{1+\sigma} y_{n-1}$$

$$h_n y'_n = \frac{1}{\sigma(\sigma+1)}\left[y_{n+1} + (\sigma^2-1) y_n - \sigma^2 y_{n-1}\right] - \frac{h_n^2}{6}\,\frac{\sigma(\sigma^2+\sigma+1)}{(1+\sigma)(\sigma^2+3\sigma+1)}(f_{n+1} - f_{n-1})$$

Again the difference scheme (4.243) when applied to the boundary value problem (4.87) is convergent if σ satisfies the condition (4.242).

4.9.3 Results from computation

We have used the variable steplength method (4.243) to solve numerically the following boundary value problems:

(i) $\epsilon y'' = y'$, $y(0) = 1$, $y(1) = 0$
with the analytic solution
$y(x) = [1 - \exp(-\epsilon^{-1}(1+x))]/[1 - \exp(-\epsilon^{-1})]$

(ii) $\epsilon y'' + 2y' + y = -3$, $y(-1) = 1$, $y(1) = 2$
with the analytic solution

$$y(x) = \frac{[(4\exp(-m_2) - 5\exp(m_2))\exp(-m_1 x) - (4\exp(-m_1) - 5\exp(m_2))\exp(-m_2 x)]}{[\exp(m_1 - m_2) - \exp(-(m_1 - m_2))]}$$

$m_1 = \epsilon^{-1}[1 - \sqrt{1-\epsilon}]$, $m_2 = \epsilon^{-1}[1 + \sqrt{1-\epsilon}]$

(iii) $\epsilon y'' = \left(y - \frac{1}{2}\right) y'$, $y(-\infty) = 1$, $y(\infty) = 0$

with the analytic solution

$$y(x) = \frac{1}{2}\left[1 - \tanh\left(\frac{x}{4\epsilon}\right)\right] \tag{4.244}$$

where ϵ is a very small constant. The problems (4.244) possess a small interval in which the solution is changing most rapidly. This interval is called the *boundary layer*. The boundary layer may occur at one end or at both the ends or at the centre. In order to get an accurate numerical solution in the interval $a \leq x \leq b$ economically we choose a small steplength $h \ll \epsilon$ in the boundary layer and a much larger steplength elsewhere. The starting value of the steplength is given by

$$h_1 = (b-a)(\sigma-1)/(\sigma^N - 1), \ \sigma > 1 \tag{4.245}$$

or

$$h_1 = (b-a)(1-\sigma)/(1-\sigma^N), \ \sigma < 1 \tag{4.246}$$

The value $\sigma > 1$ gives more mesh points at small values of x while $\sigma < 1$ gives more mesh points at larger values of x. In most of the boundary value problems it is possible to know in advance the location of the boundary layer and the value of σ may be chosen suitably. In more general cases, in which the boundary layer is not known a priori we can compute the solution for some steplength h, repeat the calculation with another value of h and see whether the solution changes by more than an acceptable amount i.e., $| y_{i+1} - y_i | > \delta$, where δ is a prescribed limit.

In the boundary value problem (4.244i) the boundary layer exists near the right hand boundary $x = 1$. We choose $\sigma = 0.6$ and this gives more mesh points near $x = 1$. For $N = 8$, $\epsilon = 10^{-2}$, the solution values are shown in Figure 4.3(a).

The boundary layer in (4.244 ii) is near the point $x = -1$. We choose $\sigma = 1.2$ and this will give more mesh points near the left hand boundary. For $N = 100$, $\epsilon = 10^{-6}$ the solution values are shown in Figure 4.3(b).

We solve the boundary value problem (4.244 iii) over the interval $[-5, 5]$. The boundary layer exists near the origin. We choose a symmetric mesh about the origin. We take $\sigma > 1$ for the interval $[0, 5]$, while for the interval $[-5, 0]$ the reflection is used. The total number of mesh points in the interval $[-5, 5]$ are $2N+1$. For $N = 8$, $\epsilon = 1/24$, the resulting system of equations are solved with the Newton-Raphson iteration method. The solution values are shown in Figure 4.3(c).

