Numerical solutions of two-point boundary value problems in Chebyshev series

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NUMERICAL SOLUTIONS OF TWO-POINT BOUNDARY VALUE PROBLEMS IN CHEBYSHEV SERIES

By

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To my wife Samia

and my daughter Dalia

ABSTRACT

Series expressed in terms of Chebyshev polynomials are applied using Lie series to the iterative solution of ordinary differential equations. After a discussion of initial value problems, the method is then used to solve two-point boundary value problems and an improved method of shooting type is derived and tested.

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Introduction

This thesis is concerned with the application of series methods to the solution of ordinary differential equations. Series of Chebyshev polynomials are used in conjunction with Lie series.

In Chapter I a brief account is given of the Lie series approach and an account of previous work on application of Lie series to numerical solution of initial value problems. A quick review is also given of the properties of Chebyshev polynomials and the methods which have previously been used to obtain solutions of initial value problems in terms of them.

In Chapter II Lie series are presented in Chebyshev form and applied to the iterative solution of initial value problems. The theory of the method is discussed and numerical results are analysed.

In Chapter III an account is given of various shooting type methods previously used in solving linear and non-linear boundary value problems and comparisons between them.

In Chapter IV the Lie series method is applied to some of the methods mentioned in Chapter III and the numerical behaviour is tested. A new method for solving non-linear boundary value problems is then derived and applied to a set of test examples. A detailed discussion is given of the comparative performance of this method under various conditions.

Finally, a new continuation procedure based on this method is suggested for future investigation.

CONTENTS

CHAPTER I

BASIC RESULTS

The first section of this chapter gives a brief account of the Lie series approach to differential equations as developed in W.Grobner and H.Knapp (1967) and H.Knapp, G.Wanner (1968).

In the second section an account is given of previous work on application of Lie series to numerical solution of initial value differential equations.

Since in this thesis the Lie series are expressed in terms of Chebyshev polynomials, a brief account is given in the third section of the properties of such polynomials and the methods which have previously been used to obtain solutions of initial value differential equations in terms of them.

1.1 Theory of Lie Series

1.1.1. Definition of Lie Series

By D we denote a linear differential operator

$$D = \theta_1(z)\frac{\partial}{\partial z_1} + \theta_2(z)\frac{\partial}{\partial z_2} + \cdots\cdots\cdots + \theta_n(z)\frac{\partial}{\partial z_n} \qquad 1.1.1.$$

the coefficients of which, $\theta_i(z)$, represent functions of Complex variables $z_1, z_2, \ldots, z_n$, which are all assumed to be holomorphic in the neighbourhood of one and the same point. If then f(z) is any function which is holomorphic in the neighbourhood of the same point, it is possible to apply the operator D to f(z) and obtain

$$DF(z) = \theta_1(z)\frac{\partial F}{\partial z_1} + \theta_2(z)\frac{\partial F}{\partial z_2} + \cdots\cdots\cdots + \theta_n(z)\frac{\partial F}{\partial z_n} \qquad 1.1.2$$

which is holomorphic and also $D^2F = D(DF)$, ... , $D^\nu F = D(D^{\nu-1}F)$ are also holomorphic.

A series of the following kind

$$e^{tD}F(z) = \sum_{\nu=0}^{\infty}\frac{t^\nu}{\nu!}D^\nu F(z)$$

$$= F(z) + tDF(z) + \frac{t^2}{2!}D^2F(z) + \cdots\cdots\cdots \qquad 1.1.3$$

is here called a Lie-series.

A Convergence proof with the help of Cauchy majorants can be found in W.Grobner, H.Knapp (1967).

1.1.2. The Commutation theorem (W.Grobner and H.Knapp (1967))

Consider the function $F(x, y_1(x), \cdots, y_n(x)) = F(x, y(x))$, and specialise to the usual definition of D as the differentiation operator so writing

$$\frac{d}{dx} F(x, y(x)) = [DF]_{x, y(x)}$$

and $$\frac{d^r}{dx^r} F(x, y(x)) = [D^r F]_{x, y(x)} \qquad \text{1.1.4}$$

where $$DF(x, y_1(x), \cdots, y_n(x)) = \frac{\partial F}{\partial x} + \sum_{k=1}^{n} \left(\frac{\partial F}{\partial y_k}\right)\left(\frac{dy_k}{dx}\right)$$

The Taylor expansion of the function $F(x, y(x))$ at the point x_0 can be written in the form

$$F(x, y(x)) = \sum_{r=0}^{\infty} \frac{(x - x_0)^r}{r!} [D^r F]_{x_0, y_0} \qquad \text{1.1.5}$$

where y_0 denotes $y(x_0)$

and so $$y_i(x) = \sum_{r=0}^{\infty} \frac{(x - x_0)^r}{r!} [D^r y_i]_{x_0, y_0}, \quad (i = 1, 2, \cdots, n) \qquad \text{1.1.6}$$

$$x = \sum_{r=0}^{\infty} \frac{(x - x_0)^r}{r!} [D^r x]_{x_0, y_0}$$

Then (1.1.5) gives the Commutation theorem

$$\sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} [D^r F(x, y)]_{x_0, y_0} = F\left(\sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} [D^r x]_{x_0, y_0}, \sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} [D^r y]_{x_0, y_0}\right) \qquad \text{1.1.7}$$

The substitutions $x_0 \longrightarrow x$, $y_0 \longrightarrow y$, $x \longrightarrow t - x_0 + x$ yield

$$\sum_{r=0}^{\infty} \frac{(t-x_0)^r}{r!} [D^r F(x, y)] = F\left(\sum_{r=0}^{\infty} \frac{(t-x_0)^r}{r!} D^r x, \sum_{r=0}^{\infty} \frac{(t-x_0)^r}{r!} D^r y\right) \qquad \text{1.1.8}$$

Thus the function symbol F can be commuted with the expression

$$\sum_{r=0}^{\infty} \frac{(t-x_0)^r}{r!} D^r \qquad \text{1.1.9}$$

All the formulae are valid in the common domain of Convergence.

1.1.3 Solution of differential equations in Lie series

Consider the system of ordinary differential equations

$$y_i'(x) = P_i(x, y_1(x), y_2(x), \ldots, y_n(x)) = P_i(x, y(x)) \quad ; \quad (i = 1, 2, \ldots, n) \qquad 1.1.10$$

with initial condition

$$y_i(x_0) = y_{i0} \quad ; \quad (i = 1, 2, \ldots, n) \qquad 1.1.11$$

The method in question is a perturbation method, so assume another system of differential equations

$$\hat{y}_i'(x) = \hat{P}_i(x, \hat{y}_1(x), \hat{y}_2(x), \ldots, \hat{y}_n(x)) = \hat{P}_i(x, \hat{y}(x)) \quad ; \quad (i = 1, 2, \ldots, n) \qquad 1.1.12$$

whose solutions $\hat{y}_1(x), \hat{y}_2(x), \ldots, \hat{y}_n(x)$ are known functions of x with the same initial values

$$\hat{y}_i(x_0) = y_{i0} \quad ; \quad (i = 1, 2, \ldots, n) \qquad 1.1.13$$

It is always easy to give such a further system with known solutions. Choose $\hat{y}_1(x), \hat{y}_2(x), \ldots, \hat{y}_n(x)$ such that they have the correct initial values, then differentiate them with respect to x and let these derivatives be the functions

$$\hat{P}_1(x), \hat{P}_2(x), \ldots, \hat{P}_n(x)$$

We introduce the following differential operators

$$D \equiv \frac{\partial}{\partial x} + \sum_{k=1}^{n} P_k(x, y_1(x), \ldots, y_n(x)) \frac{\partial}{\partial y_k} \qquad 1.1.14$$

belonging to the given system (1.1.10);

$$D_1 \equiv \frac{\partial}{\partial x} + \sum_{k=1}^{n} \hat{P}_k(x, y_1(x), \ldots, y_n(x)) \frac{\partial}{\partial y_k} \qquad 1.1.15$$

belonging to the chosen system (1.1.12); and

$$D_2 \equiv \sum_{k=1}^{n} \left\{ P_k(x, y_1(x), \cdots, y_n(x)) - \hat{P}_k(x, y_1(x), \cdots, y_n(x)) \right\} \frac{\partial}{\partial y_k} \equiv D - D_1 \qquad 1.1.16$$

Now let $P_i(x, y(x))$ and $\hat{P}_i(x, y)$, $(i = 1, 2, \cdots, n)$ be continuous functions in the Compact domain

$$B = \left\{ (x, y_1, \cdots, y_n) \,\middle|\, x \in [x_0, x_0 + a];\ |y_i - y_{i0}| \le b \ (i = 1, \cdots, n) \right\} \qquad 1.1.17$$

of the $(x, y_1, \cdots, y_n)$ - space; then they are bounded in B

i.e. $|P_i(x, y)| \le A_0$; $|\hat{P}_i(x, y)| \le C_0$, $(i = 1, \cdots, n)$ 1.1.18

and Peano -theorem guarantees the existence of corresponding solutions $y_i(x)$ of (1.1.10) and $\hat{y}_i(x)$ of (1.1.12), $(i = 1, \cdots, n)$ at least for

$$x \in [x_0, x_0 + h^*] \ ; \ h^* = \min\left(a, \frac{b}{A_0}, \frac{b}{C_0}\right) \qquad 1.1.19$$

Theorem (1): (Main formula) Knapp (1964)

If $P_i(x, y)$ and $\hat{P}_i(x, y)$, $(i = 1, 2, \cdots, n)$ are analytic in B, then the following formulae hold at least for $x \in [x_0, x_0 + h^*]$. The solution can be given as an infinite Lie series

$$y_i(x) = \hat{y}_i(x) + \sum_{r=0}^{\infty} \int_{x_0}^{x} \frac{(x-t)^r}{r!} \left[D_2 D^r y_i \right]_{t, \hat{y}(t)} dt \ ; (i = 1, \cdots, n) \qquad 1.1.20$$

or as a finite Lie series with remainder,

$$y_i(x) = \overline{y}_i(x) + R_{is}(x) \qquad 1.1.21$$

where $$\overline{y}_i(x) = \hat{y}_i(x) + \sum_{r=0}^{s} \int_{x_0}^{x} \frac{(x-t)^r}{r!} \left[D_2 D^r y_i \right]_{t, \hat{y}(t)} dt \qquad 1.1.22$$

and $$R_{is}(x) = \int_{x_0}^{x} \frac{(x-t)^s}{s!} \left\{ \left[D^{s+1} y_i \right]_{t, y(t)} - \left[D^{s+1} y_i \right]_{t, \hat{y}(t)} \right\} dt \qquad 1.1.23$$

Proof

Taylor expansions of $y_i(x)$ & $\hat{y}_i(x)$ are

$$y_i(x) = \sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} \left[D^r y_i \right]_{x_0, y_0} \qquad \text{1.1.24}$$

$$\hat{y}_i(x) = \sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} \left[D_1^r y_i \right]_{x_0, y_0} \qquad \text{1.1.25}$$

The relation

$$D^r = (D_1 + D_2)^r = D_1^r + \sum_{\alpha=0}^{r-1} D_1^{r-\alpha-1} D_2 D^{\alpha} \qquad \text{1.1.26}$$

is easily proved by induction. Hence inserting (1.1.26) into (1.1.24) gives

$$y_i(x) = \sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} \left[\left(D_1^r + \sum_{\alpha=0}^{r-1} D_1^{r-\alpha-1} D_2 D^{\alpha} \right) y_i \right]_{x_0, y_0}$$

$$= \hat{y}_i(x) + \sum_{r=0}^{\infty} \sum_{\alpha=0}^{r-1} \frac{(x-x_0)^r}{r!} \left[D_1^{r-\alpha-1} D_2 D^{\alpha} y_i \right]_{x_0, y_0}$$

Then a change in the order of summation produces

$$y_i(x) = \hat{y}_i(x) + \sum_{\alpha=0}^{\infty} \sum_{r=\alpha+1}^{\infty} \frac{(x-x_0)^r}{r!} \left[D_1^{r-\alpha-1} D_2 D^{\alpha} y_i \right]_{x_0, y_0} \qquad \text{1.1.27}$$

This formula contains expressions of the form

$$\sum_{r=\alpha+1}^{\infty} \frac{(x-x_0)^r}{r!} \left[D_1^{r-\alpha-1} g(x,y) \right]_{x_0, y_0}$$

which can be simplified with the help of the Commutation theorem (1.1.8) using the relation

$$\frac{(x-x_0)^r}{r!} = \int_{x_0}^{x} \frac{(x-t)^{\alpha}}{\alpha!} \frac{(t-x_0)^{r-\alpha-1}}{(r-\alpha-1)!} \, dt \,, \qquad \text{1.1.28}$$

($\alpha \geq 0$, $(r-\alpha-1) \geq 0$, integers)

$$\sum_{r=\alpha+1}^{\infty} \frac{(x-x_0)^r}{r!} \left[D_1^{r-\alpha-1} g(x,y) \right]_{x_0,y_0} = \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} \sum_{r=\alpha+1}^{\infty} \frac{(t-x_0)^{r-\alpha-1}}{(r-\alpha-1)!} \left[D_1^{r-\alpha-1} g(x,y) \right]_{x_0,y_0} dt$$

$$= \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} g\left(t, \sum_{r=\alpha+1}^{\infty} \frac{(t-x_0)^{r-\alpha-1}}{(r-\alpha-1)!} \left[D_1^{r-\alpha-1} y \right]_{x_0,y_0}\right) dt$$

$$= \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} g(t, \hat{y}(t))\, dt \qquad 1.1.29$$

Finally insert this into (1.1.27)

$$y_i(x) = \hat{y}_i(x) + \sum_{\alpha=0}^{\infty} \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} \left[D_2 D^\alpha y_i \right]_{t,\hat{y}(t)} dt \qquad 1.1.30$$

the formula which originally was proved by W.Grobner. It may be noted that putting $\hat{y}_i(x) = y_{i0}, \hat{P}=0$ this reduces to the Taylor series form of the solution, and so (1.1.30) is a non-trivial generalisation of Taylor series. To prove (1.1.21) operate on both sides of (1.1.26) with D_1^{r-s-1} giving

$$D_1^{r-s-1} D^{s+1} = D_1^r + \sum_{\alpha=0}^{s} D_1^{r-\alpha-1} D_2 D^\alpha$$

Rearranging and using $D = D_1+D_2$ gives

$$(D_1+D_2)^r = D_1^r + \sum_{\alpha=0}^{s} D_1^{r-\alpha-1} D_2 D^\alpha + (D^{r-s-1} - D_1^{r-s-1}) D^{s+1}, (r>s) \qquad 1.1.31$$

we next insert (1.1.26) for r≤s and (1.1.31) for (r>s) into (1.1.24) and again change the order of summation

$$y_i(x) = \sum_{r=0}^{\infty} \frac{(x-x_0)^r}{r!} \left[D_1^r y_i \right]_{x_0,y_0} + \sum_{r=0}^{s} \sum_{\alpha=0}^{r-1} \frac{(x-x_0)^r}{r!} \left[D_1^{r-\alpha-1} D_2 D^r y_i \right]_{x_0,y_0}$$

$$+\sum_{r=s+1}^{\infty}\sum_{\alpha=0}^{s}\frac{(x-x_0)^r}{r!}\left[D_1^{r-\alpha-1}D_2D^{\alpha}y_i\right]_{x_0,y_0}+\sum_{r=s+1}^{\infty}\frac{(x-x_0)^r}{r!}\left[\left(D^{r-s-1}-D_1^{r-s-1}\right)D^{s+1}y_i\right]_{x_0,y_0}$$

i.e. $$y_i(x)=\hat{y}_i(x)+\sum_{\alpha=0}^{s}\sum_{r=\alpha+1}^{\infty}\frac{(x-x_0)^r}{r!}\left[D_1^{r-\alpha-1}D_2D^{\alpha}y_i\right]_{x_0,y_0}$$

$$+\sum_{r=s+1}^{\infty}\frac{(x-x_0)^r}{r!}\left[\left(D^{r-s-1}-D_1^{r-s-1}\right)D^{s+1}y_i\right]_{x_0,y_0} \qquad 1.1.32$$

inserting (1.1.29) into (1.1.32) we obtain

$$y_i(x)=\bar{y}_i(x)+R_{is}(x)$$

where

$$\bar{y}_i(x)=\hat{y}_i(x)+\sum_{\alpha=0}^{s}\int_{x_0}^{x}\frac{(x-t)^{\alpha}}{\alpha!}\left[D_2D^{\alpha}y_i\right]_{t,g(t)}dt$$

and $$R_{is}(x)=\int_{x_0}^{x}\frac{(x-x_0)^s}{s!}\left\{\left[D^{s+1}y_i\right]_{t,y(t)}-\left[D^{s+1}y_i\right]_{t,g(t)}\right\}dt$$

An analogous proof for the non-analytic case when $P_i(x,y)$ and $\hat{P}_i(x,y)$ are only s-times continuously differentiable ($s\geq 0$) is given in H.Knapp & G.Wanner (1968).

1.1.4 Order of the remainder term

Theorem (2):

If in addition to the assumptions of theorem (1)

$$\left|\left[D^sP_i(x,y_1,\ldots,y_n)\right]_{x,y^*}-\left[D^sP_i(x,y_1,\ldots,y_n)\right]_{x,y^{**}}\right|\leq K_s\sum_{k=1}^{n}|y_k^*-y_k^{**}| \qquad 1.1.33$$

for $(x,y_1^*,\ldots,y_n^*)\in B$ and $(x,y_1^{**},\ldots,y_n^{**})\in B$

(i.e.Lipschitz Condition for the functions $D^sP_1,\ldots,D^sP_n$ with Constants K_s in B)

and $$|y_i(x)-\hat{y}_i(x)|\leq M\frac{|x-x_0|^{m+1}}{(m+1)!} \quad \text{for} \quad x\in[x_0,x_0+h^*] \qquad 1.1.34$$

(M a Constant, m an integer), then

$$\left| y_i(x) - \bar{y}_i(x) \right| \leq M \frac{K_s \, n \, |x - x_0|^{m+s+2}}{(m+s+2)!} \quad \text{for} \quad x \in [x_0, x_0 + h^*] \qquad 1.1.35$$

To prove this, note that

$$D^{s+1} y_i(x) = D^s \left(D y_i(x) \right) = D^s P_i$$

Thus

$$\left| y_i(x) - \bar{y}_i(x) \right| = \left| R_{i,s}(x) \right| = \left| \int_{x_0}^{x} \frac{(x-t)^s}{s!} \left\{ [D^{s+1} y_i]_{t, y(t)} - [D^{s+1} y_i]_{t, \hat{y}(t)} \right\} dt \right|$$

$$\leq \left| \int_{x_0}^{x} \frac{|x-t|^s}{s!} K_s \sum_{k=1}^{n} \left| y_k(t) - \hat{y}_k(t) \right| dt \right|$$

$$\leq \left| \int_{x_0}^{x} \frac{|x-t|^s}{s!} K_s \, n \, M \frac{|t - x_0|^{m+1}}{(m+1)!} dt \right|$$

and using the formula (1.1.28) we get (1.1.35)

1.1.5 Iterative process

If the remainder term is dropped, the formula (1.1.22) can be used as an iterative process G_s by taking $\bar{y}(x)$ as the new $\hat{y}(x)$ and repeating the calculation, that is by writing

$$_{\nu+1} y_i(x) = {}_{\nu} y_i(x) + \sum_{\alpha=0}^{s} \int_{x_0}^{x} \frac{(x-t)^{\alpha}}{\alpha!} \left[{}_{\nu} D_2 \, D^{\alpha} y_i \right]_{t, \, {}_{\nu} y(t)} dt \qquad 1.1.36$$

where

$$_{\nu} D_2 \equiv \sum \left\{ P_k(x, y_1, \ldots, y_n) - {}_{\nu} P_k(x) \right\} \frac{\partial}{\partial y_k} \qquad 1.1.37$$

It has been shown (H.Knapp and G.Wanner (1968)) that

(i) If the functions $D^s P_i$ are continuous and satisfy Lipschitz condition (1.1.33) in B then

$$\lim_{\nu \to \infty} {}_{\nu} y_i(x) = y_i(x) \quad \text{in an interval} \quad x \in [x_0, x_0 + h] \qquad 1.1.38$$

(ii) If $|y_i(x) - {}_0y_i(x)| \le 2\bar{b}$, $\bar{b} \le b$, $x \in [x_0, x_0+h]$, then

$$|y_i(x) - {}_\nu y_i(x)| \le 2\bar{b}\,\frac{(K_s n\,|x-x_0|^{s+1})^\nu}{[(s+1)\nu]!} \quad , (i=1,\dots,n) \, , (\nu=1,2,\dots) \qquad 1.1.39$$

(iii) If ${}_0y_i(x)$ is the first m terms of Taylor series, then this result may be improved, if

$$|y_i(x) - {}_0y_i(x)| \le M\,\frac{|x-x_0|^{m+1}}{(m+1)!} \quad \text{for} \quad x \in [x_0, x_0+h] \qquad 1.1.40$$

then $$|y_i(x) - {}_\nu y_i(x)| \le M\,|x-x_0|^{m+1}\,\frac{(K_s n\,|x-x_0|^{s+1})^\nu}{[m+1+(s+1)\nu]!} \qquad 1.1.41$$

(iv) If $$\left.\begin{matrix} |{}_1y_i(x) - {}_0y_i(x)| \le M\,\dfrac{|x-x_0|^{m+1}}{(m+1)!} \\ (i=1,\dots,n) \\ x \in [x_0, x_0+h] \end{matrix}\right\} \dots\dots \quad 1.1.42$$

then $$|y_i(x) - {}_\nu y_i(x)| \le M\,|x-x_0|^{m+1} \sum_{\rho=\nu}^{\omega} \frac{(K_s n\,|x-x_0|^{s+1})^\rho}{[m+1+(s+1)\rho]!} \qquad 1.1.43$$

(v) As a generalisation, the above results hold for s-times differentiable functions, with $G_{\bar{s}}$, $\bar{s} \le s$ or with $G_{s_1, s_2, \dots, s_n}$ which is defined as

$${}_{\nu+1}y_i(x) = {}_\nu y_i(x) + \sum_{\alpha=0}^{s_i} \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} \left[{}_\nu D_2\, D^\alpha y_i\right]_{t,\,{}_\nu y(t)} dt \qquad 1.1.44$$

where $0 \le s_i \le s$; s_i integers ($i = 1, \dots, n$)

These iterative processes may be considered also as derivable directly from Taylor series by estimating the remainder term, thus with $s = 0$ the process G_0 :

$$\begin{aligned} {}_{\nu+1}y_i(x) &= {}_\nu y_i(x) + \int_{x_0}^{x} \left[f_i(t, {}_\nu y(t)) - {}_\nu f_i(t, {}_\nu y(t))\right] dt \\ &= {}_\nu y_i + \int_{x_0}^{x} f(t, {}_\nu y(t))\, dt - ({}_\nu y(x) - {}_\nu y(x_0)) \\ &= y_{i0} + \int_{x_0}^{x} f(t, {}_\nu y(t))\, dt \end{aligned}$$

is simply the Picard iterative process. Similarly

$$G_1 : {}_{n+1}y_i(x) = y_{i0} + (x-x_0)P_i(x_0,y_0) + \int_{x_0}^{x}\int_{x_0}^{t_1} [DP_i]_{t,\,y(t)}\, dt\, dt_1 ,$$

$$G_2 : {}_{n+1}y_i(x) = y_{i0} + (x-x_0)P_i(x_0,y_0) + \frac{(x-x_0)^2}{2}[DP]_{x_0,y_0} + \int_{x_0}^{x}\int_{x_0}^{t_2}\int_{x_0}^{t_1} [D^2P_i]_{t,\,y(t)}\, dt\, dt_1\, dt_2$$

and in general

$$G_n : {}_{n+1}y_i(x) = y_{i0} + (x-x_0)P_i(x_0,y_0) + \cdots\cdots + \int_{x_0}^{x} \frac{(x-t)^n}{n!}[D^nP_i]_{t,\,y(t)}\, dt \qquad 1.1.45$$

The advantages that these can have over Taylor series are well known, for example $y' = x^{100} + y^{100}$, $y(0)=0$ produces, with $s=1$ and $\hat{y} = \frac{x^{101}}{101}$ a first iterate

$$\bar{y}(x) = \hat{y}(x) + \int_0^x \frac{t^{10100}}{(101)^{100}}\, dt + \int_0^x (x-t)\cdot 100 \cdot \frac{t^{20099}}{(101)^{199}}\, dt + \cdots$$

$$= \frac{x^{100}}{101} + \frac{x^{10101}}{10101(101)^{100}} + \frac{x^{20101}}{20101.201.(101)^{199}} + \cdots$$

containing more than 30,000 Taylor terms.

It may be noted that these iterative processes for $s=0,1,2$ have been used in a somewhat different form, by Nicolovius (1961) in connection with boundary value problems and some practical experience of his work is reported later. Wright (1964) reports some experience with $s=1$ using ChebysheΦ series and this will be discussed in chapter II. The same iterative processes can be shown to arise from the Zadunaisky approach to the solution of differential equations as follows. Consider the first order non-linear initial value problem

$$y' = f(x,y), \quad y(x_0) = \alpha \qquad , \; x \in [x_0,\, x_N]$$

(i) solving by Picard, using $\hat{y}(x)$ as an approximation, gives

$$\bar{y} = \alpha + \int_{x_0}^{x} f(t, \hat{y}(t))\, dt$$

ii) we try to find an equation which has $\bar{y}$ as exact solution such as

$$y' = f(x,y) + \bar{y}' - f(x,\bar{y})$$

iii) Solving this by Picard with the same initial $\hat{y}$ would give

$$\bar{y}_2 = \alpha + \int_{x_0}^{x} (f(t,\hat{y}) + \bar{y}' - f(t,\bar{y}))\, dt$$
$$= 2\,\bar{y}(x) - \alpha - \int_{x_0}^{x} f(t,\bar{y})\, dt$$

iv) So a better estimate of the original solution is

$$\bar{y} + (\bar{y} - \bar{y}_2) = \alpha + \int_{x_0}^{x} f(t,\bar{y})\, dt$$

which is exactly Picard iteration process.

Similarly if we consider sth term Lie series, Zadunaisky approach yields Lie series iterative process.

1.2 Practical experience with Lie Series

Knapp and Wanner (1968) reported the numerical performance of Lie series used non iteratively. In their calculations they applied (1.1.22) using Gaussian quadrature, with $\hat{y}(x)$ taken as the first (m+1) term of Taylor series, to advance a step length h, and repeated for a succession of steps. Three different types of step size control were used

i) Constant step size

ii) Step size control which keeps the local truncation error of specified size. For this they estimated the truncation error of Lie series using the relation

$$R^{*}_{is}(x) = \int_{x_0}^{x} \frac{(x-t)^s}{s!} \left\{ [D^{s+1} y_i]_{t,\bar{y}(t)} - [D^{s+1} y_i]_{t,\hat{y}(t)} \right\} dt \qquad 1.2.1.$$

The use of such estimation is justified by showing that its order is lower than that of the ignored part of the remainder term. The step h was then fixed so as to keep $\max_i \left| R_{is}(x+h) \right|$ within a given tolerance.

iii) Optimal step size control, which takes into account the stability properties of the differential equations by multiplying the desired error size in each step by the connection matrix. The elements of such matrix $H(x) = \left(\frac{\partial y_i(x)}{\partial y_{k0}} \right)$ 1.2.2 are the derivatives of the solution $y_i(x)$ with respect to the initial values y_{k0}. The connection matrix can be calculated by differentiating (1.1.24) term by term

$$H_{ik}(x) = \frac{\partial y_i(x)}{\partial y_{k0}} = \sum_{r=0}^{\infty} \frac{(x - x_0)^r}{r!} \left[\frac{\partial}{\partial y_k} D^r y_i \right]_{x_0, y_0} \qquad 1.2.3$$

In the course of a step by step integration of the equation using the intervals $x_0 < x_1 < \cdots < x_N$, formula (1.2.3) yields the local connection matrices,

$$C(x_j) = \left(\frac{\partial y_i(x_j)}{\partial y_k(x_{j-1})} \right) \qquad 1.2.4$$

Because of the chain rule these matrices are multiplied up yielding

$$H(x_N) = C(x_N) \cdots\cdots C(x_2) \cdot C(x_1) \qquad 1.2.5$$

the desired connection matrix.

Assume the differential equations are to be integrated over the range $[x_0, x_N]$ using N steps $x_0 < x_1 < \cdots < x_N$ with the step size $h_j = x_j - x_{j-1}$. If e_j is the error vector made at the point x_j, then its propagation at x_N is given by

$$e_j^{(N)} = H(x_N) \cdot H^{-1}(x_j) \cdot e_j \qquad 1.2.6$$

In the special case n = 1 (one equation only), $e_j = \phi_j . h_j^{p+1}$ where p = m + S + 1 is the order of the method. Then by minimising

$$\sum_{j=1}^{N} e_j^{(N)} = \sum_{j=1}^{N} H(x_N) \cdot H^{-1}(x_j)\, e_j \qquad 1.2.7$$

under the condition that $$\sum_{j=1}^{N} h_j = x_N - x_0 \qquad 1.2.8$$

one can show that the optimal step size control has to keep

$$\frac{H^{-1}(x_j)\, e_j}{h_j} \approx \gamma \qquad 1.2.9$$

where e_j is the truncation error (1.2.1) and γ is a specified tolerance.

1.2.1 Computational results

Results are reported for varying m,s but keeping the total order m + s + 1 constant, and for varying k, the number of Gaussian nodes

Example (1) Test of the accuracy under variation of m and s with m+s = 18

$y' = 1 - e^{-y}\,(\sin x - \cos x)$, $y(0) = 0$

exact solution $y(x) = \log(\sin x + e^{x})$

h	m	s	actual error of $\hat{y}(h)$	actual error of $\bar{y}(h)$	error estimation for $\bar{y}(h)$ (local truncation error)
0.125	18	0	7.2×10^{-15}	3.1×10^{-17}	3.1×10^{-17}
	13	5	2.3×10^{-15}	1.45×10^{-20}	1.0×10^{-20}
	8	10	8.2×10^{-8}	4.9×10^{-21}	1.5×10^{-21}
0.250	18	0	3.25×10^{-9}	2.0×10^{-11}	1.9×10^{-11}
	13	5	3.19×10^{-7}	6.6×10^{-15}	3.3×10^{-15}
	8	10	3.62×10^{-5}	1.8×10^{-15}	0.2×10^{-15}
0.500	18	0	1.3×10^{-3}	6.3×10^{-6}	6.2×10^{-6}
	13	5	4.1×10^{-3}	1.1×10^{-9}	4.7×10^{-10}
	8	10	1.5×10^{-2}	3.5×10^{-10}	0.08×10^{-10}

The Taylor series converging only for $h \leq 0.5885$, gives poor results for $h = 0.5$, in spite of this the Lie series correction yields good results. As can be seen the estimation of the local truncation error works satisfactorily here.

Another comparison between Lie series and simple power series based on the computational effort in using Gaussian quadrature is introduced by Stetter (1973) and will be mentioned later in this section.

Example (8) test of the accuracy using different step size controls.

$y' = -xy^3$, $x_o = -1$, $y(-1) = y_o = 0.9999\ 9999\ 995$

$y(o) = ?$, $y(1) = ?$

Answer is $y(o) = 100\ 000$

$y(1) = 0.9999\ 9999\ 995$

Results for m = 15, s = 3, k = 2 where k is the number of nodes in the Gaussian quadrature.

step size control	γ	h	x	actual error of y (x)	error estimation of y (x)	Steps
normal	10^{-12}	0.29...0.0000023	0 1	$1.6 \times 10^{+2}$ 1.7×10^{-13}	....	46 107
optimal	10^{-14}	0.24...0.0000060	0 1	5.1×10^{-0} 5.4×10^{-15}	9.6×10^{-0} 20.0×10^{-15}	32 80

This example has an extremely varying error function, because of this constant step size is not advisable.

1.2.2 The advantage of the Lie series method over the simple power series method

A comparison of the computational effort involved in this way of applying series has been mentioned in Stetter (1973).

Let s be the number of terms in Lie series, m the order of Taylor series representing $\hat{y}(x)$, k is the number of nodes of the Gaussian quadrature, then it has been proved (see Stetter (1973)) that the order of Convergence of Lie series method is

$$P = m + \min(s, 2k) \qquad 1.2.10$$

This result raises the question of whether this method gives any advantage over a simple power series method of order m + s.

The Computational effort for evaluation of the coefficients of $\hat{y}(x)$ is proportional to m^2, the Computational effort for evaluation of Lie series is proportional to $2 \cdot s^2$ for each node, thus the total effort is proportional to $m^2 + 2ks^2$.

From (1.2.7) we should choose $k \geq s/2$, so that we have an effort like $m^2 + s^3$ for a Convergence of order $P = m + s$. This indicates that (for large m), the highest order for a given effort is not achieved with s=o (i.e. power series method), but roughly with $3s^2 = 2m$, thus the following choices of m, s, k should be reasonable.

m	s	k
1 - 4	1	1
4 - 10	2	1 or 2
10 - 20	3	2

Furthermore, as shown in (1. 2. 1) for constant p = m+s the actual errors tend to decrease with increasing s and correspondingly decreasing m.

1.3 Chebyshev polynomials and their use in solving ordinary differential equations

In this section we are going to quote some properties of Chebyshev polynomials and the approximation of any function f(x), $x \in [-1,1]$ in terms of them. This kind of approximation is known to be a *least squares* approximation. We are also going to mention some of the iterative methods for solving ordinary differential equations in Chebyshev series.

1.3.1 Properties of Chebyshev polynomials

(i) Definitions

$$\left.\begin{aligned} T_r(x) &= \cos(r \cos^{-1} x) \qquad -1 \leq x \leq 1 \\ T_r^*(x) &= T_r(2x-1) \qquad 0 \leq x \leq 1 \end{aligned}\right\} \quad \ldots\ldots\ldots \quad 1.3.1$$

(ii) Recurrence relation

$$T_{r+1}(x) - 2x\,T_r(x) + T_{r-1}(x) = 0 \qquad 1.3.2$$

(iii) Product formula

$$T_r(x)\cdot T_s(x) = \frac{1}{2}\left\{ T_{r+s}(x) + T_{|r-s|}(x) \right\} \qquad 1.3.3$$

(iv) Differentiation

$$f(x) = \sum_{r=0}^{\infty}{}' A_r T_r(x) \quad , \quad f'(x) = \sum_{r=0}^{\infty}{}' C_r T_r(x)$$

then

$$\left.\begin{aligned} C_{2r} &= \sum_{s=r}^{\infty} 2(2s+1) A_{2s+1} \\ C_{2r+1} &= \sum_{s=r}^{\infty} 2(2s+2) A_{2s+2} \end{aligned}\right\} \quad ; \; r = 0, 1, \ldots \qquad \ldots\ldots \; 1.3.4$$

For the truncated series

$$P(x) = \sum_{r=0}^{N}{}' A_r T_r(x) \quad , \quad P'(x) = \sum_{r=0}^{N-1}{}' C_r T_r(x)$$

$$\left.\begin{aligned} C_{N-1} &= 2N A_N \\ C_{N-2} &= 2(N-1) A_{N-1} \\ C_{r-1} &= 2r A_r + C_{r+1} \quad ; \; r = 1, 2, \ldots, N-2 \end{aligned}\right\} \qquad \ldots\ldots \; 1.3.5$$

(v) Integration

$$\int T_r(x)\,dx = \begin{cases} T_1(x) & , \; r = 0 \\ \frac{1}{4} T_2(x) & , \; r = 1 \\ \frac{1}{2}\left[\frac{T_{r+1}(x)}{r+1} - \frac{T_{r-1}(x)}{r-1} \right] & , \; r > 1 \end{cases} \qquad 1.3.6$$

(vi) Orthogonal properties

$$\int_{-1}^{1} \frac{T_r(x)\,T_s(x)}{\sqrt{1-x^2}}\,dx = \begin{cases} \pi & \text{for} \quad r = s = 0 \\ \pi/2 & \text{for} \quad r = s \neq 0 \\ 0 & \text{for} \quad r \neq s \end{cases} \qquad 1.3.7$$

for $N > 0$, $r, s \leq N$

$$\sum_{j=0}^{N}{}'' T_r(x_j)\,T_s(x_j) = \begin{cases} N & r=s=0 \text{ or } N \\ N/2 & r=s\neq 0 \text{ or } N \\ 0 & r\neq s \end{cases} \qquad 1.3.8$$

where $x_j = \cos\frac{j\pi}{N}$, $j = 0, 1, \ldots, N$

(vii) Calculation of Chebyshev Coefficients

(a) If f(x) is continuous and of bounded variation in the range $[-1,1]$ then f(x) can be expressed as the following infinite series

$$P(x) = \tfrac{1}{2}A_0 T_0(x) + A_1 T_1(x) + \cdots\cdots = \sum_{r=0}^{\infty}{}' A_r T_r(x)$$

where

$$A_r = \frac{2}{\pi}\int_{-1}^{1}\frac{P(x)\,T_r(x)}{\sqrt{1-x^2}}\,dx$$

$$= \frac{2}{\pi}\int_{0}^{\pi} P(\cos\theta)\cos r\theta\,d\theta \qquad 1.3.9$$

This is a familiar representation in the theory of Fourier series.

(b)

If $$C_r = \frac{2}{N}\sum_{k=0}^{N}{}'' P(x_k)\,T_r(x_k) \;, \quad r = 0, 1, \ldots, N$$

$$= \frac{2}{N}\sum_{k=0}^{N}{}'' P\left(\cos\frac{k\pi}{N}\right)\cdot\cos\left(\frac{rk\pi}{N}\right) \qquad 1.3.10$$

where $$x_k = \cos\frac{k\pi}{N} \;, \quad k = 0, 1, \ldots, N \qquad 1.3.11$$

then the expression

$$P_n(x) = \sum_{r=0}^{n}{}' C_r T_r(x) \;, \quad n < N \qquad 1.3.12$$

is the polynomial of discrete least squares best fit

i.e. that which minimises

$$\sum_{k=0}^{N}{}''\left\{P(x_k) - \sum_{r=0}^{n}{}' C_r T_r(x_k)\right\}^2$$

and the minimum is

$$\sum_{k=0}^{N}{}'' \left\{ f^2(x_k) - \sum_{r=0}^{n} C_r^2 T_r^2(x_k) \right\}$$

In particular the function

$$P_N(x) = \sum_{r=0}^{N}{}'' C_r T_r(x) \qquad 1.3.13$$

is the polynomial of degree N which fits f(x) exactly at the data points x_k of (1.3.11) with k = o,1,...., N.

For the rest of the properties and related proofs see Fox and Parker (1968), Clenshaw (1962).

1.3.2 Chebyshev Solution of non-linear ordinary differential equations

(i) The Picard method

This method (Wright, 1964, Clenshaw and Norton 1963) solves the first order differential equation

$$y'(x) = f(x,y) \quad , \quad x \in [-1,1] \qquad 1.3.14)$$

with the initial condition $y(x_o) = \alpha$ by means of Picard iteration

$$y^{(r+1)}(x) = \alpha + \int_{x_0}^{x} f(t, y^{(r)})\, dt \qquad 1.3.15$$

If at some stage we have an approximation

$$y^{(r)}(x) = \sum_{s=0}^{N}{}' A_s^{(r)} T_s(x) \qquad 1.3.16$$

we can find the corresponding approximation

$$f^{(r)} = f(x, y^{(r)}) = \sum_{s=0}^{N}{}' B_s^{(r)} T_s(x) \qquad 1.3.17$$

The B's can be determined exactly in some cases, e.g. if f is linear with polynomial coefficients, or can be found by collocation at a prescribed set of points using (1.3.10), then using the known formula (1.3.6) for integrating a finite Chebyshev series together with (1.3.15) we get

$$y^{(r+1)} = \sum_{s=0}^{N}{}' A_s^{(r+1)} T_s(x) \qquad 1.3.18$$

which could be used at the next step. The error analysis will be mentioned in the next chapter.

(ii) Newton's method

Expanding about the solution at the rth stage gives

$$y'^{(r+1)} = F(x, y^{(r)}) + (y^{(r+1)} - y^{(r)}) F_y(x, y^{(r)})$$

i.e. $$y'^{(r+1)} - y^{(r+1)} F_y(x, y^{(r)}) = F(x, y^{(r)}) - y^{(r)} F_y(x, y^{(r)}) \qquad 1.3.19$$

a linear differential equation in $y^{(r+1)}$, which can be solved using the method of superposition.

Norton (1964) used Chebyshev series in the following manipulations

$$y^{(r+1)}(x) = \sum_{s=0}^{N}{}' A_s^{(r+1)} T_s(x)$$

$$y^{(r)}(x) = \sum_{s=0}^{N} A_s^{(r)} T_s(x)$$

$$y'^{(r+1)}(x) = \sum_{s=0}^{N-1}{}' A_s'^{(r+1)} T_s(x)$$

$$F(x, y^{(r)}) = \sum_{s=0}^{N-1}{}' B_s T_s(x)$$

$$F_y(x, y^{(r)}) = \sum_{s=0}^{N-1}{}' C_s T_s(x)$$

then substituting in (1.3.19), using 1/2 C_0 as an approximation to $f_y(x, y^{(r)})$ and equating coefficients of $T_s(x)$ we get

$$A_s'^{(r+1)} = B_s + \tfrac{1}{2} C_0 (A_s^{(r+1)} - A_s^{(r)})$$

using the relation

$$2sA_s = A'_{s-1} - A'_{s+1} \quad , s = 1, 2, \ldots, N$$

we get the set of linear equations

$$\tfrac{1}{2} C_0 (A_{s-1}^{(r+1)} - A_{s+1}^{(r+1)}) - 2sA_s^{(r+1)} = P_s$$

where $$P_s = (B_{s+1} - B_{s-1}) + \tfrac{1}{2} C_0 (A_{s-1}^{(r)} - A_{s+1}^{(r)}) \quad , s = 1, 2, \ldots, N$$

$A_s^{(r+1)}$, $A_s^{(r)}$ for $s > N$ we assumed to be zeros and the equations are

solved successively. A modification of this method in the case when c_o is small, is mentioned in Norton (1964).

In the next chapter the use of Chebyshev series in Lie series will be developed and analogous formulae to those in (1.3.1) (i) will be produced and used as a basis for an iterative method of solution of differential equations. The error analysis for this method has been given in this chapter and will be applied to results obtained.

CHAPTER II

SOLUTION OF NON-LINEAR INITIAL VALUE PROBLEMS IN CHEBYSHEV SERIES USING LIE SERIES METHOD

2.1 Lie series in Chebyshev form

2.1.1. Relations for infinite Chebyshev series

Consider the non-linear initial value problem

$$y'(x) = f(x,y), \qquad x \in [-1,1]$$
$$y(x_o) = y_o \qquad \text{2.1.1}$$

Let the auxiliary initial value problem be

$$y'(x) = \hat{f}(x,y), \qquad x \in [-1,+1]$$
$$y(x_o) = y_o \qquad \text{2.1.2}$$

with a known solution $y = \hat{y}(x)$. If the differential operators D, D_1, D_2 are as defined in (1.2.5 - 7), the truncated Lie series is of the form

$$\bar{y}(x) = \hat{y}(x) + \sum_{\alpha=0}^{s} \int_{x_0}^{x} \frac{(x-t)^{\alpha}}{\alpha!} \left\{ D_2 D^{\alpha} y \right\}_{t, \hat{y}(t)} dt \qquad \text{2.1.3}$$

and the remainder is

$$R_s^{*}(x) = \int_{x_0}^{x} \frac{(x-t)^{s}}{s!} \left\{ (D^s f)_{t, y(t)} - (D^s f)_{t, \hat{y}(t)} \right\} dt \qquad \text{2.1.4}$$

now (2.1.3) can take the form

$$\bar{y}(x) = \hat{y}(x) + \int_{x_0}^{x} [D_2 y]_{t, \hat{y}(t)} dt + \int_{x_0}^{x} \int_{x_0}^{t_1} [D_2 D y]_{t, \hat{y}(t)} dt dt_1$$

$$+ \cdots\cdots + \int_{x_0}^{x} \int_{x_0}^{t_s} \cdots\cdots \int_{x_0}^{t_1} [D_2 D^s y]_{t, \hat{y}(t)} dt\, dt_1 \cdots dt_s \qquad \text{2.1.5}$$

where

$$\left.\begin{aligned} D_2 y &= f(x,y) - \hat{f}(x,y) \\ D_2(Dy) &= [f(x,y) - \hat{f}(x,y)] \frac{\partial f}{\partial y} \\ D_2(D^2 y) &= [f(x,y) - \hat{f}(x,y)] \frac{\partial (Df)}{\partial y} \\ &\cdots\cdots\cdots \end{aligned}\right\} \cdots\cdots\cdots\cdots \qquad \text{2.16}$$

and so on

The functions involved may all be expressed as Chebyshev series

$$\left.\begin{aligned} \bar{y}(x) &= \sum_{r=0}^{\infty}{}' \bar{A}_r T_r(x) \\ \hat{y}(x) &= \sum_{r=0}^{\infty}{}' \hat{A}_r T_r(x) \\ [D_2 D^{\alpha} y]_{x,\hat{y}(x)} &= \sum_{r=0}^{\infty}{}' \hat{B}_{\alpha r} T_r(x), \quad \alpha = 0,1,\ldots \end{aligned}\right\} \quad \ldots\ldots\ldots \quad 2.1.7$$

substituting in (2.1.5) we get

$$\begin{aligned} \sum_{r=0}^{\infty}{}' \bar{A}_r T_r(x) = \sum_{r=0}^{\infty}{}' \hat{A}_r T_r(x) &+ \int_{x_0}^{x} \left(\sum_{r=0}^{\infty}{}' \hat{B}_{0r} T_r(t) \right) dt \\ &+ \int_{x_0}^{x}\int_{x_0}^{t_1} \left(\sum_{r=0}^{\infty}{}' \hat{B}_{1r} T_r(t) \right) dt\, dt_1 + \ldots\ldots\ldots \\ &+ \int_{x_0}^{x}\int_{x_0}^{t_2} \cdots \int_{x_0}^{t_1} \left(\sum_{r=0}^{\infty}{}' \hat{B}_{sr} T_r(t) \right) dt\, dt_1 \cdots dt_s \end{aligned} \quad 2.1.8$$

Now performing the integrals in the R.H.S. of (2.1.8) using (1.3.6) and comparing the coefficients of Chebyshev polynomials in the two sides produces the infinite set of equations

$$\underset{\sim}{\bar{A}} = \underset{\sim}{\hat{A}} + R_0 \underset{\sim}{\hat{B}}_0 + R_1 \underset{\sim}{\hat{B}}_1 + \ldots\ldots\ldots + R_s \underset{\sim}{\hat{B}}_s \quad 2.1.9$$

where $\underset{\sim}{\bar{A}} = (\bar{A}_1, \bar{A}_2, \ldots\ldots)^T$, $\underset{\sim}{\hat{A}} = (\hat{A}_1, \hat{A}_2, \ldots\ldots)^T$,

$\underset{\sim}{\hat{B}}_r = (\hat{B}_{r1}, \hat{B}_{r2}, \ldots\ldots)^T$, dependent on $\underset{\sim}{\hat{A}}$

and $R_0, R_1, \ldots\ldots\ldots, R_s$ are matrices derived as follows:

For the matrix R_0 consider the first integral

$$\int_{x_0}^{x} \sum_{r=0}^{\infty}{}' \hat{B}_{0r} T_r(t)\, dt = \sum_{r=0}^{\infty}{}' A_r^{(0)} T_r(x)$$

$$= \left[\frac{1}{2}\hat{B}_{00} T_1(t) + \frac{1}{4}\hat{B}_{01} T_2(t) + \sum_{r=2}^{\infty} \frac{\hat{B}_{0r}}{2}\left(\frac{T_{r+1}(t)}{r+1} - \frac{T_{r-1}(t)}{r-1} \right) \right]_{x_0}^{x} \qquad 2.1.10$$

so $\underset{\sim}{A}^{(0)} = R_0 \underset{\sim}{\hat{B}}_0$, where

$$R_0 = \begin{bmatrix} -T_1(x_0) & -\frac{T_2(x_0)}{2} & \left(T_1(x_0) - \frac{T_3(x_0)}{3}\right) & \cdots\cdots & \left(\frac{T_{r-1}(x_0)}{r-1} - \frac{T_{r+1}(x_0)}{r+1}\right) \cdots \\ \frac{1}{2} & 0 & -\frac{1}{2} & & \\ & \frac{1}{4} & 0 & -\frac{1}{4} & \\ & & \cdots\cdots & & \\ & & & \frac{1}{2r} \quad 0 \quad \frac{-1}{2r} & \cdots \\ & & & \cdots\cdots & \end{bmatrix} \qquad (2.1.11)$$

In general if $\sum_{r=0}^{\infty}{}' A_r^{(s)} T_r(x) = \int_{x_0}^{x}\int_{x_0}^{t_s} \cdots\cdots \int_{x_0}^{t_1} \sum_{r=0}^{\infty}{}' \hat{B}_{sr} T_r(t)\, dt_1 \cdots dt_s$

then $\underset{\sim}{A}^{(s)} = R_0^{s+1} \underset{\sim}{\hat{B}}_s$

i.e. $R_1 = R_0^2$, $R_2 = R_0^3$, $\cdots\cdots$, $R_s = R_0^{s+1}$ 2.1.12

In particular

$$R_0^2 = \begin{bmatrix} \left(\frac{1}{2} + \frac{T_2(x_0)}{4}\right) & \left(\frac{T_1(x_0)}{2} + \frac{T_3(x_0)}{6}\right) & \left(\frac{T_4(x_0)}{8} - \frac{T_0(x_0)}{2}\right) & \cdots\cdots & \frac{1}{2}\left(\frac{T_{r+2}(x_0)}{r+2} - \frac{T_{r-2}(x_0)}{r-2}\right) \cdots \\ -\frac{T_1(x_0)}{2} & -\left(\frac{1}{8} + \frac{T_2(x_0)}{4}\right) & \left(\frac{3T_1(x_0) - T_3(x_0)}{6}\right) & \left(\frac{1}{8} + \frac{T_2}{4} - \frac{T_4}{8}\right) \cdots & -\frac{1}{2}\left(\frac{T_{r+1}(x_0)}{r+1} - \frac{T_{r-1}(x_0)}{r-1}\right) \cdots \\ \frac{1}{8} & 0 & -\frac{1}{6} & 0 \quad \frac{1}{24} & \\ & & \cdots\cdots & & \\ & & & \frac{1}{4r(r-1)} \quad 0 \quad \frac{-1}{2(r^2-1)} \quad 0 \quad \frac{1}{4r(r+1)} \quad 0 & \cdots \\ & & & \cdots\cdots & \end{bmatrix}$$

2.1.13

and

$$R_0^3 = \begin{bmatrix} \left(\frac{-9T_1 - T_3}{24}\right) & -\left(\frac{6+8T_2+T_4}{24}\right) & \left(\frac{10T_1-5T_3-T_5}{40}\right) & \left(\frac{18-2T_6-9T_4+18T_2}{96}\right) & \cdots\cdots & -\frac{1}{8}\left(\frac{T_{r+3}}{r+3}+\frac{3T_{r+1}}{r+1}-\frac{3T_{r-1}}{r-1}-\frac{T_{r-3}}{r-3}\right)\cdots \\ \left(\frac{3+2T_2}{16}\right) & \left(\frac{3T_1+T_3}{12}\right) & \left(\frac{T_4}{16}-\frac{1}{16}\right) & \left(\frac{T_5-5T_1}{20}\right) & \left(\frac{2T_6-6T_2-1}{48}\right)\cdots\cdots & \frac{1}{4}\left(\frac{T_{r+2}}{r+2}-\frac{T_{r-2}}{r-2}\right)\cdots \\ -\frac{T_1}{8} & -\left(\frac{1}{24}+\frac{T_2}{16}\right) & -\left(\frac{T_3-3T_1}{24}\right) & \left(\frac{3-2T_4+6T_2}{64}\right) & \left(\frac{5T_3-3T_5}{120}\right) & \left(\frac{6T_4-4T_6-1}{192}\right)\cdots \frac{-1}{8}\left(\frac{T_{r+1}}{r+1}-\frac{T_{r-1}}{r-1}\right)\cdots \\ \frac{1}{48} & 0 & \frac{-1}{32} & 0 & \frac{1}{80} & 0 & \frac{-1}{480} & 0 \\ 0 & \frac{1}{192} & 0 & \frac{-3}{320} & 0 & \frac{1}{192} & 0 & \frac{-1}{960} \quad \cdots \\ & & & \cdots\cdots & & & & \\ & & \frac{1}{8r(r-1)(r-2)} & 0 & \frac{-3}{8r(r+1)(r+2)} & 0 & \frac{3}{8r(r-1)(r+1)} & 0 \quad \frac{-1}{8r(r+1)(r+2)} \quad 0\cdots \\ & & & \cdots\cdots & & & & \end{bmatrix}$$

2.1.14

2.1.2. Iteration process

The relation (2.1.3) may be used iteratively as follows

$$y^{(i+1)}(x) = y^{(i)}(x) + \sum_{\alpha=0}^{s} \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} \left\{ D_2 D^\alpha y \right\}_{t, y^{(i)}(t)} dt \quad , (i=1,\ldots) \qquad 2.1.15$$

with $y^{(0)}(x) = \hat{y}(x)$

and in (2.1.5 - 10) we replace y(x), y(x), f(x) by $y^{(i)}(x)$, $y^{(i+1)}(x)$, $f^{(i)}(x)$ respectively.

In practice we use a truncated Chebyshev series of order N, so

$$\left.\begin{aligned} y^{(i)}(x) &= \sum_{r=0}^{N\,\prime} A_r^{(i)} T_r(x) \\ y^{(i+1)}(x) &= \sum_{r=0}^{N\,\prime} A_r^{(i+1)} T_r(x) \quad , \; i = 0,1,\ldots \\ \left[D_2 D^\alpha y\right]_{x, y^{(i)}(x)} &= \sum_{r=0}^{\prime} B_{\alpha r}^{(i)} T_r(x) \quad , \; \alpha = 0,1,\ldots \end{aligned}\right\} \quad \ldots\ldots \; 2.1.16$$

where $A_r^{(i)} = 0$ for r>N, (i=0,1,...) and since the B's are the coefficients

of derivatives, then neglecting $B^{(i)}_{jr}$ for $r > N-j-1$ 2.1.17

The relation (2.1.9) becomes

$$\underset{\sim}{A}^{(i+1)} = \underset{\sim}{A}^{(i)} + R_{0N}\underset{\sim}{B}^{(i)}_{0} + R_{1N}\underset{\sim}{B}^{(i)}_{1} + \cdots\cdots + R_{sN}\underset{\sim}{B}^{(i)}_{s} \qquad 2.1.18$$

where the matrices R_{jN}, $(j=0,1,\ldots,s)$ are of order (N+1) X (N+1).

The matrix R_{0N} is the top left corner of R_0 in (2.1.12) with

$$R_{0N}(1,N+1) = \frac{T_{N-1}(x_0)}{N-1}$$

Similar to (2.1.13) one may replace $R_{1N}, R_{2N},\ldots,R_{sN}$ by $R^2_{0N},\ldots R^{s+1}_{0N}$ but in our case the use of truncated Chebyshev series will make the matrices $R^2_{0N}, R^3_{0N},\ldots$ slightly different from the matrices $R_{1N}, R_{2N},\ldots$ The difference occurs due to the appearance of terms like $T_r(x)$, $r>N$ in the matrices $R^2_{0N}, R^3_{0N}, \ldots$ while we replace these terms by zeros in R_{1N}, R_{2N}, for example the difference between R^2_{0N} and R_{1N} occurs in the location (1,N) when $R^2_{0N}(1,N) - R_{1N}(1,N) = \frac{T_{N+1}(x_0)}{2N}$ But from (2.1.17,18) this term is multiplied by $B^{(i)}_{1,N-1}$ which is zero. This justifies the use of R^2_{0N} in place of R_{1N}. Similar comparisons between R^r_{0N} and $R_{r-1,N}$, $r = 3,4\ldots$ justify the use of $R_{0N}, R^2_{0N}, \ldots$ R^{s+1}_{0N} in place of $R_{0N}, R_{1N}, \ldots, R_{sN}$ in the products $R\underset{\sim}{B}$

The iterative procedure works as follows:

(i) Work out the analytic expression for $f_y(x,y), (Df)_y, \ldots$

(ii) Starting with $y^0 = \hat{y}(x)$ as the Taylor series expansion of y about $x = x_0$ using the derivatives already calculated in (i), differentiate to get $\hat{f}(x)$

(iii) From (ii) we can find $A^{(0)}_r$, $r = 0,1,\ldots,N$ using (1.3.10)

(iv) Evaluate $\hat{f}$, f, f_y, $(Df)_y$ ..... at $x_k = \cos\frac{k\pi}{N}$, $y^{(0)}_{(x_k)}, k = 0,1,\ldots,N$

(v) Use (2.1.6) to find the values of $D_2 y$, $D_2(Dy)$ $D_2(D^2y)$, ... at x_k, $k = 0,1,\ldots,N$

(vi) Use (1.3.10), to find $\underset{\sim}{B}_0^{(0)}$, $\underset{\sim}{B}_1^{(0)}$, ...