We may conclude that the variable mesh method (4.243) is well suited for solving boundary layer problems. A priori knowledge of the location of he boundary layer is very helpful in producing accurate results with relatively little effort.

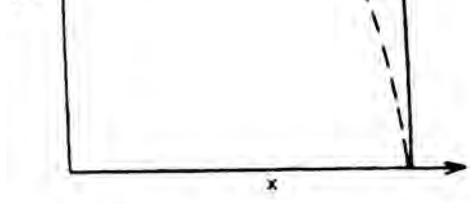


Fig. 4.3(a) Solution of $\epsilon y'' = y'$, $y(0) = 1$, $y(1) = 0$, $\epsilon = 10^{-2}$

——— exact, …… computed ($\sigma = 0.61$),

– – – computed ($\sigma = 1.0$)

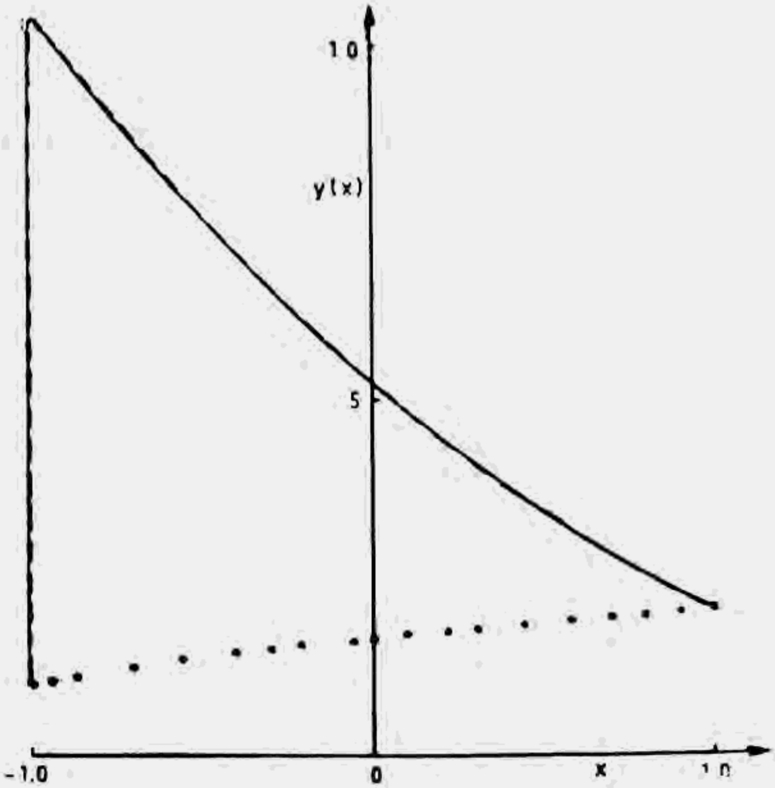


Fig. 4.3(b) Solution of $\epsilon y''+2y'+y=-3$, $y(-1)=1$, $y(1)=2$, $N=100$, $\epsilon=10^{-6}$
—— exact, ... computed ($\sigma=1.0$), – – –computed ($\sigma=1.2$)