(vii)Substitute into (2.1.18) to get $\underset{\sim}{A}^{(1)}$

(viii) Repeat until the difference between two successive evaluations $\underset{\sim}{A}^{(i)}$, $\underset{\sim}{A}^{(i+1)}$ is less than a specified tolerance.

The predicted error improvement in i steps (for N sufficiently large) is an increase from $O(|x - x_0|^{m+1}$ in $y^{(0)}$ to $O(|x - x_0|^{m+1+i(s+1)})$ in $y^{(i)}$. For this iterative process we use the notation G_{sN} to indicate the dependence on s (number of terms in Lie series) and N (number of terms in Chebyshev series).

2.2 Error Analysis for the iterative process G_{sN}

Consider the system of n first order non-linear differential equations

$$\left.\begin{aligned} y_i'(x) &= P_i(x, y_1(x), \ldots, y_n(x)) \\ y_i(x_0) &= y_{i0} \end{aligned}\right\} : (i = 1, 2, \ldots, n) \quad \ldots\ldots \quad 2.2.1$$

let $y^{(k)}$ be the kth iteration on $y^{(0)}$, then

$$y_i^{(k+1)}(x) = y_i^{(k)}(x) + \sum_{\alpha=0}^{s} \int_{x_0}^{x} \frac{(x-t)^\alpha}{\alpha!} \left\{ D_2 D^\alpha y_i \right\}_{t, y^{(k)}(t)} dt \qquad 2.2.2$$

let y_i^* be the exact solution

i.e. $$y_i^*(x) = y_i^{(k+1)}(x) + \int_{x_0}^{x} \frac{(x-t)^s}{s!} \left[(D^s P_i)_{t, y^*(t)} - (D^s P_i)_{t, y^{(k)}(t)} \right] dt \qquad 2.2.3$$

then the error of the (k+1)th iterate is

$$y_i^*(x) - y_i^{(k+1)}(x) = \int_{x_0}^{x} \int_{x_0}^{t_s} \cdots \int_{x_0}^{t_1} \left[(D^s P_i)_{t, y^*(t)} - (D^s P_i)_{t, y^{(k)}(t)} \right] dt\, dt_1 \cdots dt_s \qquad 2.2.4$$

$$\left.\begin{aligned} \text{let} \quad y_i^* &= \sum_{r=0}^{N'} A_{ir}^* T_r(x) \text{ approximately} \\ y_i^{(k)} &= \sum_{r=0}^{N'} A_{ir}^{(k)} T_r(x) \\ (D^s P_i)_{y^*(x)} &= \sum_{r=0}^{N'} B_{ir}^* T_r(x) \\ (D^s P_i)_{y^{(k)}(x)} &= \sum_{r=0}^{N'} B_{ir}^{(k)} T_r(x) \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots \quad 2.2.5$$

Since in this section we are using only the sth derivation of f_i we use the notation B_{ir} for the coefficients of $D^s f_i$ dropping the suffix s.

From (2.2.4), (2.2.5)

$$\underset{\sim}{A}_i^* - \underset{\sim}{A}_i^{(k+1)} = R_{SN}\left(\underset{\sim}{B}_i^* - \underset{\sim}{B}_i^{(k)}\right) \qquad 2.2.6$$

where R_{SN} is the matrix defined in (2.1.18), and so if $\underset{\sim}{B}_i$ satisfies the Lipschitz Condition

$$\|\underset{\sim}{B}_i^* - \underset{\sim}{B}_i^{(k)}\| \leq K_{i1}\|\underset{\sim}{A}_1^* - \underset{\sim}{A}_1^{(k)}\| + K_{i2}\|\underset{\sim}{A}_2^* - \underset{\sim}{A}_2^{(k)}\| + \cdots + K_{in}\|\underset{\sim}{A}_n^* - \underset{\sim}{A}_n^{(k)}\|, \qquad 2.2.7$$

then $$\|\underset{\sim}{A}_i^* - \underset{\sim}{A}_i^{(k+1)}\| \leq \|R_{SN}\| \sum_{j=1}^{n} K_{ij}\|\underset{\sim}{A}_j^* - \underset{\sim}{A}_j^{(k)}\|$$

i.e.

$$\begin{bmatrix} \|\underset{\sim}{A}_1^* - \underset{\sim}{A}_1^{(k+1)}\| \\ \|\underset{\sim}{A}_2^* - \underset{\sim}{A}_2^{(k+1)}\| \\ \vdots \\ \|\underset{\sim}{A}_n^* - \underset{\sim}{A}_n^{(k+1)}\| \end{bmatrix} \leq \|R_{SN}\| \begin{bmatrix} K_{11} & K_{12} & \cdots & K_{1n} \\ K_{21} & K_{22} & \cdots & K_{2n} \\ & \cdots\cdots\cdots & & \\ K_{n1} & K_{n2} & \cdots & K_{nn} \end{bmatrix} \begin{bmatrix} \|\underset{\sim}{A}_1^* - \underset{\sim}{A}_1^{(k)}\| \\ \|\underset{\sim}{A}_2^* - \underset{\sim}{A}_2^{(k)}\| \\ \vdots \\ \|\underset{\sim}{A}_n^* - \underset{\sim}{A}_n^{(k)}\| \end{bmatrix} \qquad 2.2.8$$

let $\underset{\sim}{E}^{(i)}$ be the error vector $(\|\underset{\sim}{A}_1^* - \underset{\sim}{A}_1^{(i)}\|, \ldots\ldots\ldots, \|\underset{\sim}{A}_n^* - \underset{\sim}{A}_n^{(i)}\|)^T$, then

$$\|\underset{\sim}{E}^{(k+1)}\| \leq \|R_{SN}\|\|K_s\|\|\underset{\sim}{E}^{(k)}\| \qquad 2.2.9$$

2.2.1 Lipschitz Condition and the Jacobian matrix

Any function $f(x, y_1, \ldots\ldots, y_n)$ may be approximated by $\sum_{r=0}^{N}{}'' B_r T_r(x)$

The coefficients B are obtained by a collocation process as stated in (1.3.1)(vii)

where

$$\underset{\sim}{B} = \frac{2}{N}\begin{bmatrix} \frac{1}{2}T_0(x_0) & T_0(x_1) & \cdots & T_0(x_{N-1}) & \frac{1}{2}T_0(x_N) \\ \frac{1}{2}T_1(x_0) & T_1(x_1) & \cdots & T_1(x_{N-1}) & \frac{1}{2}T_1(x_N) \\ & & \cdots\cdots & & \\ \frac{1}{2}T_N(x_0) & T_N(x_1) & \cdots & T_N(x_{N-1}) & \frac{1}{2}T_N(x_N) \end{bmatrix} \begin{bmatrix} f(x_0, y_1(x_0), \cdots, y_n(x_0)) \\ f(x_1, y_1(x_1), \cdots, y_n(x_1)) \\ \vdots \\ f(x_N, y_1(x_N) \cdots, y_n(x_N)) \end{bmatrix}$$

Hence if

$$y_i(x) = \sum_{r=0}^{N}{}' A_{ir} T_r(x)$$

then

$$\underset{\sim}{B} = \frac{2}{N} T \underset{\sim}{F}(A_1, A_2, \cdots, A_n) \qquad \text{2.2.10}$$

where T is the above matrix of Chebyshev polynomials, and $\underset{\sim}{F}$ is a vector whose components are the values of the function $f(x, y_1, \ldots, y_n)$ at $x_k = \cos\frac{k\pi}{N}$ $k = 0, 1, \ldots, N$.

Now we are going to show that a Lipschitz Condition on B similar to (2.2.7) is equivalent to the assumption that the Jacobian matrix of $\underset{\sim}{F}(\underset{\sim}{A}_1, \ldots, \underset{\sim}{A}_n)$ is of bounded norm. To show that we use the mean value theorem in the form mentioned in (M.Urabe (1967)).

$$\underset{\sim}{B}^{*} - \underset{\sim}{B}^{(k)} = \frac{2}{N} T \left\{ \underset{\sim}{F}(A_1^{*}, \cdots, A_n^{*}) - \underset{\sim}{F}(A_1^{(k)}, \cdots, A_n^{(k)}) \right\}$$

$$= \frac{2}{N} T \int_0^1 J_{\underset{\sim}{F}}\left(\underset{\sim}{A}^{(k)} + \theta(\underset{\sim}{A}^{*} - \underset{\sim}{A}^{(k)})\right) \cdot (\underset{\sim}{A}^{*} - \underset{\sim}{A}^{(k)})\, d\theta \qquad \text{2.2.11}$$

where

$$J_{\underset{\sim}{F}}(\underset{\sim}{A}) = \begin{bmatrix} \frac{\partial P_1}{\partial A_{11}} \cdots \frac{\partial P_1}{\partial A_{1n}} & \frac{\partial P_1}{\partial A_{21}} \cdots \frac{\partial P_1}{\partial A_{2n}} & \cdots & \frac{\partial P_1}{\partial A_{N1}} \cdots \frac{\partial P_1}{\partial A_{nn}} \\ \frac{\partial P_2}{\partial A_{11}} \cdots \frac{\partial P_2}{\partial A_{1n}} & \frac{\partial P_2}{\partial A_{21}} \cdots \frac{\partial P_2}{\partial A_{2n}} & \cdots & \frac{\partial P_2}{\partial A_{N1}} \cdots \frac{\partial P_2}{\partial A_{nn}} \\ \cdots\cdots & \cdots\cdots & \cdots & \cdots\cdots \\ \frac{\partial P_N}{\partial A_{11}} \cdots \frac{\partial P_N}{\partial A_{1n}} & \frac{\partial P_N}{\partial A_{21}} \cdots \frac{\partial P_N}{\partial A_{2n}} & \cdots & \frac{\partial P_N}{\partial A_{N1}} \cdots \frac{\partial P_N}{\partial A_{nn}} \end{bmatrix} \qquad \text{2.2.12}$$

$$= \left[J_{\underset{\sim}{F},1}(\underset{\sim}{A}) \quad J_{\underset{\sim}{F},2}(\underset{\sim}{A}) \quad \cdots\cdots \quad J_{\underset{\sim}{F},n}(\underset{\sim}{A}) \right] \qquad 2.2.13$$

i.e.

$$\underset{\sim}{B}^{*} - \underset{\sim}{B}^{(k)} = \frac{2}{N} T \left\{ \int_0^1 J_{F,1}\left(\underset{\sim}{A}^{(k)} + \theta(\underset{\sim}{A}^{*} - \underset{\sim}{A}^{(k)})\right) \cdot (\underset{\sim}{A}_1^{*} - \underset{\sim}{A}_1^{(k)})\, d\theta + \right.$$

$$\left. \cdots\cdots + \int_0^1 J_{F,n}\left(\underset{\sim}{A}^{(k)} + \theta(\underset{\sim}{A}^{*} - \underset{\sim}{A}^{(k)})\right) \cdot (\underset{\sim}{A}_n^{*} - \underset{\sim}{A}_n^{(k)})\, d\theta \right\} \qquad 2.2.14$$

if $\| J_{F,i}(\underset{\sim}{A}) \| \leq K_i$ then

$$\left\| \int_0^1 J_{F,i}\left(\underset{\sim}{A}^{(k)} + \theta(\underset{\sim}{A}^{*} - \underset{\sim}{A}^{(k)})\right) d\theta \right\| \leq K_i \quad , \quad i = 1, 2, \cdots, n$$

and $$\| \underset{\sim}{B}^{*} - \underset{\sim}{B}^{(k)} \| \leq \frac{2}{N} \| T \| \left\{ K_1 \| \underset{\sim}{A}_1^{*} - \underset{\sim}{A}_1^{(k)} \| + \cdots\cdots + K_n \| \underset{\sim}{A}_n^{*} - \underset{\sim}{A}_n^{(k)} \| \right\}$$

$$= \sum_{i=1}^{n} M_i \cdot \| \underset{\sim}{A}_i^{*} - \underset{\sim}{A}_i^{(k)} \| \quad , \quad M_i \text{ are Constants} \qquad 2.2.15$$

i.e. The condition that the Jacobian matrix $J_{\underset{\sim}{F}}(\underset{\sim}{A})$ is of bounded norm implies the Lipschitz Condition (2.2.15).

From (2.2.9) a sufficient condition for convergence of the iterative process $G_{s,N}$ is

$$\| R_{sN} \| \| K_s \| < 1 \qquad 2.2.16$$

2.3 The Behaviour of the matrix $R_{s\,N}$

We investigate the behaviour of the maximum eigenvalue and the norm of the matrices $R_{s\,N}$, first when s is fixed and N variable and second for fixed N and variable s.

2.3.1 Fixed s and variable N

Consider the matrix $R_{o\,N} = (r_{ij})$ with $x_o = o$, and let

$$a_i = \sqrt{\sum_{j=1}^{N+1} |r_{ij}|^2} \qquad 2.3.1$$

then $a_i = 1/\sqrt{2}(i-1) \quad . \quad i = 2, \cdots\cdots, N$

$a_{N+1} = 1/2N$

$a_1^2 = \left(\frac{1}{2}\right)^2 + \left(\frac{3}{4}\right)^2 + \left(\frac{5}{12}\right)^2 + \cdots = \left(\frac{1}{2}\right)^2 + \sum_1^{N/2} \left(\frac{2S+1}{2S(S+1)}\right)^2$

$= \frac{1}{4}\left[1 + \sum\left(\frac{1}{S^2} + \frac{1}{(S+1)^2} + \frac{2}{S(S+1)}\right)\right] \leq N+1$

Then from Hadamard's theorem (see Cohen (1973)).

$$|\det R_{oN}| \leq \prod_1^{N+1} a_i$$

using $N! > e^{-N} N^N (\sqrt{2\pi N} - 2)$

then $$|\det R_{oN}| \leq \left(\frac{1}{\sqrt{2}}\right)^{N+1} \frac{e^N}{N^N(\sqrt{2\pi N} - 2)} \cdot \sqrt{N+1} \qquad 2.3.2$$

So if λ_i , $(i = 1, \cdots, N+1)$ are the eigenvalues of R_{oN} then

$$\min|\lambda_i| \leq |\det R_{oN}|^{1/N} \leq \frac{\text{const}}{N}$$

For N even and $x_o = o$ the characteristic equation takes the form

$$-2^N N!\,\lambda^{N+1} + 2^{N-2}(N-1)!\,\lambda^{N-1} \cdot \frac{N-4}{2!}(N-2)!\,\lambda^{N-3} + \frac{N-6}{3!}(N-3)!\,\lambda^{N-5} - \cdots\cdots + (-1)^{\frac{N}{2}+1}\lambda = 0$$

from the first two terms $\max|\lambda| \sim \frac{1}{2\sqrt{N}}$ and from the first 3-terms $\max|\lambda| \sim \frac{1}{2\sqrt{2}N}$

In general $$\max|\lambda| \leq \frac{C}{\sqrt{N}} \qquad 2.3.3$$

where C is a constant depending on the point where the initial conditions are taken and C is small for $x_o = o$ and larger for $x_o = 1$. From (2.3.3) we can see that the maximum eignvalue decreases as N increases.

Tables (1), (2) show the behaviour of the maximum eigenvalue and the spectral norm as N increases, the initial conditions being taken at $x_o = o$ and $x_o = 1$ respectively. Both tables show that the maximum eignvalue decreases as N increases and it takes lower values when $x_o = o$. From table (1) we can notice

that the spectral norm can increase with N and this is understandable since the norm is always a larger bound.

Table (I) $x_o = o$

N	Max.eig.val.	spectral norm
10	0.117 973	1.110 739
15	0.085 396	1.136 349
20	0.065 304	1.151 607
25	0.054 101	1.158 971
30	0.045 430	1.164 917
35	0.039 742	1.168 372
40	0.034 804	1.171 523
45	0.031 378	1.173 573
50	0.028 239	1.175 472

Table 2 $x_o = 1$

N	Max.eig.val.	spectral norm
10	0.186 720	1.492 437
15	0.131 301	1.490 793
20	0.100 855	1.490 235
25	0.082 190	1.489 982
30	0.069 231	1.489 845
35	0.059 842	1.489 763
40	0.055 832	1.489 710
45	0.055 335	1.489 674
50	0.053 332	1.489 648

The larger maximum eigenvalue for $x_o=1$ can of course make the difference between converging and diverging; thus, for example the iterative process $G_{o,50}$ diverges when applied to

$$y'(x) = 20y \quad , \quad y(1) = 1$$

while for

$$y' = 20y \quad , \quad y(0) = e^{-20}$$

the same iterative process converged in 44 iterations.

2.3.2 Fixed N and variable s

Let the maximum eigenvalue of the matrix R_{sN} be denoted by ρ_{sN}. Since $R_{sN} = R_{oN}^{s+1}$, $\rho_{sN} = \rho_{oN}^{s+1}$ then for any fixed N the maximum eigenvalues go down as s increases. Table (3) shows the values and also the spectral norms.

Table 3

N	s	$\rho_{sN} = (\rho_{oN})^{s+1}$	Spectral norm
10	0	0.117 973 542 12	1.110 739 308 49
	1	0.013 917 756 64	0.529 326 736 87
	2	0.001 641 927 04	0.163 067 253 78
	3	0.000 193 703 94	0.048 305 606 44
	4	0.000 022 851 94	0.008 128 705 15
50	0	0.028 239 674 82	1.175 472 641 69
	1	0.000 911 599 55	0.529 950 921 09
	2	0.000 025 545 70	0.196 693 122 16
	3	0.000 001 279 43	0.048 890 934 63
	4	0.000 000 041 86	0.010 057 373 06

From the results of this and previous section it follows that the iterative process $G_{s,N}$ should have its behaviour governed by the product $\| R_{s\,N} \| \, \| K_s \|$ where $\| R_{s.N} \|$ is smaller for larger s, fixed N and for larger N, fixed s. The behaviour of $\| K_s \|$ is dependent on the function f_i. This is the result in Chebyshev series which corresponds to the results (1.1.35), (1.1.41).

Note on linear differential equations with constant coefficients

Consider the linear differential equation

$$y'(x) = F(x,y) = \lambda y + f(x) \qquad 2.3.4$$

now $D^s F(x,y) = \lambda^{s+1} y + \lambda^s P(x) + \lambda^{s-1} P'(x) + \cdots \to P^{(s)}(x)$

then from (2.2.4)

$$y^*(x) - y^{(1)}(x) = \int_{x_0}^{x}\int_{x_0}^{t_s}\cdots\int_{x_0}^{t_1} \lambda^{s+1}\left(y^*(t) - y^{(0)}(t)\right) dt\, dt_1 \cdots dt_s \qquad 2.3.5$$

If $y^* = \sum_{r=0}^{N}{}' A_r^* T_r(x)$

$$y^{(i)} = \sum_{r=0}^{N}{}' A_r^{(i)} T_r(x)$$

then substituting in (2.3.5), performing the integrals and equating the coefficients of $T_n(x)$ in both sides we get

$$\underset{\sim}{A}^* - \underset{\sim}{A}^{(1)} = \left(\lambda R_{0,N}\right)^{s+1} \left(\underset{\sim}{A}^* - \underset{\sim}{A}^{(0)}\right) \qquad 2.3.6$$

where $R_{0,N}$ is the matrix defined in section (2.1.2).

Proceeding with the iterative process we get

$$\underset{\sim}{A}^* - \underset{\sim}{A}^{(r)} = \left[\left(\lambda R_{0,N}\right)^{s+1}\right]^r \left(\underset{\sim}{A}^* - \underset{\sim}{A}^{(0)}\right) \qquad 2.3.7$$

which is the actual error after r iterations.

In the non linear case it is difficult to get an explicit expression for the actual error, but we can find an expression for the error bound as in (2.2.9).

2.3.3. The accuracy of the iterative processes

Each of the following examples is solved using the iterative processes $G_{0,N}, \ldots\ldots, G_{3,N}$

(i) $y' = 20y \qquad y(0) = e^{-20} \qquad x \in [-1,1]$

Exact solution $y = e^{20(x-1)}$

(ii) $y' = \frac{1}{2} e^{-y}$, $y(-1) = o$, $x \in [-1,1]$

Exact solution $y = \log (\frac{3+x}{2})$

(iii) $y' = y^2$, $y(-1) = o$, $x \in [-1,1]$

Exact solution $y = \frac{2}{3-2x}$

(iv) $y' = \frac{1}{2} (1 - e^{-y}(\text{Sin } (\frac{x+1}{2}) - \text{Cos } (\frac{x+1}{2})))$, $y(-1) = o$, $x \in [-1,1]$

Exact solution $y = \log (\text{Sin } (\frac{x+1}{2}) + \exp (\frac{x+1}{2}))$

(v) $y' = 1 - y^2$, $y(o) = o$, $x \in [-1,1]$

Exact solution $y = \text{Sin } x$

(vi) $y' = 1+y^2$, $y(o) = o$, $x \in [-1,1]$

Exact solution $y = \tan x$

In each of these we used N = 50 and the program stops when all the coefficients A in two successive iterations agree to a specified tolerance E. In example (i) E was 10^{-6}, in all the rest 10^{-11}.

Table (4) shows the number of iterations needed to achieve such accuracy.

In figures (1) - (6) the L_2 norm of the error vector $E_{s,r}$ calculated after r iterations using the iterative process $G_{s,N}$ is plotted against the product $r(s+1)$

TABLE 4

Iterative process $G_{s,N}$	Number of iterations					
	EQ(i)	EQ(ii)	EQ(iii)	EQ(iv)	EQ(v)	EQ(vi)
$G_{o,50}$	40	10	19	8	9	13
$G_{1,50}$	20	6	11	6	5	8
$G_{2,50}$	14	4	8	5	3	6
$G_{3,50}$	11	4	6	4	3	5

In example (i) (the linear case with constant coefficients), the four error curves coincide (and this can easily be justified from (2.3.7)) while in the rest of the examples the graphs show that the errors for constant r(s+1) are slightly larger for larger s.

Some of these examples are solved by K.Wright (1964) using picard andNicolovius methods which are equivalent to $G_{0,N}$, $G_{1,N}$ respectively. A small N was used and tolerance 10^{-6} and the next table shows his results.

TABLE 5

EQ	No. of iterations		N
	picard	Nicolovius	
(ii)	12	11	9
(v)	8	6	7
(vi)	17	33	12

Using the same number N and the same tolerance we get the following results for the number of iterations.

TABLE 6

EQ	No. of iterations				N
	$G_{0,N}$	$G_{1,N}$	$G_{2,N}$	$G_{3,N}$	
(ii)	8	5	4	4	9
(v)	7	5	5	5	7
(vi)	9	8	7	9	12

These tables show that it is possible to get for larger s when N is fairly small slower convergence.

2.3.4. Computational effort

A more valid criterion for assessing the value of using Lie series for this type of problem is by considering the number of function evaluations necessary to achieve a given accuracy. In $G_{s,N}$ we use N + 1 collocation points and the processes $G_{0,N}$, $G_{1,N}$, $G_{2,N}$, $G_{3,N}$

demand at each iteration the evaluation of the functions shown in the following table.

TABLE 7

Iteration process	Functions evaluated	No.of functions
$G_{o,N}$	$\hat{y}$, $\hat{f}$, f	3
$G_{1,N}$	$\hat{y}$, $\hat{f}$, f, fy	4
$G_{2,N}$	$\hat{y}$, $\hat{f}$, f, fy, fxy, fyy	6
$G_{3,N}$	$\hat{y}$, $\hat{f}$, f, fx, fy, fxy, fyy, fxxy, fxyy, fyyy	10

The following table shows the predicted effort needed to achieve a fixed order of $3+12r$, starting with $\hat{y}$ as Taylor series of order 2 denoting the number of function evaluations of the iterative process $G_{s,N}$ by V_s

TABLE 8

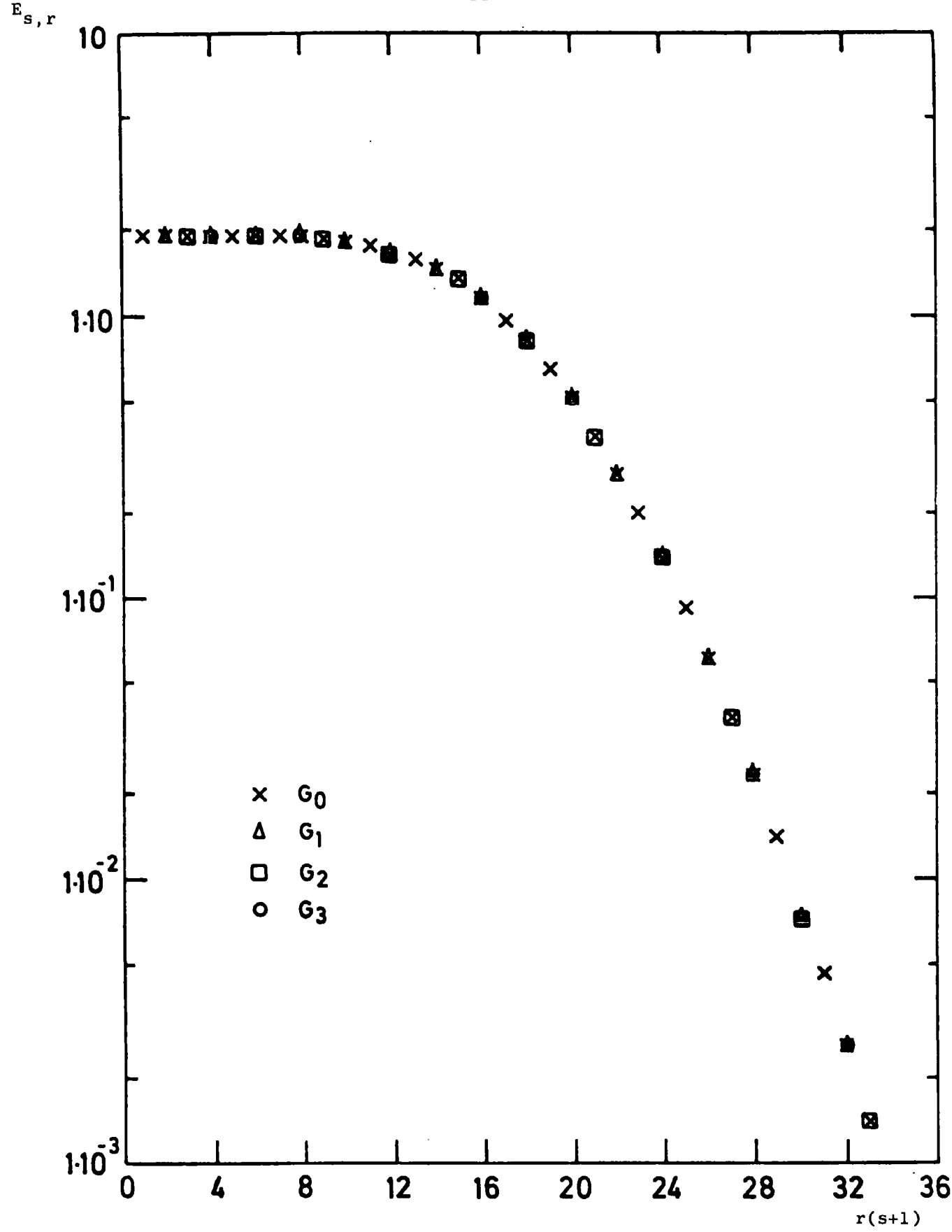
Iterative process $G_{r,N}$	No. of iterations needed	No.of function evaluations	Ratio
$G_{o,N}$	12r	36 r (N+1)	1
$G_{1,N}$	6r	24 r (N+1)	.67
$G_{2,N}$	4r	24 r (N+1)	.67
$G_{3,N}$	3r	30 r (N+1)	.83

Since the behaviour of the accuracy is slightly different from the behaviour of the order of the error shown by the graphs, then one may not expect to get the same relation between Computational efforts of $G_{o,N}$,...., $G_{3,N}$ shown in table (8) for a fixed accuracy. To show that we use the practical results in table (4) and the computational efforts in table (7) to estimate the Computational effort used to achieve the specified

accuracy for each example, and this is shown in table (9).

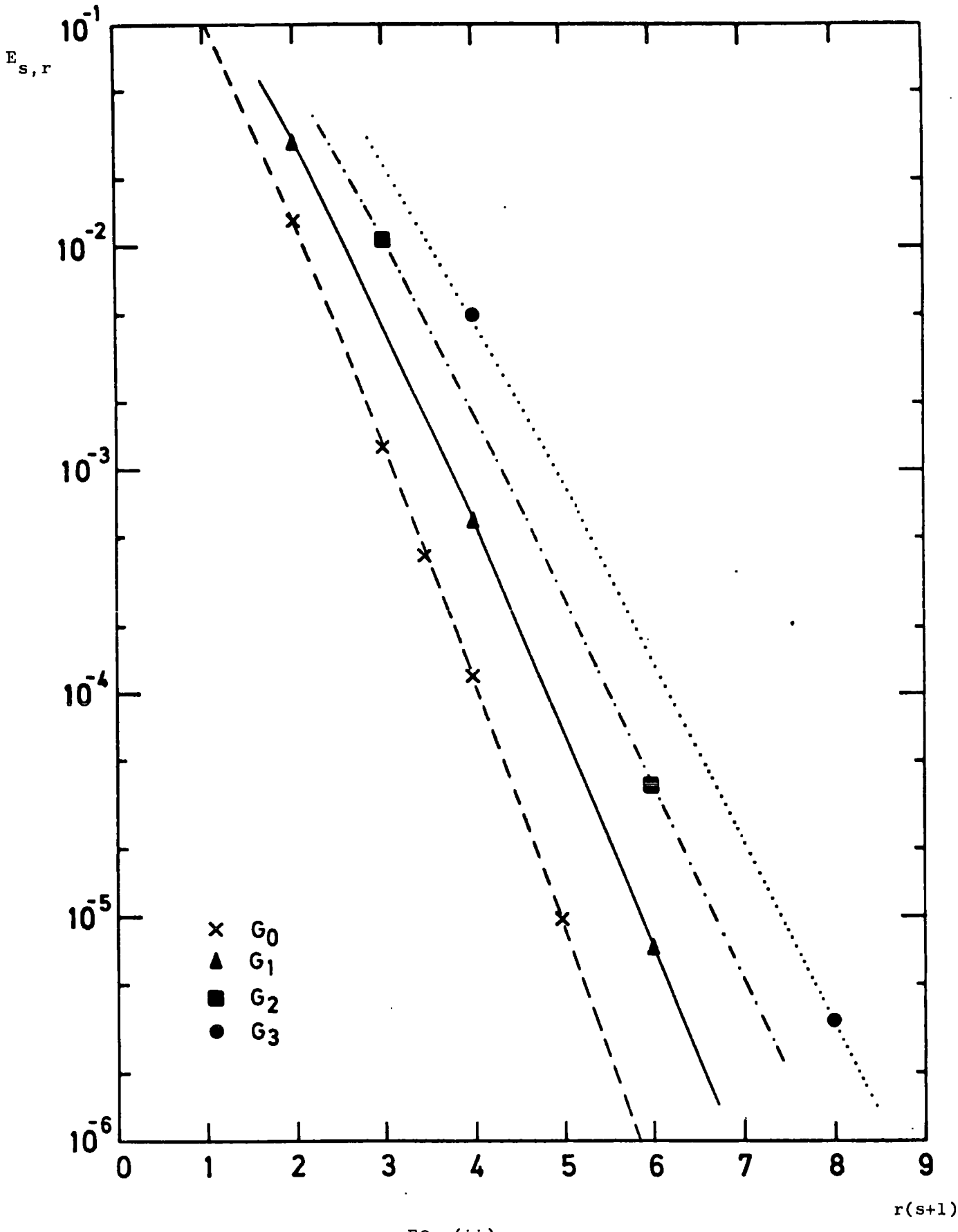
TABLE 9

	EQ(i)	EQ(ii)	EQ(iii)	EQ(iv)	EQ(v)	EQ(vi)	Predicted Ratios
V_o	6120	1530	2907	1224	1377	1989	
V_1/V_o	0.67	0.80	0.77	1	0.73	0.82	0.67
V_2/V_o	0.70	0.80	0.84	1.25	0.67	0.92	0.67
V_3/V_o	0.92	1.33	1.05	1.67	1.11	1.28	0.83
Best Iterative process	$G_{1,50}$	$G_{1,50}$ or $G_{2,50}$	$G_{1,50}$	$G_{o,50}$ or $G_{1,50}$	$G_{2,50}$	$G_{1,50}$	



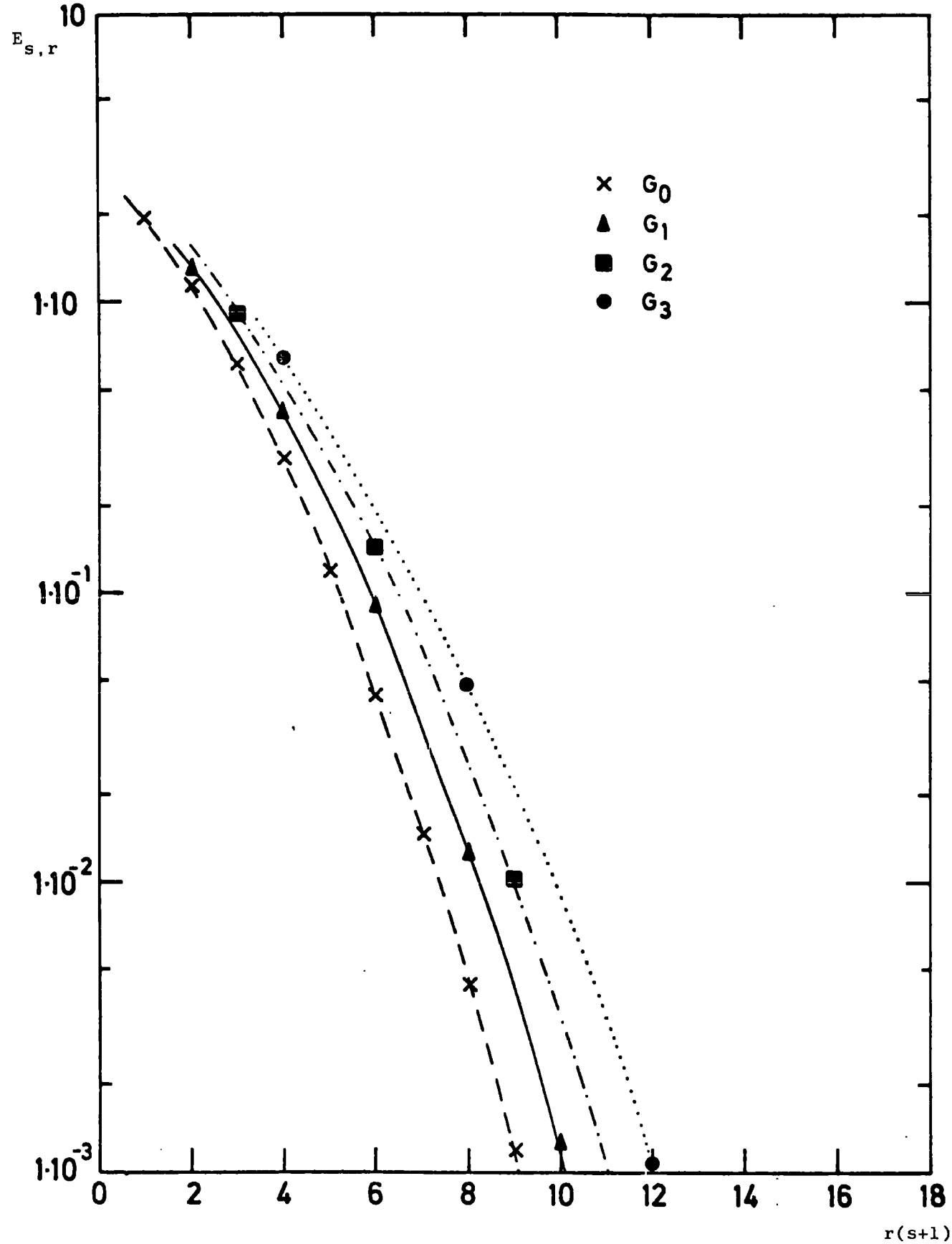
EQ. (i)

Graph (1)



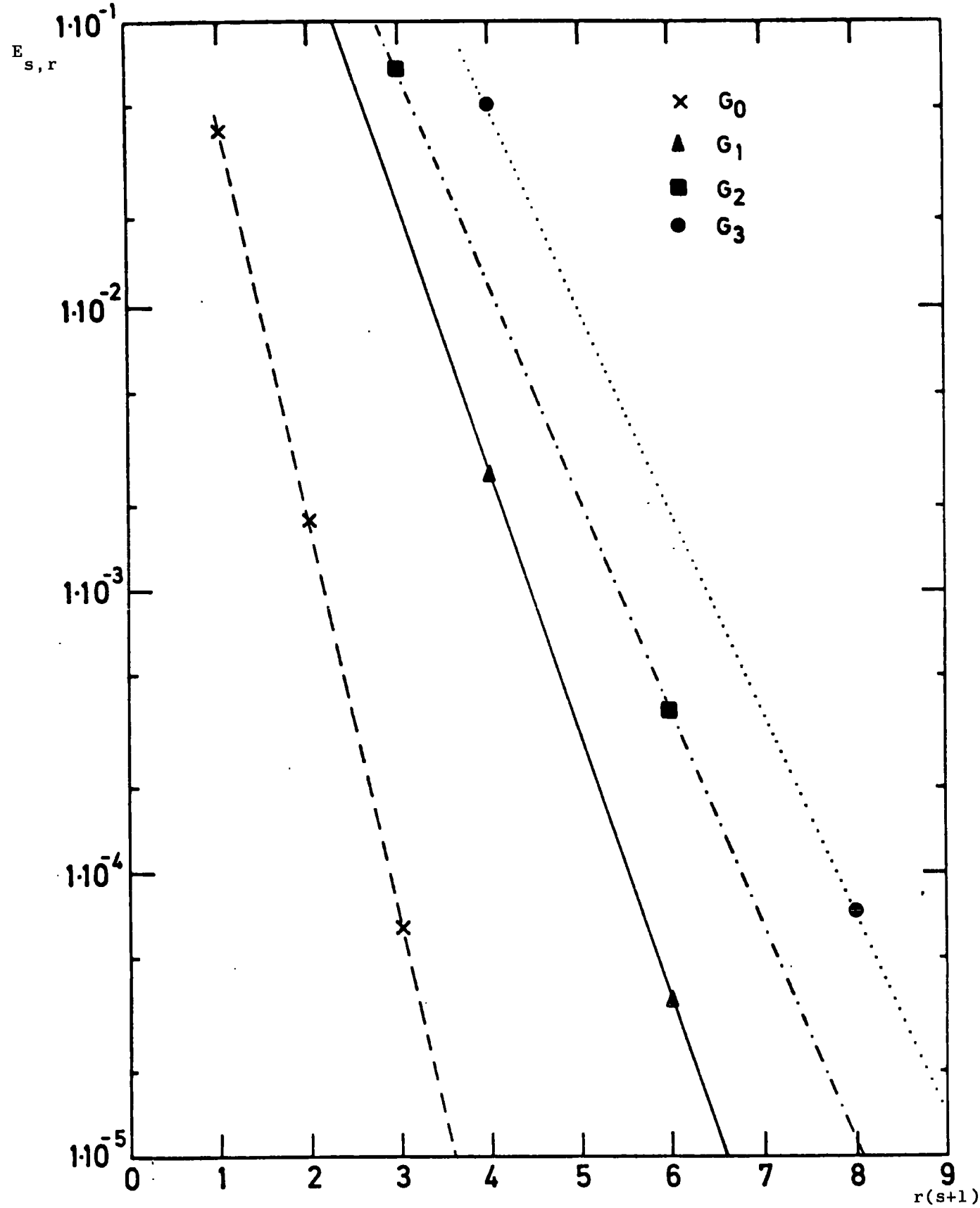
EQ. (ii)

Graph (2)



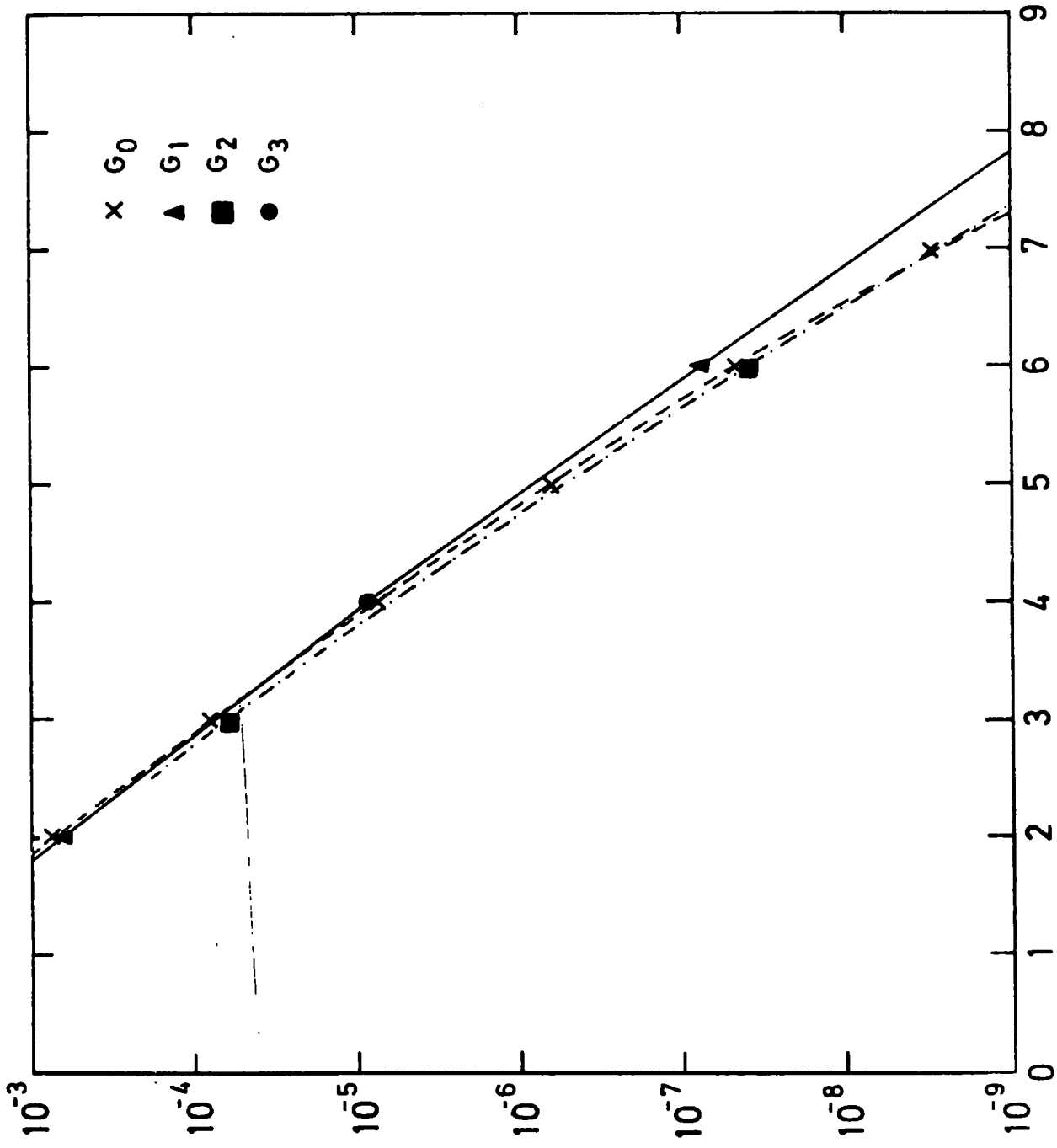
EQ. (iii)

Graph (3)


$E_{s,r}$
$1\cdot10^{-1}$
$1\cdot10^{-2}$
$1\cdot10^{-3}$
$1\cdot10^{-4}$
$1\cdot10^{-5}$
0
1
2
3
4
5
6
7
8
9
r(s+1)
G_0
G_1
G_2
G_3

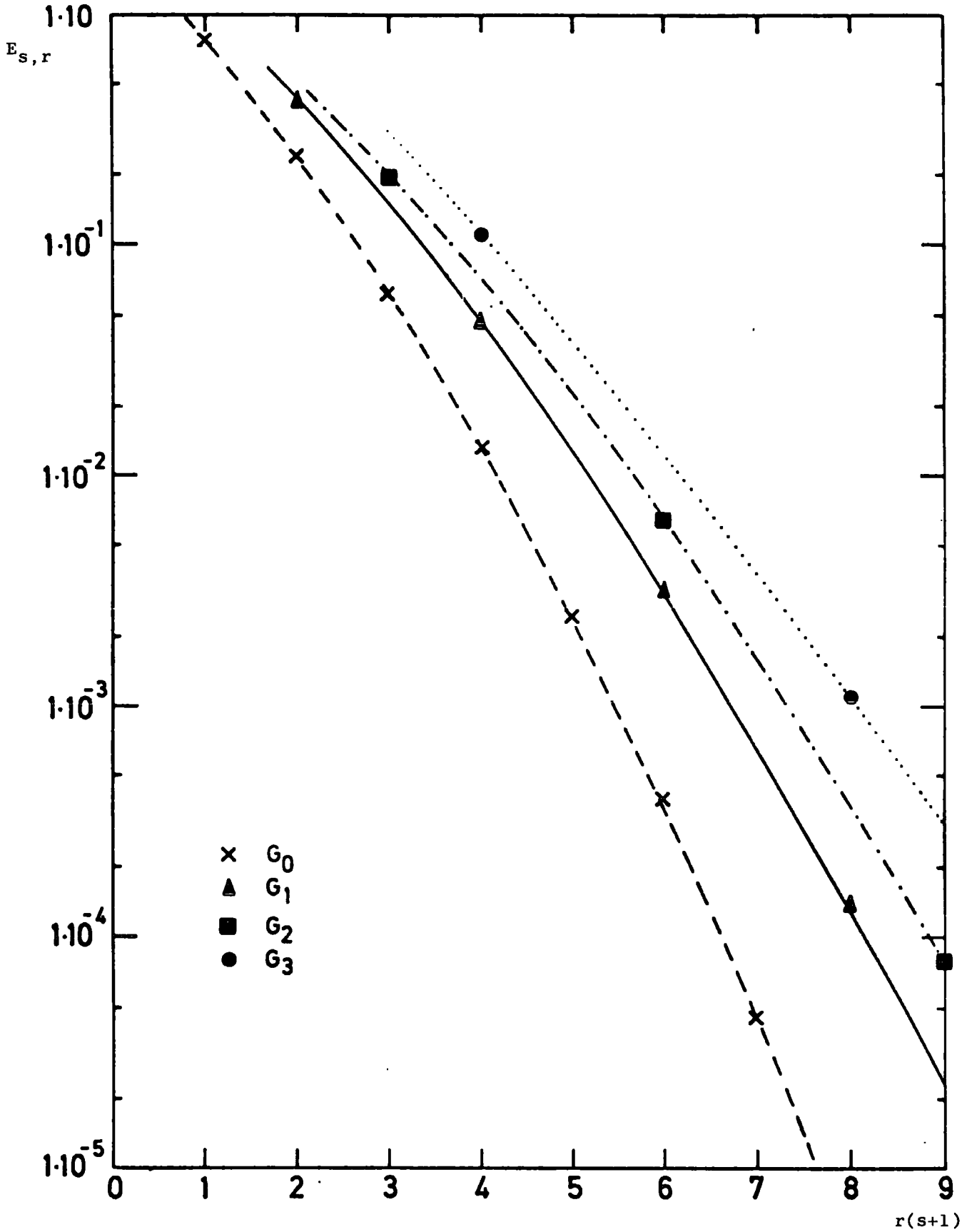
EQ. (iv)

Graph (4)



EQ(v)

Graph (5)


1·10
$E_{s,r}$
$1\cdot10^{-1}$
$1\cdot10^{-2}$
$1\cdot10^{-3}$
$1\cdot10^{-4}$
$1\cdot10^{-5}$
0
1
2
3
4
5
6
7
8
9
r(s+1)
G_0
G_1
G_2
G_3

EQ. (vi)

Graph (6)

CHAPTER III

A SURVEY OF NUMERICAL METHODS FOR TWO-POINT BOUNDARY VALUE PROBLEMS IN ORDINARY DIFFERENTIAL EQUATIONS

There are now very many suggested methods for solving linear and non-linear boundary value problems, a recent comprehensive survey is given by Aktas and Stetter (1977). In this chapter we review only the methods which have some bearing on the project of this thesis, using the classification suggested by the above paper. The following standard notation will be used.

(A) For linear two-point boundary value problems we consider the set of n linear ordinary differential equations

$$\dot{\underset{\sim}{y}} = A(x)\,\underset{\sim}{y}(x) + \underset{\sim}{f}(x) \qquad x \in [x_0, x_N] \qquad 3.1.1$$

where A(x) is an nxn matrix with elements $A_{ij}(x)$, $i,j = 1,2,\ldots,n$,

$$\underset{\sim}{y}(x) = (y_1(x), y_2(x), \ldots\ldots\ldots, y_n(x))^T$$

$$\underset{\sim}{f}(x) = (f_1(x), f_2(x), \ldots., f_n(x))^T$$

The boundary conditions are assumed to be separable with initial conditions

$$y_i(x_0) = c_i \quad , i = 1,2,\ldots.,r \qquad 3.1.2$$

and terminal conditions

$$y_{i_m}(x_N) = C_{i_m} \quad , m = 1,2,\ldots.,n-r \qquad 3.13$$

(B) For non-linear two-point boundary value problems we consider only the second order non-linear differential equation

$$y'' = f(x,y,y') \quad , x \in [x_0, x_N] \qquad 3.1.4$$

or

$$\begin{aligned} y' &= z \\ z' &= f(x,y,z) \end{aligned} \quad , x \in [x_0, x_N] \qquad 3.1.5$$

with the boundary conditions

$$y(x_0) = \alpha \quad , y(x_N) = \beta \qquad 3.1.6$$

The methods described are:

3.1 Quasilinearization which allows (B) to be put into the form (A)

3.2 Shooting methods, including for (A) the method of adjoints and method of sweeps, and for (B) Newton Raphson correction

3.3 Parallel shooting or Multiple shooting

3.4 Series methods, concentrating on Chebyshev collocation methods such as Picard method and Newton's method

3.5 Analytic methods including two types of continuation methods

3.6 Nicolovius method

3.1 Quasilinearization

In this technique we linearize the non-linear boundary value problems around a nominal solution satisfying the boundary conditions, then solve a sequence of linear boundary value problems in which the solution of the $k^{\underline{th}}$ one is the nominal profile for the $(k+1)^{\underline{st}}$. In the limit the solutions of the linear two-point boundary value problems converge to the solution of the non-linear boundary value problem. Consider the problem (B), let $(y^{(k)}, z^{(k)})$ be an approximate solution satisfying the boundary conditions. Expanding the R.H.S. of (3.1.5) in the neighbourhood of $(y^{(k)}, z^{(k)})$ we get

$$y'^{(k+1)} = z^{(k+1)}$$

$$z'^{(k+1)} = P(x, y^{(k)}, z^{(k)}) + \left(\frac{\partial P}{\partial y}\right)_{y^{(k)}, z^{(k)}} \cdot (y^{(k+1)} - y^{(k)}) + \left(\frac{\partial P}{\partial z}\right)_{y^{(k)}, z^{(k)}} (z^{(k+1)} - z^{(k)})$$

i.e.
$$\begin{bmatrix} y'^{(k+1)} \\ z'^{(k+1)} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ (P_y)_{y^{(k)}, z^{(k)}} & (P_z)_{y^{(k)}, z^{(k)}} \end{bmatrix} \begin{bmatrix} y^{(k+1)} \\ z^{(k+1)} \end{bmatrix} + \begin{bmatrix} 0 \\ (P - P_y \cdot y - P_z z)_{y^{(k)}, z^{(k)}} \end{bmatrix} \qquad 3.1.7$$

with $y^{(k+1)}(x_0) = \alpha$, $y^{(k+1)}(x_N) = \beta$ 3.1.8

Solving this linear system using any of the methods used for linear systems gives $(y^{(k+1)}, z^{(k+1)})$, and this can then be repeated until the process converges to the exact solution. A discussion about the conditions under which this method converges and the rate of convergence is mentioned in Roberts and Shipman (1972).

3.2 Shooting Methods

By shooting methods we mean the methods which solve systems of initial value problems instead of solving boundary value ones. In this section we are going to discuss two of the methods used only for linear boundary value problems, that is the method of adjoints and method of sweeps, and one general method, Newton Raphson solution.

3.2.1 Method of adjoints

The idea of this method as developed by Goodman and Lance (1956) is to make use of the adjoint equations, defined as a set of homogenous linear ordinary differential equations whose matrix of coefficients is the negative transpose of the matrix of the original set. For the system of equations (3.1.1) the adjoint equations are

$$\dot{\underset{\sim}{P}} = -A^{T}(x)\ \underset{\sim}{P} \qquad 3.2.1$$

Multiplying the i^{th} equation of 3.1.1. by P_i and the i^{th} equation 3.2.1 by y_i, adding the resulting equations and summing over all n we get

$$\sum_{i=1}^{n} \frac{d}{dx}\ P_i(x)\, y_i(x) = \sum_{i=1}^{n} P_i(x)\, P_i(x) \qquad 3.2.2$$

Integrating over $[x_0, x_N]$, we get

$$\sum_{i=1}^{n} P_i(x_N)\, y_i(x_N) - \sum_{i=1}^{n} P_i(x_0)\, y_i(x_0) = \int_{x_0}^{x_N} \left(\sum_{i=1}^{n} P_i(x)\, P_i(x) \right) dx \qquad 3.2.3$$

Equation 3.2.3 is the fundamental identity of this method. To utilise this identity integrate backward (3.2.1) (n-r) times with terminal conditions

$$\left.\begin{aligned} P_i^{(m)}(x_N) &= 1 \quad , \quad i = im \\ &= o \quad , \quad i \neq im \end{aligned}\right\} \quad m = 1, 2, \ldots, n-r$$

i.e. $$P_i^{(m)}(x_N) = \delta_i^{im} \qquad 3.2.4$$

where the subscript m refers to the $m^{\underline{th}}$ backward integration of the adjoint equations and the im refers to the subscripts on the specified terminal conditions $y_{im}(x_N)$. Now

$$P_{i_{im}}^{(m)}(x_N)\; y_{i_{im}}(x_N) = 1. \; y_{i_{im}}(x_0) = C_{i_{im}} \qquad 3.2.5$$

and (3.2.3) takes the form

$$\sum_{i=r+1}^{n} P_i^{(m)}(x_0)\, y_i(x_0) = y_{im}(x_N) - \sum_{i=1}^{r} P_i^{(m)}(x_0)\, y_i(x_0) - \int_{x_0}^{x_N} \sum_{i=1}^{n} P_i^{(m)}(x)\, f_i(x)\, dx \qquad 3.2.6$$

The R.H.S. of (3.2.6) is known for the (n-r) specified $y_{im}(x_N)$ and corresponding $P_{im}(x_N)$, hence this yields a set of (n-r) linear algebraic equations in the (n-r) unknowns $y_{r+1}(x_0), \ldots, y_n(x_0)$. In matrix form

$$\begin{bmatrix} y_{r+1}(x_0) \\ y_{r+2}(x_0) \\ \vdots \\ y_n(x_0) \end{bmatrix} = \begin{bmatrix} P_{r+1}^{(1)}(x_0) & \cdots & P_n^{(1)}(x_0) \\ P_{r+1}^{(2)}(x_0) & \cdots & P_n^{(2)}(x_0) \\ & \cdots & \\ P_{r+1}^{(n-r)}(x_0) & \cdots & P_n^{(n-r)}(x_0) \end{bmatrix}^{-1} \times \begin{bmatrix} y_{i_1}(x_N) - \sum_{1}^{r} P_i^{(1)}(x_0)\, y_i(x_0) - \int_{x_0}^{x_N} \sum_{1}^{n} P_i^{(1)}(x)\, f_i(x)\, dx \\ \cdots \\ y_{i_{n-r}}(x_N) - \sum_{1}^{r} P_i^{(n-r)}(x_0)\, y_i(x_0) - \int_{x_0}^{x_N} \sum_{1}^{n} P_i^{(n-r)}\, f_i\, dx \end{bmatrix} \qquad 3.2.7$$

Then after calculating the missing initial conditions $y_i(x_0)$, i = r+1..., n

we can integrate forward to get the required solutions.