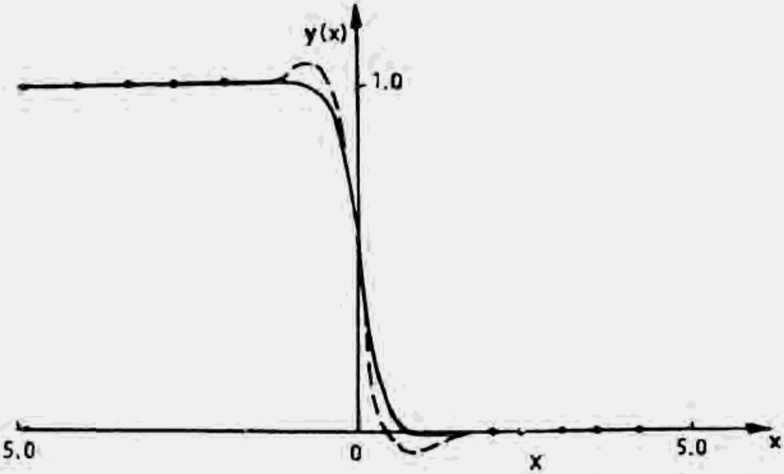


Fig. 4.3(c) Solution of $\epsilon y''=(y-1/2)y'$, $y(-\infty)=1$, $y(\infty)=0$, $N=8$, $\epsilon=1/24$
—— exact, ... computed ($\sigma=1.1$), – – – computed ($\sigma=1.0$)

Bibliographical Note

The texts listed at 12, 46, 87, 113, 114, 121 and 152 deal with the difference methods for two point boundary value problems. The shooting method has been described in 152 and 205. The difference methods for linear and non-linear boundary value problems in ordinary differential equations are treated in 139, 153, 154 and 226. The linear two-point boundary value problem in an infinite interval is solved in 206. The general two-point boundary value problem is studied in 8, 38, 39, 40, 41, 227 and 231. The high accuracy difference methods are given in 36, 37, 115, 240, 243 and 245. The error bounds for the solution are available in 242, 244, 246, 247, and 248. The five-band system arising in the fourth order boundary value problems is discussed in 48, 134, 149 and 241.

The matrix methods for solving the system of equations are given in 76 and 251.

The eigenvalue problems are discussed in 151 and 157. The variable step methods are given in 112, 196 and 234.

Problems

1. The nth order linear two point boundary value problem

$$L[y(x)] = \sum_{i=0}^{n} f_i(x) y^{(i)}_{(x)} = r(x)$$

$$\sum_{i=0}^{n-1} (\alpha_{\nu, i}\, y^{(i)}_{(a)} + \beta_{\nu, i}\, y^{(i)}_{(b)}) = \gamma_\nu,\ \nu = 0(1)n-1$$

may be replaced by at most $n+1$ initial value problems of the form

$$L[y_{n+1}(x)] = r(x)$$

$$y^{(\nu)}_{n+1}(a) = 0, \qquad \nu = 0(1)n-1$$

$$L[y_k(x)] = 0$$

$$y_k^{(\nu)}(a) = \begin{cases} 0\ , & \nu \neq k-1 \\ 1\ , & \nu = k-1 \end{cases} \qquad \begin{array}{l} \nu = 0(1)n-1 \\ k = 1(1)n \end{array}$$

where

$$y(x) = y_{n+1}(x) + \sum_{k=1}^{n} \lambda_k y_k(x)$$

The constants $\lambda_1, \lambda_2, \ldots, \lambda_n$ are determined by satisfying the boundary conditions.

Reduce the following boundary value problems to the initial value problems:

(i) $\epsilon y'' + ky' = 0 \qquad (\,|\,k\,| > 0,\ \epsilon > 0)$

$y(0) = \alpha,\ y(1) = \beta$

(ii) $y''' + ky'' = 0, \qquad (k > 0)$

$y(0) = 0,\ y'(0) = \beta,\ y'(\infty) = 1$

(iii) $y^{(iv)}-k_1 y'''+k_2y''=0$

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

(iv) $y^{(iv)}-k^4y=q,\ (q, k>0)$

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

Also determine the missing initial conditions with the help of the analytic solution of the initial value problems.

2. Reduce the third order boundary value problem

$$y'''-k^2y'+a=0 \qquad (a>0)$$
$$y'(0)=0,\ y\left(\frac{1}{2}\right)=0,\ y'(1)=0$$

to the initial value problems.
Also determine the missing initial conditions.