Detailed discussion of this method with implicit boundary conditions and solved examples can be found in Roberts and Shipman (1972).

3.2.2 Method of sweeps

Consider the set of two equations

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \end{bmatrix} = A(x) \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} + \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \qquad 3.2.8$$

where $A(x) = \begin{bmatrix} a_{11}(x) & a_{12}(x) \\ a_{21}(x) & a_{22}(x) \end{bmatrix}$

with the boundary conditions

$$y_1(x_0) = \alpha \quad , \quad y_1(x_N) = \beta \qquad 3.2.9$$

The method of sweeps (Scott (1975) or factorization method or method of Gelfand and Lorkustskiyevskii (Berezin and Zhidkov (1965)) is a method which uses a Riccati transformation to help in finding the missing initial conditions. Now consider the Riccati transformation

$$y_1(x) = r_1(x)\, y_2(x) + r_2(x) \qquad 3.2.10$$

Substituting in (3.2.8) we get

$$y_2(x) \left\{ a_{12} + [a_{11} - a_{22}]\, r_1(x) - a_{21} r_1^2(x) - r_1'(x) \right\}$$

$$+ \left\{ [a_{11} - a_{21} r_1(x)]\, r_2(x) - P_2(x) r_1(x) + P_1(x) - r_2'(x) \right\} = 0$$

this is true if

$$r_1' = a_{12} + (a_{11} - a_{22}) r_1 - a_{21} r_1^2 \qquad 3.2.11$$

$$r_2' = [a_{11} - a_{21} r_1]\, r_2 - P_2(x) r_1(x) + P_1(x) \qquad 3.2.12$$

with the initial conditions

$$r_1(x_N) = 0 \quad , \quad r_2(x_N) = \beta \qquad 3.2.13$$

Solving (3.2.11-13), for $v_1(x)$, and $v_2(x)$ then (3.2.10) gives from (3.2.10)

$$y_2(x_0) = [\alpha - v_2(x_0)] / v_1(x_0) \qquad 3.2.14$$

From (3.2.9), (3.2.14) we integrate (3.2.8) forward to get the required solution.

3.2.3 Newton-Raphson method

Consider the non linear boundary value problem (3.1.4) - (3.1.6). A formal approach to the exact solution of the problem is obtained by considering a related initial value problem, say

$$u'' = f(x, u, u') \quad , \quad x \in [x_0, x_N] \qquad 3.2.15$$

or

$$\left.\begin{aligned} u' &= v \\ v' &= f(x, u, v) \quad , \quad x \in [x_0, x_N] \end{aligned}\right\} \cdots\cdots \qquad 3.2.16$$

with the initial conditions

$$u(x_0) = \alpha \quad , \quad v(x_0) = s \qquad 3.2.17$$

We denote the solution of (3.2.16) by

$$u = u(x,s) \qquad 3.2.18$$

to point out the dependence on s.

Evaluating the solution at $x = x_N$ we try to find s such that

$$\phi(s) = u(x_N, s) - \beta = 0 \qquad 3.2.19$$

If s* is the exact solution of (3.2.19), then

$$y = u(x,s^*) \qquad 3.2.20$$

is the solution of (3.1.4).

To solve (3.2.19) one may use Newton's iterative process

$$s^{\nu+1} = s^{\nu} - \left[\left(\frac{\partial \phi(s)}{\partial s} \right)_{s^{\nu}} \right]^{-1} \phi(s^{\nu}) \quad , \quad (\nu = 0, 1, \cdots) \qquad 3.2.21$$

where $\phi(s^{\nu})$ could be evaluated using (3.2.16-19) with $s = s^{\nu}$

and $\left(\frac{\partial \phi(s)}{\partial s}\right)_{s^\nu}$ is the solution of

$$\left.\begin{aligned} P'(x, s^\nu) &= Q(x, s^\nu) \\ Q'(x, s^\nu) &= \left(\frac{\partial f}{\partial u}\right)_{s^\nu} \cdot P(x, s^\nu) + \left(\frac{\partial f}{\partial v}\right)_{s^\nu} \cdot Q(x, s^\nu) \end{aligned}\right\} \quad \text{3.2.22}$$

evaluated at $x = x_N$, where

$$P = \frac{\partial u}{\partial s} \quad , \quad Q = \frac{\partial v}{\partial s} \qquad \text{3.2.23}$$

satisfying the initial conditions

$$P(x_0, s^\nu) = 0 \quad , \quad Q(x_0, s^\nu) = 1 \qquad \text{3.2.24}$$

3.2.4 Difficulties of shooting methods

The application of a shooting method may be faced by two main difficulties. First, well conditioned boundary value problems may lead to unstable initial value problems with rapidly growing solutions. This causes a loss in accuracy in solving the corresponding system $\phi(s) = 0$. In some cases greater accuracy in calculations may overcome this difficulty. This is not always practical, and later in this chapter we will discuss the parallel shooting method which can frequently reduce this difficulty.

The second difficulty arises from the dependence of shooting methods on assuming the missing initial conditions and integrating the differential equation over the given interval. It is of crucial importance that the resulting initial value problem has a solution over this interval. In some ill-conditioned or sometimes called sensitive problems, one can only choose the missing initial conditions within a very small neighbourhood of the exact ones. For example the problem

$$y''(x) = 16 \sinh 16y \quad , \qquad y(0) = y(1) = 0$$

is given by Keller (1968); the exact solution is $y(x) = 0$, and the true

initial condition is $y'(o) = o$, yet if we choose $s > 10^{-7}$ the solution of the initial value problem is singular in $[o,1]$. Continuation methods and parallel shooting frequently help to overcome this difficulty as will be shown later in this chapter.

3.2.5 Relation between method of adjoints, method of sweeps and Newton Raphson method for linear equations

Consider the linear boundary value problem (3.2.8-9). Let the fundamental solution be $\begin{bmatrix} Y_{11} \\ Y_{12} \end{bmatrix}$, $\begin{bmatrix} Y_{21} \\ Y_{22} \end{bmatrix}$ where

$$\begin{bmatrix} Y_{11}(x_0) \\ Y_{12}(x_0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} Y_{21}(x_0) \\ Y_{22}(x_0) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad 3.2.25$$

Then the particular solution is

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = c_1 \begin{bmatrix} Y_{11} \\ Y_{12} \end{bmatrix} + c_2 \begin{bmatrix} Y_{21} \\ Y_{22} \end{bmatrix} + \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} \qquad 3.2.26$$

where $$\begin{bmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} + \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} \qquad 3.2.27$$

and $$\begin{bmatrix} \dot{Y}_{11} \\ \dot{Y}_{12} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} Y_{11} \\ Y_{12} \end{bmatrix}; \quad \begin{bmatrix} \dot{Y}_{21} \\ \dot{Y}_{22} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} Y_{21} \\ Y_{22} \end{bmatrix} \qquad 3.2.28$$

Substituting the boundary condition in (3.2.26) we get

$$c_1 = \alpha - \eta_1(x_0), \quad c_2 = \frac{1}{Y_{21}(x_N)} \left[\beta - (\alpha - \eta_1(x_0)) Y_{11}(x_N) - \eta_1(x_N) \right] \qquad 3.2.29$$

Then the missing initial condition is

$$y_2(x_0) = s^* = \frac{\beta - \eta_1(x_N) - [\alpha - \eta_1(x_0)] Y_{11}(x_N)}{Y_{21}(x_N)} + \eta_2(x_0) \qquad 3.2.30$$

(i) Newton-Raphson method

Assuming the missing initial condition $y_2(x_o)=s$, then the approximate solution at $x = x_N$ is

$$\bar{y}_1 = [\alpha - \eta_1(x_0)]\, Y_{11}(x_N) + [s - \eta_2(x_0)]\, Y_{21}(x_N) + \eta_1(x_N) \qquad 3.2.31$$

The correction equation is just (3.2.28), so $\frac{\partial y_1}{\partial s}$ is just Y_{21}, so ordinary shooting produces

$$s_{corrected} = s - \frac{\bar{y}_1(x_N) - \beta}{Y_{21}(x_N)} \qquad 3.2.32$$

substituting from (3.2.31) we can easily see that $s_{corrected} = s^*$ i.e. Newton-Raphson method gives the correct value of the missing initial condition in one iteration.

(ii) Method of adjoints

For equation (3.2.8), the adjoint equations are

$$\begin{bmatrix} \dot{P}_1 \\ \dot{P}_2 \end{bmatrix} = - \begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \qquad 3.2.33$$

and we consider the particular solution satisfying

$$P_1(x_N) = 1 \quad , \quad P_2(x_N) = 0 \qquad 3.2.34$$

the relation between any solution y(x) of (3.2.8) or (3.2.27) and any solution P of the adjoint system (3.2.33) is

$$\left[y_1 P_1 + y_2 P_2 \right]_{x_0}^{x_N} = \int_{x_0}^{x_N} \left(P_1 P_1 + P_2 P_2 \right) dx$$

Hence in particular

$$\eta_1(x_N) - \eta_1(x_0)\, P_1(x_0) - \eta_2(x_0)\, P_2(x_0) = \int_{x_0}^{x_N} \left(P_1 P_1 + P_2 P_2 \right) dx \qquad 3.2.35$$

similarly the relation between any solution Y of (3.2.28) and any solution P of (3.2.33) is

$$\left[Y_1 P_1 + Y_2 P_2 \right]_{x_0}^{x_N} = 0 \qquad 3.2.36$$

Hence in particular for $P_1(x_N) = 1$, $P_2(x_N) = 0$

$$\left.\begin{aligned} P_1(x_0) &= Y_{11}(x_N) \\ P_2(x_0) &= Y_{21}(x_N) \end{aligned}\right\} \qquad 3.2.37$$

Now the method of adjoints states that

$$y_2(x_0) = \frac{1}{P_2(x_0)} \left[\beta - \alpha P_1(x_0) - \int_{x_0}^{x_N} (F_1 P_1 + F_2 P_2)\, dx \right] \qquad 3.2.38$$

substituting from (3.2.35) into (3.2.37) gives

$$y_2(x_0) = \left[\beta - \alpha Y_{11}(x_N) - \eta_1(x_N) + \eta_1(x_0) Y_{11}(x_N) + \eta_2(x_0) Y_{21}(x_N) \right] \Big/ Y_{21}(x_N)$$

and this is the same value again as in (3.2.30). Hence for linear equations adjoint method and Newton's shooting give the true value immediately.

(iii) Method of sweeps and Method of adjoints

In equations (3.2.11) - (3.2.14), if we put

$$r_1(x) = \frac{-P_2(x)}{P_1(x)} \quad , \quad r_2(x) = \frac{1}{P_1(x)} \left(\beta + \int_{x_N}^{x} (F_1 P_1 + F_2 P_2)\, dt \right)$$

This gives the equations (3.2.33), (3.2.34) and (3.2.38) i.e. method of sweeps gives the same results as the method of adjoints.

A comparison of the numerical behaviour of these two methods will be mentioned in the next chapter.

3.3 Parallel shooting method

The idea of this method as mentioned in Keller (1968) and Cebici & Keller (1971) is to divide the interval $[x_0, x_N]$ into sub intervals, solving appropriate initial value problems over each sub interval, and then simultaneously adjusting the initial data in order to satisfy the given boundary conditions and appropriate continuity conditions at the mesh points.

Consider the boundary value problem (3.1.5), (3.1.6) and divide the interval $[x_0, x_N]$ into the sub-intervals $[x_0, x_1] \cdots [x_{N-1}, x_N]$. To start the iterative process, the following sets of initial conditions must be assumed:

$$\begin{bmatrix} y(x_0) \\ z(x_0) \end{bmatrix} = \begin{bmatrix} \alpha \\ s \end{bmatrix} , \quad \begin{bmatrix} y(x_r) \\ z(x_r) \end{bmatrix} = \begin{bmatrix} \lambda_r \\ \mu_r \end{bmatrix} , \quad r = 1, 2, \cdots, N-1 \qquad 3.3.1$$

solving over each subinterval we get the solutions

$$\left.\begin{aligned} & y_0(x, s) \ , \ z_0(x, s) \quad \text{for} \quad x \in [x_0, x_1] \\ & y_r(x, \lambda_r, \mu_r) \ , \ z_r(x, \lambda_r, \mu_r) \quad \text{for} \quad x \in [x_r, x_{r+1}], \\ & \qquad\qquad\qquad\qquad\qquad\qquad r = 1, 2, \cdots, N-1 \end{aligned}\right\} \qquad 3.3.2$$

These solutions must satisfy the continuity conditions

$$\left.\begin{aligned} & \begin{bmatrix} y_0(x_1, s) \\ z_0(x_1, s) \end{bmatrix} = \begin{bmatrix} \lambda_1 \\ \mu_1 \end{bmatrix} = \begin{bmatrix} y_1(x_1, \lambda_1, \mu_1) \\ z_1(x_1, \lambda_1, \mu_1) \end{bmatrix} \\ & \begin{bmatrix} y_{r-1}(x_r, \lambda_{r-1}, \mu_{r-1}) \\ z_{r-1}(x_r, \lambda_{r-1}, \mu_{r-1}) \end{bmatrix} = \begin{bmatrix} \lambda_r \\ \mu_r \end{bmatrix} = \begin{bmatrix} y_r(x_r, \lambda_r, \mu_r) \\ z_r(x_r, \lambda_r, \mu_r) \end{bmatrix}, \quad r = 2, \cdots, N-1 \end{aligned}\right\} \qquad 3.3.3$$

and the boundary conditions

$$y_{N-1}(x_N, \lambda_{N-1}, \mu_{N-1}) = \beta \qquad 3.3.4$$

i.e. in a vector form

$$\phi(\underset{\sim}{s}) = \begin{bmatrix} \phi_1(\underset{\sim}{s}) \\ \phi_2(\underset{\sim}{s}) \\ \phi_3(\underset{\sim}{s}) \\ \phi_4(\underset{\sim}{s}) \\ \vdots \\ \phi_{2N-1}(\underset{\sim}{s}) \end{bmatrix} = \begin{bmatrix} y_0(x_1, s) - \lambda_1 \\ z_0(x_1, s) - \mu_1 \\ y_1(x_2, \lambda_1, \mu_1) - \lambda_2 \\ z_2(x_2, \lambda_1, \mu_1) - \mu_2 \\ \\ y_{N-1}(x_N, \lambda_{N-1}, \mu_{N-1}) - \beta \end{bmatrix} \qquad 3.3.5$$

where $$\underset{\sim}{s} = (s, \lambda_1, \mu_1, \ldots\ldots, \lambda_{N-1}, \mu_{N-1})^T \qquad 3.3.6$$

solving (3.3.5) using Newton's method

$$\underset{\sim}{s}^{r+1} = \underset{\sim}{s}^{r} - \left[\left(\frac{\partial \underset{\sim}{\phi}(\underset{\sim}{s})}{\partial \underset{\sim}{s}} \right)_{\underset{\sim}{s}^r} \right]^{-1} \underset{\sim}{\phi}(\underset{\sim}{s}^r) \qquad 3.3.7$$

To find the Jacobian matrix $\left(\frac{\partial \underset{\sim}{\phi}(\underset{\sim}{s})}{\partial \underset{\sim}{s}} \right)_{\underset{\sim}{s}^r}$ we solve

$$\left.\begin{aligned} P' &= Q \\ Q' &= P_y P + P_z Q \end{aligned}\right\} \qquad 3.3.8$$

once with the initial condition $P(x_0) = 0$, $Q(x_0) = 1$

and the solution is denoted by $P_0(x)$, $Q_0(x)$ for $x \in [x_0, x_1]$

and twice with the initial conditions $\begin{bmatrix} P(x_r) \\ Q(x_r) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$; $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

and the solutions are denoted by $\begin{bmatrix} P_r^{(1)}(x) \\ Q_r^{(1)}(x) \end{bmatrix}$ & $\begin{bmatrix} P_r^{(2)}(x) \\ Q_r^{(2)}(x) \end{bmatrix}$ respectively

for $x \in [x_r, x_{r+1}]$, $r = 1, 2, \ldots\ldots, N-1$,

where $$P_0(x) = \frac{\partial y_0}{\partial s} \quad , \quad P_r^{(1)}(x) = \frac{\partial y_r}{\partial \lambda_r} \quad , \quad P_r^{(2)}(x) = \frac{\partial y_r}{\partial \mu_r}$$

$$Q_0(x) = \frac{\partial z_0}{\partial s} \quad , \quad Q_r^{(1)}(x) = \frac{\partial z_r}{\partial \lambda_r} \quad , \quad Q_r^{(2)}(x) = \frac{\partial z_r}{\partial \mu_r}$$

Then $$J^{(r)} = \left(\frac{\partial \underset{\sim}{\phi}(\underset{\sim}{s})}{\partial \underset{\sim}{s}} \right)_{\underset{\sim}{s}^r} = \begin{bmatrix} P_0(x_1) & -1 & 0 & & \\ Q_0(x_1) & 0 & -1 & & \\ & P_1^{(1)}(x_2) & P_1^{(2)}(x_2) & -1 & 0 \\ & Q_1^{(1)}(x_2) & Q_1^{(2)}(x_2) & 0 & -1 \\ & & \ldots\ldots\ldots & & \\ & & & P_{N-1}^{(1)}(x_N) & P_{N-1}^{(2)}(x_N) \end{bmatrix}$$

and substituting in (3.3.7) gives $S^{\nu+1}$, the whole process is repeated until it converges to the required solution.

The difficulties facing ordinary shooting have been mentioned in (3.2.4). Keller (1968) showed that parallel shooting yields an exponential reduction in the error growth factor, which helps to overcome the problem of fast growing solutions. For the case of sensitive problems where the difficulty lies in guessing the missing initial conditions, Weiss (1973) shows that parallel shooting yields an exponential increase in the domain of attraction for the initial guess. On the other hand we need to guess many parameters compared with few in the case of ordinary shooting. This may make the problem more difficult. To overcome this difficulty we are going to discuss in the next chapter a starting procedure to help provide approximations to the missing initial conditions.

For the linear boundary value problems George and Gunderson (1972) discussed the determination of the subinterval lengths taking into consideration the conditioning of the final matrix used to determine all the shooting parameters.

3.4 Series methods

In a series method, the solution of a boundary value problem is expressed by a finite series. The most common application of the series methods are using Chebyshev series or Fourier series. Concentrate on Chebyshev collocation methods for solving boundary value problems such as Picard method (Clenshaw and Norton (1963) and Wright (1964) and Newton's method (Norton (1964)).

3.4.1 The Picard method

Consider the second order non linear boundary value problem (3.1.4) with $x\in[-1,1]$ and the boundary conditions

$$y(-1)=\alpha \quad , \quad y(1)=\beta \qquad 3.4.1$$

Integrating $$y''_{i+1} = P(x, y_i, y_i') \qquad 3.4.2$$

we can define an iterative process

$$y_{i+1}(x) = \lambda + \mu x + \iint F(x, y_i, y_i')\,(dx)^2 \qquad 3.4.3$$

where λ and μ are evaluated such that

$$y_{i+1}(-1) = \alpha, \quad y_{i+1}(1) = \beta \qquad 3.4.4$$

For a general index we have $y_i(x)$ satisfying the boundary conditions (3.4.1), and its derivative $y_i'(x)$. From the values $y_i(x_s)$, $y_i'(x_s)$ and $f(x_s, y_i(x_s), y_i'(x_s))$ where $x_s = \cos\frac{s\pi}{N}$, $s = 0,1,\ldots,N$ then using (1.3.10) we can compute the coefficients a_r, a_r', B_r where

$$\begin{aligned} y_i(x) &= \sum_{r=0}^{N}{}' a_r T_r(x) \\ y_i'(x) &= \sum_{r=0}^{N-1}{}' a_r' T_r(x) \\ F(x, y_i, y_i') &= \sum_{r=0}^{N-2}{}' B_r T_r(x) \end{aligned} \qquad 3.4.5$$

Let $y_{i+1}(x) = \sum_{r=0}^{N}{}' A_r T_r(x)$, $y_{i+1}'(x) = \sum_{r=0}^{N-1}{}' A_r' T_r(x)$ 3.4.6

then substituting from (3.4.5) into (3.4.3) we get

$$\sum_{r=0}^{N}{}' A_r T_r(x) = \lambda T_0(x) + \mu T_1(x) + \iint \left(\sum_{r=0}^{N-2}{}' B_r T_r(x) \right) (dx)^2 \qquad 3.4.7$$

and from the boundary conditions (3.4.4)

$$\begin{aligned} A_0 &= \alpha + \beta - 2(A_2 + A_4 + \cdots\cdots) \\ A_1 &= \alpha - \beta - (A_1 + A_3 + \cdots\cdots) \end{aligned} \qquad 3.4.8$$

Using (1.3.6) in (3.4.7) and equating coefficients of $T_r(x)$ in both sides we get the new set of coefficients A_r, $r = 0,1,\ldots,N$, repeating until the process converges to the required solution.

This method fails to converge in many problems; to explain, the following notation is used. The iterative process (3.4.3) is written as

$$y_{k+1} = F(y_k) = A + Bx + \iint F(x, y_k, y_k')\,(dx)^2 \qquad 3.4.9$$

This is equivalent to

$$F(y_k) = \frac{\alpha+\beta}{2} + \left(\frac{\beta-\alpha}{2}\right)x + \int_{-1}^{1} G(x,t)\, P\{t, y_k(t), y_k'(t)\}\, dt \qquad 3.4.10$$

where G(x,t) is the Green's function of the reduced problem

$$L(y) \equiv y'' = r(x) \quad , \quad y(-1) = y(1) = 0 \qquad 3.4.11$$

So: if $y^*(x)$ is the exact solution of 3.1.4

$$F(y^*) - F(y_k) = \int_{-1}^{1} G(x,t)\left[P\{t, y^*(t), y^{*\prime}(t)\} - P\{t, y_k(t), y_k'(t)\}\right] dt \qquad 3.4.12$$

and $F(y^*) = y^*$ so this is $y^* - y_{k+1}$

The convergence of the process now depends on the behaviour of the right hand integral: for example, if

$$P(x, y, y') = -\mu^2 y \qquad 3.4.13$$

then (3.4.12) becomes,

$$y^* - y_{k+1} = -\mu^2 \int_{-1}^{1} G(x,t)\,[\,y^*(t) - y_k(t)\,]\, dt \qquad 3.4.14$$

Since $y^*(x) - y_k(x) = 0$ at $x = \pm 1$ it has an expansion in terms of the eigenfunction of 3.4.11, i.e. as a series

$$y^*(x) - y_k(x) = \sum_{n=0} C_n \cos(2n+1)\frac{\pi x}{2} \qquad 3.4.15$$

and then $$\int_{-1}^{1} G(x,t) \cos(2n+1)\frac{\pi t}{2}\, dt = \frac{-4}{(2n+1)^2\pi^2} \cos(2n+1)\frac{\pi x}{2}$$

so that ultimately $|\, y^* - y_{k+1}\,| > |y^* - y_k|$ if $\frac{4\mu^2}{\pi^2} > 1$ 3.4.16

that is the process will then diverge. This treatment is given in Collatz (1960).

3.4.2 Newton's method

This method is using the idea of quasilinearization with the method of superposition and expressing the solution in terms of Chebyshev polynomials. Consider the non linear boundary value problem (3.1.4), (3.1.6). Expanding the R.H.S. in Taylor series about $y_i(x)$, $y_i'(x)$, we get Newton's iterative process.

$$y_{i+1}'' - g(x)\,y_{i+1}' - h(x)\,y_{i+1} = f(x, y_i, y_i') - g(x)\,y_i' - h(x)\,y_i \qquad 3.4.17$$

where $$g(x) = \frac{\partial f}{\partial y'}(x, y_i, y_i')$$

and $$h(x) = \frac{\partial f}{\partial y}(x, y_i, y_i')$$

Norton (1964) used Chebyshev polynomials in the following modifications

let $$y_i(x) = \sum_{r=0}^{N}{}' a_r T_r(x) \quad , \quad y_{i+1}(x) = \sum_{r=0}^{N}{}' A_r T_r(x)$$

$$y_i'(x) = \sum_{0}^{N-1}{}' a_r' T_r(x) \quad , \quad y_{i+1}'(x) = \sum_{r=0}^{N}{}' A_r' T_r(x)$$

$$f(x, y_i, y_i') = \sum_{0}^{N-2}{}' b_r T_r(x) \quad , \quad y_{i+1}''(x) = \sum_{r=0}^{N}{}' A_r'' T_r(x)$$

$$h(x) = \sum_{0}^{N}{}' c_r T_r(x) \quad , \quad g(x) = \sum_{r=0}^{N}{}' c_r' T_r(x)$$

For simplicity h(x) and g(x) are approximated by $\frac{1}{2} c_0$, $\frac{1}{2} c_0'$ respectively. Substituting in (3.4.17) and equating coefficients of $T_r(x)$ we get

$$A_r'' - \tfrac{1}{2} c_0' A_r' - \tfrac{1}{2} c_0 A_r = d_r \quad , \quad r = 0, 1, \ldots, N \qquad 3.4.18$$

where $$d_r = b_r - \tfrac{1}{2} c_0' a_r' - \tfrac{1}{2} c_0 a_r \qquad 3.4.19$$

From (3.4.18)

$$(A_{r-1}'' - A_{r+1}'') - \tfrac{1}{2} c_0' (A_{r-1}' - A_{r+1}') - \tfrac{1}{2} c_0 (A_{r-1} - A_{r+1}) = d_{r-1} - d_{r+1} \qquad 3.4.20$$

using the relations

$$2r\,A_r' = A_{r-1}'' - A_{r+1}'' \quad , \quad 2r\,A_r = A_{r-1}' - A_{r+1}' \qquad 3.4.21$$

we get the recurrence equations

$$C_0 A_{r-1} = C_0 A_{r+1} + 2r\,(2A'_r - C_0 A_r) + 2(d_{r+1} - d_{r-1})$$
$$A'_{r-1} = A'_{r+1} + 2r A_r \qquad 3.4.22$$

for $r = N, N-1, \ldots\ldots, 1$

Every solution of the system may be expressed as the sum of a particular solution E_r, E'_r $(r=o,1,\ldots,N)$ and a linear combination of four independent solutions of the corresponding homogenous system.

$$C_0 B_{r-1} = C_0 B_{r+1} + 2r\,(2B'_r - C'_0 B_r)$$
$$B'_{r-1} = B_{r+1} + 2r B_r \qquad 3.4.23$$

let F_r, F'_r and G_r, G'_r are two solutions of (3.4.23), then

$$A_r = E_r + \mu F_r + \gamma G_r$$

where μ and γ are determined with the aid of the boundary conditions. Where c_o is small it is difficult to produce linearly independent solutions and a modification to this procedure is mentioned in Norton (1964).

3.5 Analytic methods

These approaches replace the given boundary value problem by some analytically equivalent mathematical problem and attempt to solve the new problem numerically. From these methods we are going to choose the continuation method which is closely related to the application of shooting techniques. In these methods two approaches are discussed (Roberts and Shipman (1972)). The first approach is to perturb the integration interval $[x_o, x_N]$ and the second is to perturb the differential equation itself.

3.5.1 Continuation method (perturbed interval)

Consider the non linear boundary value problem (3.1.4), (3.1.6)

(i) start by choosing the missing initial conditions, i.e. the initial conditions becomes $y(x_o) = \alpha$, $y'(x_o) = s$ 3.5.1

(ii) Integrate (3.1.4) forward until overflow problems or numerical difficulties appear. Choose the final value of x as x_1 such that the solution has a good behaviour in $[x_0, x_1]$

(iii) Solve eqn. (3.1.4) over $[x_0, x_1]$ with the boundary conditions

$$y(x_0) = \alpha \quad , \quad y(x_1) = \beta$$ using shooting method

(iv) To extend the interval from $[x_0, x_1]$ to $[x_0, x_2]$ let the initial conditions resulting from the solution in (iii) be $y(x_0) = \alpha$ $y'(x_0) = s_1$. Then solving (3.1.19) over $[x_0, x_2]$ with the boundary condition $y(x_0) = \alpha$, $y(x_2) = \beta$

(v) Repeat for the terminal values x_1, x_2.... until $x = x_N$ at this value the original problem will have been solved. Detailed discussion and solved examples can be found in Roberts and Shipman (1972).

3.5.2. Continuation method (perturbed differential equation)

Consider the boundary value problem (3.1.4). The application of this technique starts by writing the R.H.S. of (3.1.4) in the form

$$f(x, y, y') = P(x, y, y') + Q(x, y, y') \qquad 3.5.2$$

such that the boundary value problem

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

with the boundary conditions (3.1.6) is solvable numerically. Then we solve the sequence of two-point boundary value problems

$$y'' = P + \mu_k Q \quad , \quad k = 0, 1, \ldots, N$$

where $\mu_0 = 0$, $\mu_{k+1} = \mu_k + \Delta\mu_k$

and the missing initial conditions for the solution of the k^{th} problem are taken as the initial conditions for the shooting method solution of the $(k+1)^{\text{st}}$ problem. If a sequence $\Delta\mu_k$ can be found such that each problem (3.1.4), (3.1.6) has a solution and such that $\mu_N = 1$, for some N, then the required problem will have been solved.

3.6 Nicolovius method

Nicolovius (1961) suggested an iterative method for solving linear and non linear boundary value problems using Taylor series with integrated remainder. To describe the method consider the system of n non-linear boundary value problems

$$\underset{\sim}{y}'(x) = \underset{\sim}{f}(x, \underset{\sim}{y}) \qquad 3.6.1$$

with the boundary conditions

$$\underset{\sim}{U}(\underset{\sim}{y}(x_0), \underset{\sim}{y}(x_N)) = 0 \qquad 3.6.2$$

Use a Taylor series expansion about some point $x=x_1$, including the remainder term in integral form and using the notation

$$P_{i\cdot}(x, \underset{\sim}{y}) = P_{i,1}(x, \underset{\sim}{y})$$

$$\frac{d^j}{dx^j} P_{i\cdot} = P_{i,j+1}(x, \underset{\sim}{y})$$

then the exact equation is

$$y_{i\cdot}(x) = y_{i\cdot}(x_1) + \sum_{j=1}^{P_i-1} \frac{(x-x_1)^j}{j!} P_{i,j}(x_1, \underset{\sim}{y}(x_1)) + \frac{1}{(P_i-1)!} \int_{x_1}^{x} P_{i,P_i}(t, \underset{\sim}{y}(t))(x-t)^{P_i-1}\, dt$$

This can be written as an iterative formula implicit in $y_i^{(k)}$ in the form

$$y_{i\cdot}^{(k)}(x) - y_{i\cdot}^{(k)}(x_1) - \sum_{j=1}^{P_i-1} \frac{(x-x_1)^j}{j!} P_{i,j}(x_1, \underset{\sim}{y}^{(k)}(x_1)) = \frac{1}{(P_i-1)!} \int_{x_1}^{x} P_{i,P_i}(t, \underset{\sim}{y}^{(k-1)}(t))(x-t)^{P_i-1}\, dt \qquad 3.6.3$$

The derivate $P_{i,j}(x_1, \underset{\sim}{y}^{(k)}(x_1))$ can all be written in terms of n unknown $y_{i\cdot}^{(k)}(x_1)$ (or a smaller number if x_1 is one of the end points and some values of y_i are given there). Then substituting $x = x_0$, $x = x_N$ in (3.6.3) and using the boundary condition (3.6.2) gives a set of non-

linear equations for the unknown $y_i^{(k)}(x_1)$. The integrals are evaluated in terms of the previous iterate which determines the profiles

In the case of a single higher order differential equation, consider the non-linear boundary value problem (3.1.4) with the boundary conditions (3.4.1). Then expanding the solution about x = o and similar to (3.6.3) we get the following iterative formula

$$y^{(k)}(x) = y^{(k)}(0) + x\,y'^{(k)}(0) + \sum_{j=2}^{p} \frac{x^j}{j!} D^{j-2} F(0, y^{(k)}(0), y'^{(k)}(0)) + \frac{1}{p!} \int_0^x D^{p-1} F(t, y^{(k-1)}(t), y'^{(k-1)}(t))\,(x-t)^p\,dt \qquad 3.6.4$$

Using the boundary conditionswe get

$$\alpha = y^{(k)}(0) - y'^{(k)}(0) + \sum_{j=2}^{p} \frac{(-1)^j}{j!} D^{j-2} F(0, y^{(k)}(0), y'^{(k)}(0)) + \frac{1}{p!} \int_{-1}^{0} D^{p-1} F(t, y^{(k-1)}(t), y'^{(k-1)}(t))\,(t+1)^p\,dt \qquad 3.6.5$$

$$\beta = y^{(k)}(0) + y'^{(k)}(0) + \sum_{j=2}^{p} \frac{1}{j!} D^{j-2} F(0, y^{(k)}(0), y'^{(k)}(0)) + \frac{1}{p!} \int_0^1 D^{p-1} F(t, y^{(k-1)}(t), y'^{(k-1)}(t))\,(1-t)^p\,dt \qquad 3.6.6$$

From (3.6.5) and (3.6.6) we solve to get $y^{(k)}(0)$, $y'^{(k)}(0)$ and substitute them in (3.6.4) to get the required approximate solution.

To show how the method was practically used, the next example is given by Nicolvius with n = 2, p = 3, $y_1 = y$, $y_2 = z$, $f_{i,j} = f_j$, $f_{2,j} = g_j$

$$\left.\begin{aligned} y' &= P_1(x,y,z) = z + \tfrac{1}{10} y^2, \quad y(-1) = 0 \\ z' &= g_1(x,y,z) = -y + \tfrac{1}{10} yz, \quad z(1) = -\tfrac{1}{2} \end{aligned}\right\} \qquad 3.6.7$$

$$y'' = P_2(x,y,z) = -y + \tfrac{3}{10} yz + \tfrac{1}{50} y^3$$

$$z'' = g_2(x,y,z) = -z - \tfrac{1}{5} y^2 + \tfrac{1}{10} z^2 + \tfrac{1}{50} y^2 z$$

$$y''' = P_3(x,y,z) = -z - \tfrac{2}{5} y^2 + \tfrac{3}{10} z^2 + \tfrac{3}{25} y^2 z + \tfrac{3}{500} y^4$$

$$z''' = g_3(x,y,z) = y - \frac{7}{10}yz - \frac{3}{50}y^3 + \frac{3}{50}yz^2 + \frac{3}{500}y^3z$$

$$y^{IV} = P_4(x,y,z) = y - \frac{3}{2}yz - \frac{1}{5}y^3 + \frac{3}{10}yz^2 + \frac{3}{50}y^3z + \frac{3}{1250}y^5$$

$$z^{IV} = g_4(x,y,z) = z + \frac{4}{5}y^2 - \frac{7}{10}z^2 - \frac{11}{25}y^2z + \frac{3}{50}z^3 - \frac{3}{125}y^4 + \frac{9}{250}y^2z^2 + \frac{3}{1250}y^4z$$

For $x_0 = 0$, $P_1 = P_2 = 4$, we get from (3.6.3) with these functions the iteration formulae

$$\left.\begin{aligned} y_k(x) &= y_k(0) + \sum_{j=1}^{3} \frac{x^j}{j!} P_j(0, y_k(0), z_k(0)) \\ &\quad + \frac{1}{6}\int_0^x P_4(t, y_{k-1}(t), z_{k-1}(t))(x-t)^3\,dt \\ z_k(x) &= z_k(0) + \sum_{j=1}^{3} \frac{x^j}{j!} g_j(0, y_k(0), z_k(0)) \\ &\quad + \frac{1}{6}\int_0^x g_4(t, y_{k-1}(t), z_{k-1}(t))(x-t)^3\,dt, \\ &\qquad (k = 1, 2, \ldots) \end{aligned}\right\} \quad 3.6.5$$

substituting P_j, g_j $(j = 1, 2, 3)$ in the R.H.S. of (3.6.5) and using the boundary conditions in (3.6.4) we get

$$0 = \frac{1}{2}y(0) + \frac{5}{6}z(0) - \frac{1}{30}y^2(0) + \frac{3}{20}y(0)z(0) - \frac{1}{20}z^2(0) + \frac{1}{100}y^3(0) - \frac{1}{50}y^2(0)z(0) - \frac{1}{1000}y^4(0) - \frac{1}{6}\int_0^{-1} P_4(t, y_{k-1}(t), z_{k-1}(t))(1+t)^3\,dt$$

$$-\frac{1}{2} = \frac{1}{2}z(0) - \frac{5}{6}y(0) - \frac{1}{60}y(0)z(0) - \frac{1}{10}y^2(0) + \frac{1}{20}z^2(0) + \frac{1}{100}y^2(0)z(0) - \frac{1}{100}y^3(0) + \frac{1}{100}y(0)z^2(0) + \frac{1}{1000}y^3(0)z(0) + \frac{1}{6}\int_0^1 g_4(t, y_{k-1}(t), z_{k-1}(t))(1-t)^3\,dt$$

Solving these two equations iteratively for $y(0)$, $z(0)$

$$y_k(0) = F(y_k(0), z_k(0)) + \frac{15}{16} + \frac{3}{16}\int_{-1}^{0} P_4(t, y_{k-1}(t), z_{k-1}(t))(1+t)^3\,dt + \frac{5}{16}\int_0^1 g_4(t, y_{k-1}(t), z_{k-1}(t))(1-t)^3\,dt \quad 3.6.6$$

$$z_k(0) = G(y_k(0), z_k(0)) + \frac{9}{16} + \frac{5}{16}\int_{-1}^{0} P_4(t, y_{k-1}(t), z_{k-1}(t))(1+t)^3\,dt + \frac{3}{16}\int_0^1 g_4(t, y_{k-1}(t), z_{k-1}(t))(1-t)^3\,dt \quad 3.6.7$$

where $F(x,y) = -\frac{9}{40}y^2 + \frac{11}{80}yz + \frac{3}{80}z^2 - \frac{3}{400}y^3 - \frac{3}{800}y^2z + \frac{3}{160}yz^2 - \frac{3}{1600}y^4 + \frac{9}{8000}y^3z$

$$G(Y,Z) = -\frac{7}{40}Y^2 + \frac{21}{80}YZ - \frac{3}{80}Z^2 + \frac{3}{400}Y^3 - \frac{21}{800}Y^2Z + \frac{9}{800}YZ^2 - \frac{3}{1600}Y^4 + \frac{9}{8000}Y^3Z$$

For a general index we have $y_{k-2}(x)$, $z_{k-2}(x)$ and $y_{k-1}(0)$, $z_{k-1}(0)$, we use (3.6.5) to get $y_{k-1}(x)$, $z_{k-1}(x)$ and substituting in (3.6.6), (3.6.7) and evaluating the integrals we get two non-linear equations in the unknowns $y_k(0)$, $z_k(0)$. Solving to determine them and using (3.6.5) gives $y_k(x)$, $z_k(x)$ and the process is repeated until convergences.

The above example is one which fails to converge using the ordinary Picard method (corresponding to $p_1 = p_2 = 1$) but converges with the values given. Further discussion of this method is given in the next chapter.

CHAPTER IV

A series approach for solving two-point boundary value problems

Introduction

In the first part of this chapter, section 4.1, we report practical experience in applying the Lie series method in Chebyshev form to some of the shooting techniques mentioned in chapter III. The method is here simply used as an alternative way of solving initial value problems, and its performance can be analysed in the same way as has already been done in chapter II. Details of the techniques used are given in (4.1) and practical experience in (4.2).

In the remainder of this chapter we derive an improved method for solving boundary value problems using Lie series, based on alternative ways of successively improving the solution series. This method can be described as a function continuation one in which acceptable series solutions are derived iteratively using intermediate approximations of various types and orders. The method is described and the errors at different stages are discussed in (4.3). Practical implementation and results are given in (4.4). The results are discussed and conclusions drawn in (4.5). Comparisons with other methods and suggestions for further work are given in (4.6).

Note on practical examples

The following examples are solved throughout this chapter using various methods.

(i) $y'' = (y'^2 - y^2)\, e^{-x} - xe^{x}$, $x \in [o, \frac{1}{2}]$

$y(o) = 1$, $y(\frac{1}{2}) = \frac{3}{2} e^{\frac{1}{2}}$

Exact solution $y = (1+x)e^{x}$

(ii) $y'' = 16 \operatorname{Sinh} 16y$, $x \in [o, 1]$

$y(o) = o$, $y(1) = o$

Exact solution $y(x) = o$

(iii) $y'' = \frac{1}{4} e^{y}$, $x \in [-1,1]$

$y(-1) = o$, $y(1) = o$

(iv) $y'' = -\frac{1}{4} e^{y}$, $x \in [-1,1]$

$y(-1) = o$, $y(1) = o$

(v) $y'' = \frac{3}{2} y^{2}$, $x \in [o,1]$

$y(o) = 4$, $y(1) = 1$

Exact solution $y(x) = \frac{4}{(1+x)^2}$

(vi) $y'' = -o.7y - (3\cot x + 2 \tan x)y'$, $x \in [\frac{\pi}{6} , \frac{\pi}{3}]$

$y(\frac{\pi}{6}) = o$, $y(\frac{\pi}{3}) = 5$

4.1 Lie series method for a single higher order differential equation

Consider the non-linear differential equation of order n

$$y^{(n)}(x) = P(x, y, y', \cdots, y^{(n-1)}) \quad , \quad x \in [-1,1] \qquad 4.1.1$$

or

$$\left.\begin{aligned} y_1' &= y_2 \\ y_2' &= y_3 \\ &\vdots \\ y_n' &= P(x, y_1, y_2, \cdots, y_n) \\ &= P(x, \underset{\sim}{y}) \end{aligned}\right\} \quad , \; x \in [-1,1] \qquad \cdots\cdots\cdots\cdots \qquad 4.1.2$$

where $\underset{\sim}{y} = (y_1, y_2, \cdots, y_n)^T$

and let the auxiliary system be

$$\left.\begin{aligned} \hat{y}_1' &= \hat{y}_2 \\ \hat{y}_2' &= \hat{y}_3 \\ &\vdots \\ \hat{y}_n' &= \hat{P}(x, \hat{y}_1, \cdots, \hat{y}_n) \\ &= \hat{P}(x, \underset{\sim}{\hat{y}}) \end{aligned}\right\} \quad ; \; x \in [-1,1] \qquad \cdots\cdots\cdots\cdots \qquad 4.1.3$$

where $\hat{\underset{\sim}{y}} = (\hat{y}_1, \hat{y}_2, \ldots\ldots, \hat{y}_n)^T$

Then the truncated Lie series expression (2.1.3) becomes

$$\overline{y}_1(x) = \hat{y}_1(x) + \int_{-1}^{x} [y_2 - \hat{y}_2]_{t, \hat{\underset{\sim}{y}}(t)} dt + \int_{-1}^{x} (x-t)[y_3 - \hat{y}_3]_{t, \hat{\underset{\sim}{y}}(t)} dt + \ldots\ldots$$

$$+ \int_{-1}^{x} \frac{(x-t)^{n-2}}{(n-2)!} [y_n - \hat{y}_n]_{t, \hat{\underset{\sim}{y}}(t)} dt + \int_{-1}^{x} \frac{(x-t)^{n-1}}{(n-1)!} [f - \hat{f}]_{t, \hat{\underset{\sim}{y}}(t)} dt + \ldots + \int_{-1}^{x} \frac{(x-t)^s}{s!} [D_2 D^s y_1]_{t, \hat{\underset{\sim}{y}}(t)} dt$$

$$\overline{y}_1(x) = \hat{y}_1(x) + \sum_{r=n-1}^{s} \int_{-1}^{x} \frac{(x-t)^r}{r!} [D_2 D^r y_1]_{t, \hat{\underset{\sim}{y}}(t)} dt \qquad 4.1.4$$

and for a general index i we get

$$\overline{y}_i(x) = \hat{y}_i(x) + \sum_{r=n-i}^{s-i+1} \int_{-1}^{x} \frac{(x-t)^r}{r!} [D_2 D^r y_i]_{t, \hat{\underset{\sim}{y}}(t)} dt \qquad 4.1.5$$

For the second order case

$$\left.\begin{aligned} y' &= z \\ z' &= f(x, y, z) \quad , \; x \in [-1, 1] \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots\ldots\ldots \qquad 4.1.6$$

$$\overline{y} = \hat{y} + \sum_{r=1}^{s} \int_{-1}^{x} \frac{(x-t)^r}{r!} [D_2 D^r y]_{t, \hat{y}, \hat{z}} dt \qquad 4.1.7$$

$$= \hat{y} + \int_{-1}^{x} (x-t)(f - \hat{f})_{t, \hat{y}, \hat{z}} dt + \int_{-1}^{x} \frac{(x-t)^2}{2} [f_z (f - \hat{f})]_{t, \hat{y}, \hat{z}} dt + \ldots\ldots$$

$$\overline{z} = \hat{z} + \sum_{r=0}^{s-1} \int_{-1}^{x} \frac{(x-t)^r}{r!} [D_2 D^r z]_{t, \hat{y}, \hat{z}} dt \qquad 4.1.8$$

$$= \hat{z} + \int_{-1}^{x} (f - \hat{f})_{t, \hat{y}, \hat{z}} dt + \int_{-1}^{x} (x-t)[f_z (f - \hat{f})]_{t, \hat{y}, \hat{z}} dt + \ldots$$

4.2 Application of Lie series method to initial value methods for solving non-linear boundary value problems

In this section we are going to use the Lie series method ($G_{s,N}$) in Chebyshev form with y(x) taken as the first four terms of Taylor series to solve the initial value problems appearing in shooting techniques. The use of Chebyshev polynomials also simplifies the integrals appearing in some methods. We compare the numerical behaviour of the Newton Raphson method with the method of adjoints and method of sweeps using quasi-linearization applied to the non-linear second order differential equation (4.1.6). we assume h is sufficiently small ($h = x_{n} - x_{0}$)

4.2.1 Application of Lie series to the method of adjointsusing quasilinearization

Consider the boundary value problem (4.1.6) with the boundary conditions

$$y(-1) = \alpha \quad , \quad y(1) = \beta \qquad 4.2.1$$

As in (3.1) we use quasilinearization about a current solution $y^{(k)}(x)$ to get the linear equation

$$\begin{bmatrix} y'^{(k+1)}(x) \\ z'^{(k+1)}(x) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ (P_y)_{y^{(k)},z^{(k)}} & (P_z)_{y^{(k)},z^{(k)}} \end{bmatrix} \begin{bmatrix} y^{(k+1)} \\ z^{(k+1)} \end{bmatrix} + \begin{bmatrix} 0 \\ [P - P_y \cdot y - P_z \cdot z]_{y^{(k)},z^{(k)}} \end{bmatrix} \qquad 4.2.2$$

with the boundary conditions

$$y^{(k+1)}(-1) = \alpha \quad , \quad y^{(k+1)}(1) = \beta \qquad 4.2.3$$

Applying the method of adjoints, the adjoint equations for (4.2.2) become

$$\left.\begin{aligned} \dot{P}_1 &= F_1(x, P_1, P_2) = -[P_y]_{y^{(k)},z^{(k)}} P_2 \\ \dot{P}_2 &= F_2(x, P_1, P_2) = -P_1 - [P_z]_{y^{(k)},z^{(k)}} P_2 \\ P_1(1) &= 1 \quad , \quad P_2(1) = 0 \end{aligned}\right\} \qquad 4.2.4$$

we solve these by $G_{2,N}$, where

$$\hat{P}_1(x) = 1 + (x-1)\,P_1(1,1,0) + \frac{(x-1)^2}{2} DP_1(1,1,0) \qquad 4.2.5$$

$$\hat{P}_2(x) = (x-1)\,P_2(1,1,0) + \frac{(x-1)^2}{2} DP_2(1,1,0) \qquad 4.2.6$$

$$\hat{P}_1 = \dot{\hat{P}}_1 \quad , \quad \hat{P}_2 = \dot{\hat{P}}_2 \qquad 4.2.7$$

$$\bar{P}_1 = \hat{P}_1 + \int_1^x (P_1 - \hat{P}_1)_{t,\hat{P}(t)}\,dt + \int_1^x (x-t)\left[(-P_y)_{y(t),z(t)}(P_2 - \hat{P}_2)\right]_{t,\hat{P}(t)}\,dt$$

$$+ \int_1^x \frac{(x-t)^2}{2}\left\{(P_y)_{y(t),z(t)}(P_1 - \hat{P}_1) + (P_y P_z - P_{xy} - P_{yy}z - P_{yz}P)_{y(t),z(t)}(P_2 - \hat{P}_2)\right\}_{t,\hat{P}}\,dt \qquad 4.2.8$$

$$\bar{P}_2 = \hat{P}_2 + \int_1^x (P_2 - \hat{P}_2)_{t,\hat{P}}\,dt + \int_1^x (x-t)\left[-(P_1 - \hat{P}_1) - (P_z)_{y(t),z(t)}(P_2 - \hat{P}_2)\right]_{t,\hat{P}}\,dt$$

$$+ \int_1^x \frac{(x-t)^2}{2}\left\{(P_z)_{y(t),z(t)}(P_1 - \hat{P}_1) + (P_y + P_z^2 - P_{xz} - P_{yz}z - P_{zz}P)_{y(t),z(t)}(P_2 - \hat{P}_2)\right\}_{t,\hat{P}}\,dt \qquad 4.2.9$$

The fundamental equation simplifies in this case to

$$Z^{(k+1)}(-1) = \frac{1}{P_2(-1)}\left[\beta - \alpha P_1(-1) - \int_{-1}^{1} [P - P_y y - P_z z]_{y(t),z(t)} P_2(x)\,dx\right] \qquad 4.2.10$$

If the integrand $P_2(x)[P - P_y y - P_z z]_{y(t),z(t)}$ is expressed in the form

$$\sum_{r=0}^{N}{}' c_r^{(k)} T_r(x) \qquad 4.2.11$$

then

$$Z^{(k+1)}(-1) = \frac{1}{P_2(-1)}\left\{\beta - \alpha P_1(-1) - \left[\frac{c_0^{(k)}}{2}T_1 + \frac{c_1^{(k)}}{4}T_2 + \sum_{2}^{N}{}' \frac{c_r^{(k)}}{2}\left(\frac{T_{r+1}}{r+1} - \frac{T_{r-1}}{r-1}\right)\right]_{-1}^{1}\right\} \qquad 4.2.12$$

Now we solve for $y^{(k+1)}(x)$, $z^{(k+1)}(x)$ using $G_{3,N}$ with the initial conditions $y^{(k+1)}(-1) = \alpha$ and $z^{(k+1)}(-1) = s^{(k+1)}$ evaluated from (4.2.12)

$$\hat{y}^{(k+1)}(x) = \alpha + (x+1)\,S^{(k+1)} + \frac{(x+1)^2}{2} P(-1,\alpha,S^{(k+1)}) + \frac{(x+1)^3}{6} DP(-1,\alpha,S^{(k+1)}) \qquad 4.2.13$$

and $$\hat{Z}^{(k+1)} = \hat{y}'^{(k+1)} \quad , \quad \hat{P}^{(k+1)} = \hat{y}''^{(k+1)} \qquad 4.2.14$$

$$\bar{y}^{(k+1)} = \hat{y}^{(k+1)} + \int_{-1}^{x} (x-t)(P-\hat{P})_{t,\hat{y},\hat{z}}\,dt + \int_{-1}^{x} \frac{(x-t)^2}{2}\left[P_z(P-\hat{P})\right]_{t,\hat{y},\hat{z}}\,dt$$

$$+ \int_{-1}^{x} \frac{(x-t)^3}{6}\left\{(P_{xz} + P_{yz}z + P_{zz}P + P_y + P_z^2)(P-\hat{P})\right\}_{t,\hat{y},\hat{z}}\,dt \qquad 4.2.14$$

and $$\bar{Z}^{(k+1)} = \bar{y}'^{(k+1)} \qquad 4.2.16$$

It will be noted that the same f - derivatives occur in 4.2.8 4.2.9 and 4.2.13, because of the use of $G_{2,N}$ in one set and $G_{3,N}$ in the other.

For the sake of comparison as will be shown later, we apply the method of adjoints in two directions. First we integrate the differential equation forward and the adjoint equations backward and we denote this direction by F and second we integrate the differential equation backward and the adjoint equations forward, this direction is denoted by B. In this case the initial conditions for (4.2.4) are

$$P_1(-1) = 1 \quad , \quad P_2(-1) = 0 \qquad 4.2.17$$

and (4.2.12) becomes

$$Z^{(k+1)}(1) = \frac{1}{P_2(1)}\left\{\alpha - \beta P_1(1) + \left[\frac{c_0^{(k)}}{2}T_1 + \frac{c_1^{(k)}}{4}T_2 + \sum_{2}^{N} \frac{c_r^{(k)}}{2}\left(\frac{T_{r+1}}{r+1} - \frac{T_{r-1}}{r-1}\right)\right]_{-1}^{1}\right\} \qquad 4.2.18$$

Each of the initial value problems is iterated until the L_∞ norm of the difference between two successive vectors of coefficients is less than a specified tolerance ε, and the same ε is used as a stopping criterion for k, the final solution $y^{(k)}(x)$ being such that $\left| y^{(k)}(1) - \beta \right| < \varepsilon$ (for case F) and $\left| y^{(k)}(-1) - \alpha \right| < \varepsilon$ (for case B). The number of terms N of Chebyshev series is kept constant in these

calculations.

The results shown in Table 1 show the number of iterations used in solving the differential equation (4.1.6) using $G_{3,N}$ and the number of iterations used to solve the adjoint equation using $G_{2,N}$.