3. The differential equation $y''=x^3(y+y')$ and the boundary conditions $y(0)=1$ and $y(0.5)=1.3$ are given.
Put $y'(0)=\alpha$ and determine by a series expansion a polynomial in x of degree 5 which approximates $y(x)$. Determine α so that the boundary condition $y(0.5)=1.3$ is satisfied.

(BIT 14(1974), 122)

4. Determine to two correct decimals the constant α such that the problem

$$y''=xy$$
$$y(0)=\alpha, \quad y'(0)=1$$

has a solution satisfying $y(1)=1$.

(BIT 15(1975), 224)

5. The function $y(x)$ satisfies

$$y''+xy=0, \quad y(1)=1, \quad y'(1)=c.$$

Determine a value for c such that $y(1.1)=y'(1.1)$. The answer shall be given to 3 correct decimals.

(BIT 17(1977), 369)

6. Find the constants $a_1, a_2, \ldots,$ in the equation

$$D=\sum_{s=1}^{\infty} a_s\mu\delta^s$$

where $h=1$, $D=$ differentiation operator, $\mu=$ mean value operator and $\delta=$ central difference operator. (BIT 7(1967), 81)

7. Find constants a, b and n such that the formula

$$h^2y_1''=a\Delta^2y_0+b\Delta^4y_0$$

will be exact for polynomials of the highest possible degree n.

(BIT 6(1966), 359)

8. Determine the constants in the following relations

$$h^{-4}\delta^4 = D^4(1+a\delta^2+b\delta^4)+0(h^6)$$
$$hD = \mu\delta+a_1\Delta^3E^{-1}+(hD)^4(a_2+a_3\mu\delta+a_4\delta^4)+0(h^7)$$

(BIT 8(1968), 59)

9. Find the coefficients a and b in the operator formula

$$\delta^2+a\delta^4 = h^2D^2(1+b\delta^2)+0(h^8) \qquad \text{(BIT 8(1968), 138)}$$

10. The differential equation $y''+x^2(y+1) = 0$ is given with boundary values $y = 0$ for $x = \pm 1$. Find approximate values of $y(0)$ and $y(1/2)$ using the second and fourth order difference schemes, with $h = 1/2$. (BIT 7(1967), 81)
11. Find difference approximations for the solution $y(x)$ of the boundary value problem

$$y''+8\sin^2 \pi x\, y = 0,\ x\in[0, 1]$$
$$y(0) = y(1) = 1$$

with step length $h = 0.25$, using second and fourth order methods. Also find an approximate value for $y'(0)$. (BIT 8(1968), 246)
12. The difference scheme

$$\delta^2 y_n = h^2\left[\frac{7}{12}y_n''+\frac{5}{24}(y_{n-r}''+y_{n+r}'')\right],\ r^2 = \frac{2}{5}$$

with *Approximation* I is used to replace the boundary value problem

$$y'' = f(x)y(x)+g(x)$$
$$y(a) = A,\ y(b) = B$$

by a system of linear equations

$$(-1+A_n)\,y_{n-1}+(2+B_n)\,y_n+(-1+C_n)\,y_{n+1} = D_n,\ 1 \leqslant n \leqslant N-1$$
$$y_0 = A,\ y_N = B$$

Determine A_n, B_n, C_n and D_n. Show that the principal part of the truncation error is given by

$$\left[\frac{19}{1512000}M_8+\frac{38-9\sqrt{10}}{86400}f_M M_6+\frac{(\sqrt{10}-2)}{3600}f_M' M_5\right]h^8$$

where $\quad M_n = \max\limits_{a\leqslant x\leqslant b} |\, y^{(n)}_{(x)} \,|,\ f_M = \max\limits_{a\leqslant x\leqslant b} |\, f(x)\,|$

and $\quad f_M' = \max\limits_{a\leqslant x\leqslant b} |\, f'(x)\,|$

13. The system of equations

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