TABLE 1

Eqn.	S_o	No.of rounds k	Direction	Tol. ε	No.of iterations Diff. Eqn.	Adj. Eqn.	N
(i)	0.4	5	F	0.1D-8	25	21	31
(i)	0.6	5	F	"	32	27	"
(i)	0.6	4	B	"	30	20	"
(iii)	0.5	5	F	0.1D-10	22	22	"
(iv)	0.5	4	F	"	16	16	"
(v)	-1	4	B	0.1D-8	31	29	"
(vi)	0	1	F	"	6	6	"

4.2.2 Application of Lie series to the method of sweeps using quasilinearization

As in (4.2.1) we start with the boundary value problem (4.1.6) with the boundary condition (4.2.1) and use quasilinearization about the current solution $y^{(h)}(x)$, $z^{(k)}(x)$ to get (4.2.2), (4.2.3). The Riccati equations become:

$$\left.\begin{aligned} \dot{r}_1 &= g_1(x, r_1, r_2) = 1 - (F_z)_{y^{(k)}, z^{(k)}} r_1 - (F_y)_{y^{(k)}, z^{(k)}} r_1^2 \\ \dot{r}_2 &= g_2(x, r_1, r_2) = -(F_y)_{y^{(k)}, z^{(k)}} r_1 r_2 - (F - F_y y - F_z z)_{y^{(k)}, z^{(k)}} r_1 \end{aligned}\right\} \quad 4.2.19$$

For the case F the initial conditions are

$$r_1(1) = 0 \quad , \quad r_2(1) = \beta \qquad 4.2.20$$

we solve (4.2.19) by $G_{2,N}$ where

$$\hat{r}_1 = (x-1)\, g_1(1,0,\beta) + \frac{(x-1)^2}{2} Dg_1(1,0,\beta) \qquad 4.2.21$$

$$\hat{r}_2 = \beta + (x-1)\, g_2(1,0,\beta) + \frac{(x-1)^2}{2} Dg_2(1,0,\beta) \qquad 4.2.22$$

$$\hat{g}_1 = \dot{\hat{r}}_1 \quad , \quad \hat{g}_2 = \dot{\hat{r}}_2 \qquad 4.2.23$$

$$\bar{r}_1 = \hat{r}_1 + \int_1^x (g_1 - \hat{g}_1)_{t,\hat{\underline{r}}}\, dt + \int_1^x (x-t)\left[-(P_z + 2P_y r_1)(g_1 - \hat{g}_1)\right]_{t,\hat{\underline{r}}(t)} dt$$
$$+ \int_1^x \frac{(x-t)^2}{2}\Big\{-\left[2P_y - P_z^2 + P_{xz} + P_{yz} z + P_{zz} F + 2r_1 (P_{xy} + P_{yy} z + P_{yz} F - 3P_y (P_z + P_y r_1))\right]$$
$$(g_1 - \hat{g}_1)\Big\}_{t,\hat{\underline{r}}(t)} dt \qquad 4.2.24$$

$$\bar{r}_2 = \hat{r}_2 + \int_1^x (g_2 - \hat{g}_2)_{t,\hat{\underline{r}}}\, dt + \int_1^x (x-t)\Big\{\left[P_y (P_{yy} - r_2) - F + P_z z\right](g_1 - \hat{g}_1) - (P_y \cdot r_1)(g_2 - \hat{g}_2)\Big\}_{t,\hat{\underline{r}}} dt$$
$$+ \int_1^x \frac{(x-t)^2}{2}\Big\{-\left[(P_{xy} + P_{yy} z + P_{yz} F) r_1 + (P_x - (P_{xy} + P_{yy} z + P_{yz} F) y - (P_{xz} + P_{yz} z + P_{zz} F) z\right)$$
$$- (P_y r_1 + F - P_y y - P_z z)(P_z + 4P_y r_1)\Big](g_1 - \hat{g}_1) - \left[(P_{xy} + P_{yy} z + P_{yz} F) r_1 + P_y g_1 - P_y^2 r_1^2\right]$$
$$(g_2 - \hat{g}_2)\Big\}_{t,\hat{\underline{r}}(t)} dt \qquad 4.2.25$$

and $$Z^{(k+1)}(-1) = \frac{\alpha - r_2(-1)}{r_1(-1)} = s^{(k+1)} \qquad 4.2.26$$

Now solve for $y^{(k+1)}(x)$, $z^{(k+1)}(-1)$ using $G_{3,N}$ with the initial condition $y^{(k+1)}(-1) = \alpha$, $z^{(k+1)}(-1) = s^{(k+1)}$ evaluated from (4.2.26), and find $y^{(k+1)}$, $y^{(k+1)}$ as in (4.2.13), (4.2.15). Again the same f-derivatives occur in both sets of equations.

For the case B the initial conditions are

$$r_1(-1) = 0 \quad , \quad r_2(-1) = \alpha \qquad 4.2.27$$

and $$Z^{(k+1)}(1) = \frac{\beta - r_2(1)}{r_1(1)} \qquad 4.2.28$$

Again, each of the initial value problems is iterated until the L_∞

norm of the difference between two successive vectors of coefficients is less than a specified tolerance ε and the same ε is used as a stopping criterion for k, the final solution $y^{(k)}(x)$ being such that $\left| y^{(k)}(1) - \beta \right| < \varepsilon$ (for the case F) and $\left| y^{(k)}(-1) - \alpha \right| < \varepsilon$ (for the case B). The number of terms N of Chebyshev series is kept constant in these calculations.

In the results shown in Table 2, the number of iterations used for solving the diff-equation (4.1.9) using $G_{3,N}$ and the number of iterations used for solving Riccati equations using $G_{3,N}$ are listed.

TABLE 2

Eq.	S_o	No.of rounds k	Direction	Tol ε	No. of iterations Diff. Eq.	Riccati Eq.	N
(i)	0.4	5	F	0.1D-8	25	44	31
(i)	0.6	-	F	"	Blows up		"
(i)	0.6	4	B	"	30	24	"
(iii)	0.5	5	F	0.1D-10	22	24	"
(iv)	0.5	4	F	"	16	21	"
(v)	-1	4	B	0.1D-8	31	32	"
(vi)	0	1	F	"	6	7	"

Note: "Blows up" here means that the solution of the Riccati equation becomes infinite in $[-1,1]$.

4.2.3 Application of Lie series to shooting method (Newton Raphson)

The Lie series method $G_{3,N}$ is used to solve the differential equation (4.1.6) with the initial conditions

$$y(-1) = \alpha \quad , \quad z(-1) = s^{(k)} \qquad 4.2.29$$

as in (4.2.13), (4.2.15) and the solution is denoted by $y^{(k)}, z^{(k)}$.

The correction equation becomes

$$\left.\begin{aligned} P'(x, s^{(k)}) &= Q(x, s^{(k)}) \\ Q'(x, s^{(k)}) &= \left(F_y\right)_{y^{(k)}, z^{(k)}} P(x, s^{(k)}) + \left(F_z\right)_{y^{(k)}, z^{(k)}} Q(x, s^{(k)}) \\ &= \mathcal{F}(x, P, Q) \\ P(-1, s^{(k)}) &= 0 \quad , \quad Q(-1, s^{(k)}) = 1 \end{aligned}\right\} \qquad 4.2.30$$

We use $G_{3,N}$ to solve (4.2.30), starting with

$$\hat{P} = (x+1) + \frac{(x+1)^2}{2}\left[\left(F_z\right)_{-1, a, s^{(k)}}\right] + \frac{(x+1)^3}{6}\left[\left(F_{zx} + F_{zy} z + F_{zz} P + F_y + F_z^2\right)_{-1, a, s^{(k)}}\right]$$

$$\hat{Q} = \dot{\hat{P}} \quad , \quad \hat{\mathcal{F}} = \dot{\hat{Q}}$$

$$\bar{P} = \hat{P} + \int_{-1}^{x} (x-t)\left(\mathcal{F} - \hat{\mathcal{F}}\right)_{t, \hat{P}, \hat{Q}} dt + \int_{-1}^{x} \frac{(x-t)^2}{2}\left(F_z\right)_{y^k, z^k}\left(\mathcal{F} - \hat{\mathcal{F}}\right)_{t, \hat{P}, \hat{Q}} dt$$

$$+ \int_{-1}^{x} \frac{(x-t)^3}{6}\left(F_{zx} + F_{zy} z + F_{zz} P + F_y + F_z^2\right)_{y^{(k)}, z^{(k)}}\left(\mathcal{F} - \hat{\mathcal{F}}\right)_{t, \hat{P}, \hat{Q}} dt$$

In this case $G_{3,N}$ is used for both sets of equations since exactly the same fderivatives occur.

The new initial condition is then found from

$$Z^{(k+1)}(-1) = s^{(k+1)} = s^{(k)} - \frac{y(1, s^{(k)}) - \beta}{P(1, s^{(k)})} \qquad 4.2.31$$

and the process is then repeated. The same criterion as before is used for the solution of the initial value problems and for stopping the process.

Table 3 shows the practical results:

TABLE 3

Eq.	S_o	N	Tol e	No.of Iterations Diff.Eq.	Corr.Eq.
(i)	0.4	31	0.1D-8	25	22
(i)	0.6	"	"	28	26
(i)	0.7	"	"	Blows up	
(ii)	0.1D-4	"	"	Blows up	
(iii)	0.5	"	"	22	18
(iv)	0.5	"	"	16	13

Note "Blows up" means that the solution $y(x,s^0)$ becomes infinite in $[-1,1]$.

4.2.4 Comparison of methods

In solving the initial value problems we used $G_{3,N}$ to solve the differential equation and the correction equation in the shooting method, since they are using the same f derivatives while we used $G_{2,N}$ to solve the Adjoint equations and Riccati equations to avoid using higher f derivatives than those which occur in solving the differential equation.

Comparing tables (1) and (3) we can easily notice that method of adjoints and shooting method have almost the same behaviour while comparison of tables (1) and (2) shows that method of adjointsis more stable than the method of sweeps specially in the case F in the non-linear case. while for the linear case they have the same behaviour.

In these three methods we have the same difficulty of choosing s_0 so as to find a starting profile. For this reason we are going to develop a new method which helps in providing a starting value for shooting techniques.

4.3 A series method for solving non-linear boundary value problems

4.3.1 General idea of the method

Consider the second order non-linear boundary value problem

$$y'' = f(x,y,y') \quad , \quad y(0)=\alpha, \quad y(h)=\beta \qquad 4.3.1$$

or

$$\left.\begin{aligned} y' &= z \\ z' &= f(x,y,z) \quad , x\in[0,h] \\ y(0) &= \alpha \quad , \quad y(h)=\beta \end{aligned}\right\} \qquad 4.3.2$$

The interval here has been taken as $[0,h]$ for convenience in describing the order of accuracy.

The related initial value problem associated with this is

$$u'' = f(x,u,u') \quad , u(0)=\alpha, \quad u'(0)=s \qquad 4.3.3$$

or
$$\left.\begin{aligned} u' &= v \\ v' &= f(x,u,v) \quad , x\in[0,h] \\ u(0) &= \alpha \quad , v(0) = s \end{aligned}\right\} \qquad 4.3.4$$

Let u(x,s) be the solution of (4.3.4), if (4.3.2) has an isolated solution, for which z(o) = s*, it is known (Keller 1968) that u(x,s) is unique, that it depends differentiably on s, and that s* is the unique solution of the equation

$$\phi(s^*) = u(h,s^*) - \beta = 0 \qquad 4.3.5$$

Note however that for u(o,s) to be finite in [o,h] it may be necessary to restrict s to some neighbourhood of s*.

Now let $u_m(x,s)$ be an approximation to u(x,s) given by a Taylor series of order m, and consider the related equation

$$\phi_m(s) = u_m(h,s) - \beta = 0 \qquad 4.3.6$$

The solution of this equation, if it exists, will be called s_m. The process to be described is in two stages:
firstly, the determination of s_m from an initial approximation s_o, and secondly, the use of s_m as a starting value for the shooting (Newton Raphson) process.

The questions which arise are then,

(i) under what conditions does such an s_m exist

(ii) its value as a start of the shooting process, which depends on its accuracy as an estimate of s*

(iii) how may s_m be determined

(iv) how does this method compare with the use of ordinary shooting starting with the same initial approximation s_o

A brief theoretical analysis of these questions will now be given.

Practical results will be given in succeeding sections.

4.3.2. Existence of s_m

For equation (4.3.6) we have for a sufficiently small h

$$u_m(x,s) = u(x,s) + R_m(x,s) \qquad 4.3.7$$

where R_m is $O(x)^{m+1} D^{m-1} f$, i.e. R_m is bounded and of known order. Since equation (4.3.5) has always a solution s*, then for large enough m, equation (4.3.6) has a solution s_m.

If u(x,s) is continuous in $N_\rho = \{(x,s) \mid x \in [0,h], |s-s^*| \le \rho\}$ and $u_m(x,s)$ is continuous in $N_{\rho_m} = \{(x,s) \mid x \in [0,h], |s-s^*| \le \rho_m\}$ then $\rho_m \ge \rho$ i.e. $N_{\rho_m} \supset N_\rho$ since any s for which u(x,s) is continuous $0 \le x \le h$ has also $u_m(x,s)$ continuous, whereas the reverse is not true.

While s_1 always exists such that $\alpha + s_1 h = \beta$, s_m may not exist for small values of $m > 1$.

4.3.3. Accuracy of s_m

Since $u_m(x,s)$ is expressed as a Taylor series of order m, then

$$u_m(x,s_m) = \alpha + x s_m + \frac{x^2}{2} f(0,\alpha,s_m) + \cdots + \frac{x^m}{m!} D^{m-2} f(0,\alpha,s_m) \qquad 4.3.8$$

and the exact solution u(x,s) can be expressed as an infinite Taylor series.

$$u(x,s^*) = \alpha + x s^* + \frac{x^2}{2} f(0,\alpha,s^*) + \cdots + \frac{x^m}{m!} D^{m-2} f(0,\alpha,s^*) + \cdots \qquad 4.3.9$$

Hence $u_m(x,s_m) - u(x,s^*) = u_m(x,s_m) - u(x,s_m) + u(x,s_m) - u(x,s^*)$

$$= O(x^{m+1}) + (s_m - s^*)(O(x))$$

since $u_m(h,s_m) = \beta = u(h,s^*)$ then

$$0 = O(h^{m+1}) + (s_m - s^*)(h + \cdots)$$

i.e. $$s_m - s^* = O(h^m) \qquad 4.3.10$$

Explicit expressions for $s_m - s^*$ using various types of series are considered in the next section.

4.3.4 Determination of s_m

To solve the equation (4.3.6) for s_m we use the Newton Raphson

iterative process

$$s_m^{\nu+1} = s_m^{\nu} - \left[u_m(h, s_m^{\nu}) - \beta \right] \Big/ \left(\frac{\partial u_m}{\partial s_m} \right)_{h, s_m^{\nu}} = G_m(s_m^{\nu}) \qquad 4.3.11$$

where $\frac{\partial u_m}{\partial s_m}$ is the solution of the differential equation

$$U'' = (f_u)_{x, s_m^{\nu}} U + (f_v)_{x, s_m^{\nu}} U' \qquad 4.3.12$$

$$U(0) = 0 \quad , \quad U'(0) = 1$$

and $U_m(x, s_m^{\nu})$ is an approximate solution of (4.3.12) expressed by a Taylor series of order m. Note that since $s_m - s^*$ is of order h^m. this equation need only be dealt with to this order. With a proper choice of s_m^o, the iterative process (4.3.11) will converge to s_m. (See graph 7)

4.3.5 Conditions for convergence

For the equation (4.3.5), Keller (1968) proves that under certain conditions $\phi(s)$ has a positive derivative for all s, hence $\phi(s) = 0$ has a unique root (see Keller (1968) theorem (1.2.6), pp.16)

So s^* can be obtained using the iterative process

$$S^{\nu+1} = G(S^{\nu}) = S^{\nu} - \frac{\phi(S^{\nu})}{\phi'(S^{\nu})} \qquad 4.3.13$$

and the rate of convergence will depend on $s^o - s^*$ and $G''(s)$.

Since from (4.3.11), $G(s) - G_m(s) = O(h^{m+1})$, then (4.3.11) and (4.3.13) have approximately the same rate of convergence. The graphs 7&8 of some practical results agree with this statement.

A general estimate of the domain of convergence of (4.3.13) is reported in Traub (1964).

If $J = \{ s \mid |s - s^*| < r \}$ and $|G''(s)| \le 2M$ for $s \in J$, then $Mr < 1$ is a sufficient condition for convergence

Alternatively if $|G(s) - G(t)| \le K |s - t| \quad \forall\, s, t \in J$ and $K < 1$, then $|s - s^*| < \frac{1}{M}$ where $|G''(s)| \le 2M$ in J

This is enough to ensure $S = G(s)$ is contraction mapping, since

$$S^{\nu+1} - S^{*} = \frac{G''(\xi)}{2} (S^{\nu} - S^{*})^2 \qquad \text{for } \xi \text{ between } S^{\nu} \text{ and } S^{*}$$

so $$|G(S_0) - G(S^{*})| \le M |S_0 - S^{*}|^2$$

$$\le M\rho |S_0 - S^{*}|$$

So we have interval of existence of solution $|S - S^{*}| < \rho$

and interval within which Newton converges $|S - S^{*}| < \frac{1}{M} \le \rho$

For the iterative process (4.3.11) if $|G_m''(s)| \le 2M_m$ and

$G_m(S) = G(S) + O(h^{m+1})$, so $2M_m \le 2M + O(h^{m+1})$

so interval of convergence for (4.3.11) is

$$|S - S_m| < \frac{1}{M} - O(h^{m+1}) \le \frac{1}{M_m}$$

This implies that the outer range for s_o is of the same order as that of ordinary shooting since $s^* - s_m = o(h^{m+1})$.

4.4 Practical applications

In this section we are going to discuss how this method is applied in practice using various combinations of series. We adopt the following notation throughout this chapter.

TLm: for the method which uses a truncated Taylor series of order m

i.e. $$u_m = u(x_0) + (x - x_0)u'(x_0) + \cdots + \frac{(x - x_0)^m}{m!} D^m u(x_0) \qquad 4.4.1$$

TPm: for the method which uses a two-point series of order m

$$u_m = A_0 + A_1(x - x_0) + A_2(x - x_0)(x - x_N) + A_3(x - x_0)^2(x - x_N) + A_4(x - x_0)^2(x - x_N)^2$$

$$+ \cdots\cdots + \begin{cases} A_m (x - x_0)^{\frac{m}{2}} (x - x_N)^{\frac{m}{2}} & \text{for m even} \\ A_m (x - x_0)^{\frac{m+1}{2}} (x - x_N)^{\frac{m-1}{2}} & \text{for m add} \end{cases} \qquad 4.4.2$$

Here the coefficients A_i, $i = 0, 1, \ldots, m$ are calculated such that $u(x)$ and $u_m(x)$ and their higher derivatives up to some order agree at both ends of the interval $[x_0, x_N]$

For example, for the differential equation

$$y'' = f(x, y, y') \qquad , x \in [x_0, x_N] \qquad 4.4.3$$

where $$\left.\begin{aligned} y(x_0) &= y_0 \quad , \quad y(x_N) = y_N \\ y'(x_0) &= s_0 \quad , \quad y'(x_N) = s_N \end{aligned}\right\} \qquad 4.4.4$$

then $y_5 = A_0 + A_1(x-x_0) + A_2(x-x_0)(x-x_N) + \cdots\cdots + A_5(x-x_0)^3(x-x_N)^2$

where using (4.4.4) and the conditions

$$\left.\begin{aligned} D^i y_5(x_0) &= D^i y(x_0) \\ D^i y_5(x_N) &= D^i y(x_N) \end{aligned}\right\} \quad , \ (i = 0,1,2) \qquad 4.4.5$$

and $x_N - x_0 = h$, we get

$$\begin{bmatrix} y_0 \\ y_N \\ s_0 \\ s_N \\ P_0 \\ P_N \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ 1 & h & & & & \\ & 1 & -h & & & \\ & 1 & h & h^2 & & \\ & & 2 & -2h & 2h^2 & \\ & & 2 & 4h & 2h^2 & 2h^3 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \end{bmatrix} \qquad 4.4.6$$

$TLL_{m,n}$: For the method which uses (n+1)-term Lie series with $\hat{u}(x)$ as a Taylor series of order m and the total order P= m+n+1

$$\text{i.e.} \quad u_p = u_m + \sum_{r=0}^{n} \int_{x_0}^{x} \frac{(x-t)^r}{r!} \left[D_2 D^r u \right]_{u_m} dt \qquad 4.4.7$$

$TPL_{m,n}$: For the method which uses (n+1)-term Lie series with $\hat{u}(x)$ as a two-point series of order m.

4.4.1 TL_m method

We have not used this method in practice since better methods are available and will be discussed in the next subsections. However it is simple to explain and to analyse, and forms a basis for the methods which follow.

Consider the non-linear boundary value problem

$$\left.\begin{aligned} y' &= z \\ z' &= F(x,y,z) \quad , \quad y(-1) = \alpha, \quad y(1) = \beta \end{aligned}\right\} \qquad 4.4.8$$

(i) Guess a value s_o for the missing initial condition

i.e. $z(-1) = s_o$ 4.4.9

(ii) Form the expressions

$$y_m(x, s_o) = \alpha + (x+1)s_o + \frac{(x+1)^2}{2} P(-1, \alpha, s_o) + \cdots + \frac{(x+1)^m}{m!} D^{m-2} P(-1, \alpha, s_o)$$

$$z_m(x, s_o) = y_m'(x, s_o)$$

(iii) Subsitute this approximate solution into the correction equation

$$\left.\begin{aligned} \dot{P} &= Q \\ \dot{Q} &= (P_y)_{y_m, z_m} P + (P_z)_{y_m, z_m} Q = F(x, P, Q) \\ P(-1) &= 0 \quad , \quad Q(-1) = 1 \end{aligned}\right\} \qquad 4.4.10$$

and form the expression

$$P_m(x, s_o) = (x+1) + \frac{(x+1)^2}{2} F(-1, 0, 1) + \cdots + \frac{(x+1)^m}{m!} D^{m-2} F(-1, 0, 1)$$

(iv) Use the iterative process

$$s_1 = s_o - [y_m(1, s_o) - \beta] / P_m(1, s_o)$$

(v) Repeat until s converges to the value s_m

(vi) Start with $s = s_m$ and apply shooting technique using an accurate initial value method.

An explicit expression for the rate of convergence of this method and for the error $s_m - s^*$ for a linear equation, is given in the appendix for the case m=3.

4.4.2 $\underline{TLL_{m,n}}$ method

We have shown that if $\bar{y}(x)$ is found from $\hat{y}(x)$ by using Lie series of order n, and if $\hat{y}(x)$ is a Taylor expansion of order m, then $\bar{y}(x)$ agrees with the Taylor expansion up to order m+n :that it is a more economical way to obtain this expansion, and that some practical experience indicates that it may be somewhat more accurate than the order indicates. Hence this series is used as a basis for finding a starting s, in practice with m=n=3. It is more efficient to use

m=n since the same f-derivatives occur in $\hat{y}$ and Lie series. The method can be described as follows.

(I) Shooting from one end

(i) Consider the non-linear boundary value problem (4.4.8) and assume the missing initial conditions $z(-1)=s_o$

(ii) Starting with $\hat{y}(x)$ as a Taylor series of order 3

i.e. $\hat{y}(x) = \alpha + (x+1)s_o + \frac{(x+1)^2}{2} F(-1,\alpha,s_o) + \frac{(x+1)^3}{6} DF(-1,\alpha,s_o)$

and $\hat{z}(x) = s_o + (x+1)F(-1,\alpha,s_o) + \frac{(x+1)^2}{2} DF(-1,\alpha,s_o)$

(iii) Iterate once on y(x) using Lie series iterative process $G_{3,N}$ to get $\bar{y}(x)$ and $\bar{z}(x)$ where

$$\bar{y}(x) = \hat{y}(x) + \int_{-1}^{x} (x-t)(F-\hat{F})_{\hat{y},\hat{z}}\,dt + \int_{-1}^{x} \frac{(x-t)^2}{2}\left[F_z(F-\hat{F})\right]_{\hat{y},\hat{z}}\,dt + \int_{-1}^{x} \frac{(x-t)^3}{6}\left[(DF)_z(F-\hat{F})\right]_{\hat{y},\hat{z}}\,dt$$

$$\bar{z}(x) = \hat{z}(x) + \int_{-1}^{x} (F-\hat{F})_{\hat{y},\hat{z}}\,dt + \int_{-1}^{x} (x-t)\left[F_z(F-\hat{F})\right]_{\hat{y},\hat{z}}\,dt + \int_{-1}^{x} \frac{(x-t)^3}{2}\left[(DF)_z(F-\hat{F})\right]_{\hat{y},\hat{z}}\,dt$$

(iv) Subsitute $\bar{y}(x)$ and $\bar{z}(x)$ into the correction equation

$$\dot{P} = Q$$
$$\dot{Q} = (F_y)_{\bar{y},\bar{z}} P + (F_z)_{\bar{y},\bar{z}} Q = F(x,P,Q)$$
$$P(-1) = 0 \quad , \quad Q(-1) = 1$$

(v) Again for the correction equation we start with $\hat{P}(x)$ taken as Taylor series of order 3

$$\hat{P}(x) = (x+1) + \frac{(x+1)^2}{2}(F_z)_{-1,\alpha,s_o} + \frac{(x+1)^3}{6}\left[(DF)_z\right]_{-1,\alpha,s_o}$$

$$\hat{Q}(x) = 1 + (x+1)(F_z)_{-1,\alpha,s_o} + \frac{(x+1)^2}{2}\left[(DF)_z\right]_{-1,\alpha,s_o}$$

(vi) Iterate once on $\hat{P}(x)$ using the same Lie series iterative process $G_{3,N}$ to get $\bar{P}(x)$ and $\bar{Q}(x)$ where

$$\bar{P}(x) = \hat{P}(x) + \int_{-1}^{x} (x-t)(F-\hat{F})_{t,\hat{P},\hat{Q}}\,dt + \int_{-1}^{x} \frac{(x-t)^2}{2}\left[(F_z)_{\bar{y},\bar{z}}(F-\hat{F})\right]_{\hat{P},\hat{Q}}\,dt + \int_{-1}^{x} \frac{(x-t)^3}{6}\left\{\left[(DF)_z\right]_{\bar{y},\bar{z}}(F-\hat{F})\right\}_{t,\hat{P},\hat{Q}}\,dt$$

$$\bar{Q}(x) = \hat{Q}(x) + \int_{-1}^{x} (F - \hat{F})_{t,\hat{P},\hat{Q}}\, dt + \int_{-1}^{x} (x-t)\left[(P_z)_{\bar{y},\bar{z}}(F-\hat{F})\right]_{t,\hat{P},\hat{Q}} dt$$

$$+ \int_{-1}^{x} \frac{(x-t)^2}{2}\left\{\left[(DP)_z\right]_{\bar{y},\bar{z}}(F-\hat{F})\right\}_{t,\hat{P},\hat{Q}} dt$$

(vii) Use the Newton iteration process

$$S_1 = S_0 - \left[\bar{y}(1,S_0) - \beta\right] / \bar{P}(1,S_0)$$

to get the new value of z(-1)

(viii) Repeat the process of one iteration for solution and one iteration for correction until the value of s converges to a value $\bar{s}$.

(ix) Start with $z(-1)=\bar{s}$ and repeat the whole procedure but in (iii) and (vi) we iterate using Lie series until it converges to a specified tolerance, that is we apply the normal Newton Raphson shooting process using Lie series as an initial value method.

An explicit expression for the condition under which the process (i ⟶ viii) converges, the rate of convergence and the error $\bar{s}$ - s* is given in the appendix for the case $TLL_{2,2}$. Table (4) shows the practical results.

TABLE 4

Eq.	S_o	No. of iterations Stage (1)	$\bar{S}$	No. of iterations Stage (2)	s*	ε_1	ε_2
(i)	0.7	7x2= 14	0.50011	30	0.5	0.1D-8	0.1D-10
(i)	0.4	6x2=12	0.50011	30	0.5	0.1D-8	0.1D-10
(ii)	0.1D-4	3x2=6	0•1D-12	1	0	0•1D-9	0.1D-16
(iii)	0.5	5x2=10	-0.231801	20	-0.2318162	0.1D-8	0.1D-10
(iv)	0.5	4x2=8	0.274716	20	0.274676	0.1D-8	0.1D-10

ε_1 is a tolerance such that the difference between two successive estimates of $\bar{s}$ is less than ε_1 and ε_2 is a tolerance used in solving the initial value

problems such that the L_∞ norm of two successive vectors of coefficients is less than ε_2 and the same tolerance is used as a stopping criterion when $|y^{(k)}_{(1)} - \beta| < \varepsilon_2$. Here stage (1) means the convergence from s_o to $\bar{s}$ and stage (2) means using shooting method to find s*; the number of iterations mentioned is the total number of iterations used for solving the differential equation and the correction equations.

To assess the effect of the number of terms taken in the series used a small experiment was done using equation (i) only and these results are shown in table (5).

TABLE 5

n	m	s_o	No. of iterations Stage (1)	$\bar{s}$	No.of iterations Stage (2)	s*	ε_1	ε_2
3	3	0.7	7x2=14	0.50011	30 (42)	0.5	0.1D-8	0.1D-10
2	3	0.7	7x2=14	0.50035	30 (42)	0.5	0.1D-8	0.1D-10
1	2	0.7	7x2=14	0.5094	43 (59)	0.5	0.1D-8	0.1D-10

In stage (2) for plane figures we use m=n=3 and for bracketed figures we use m=3, n=2.

(II) A note on Nicolovius method

It seems appropriate here to mention the Nicolovius method which is also based on Lie series and to point out where it differs from that used here. The method here converges when

$$\bar{y}(x) = \hat{y}(x) + \int_{-1}^{x} (x-t)(f-\hat{f})_{\hat{y},\hat{z}}\,dt + \int_{-1}^{x} \frac{(x-t)^2}{2}[f_z(f-\hat{f})]_{\hat{y},\hat{z}}\,dt + \int_{-1}^{x} \frac{(x-t)^3}{6}[(Df)_z(f-\hat{f})]_{\hat{y},\hat{z}}\,dt$$

and $\bar{y}(1) = \beta$ where $\bar{y}$, $\hat{y}$ both have derivative $\bar{s}$ at $x = -1$.

In the Nicolovius method, applied to this problem we will have

$$y^{(k)}(x) = \alpha + (x+1)s + \frac{(x+1)^2}{2} f(-1,\alpha,s) + \frac{(x+1)^3}{6} Df(-1,\alpha,s) + \int_{-1}^{x} \frac{(x-t)^3}{6}[D^2 f]_{y^{(k-1)},z^{(k-1)}}\,dt$$

and solve $y^{(k)}(1) = \beta$, where the integral is a known quantity from the

previous iterate, i.e. we solve for s in the first four terms only while the integral depends on the previous value of s. This method is a direct extension of the Picard method (Clenshaw and Norton (1963)) and one might expect to find the same difficulties which face the Picard method occurring here.

(III) Shooting from both ends

(i) Consider the non-linear boundary value problem (4.4.8) and assume the missing initial and terminal conditions are $z(-1)=s_o$ and $z(1)=ss_o$ and let the solution over the sub-interval $[-1,o]$ be denoted by $(y_1(x), z_1(x))$ and the solution over the sub-interval $[0,1]$ be denoted by $(y_2(x), z_2(x))$

(ii) As in I(ii) we start with $\hat{y}_1$, as a Taylor series of order 3 and $\hat{z}_1 = \hat{y}_1'$

(iii) Iterate <u>once</u> on $\hat{y}_1$ and $\hat{z}_1$ using Lie series iterative process $G_{3,N}$ to get $\bar{y}_1$ and $\bar{z}_1$ as in I(iii) and store the values $\bar{y}_1(o)$ and $\bar{z}_1(o)$

(iv) Substitute $\bar{y}_1(x)$ and $\bar{z}_1(x)$ into the correction equation as in I(iv) with P_1 and Q_1 replacing P and Q.

(v) For the correction equation we start with $\hat{P}_1$ taken as a Taylor series of order 3 and $\hat{Q}_1 = \hat{P}_1'$ as in I(v)

(vi) Iterate <u>once</u> on $\hat{P}_1$ and $\hat{Q}_1$ using the same Lie series iterative process $G_{3,N}$ to get $\bar{P}_1$ and $\bar{Q}_1$ as in I(vi) and store $\bar{P}_1(o), \bar{Q}_1(o)$

(vii) Repeat (iii), (iv), (v) and (vi) using y_2, z_2, p_2, q_2, ss_o instead of y, z, P_1, Q_1, s_o and the initial conditions are taken at 1 instead of -1 and finally store the values $\bar{y}_2(o), \bar{z}_2(o), \bar{P}_2(o), \bar{Q}_2(o)$

(viii) Use the Newton Raphson correction

$$\begin{bmatrix} S_1 \\ SS_1 \end{bmatrix} = \begin{bmatrix} S_o \\ SS_o \end{bmatrix} - \begin{bmatrix} \bar{P}_1(o) & -\bar{P}_2(o) \\ \bar{Q}_1(o) & -\bar{Q}_2(o) \end{bmatrix}^{-1} \begin{bmatrix} \bar{y}_1(o) - \bar{y}_2(o) \\ \bar{z}_1(o) - \bar{z}_2(o) \end{bmatrix}$$

(ix) Repeat until s and ss converge to $\bar{s}, \bar{ss}$, then using these as a starting values for ordinary shooting from both ends with iterating to convergence in (iii) and (vi).

The practical results are shown in Table 6.

TABLE 6

$TLL_{m,n}$ (both ends)

Eq.	s_o	ss_o	No. of iterations stage (1)	$\bar{s}$	$\overline{ss}$	No. of iterations stage (2)	s^*	ss^*	ε_1	ε_2
(i)	0.6	0.8	22 × 4 = 88	0.2499948	0.5152555	44	0.25	0.515225	0.1D-8	0.1D-10
(i)	0.4	0.6	6 × 4 = 24	0.2499948	0.5152555	44	0.25	0.515225	0.1D-8	0.1D-10
(ii)	0.1D-2	0.1D-2	4 × 4 = 16	0.1D-11	0.1D-11	2	0	0	0.1D-9	0.1D-15
(iii)	0.4	0	4 × 4 = 16	-0.115909	0.1159094	26	-0.115908	0.115908	0.1D-8	0.1D-10
(iv)	0.4	0	4 × 4 = 16	0.137336	-0.137336	26	0.137338	-0.137338	0.1D-8	0.1D-10
(v)	-3	-1	7 × 4 = 28	-2.013	-0.24026	75	-2	-0.25	0.1D-8	0.1D-10

The tolerance ε_1 is used as in Table 4 while ε_2 is a tolerance used in solving the initial value problems as in Table 4 and also used as a stopping criterion when $|y_1(0) - y_2(0)| < \varepsilon_2$ and $|z_1(0) - z_2(0)| < \varepsilon_2$.

A similar experiment to that reported in Table (5) was done for the same equation using this method and results are shown in Table (7).

4.4.3 $TPL_{m,n}$ method

For the same number of derivatives of y evaluated at both ends one can get a polynomial with order twice the order of Taylor series by using two-point series. This is suggested by Olsøn (1977) who uses two-point series in conjunction with quasilinearization and the adjoint method. For this reason we are going to apply two-point series as a replacement of Taylor series in III and discuss the practical results. In practice we used this method for m=7, n=3.

(i) As in III(i)

(ii) Generate the two-point series of order 7 as explained earlier

$$\hat{y}(x) = A_0 + A_1(x+1) + A_2(x+1)(x-1) + \cdots + A_7(x+1)^4(x-1)^3$$

$\hat{z}(x) = \hat{y}'(x)$, $\hat{y}_1(x)$ takes the values of y when $x \in [-1,0]$,

$\hat{y}_2(x)$ takes the values of y(x) for $x \in [0,1]$

and $\hat{z}_1(x) = \hat{y}_1'(x)$, $\hat{z}_2(x) = \hat{y}_2'(x)$

The steps (iii) ⟶ (ix) are exactly as in III. Table 8 shows the practical results.

A similar experiment to that reported in table (7) is done for the same example using this method and results are shown in table (9).

4.5. Comparisons between the different methods

4.5.1. Series methods and straight shooting

Corresponding to table (4) we solved the same examples under the same conditions using straight shooting, that is allowing the iterative process $G_{3,N}$ to converge in the steps (iii) and (vi). The practical results are given in table (10).

TABLE 7

$TLL_{m,n}$ (both ends)

m	n	s_o	ss_o	No. of iterations stage (1)	$\bar{s}$	$\overline{ss}$	No. of iterations stage (2)	s^*	ss^*	ε_1	ε_2
3	3	0.6	0.8	22 × 4 = 88	0.2499948	0.515255	44 (64)	0.25	0.51522	0.1D-8	0.1D-10
3	2	0.6	0.8	8 × 4 = 32	0.25007	0.51495	44 (64)	0.25	0.51522	0.1D-8	0.1D-10
2	1	0.6	0.8	8 × 4 = 32	0.25405	0.50236	62 (90)	0.25	0.51522	0.1D-8	0.1D-10

In stage (2) column the plain figures for the case m = n = 3, and the bracketed figures for m = 3, n = 2.

TABLE 8

$TPL_{m,n}$

Eq.	s_o	ss_o	No. of iterations stage (1)	$\bar{s}$	$\overline{ss}$	No. of iterations stage (2)	s^*	ss^*	ε_1	ε_2
(i)	0.6	0.8	12 × 4 = 48	0.24999999	0.5152254	22	0.25	0.51522539	0.1D-8	0.1D-10
(i)	0.4	0.6	7 × 4 = 28	0.24999999	0.5152254	22	0.25	0.51522539	0.1D-8	0.1D-10
(iii)	0.4	0	4 × 4 = 16	-0.11590816	0.11590816	20	-0.115908147	0.115908147	0.1D-8	0.1D-10
(iv)	0.4	0	5 × 4 = 20	0.1373381	-0.1373381	20	0.1373381	-0.1373381	0.1D-8	0.1D-10
(v)	-3	-1	7 × 4 = 28	-2.00054	-0.249978	50	-2	-0.25	0.1D-8	0.1D-10

The tolerances ε_1 and ε_2 again have the same significance as in Table 6.

TABLE 9

$TPL_{m,n}$

m	n	s_o	ss_o	No. of iterations stage (1)	$\bar{s}$	$\overline{ss}$	No. of iterations stage (2)	s^*	ss^*	ε_1	ε_2
7	3	0.6	0.8	12 × 4 = 48	0.25	0.51522539	22 (24)	0.25	0.5152253	0.1D-8	0.1D-10
7	2	0.6	0.8	12 × 4 = 48	0.25	0.51522539	22 (24)	0.25	0.5152253	0.1D-8	0.1D-10
5	1	0.6	0.8	19 × 4 = 76	0.24999923	0.51522582	23 (26)	0.25	0.5152253	0.1D-8	0.1D-10

In stage (2) column plain figures for the case m = 7, n = 3, and bracketed figures for m = 7, n = 2.

TABLE 10

Eq.	S_o	No. of iterations	s*	Tol.6
(i)	0.7	Blows up	0.5	0.1D-10
(i)	0.4	65	0.5	0.1D-10
(ii)	0.1D-4	Blows up	0	0.1D-10
(iii)	0.5	40	-0.2318162	0.1D-10
(iv)	0.5	29	0.2746763	0.1D-10

Comparing tables (4) and (10) we notice that

(1) For equation (i) with s_o=0.7 and equation (ii) with s_o=0.1D-4 straight shooting fails to start while the series method $TLL_{3,3}$ converged.

(2) When both methods converge to the solution, method $TLL_{3,3}$ converges faster and uses a smaller total number of iterations as the following table shows:

TABLE 11

Eq.	$TLL_{3,3}$	Shooting
(i)	42	65
(iii)	30	40
(iv)	28	29

Similarly corresponding to table6 we solved the same examples under the same conditions using shooting from both ends, that is allowing the iterative process $G_{3,N}$ to converge in the steps (iii) and (iv).
The practical results are given in table (12).
Comparing tables (6) and (12) we can find that the above two advantages are valid here also.

(1) For equation (i) with s_o=0.6, ss_o=0.8 and equation (ii) with $s_o = ss_o$ = 0.1D-2, straight shooting fails to start while $TLL_{3,3}$ converged.

TABLE 12

Eq.	s_o	ss_o	No. of iterations	s^*	ss^*	ε
(i)	0.6	0.8	Blows up	0.25	0.515225	0.1D-10
(i)	0.4	0.6	106	0.25	0.515225	0.1D-10
(ii)	0.1D-2	0.1D-2	Blows up	0	0	0.1D-10
(iii)	0.4	0	70	-0.115908	0.115908	0.1D-10
(iv)	0.4	0	56	0.137338	-0.137338	0.1D-10
(v)	-3	-1	118	-2	-0.25	0.1D-10

(2) When both methods converge to the same solution, $TLL_{3,3}$ converges faster. The following table shows the total number of iterations for the two methods.

TABLE 13

Eq	$TLL_{3,3}$	Shooting
(i)	68	106
(iii)	42	70
(iv)	42	56
(v)	103	118

Corresponding to table (8), the same examples are solved using y as a two-point series and straight shooting; the practical results are given in table (14).

A similar comparison between (14) and (8) shows that

(1) For equation (i) with $s_o = 0.6$, $ss_o = 0.8$ straight shooting failed to start while $TPL_{7,3}$ converged

(2) $TPL_{7,3}$ is again faster than straight shooting as shown in the following table of total number of iterations

TABLE 15

EQ	$TPL_{7,3}$	Shooting
(i)	50	105
(iii)	36	66
(iv)	40	52
(v)	78	114

In all the above comparisons the number of iterations can be used as a measure for comparing the effort involved since we use the same iterative process each time. Also looking at Tables (13) and (15) we note that $TPL_{7,3}$ has an edge over $TLL_{3,3}$.

To compare the rate of convergence from s_o to $\bar{s}$ and from $\bar{s}$ to s* using $TLL_{3,3}$, with the rate of convergence from s_o to s* using straight

TABLE 14

Eq.	s_o	ss_o	No. of iterations	s^*	ss^*	ε
(i)	0.6	0.8	Blows up	0.25	0.515225	0.1D-10
(i)	0.4	0.6	105	0.25	0.515225	0.1D-10
(iii)	0.4	0	66	-0.115908	0.115908	0.1D-10
(iv)	0.4	0	52	0.137338	-0.137338	0.1D-10
(v)	-3	-1	114	-2	-0.25	0.1D-10

shooting we used example (i) with $s_o=0.4$ and plotted $|s-s^*|$ against r, the number of applications of Newton correction. This is shown in graph (7) where the dotted line refers to stage (1) from s_o to $\bar{s}$ and the solid line to stage (2), and also to straight shooting. The graph shows that stage (1) and straight shooting have approximately the same rate of convergence up to $\bar{s}$ as would be expected from the analysis, and hence of course there is considerable saving in using the series process. When s has reached $\bar{s}$, there is no further gain in continuing to use stage (1) and shooting will be necessary.

A similar graph showing the relation between $\|y^{(k)} - y^*\|$ and r is also plotted for the same example and again agrees with the above statement.

4.5.2 Computational effort

In the previous section the relative advantage of this class of methods over straight shooting has been demonstrated. In this section we analyse the computational effort involved in the same way as was done in 2.3.4 , by counting the total number of function evaluations. A comparison can then be made of the efficiency of using different types and orders of $\hat{y}$ and different numbers of terms in Lie series. This has been done for straight shooting, which is of course a very similar investigation to that carried out in 2.3.4, and the results are also found to be similar. A more interesting comparison is between different distributions of computational effort between the two stages in the series method, and also between the total effort involved in the series method and in straight shooting under comparable conditions.

4.5.3. Number of function evaluations in different methods

The effort depends on

N the highest term used in Chebyshev series

r_1 the total number of iterations used in applying Lie series to differential equation

K the number of times missing initial conditions are corrected

r_2 the total number of iterations used in applying Lie series to the correction.

$J = K + 1$ when shooting from one end and $J = K + 2$ when shooting from both ends. Table 16 shows the effort in each stage in terms of these quantities allowing for the overlap where functions needed in the correction equation have already been calculated in applying Lie series to the differential equation.

4.5.4. Computational effort, straight shooting

Equation (i) is solved under various conditions and the effort involved can be calculated from table 16 . The values obtained are shown in tables 17, 18, 19.

The results from the three tables confirm for this example the general conclusion reached in 2.3.4, that $G_{2,N}$ is more efficient than $G_{3,N}$ for initial value problems. They also suggest that, again for this example $(G_{2,N}, G_{2,N})$ is better than $(G_{2,N}, G_{1,N})$, that is there is an advantage in calculating the additional function required for $G_{2,N}$ in the correction equation rather than using simply $G_{1,N}$ there. Comparisons between tables 18,19 suggest that with the same initial values calculating $\hat{y}$ as a two-point series is more efficient than using Taylor series and shooting from both ends, as would be expected.

TABLE 16

Method	$\hat{y}$	Effort for solution	$\hat{p}$	Effort for correction
$G_{3,N}$; $G_{3,N}$	TL_3	$9r_1(N+1) + J$	TL_3	$3r_2(N+1) + 2K$
	TP_7	$9r_1(N+1) + 2J$		
$G_{3,N}$; $G_{2,N}$	TL_3	$9r_1(N+1) + J$	TL_3	$3r_2(N+1) + 2K$
	TP_7	$9r_1(N+1) + 2J$		
$G_{2,N}$; $G_{2,N}$	TL_3	$5r_1(N+1) + 2J$	TL_3	$(3r_2 + K)(N+1) + 5K$
	TP_7	$5r_1(N+1) + 4J$		
$G_{2,N}$; $G_{1,N}$	TL_3	$5r_1(N+1) + 2J$	TL_3	$(3r_2 + K)(N+1) + 5K$
	TP_7	$5r_1(N+1) + 4J$	TL_2	$(3r_2 + K)(N+1)$
	TP_5	$5r_1(N+1)$		
$G_{1,N}$; $G_{1,N}$	TL_2	$4r_1(N+1)$	TL_2	$(3r_2 + 2K)(N+1)$
	TP_5	$4r_1(N+1)$		

TABLE 17

TLL (one end)

Method	s_o	$\hat{y}$	r_1	J	$\hat{p}$	r_2	k	Total effort
$G_{3.45}$; $G_{3.45}$	0.4	TL_3	35	6	TL_3	30	5	18646
$G_{3.45}$; $G_{2.45}$	0.4	TL_3	35	6	TL_3	43	5	20440
$G_{2.45}$; $G_{2.45}$	0.4	TL_3	47	6	TL_3	43	5	17006
$G_{2.45}$; $G_{1.45}$	0.4	TL_3	47	6	TL_3	83	5	22506

TABLE 18

TLL (both ends)

Method	s_o	ss_o	$\hat{y}$	r_1	J	$\hat{p}$	r_2	K	Total effort
$G_{3,45}$; $G_{3,45}$	0.4	0.6	TL_3	54	12	TL_3	52	10	29564
$G_{3,45}$; $G_{2,45}$	0.4	0.6	TL_3	54	12	TL_3	72	10	32324
$G_{2,45}$; $G_{2,45}$	0.4	0.6	TL_3	77	12	TL_3	72	10	28180
$G_{2,45}$; $G_{1,45}$	0.4	0.6	TL_3	77	12	TL_2	135	10	36824

TABLE 19

TPL (both ends)

Method	s_o	ss_o	$\hat{y}$	r_1	J	$\hat{p}$	r_2	K	Total effort
$G_{3,45}$; $G_{3,45}$	0.4	0.6	TP_7	53	12	TL_3	52	10	29162
$G_{3,45}$; $G_{2,45}$	0.4	0.6	TP_7	53	12	TL_3	62	10	30542
$G_{2,45}$; $G_{2,45}$	0.4	0.6	TP_7	61	12	TL_3	62	10	23144
$G_{2,45}$; $G_{1,45}$	0.4	0.6	TP_7	61	12	TL_2	95	10	27648

4.5.5. Computational effort, series method

In a similar way we can use the results reported in tables 5 , 7 , (9) to calculate the effort involved in solving equation (i) by series method under various conditions. The efforts in stages (1) and (2) are shown separately in tables 20, 21 , 22 .

These results can be combined to give the total effort involved in solving equation (i) under all the conditions considered, the final comparison of effort is shown in table 23 .

Note In stage (1) an unnecessary number of iterations were added due to requiring a tolerance 0.1D-8 for the accuracy of $\bar{s}$ while $\bar{s}$ is accurate to 3 decimals only in some cases. This waste of effort could be avoided by relating the tolerance with the predicted order of $\bar{s}$.

Comments

(i) From table 23 the minimum effort occurswhen m=3, n=2 in stage (1) and using $(G_{2,N}, G_{2,N})$ in stage (2) in TLL case and when m=7, n=2 and using $(G_{2,N}, G_{2,N})$ in stage (2) in TPL case; TPL shows a slight advantage when compared with TLL (both ends).

(ii) Comparing tables 17 , 18 , 19 with 23 we notice that we used worse starting value for s_o, ss_o in table 23 and still the effort was less than that of straight shooting which was shown in 17 - 19.

4.6 The series approach as a new continuation method

In the method $TLL_{m,n}$ we start by assuming the missing initial condition $z(-1) = s_o$, expressing $\hat{y}(x,s_o)$ as a series of order m and applying one iteration on $\hat{y}$ using (n + 1)-term Lie series to get $\bar{y}$ which is a series of order q = m + n

i.e. $y - \bar{y} = O(x + 1)^{m+n+1}$ (as discussed in chapter I)

TABLE 20

TLL (one end)

m	n	Stage (1)		Effort	Stage (2)									
					$G_{3,N}$					$G_{2,N}$				
		r_1	r_2		r_1	J	r_2	K	Effort	r_1	J	r_2	K	Effort
3	3	7	7	3885	18	3	12	2	9115	24	3	18	2	8112
3	2	7	7	2947	18	3	12	2	9115	24	3	18	2	8112
2	1	7	7	2898	24	4	19	3	12568	32	4	27	3	11247

TABLE 21

TLL (both ends)

m	n	Stage (1)		Effort	Stage (2)									
					$G_{3,N}$					$G_{2,N}$				
		r_1	r_2		r_1	J	r_2	K	Effort	r_1	J	r_2	K	Effort
3	3	44	44	24420	24	6	20	4	12710	36	6	28	4	12360
3	2	16	16	6736	24	6	20	4	12710	36	6	28	4	12360
2	1	16	16	6624	32	8	30	6	17408	48	8	42	6	17158

TABLE 22

TPL (both ends)

m	n	Stage 1		Effort	Stage 2									
					G_{31N}					G_{21N}				
		r_1	r_2		r_1	J	r_2	K	Effort	r_1	J	r_2	K	Effort
7	3	26	26	14456	12	4	10	2	6360	12	4	12	2	4534
7	2	26	26	10998	12	4	10	2	6360	12	4	12	2	4534
5	1	38	38	15732	13	4	10	2	6774	14	4	12	2	4994

TABLE 23

m	n	TLL (one end)		TLL (both ends)		m	n	TPL	
		A	B	A	B			A	B
3	3	13000	11997	37130	36780	7	3	20816	18990
3	2	12062	11059	19446	19096	7	2	17358	15532
2	1	15466	14145	24032	23782	5	1	22506	20726

Then we do the same for the correction equation by applying a Lie series of the same order starting with $\hat{p}$ to find $\bar{p}$ of order q, and then using Newton Raphson correction to find s_1, the new value of the missing initial condition. The process is then repeated starting with $\hat{y}(x,s_1)$ and continued until it converges to $\bar{s}$, where

$$|s^* - \bar{s}| = O(x_N - x_0)^q = O(2^q) \qquad \text{for the range } [-1,1]$$

$\bar{s}$ is then a better start for applying the shooting method than s_o. But if the problem is too sensitive then $\bar{s}$ may not be close enough to s* to enable the shooting method to be applied. In this case we have to increase the accuracy of $\bar{s}$. For this we suggest the following continuation procedure.

(i) Start by assuming $z(-1)=s_o$ and use stage (1), one iteration for solution and one iteration for correction as explained in (4.4), converging to $\bar{s}^{(1)}$.

(ii) Use $\bar{s}^{(1)}$ as a starting value for z(-1) and apply the same method with two iterations for solution and two iterations for correction until it converges to $\bar{s}^{(2)}$

(iii) Repeating the process we get the sequence $\bar{s}^{(k)}$, k = 1, 2, ... whose limit is the exact solution s^*.

Notes

(1) We may stop at any stage and apply the shooting method when $\bar{s}^{(k)}$ is a good enough approximation to s^*

(2) From the theory of Lie series, if $\bar{y}^{(k)}(x,\bar{s}^{(k)})$ is k^{th} approximation to $y(x,s^*)$ then

$$y(x,s^*) - \bar{y}^{(k)}(x,\bar{s}^{(k)}) = y(x,s^*) - \bar{y}^{(k)}(x,s^*) + \bar{y}^{(k)}(x,s^*) - \bar{y}^{(k)}(x,\bar{s}^{(k)})$$

$$= O(x+1)^{m+(n+1)k} + (s^* - \bar{s}^{(k)})(O(x+1))$$

put x = 1, then $|s^* - \bar{s}^{(k)}| = O(2)^{m-1+(n+1)k}$

The above method has been applied to example (i) and the results are shown in table 24 and plotted in graph (9).

TABLE 24.

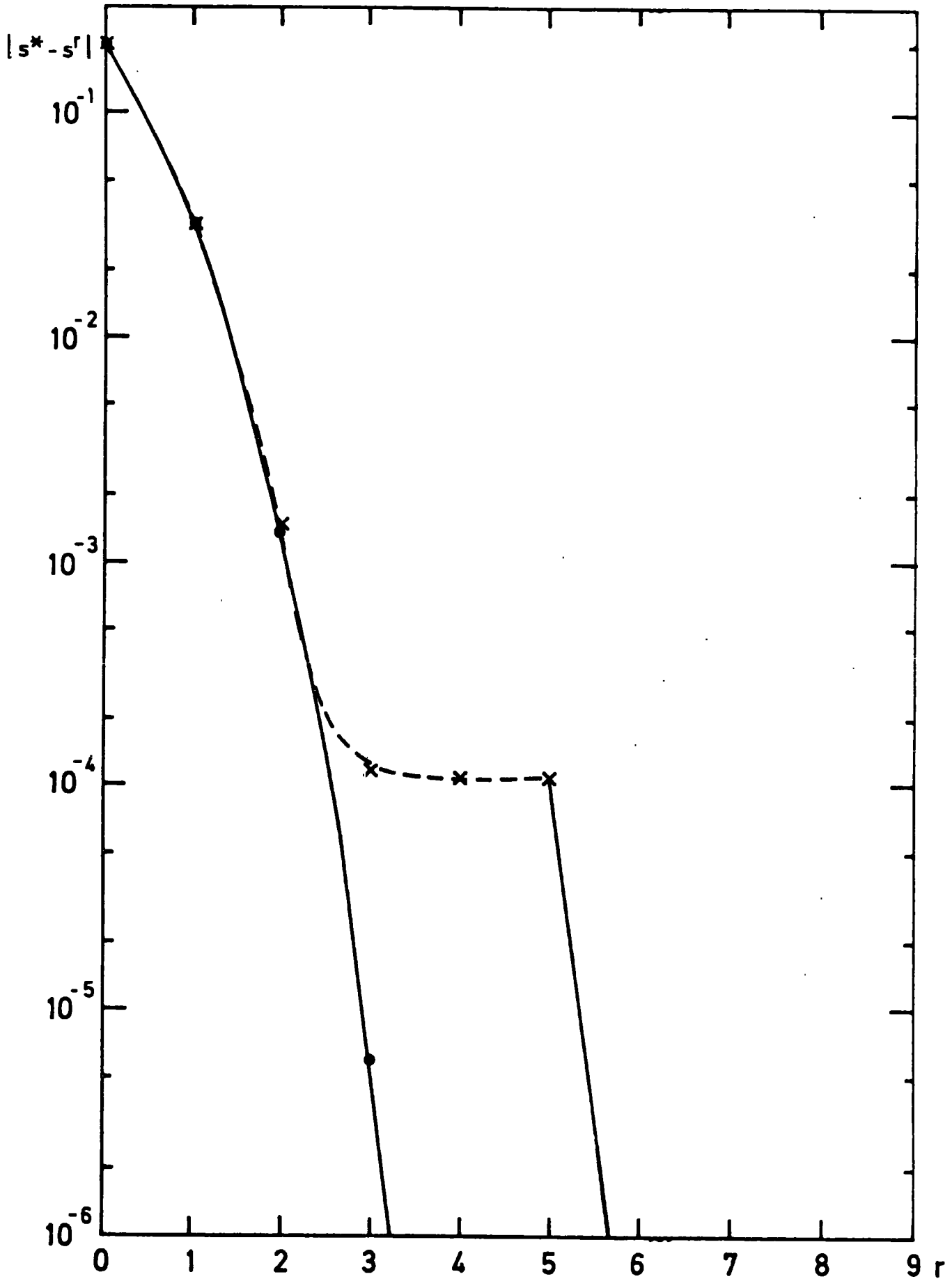
Stage No. k	Starting value $\underset{s}{-}^{(k-1)}$	No. of Iterations	Final value $\underset{s}{-}^{(k)}$
1	0.4	4 x 2 = 8	0.50011
2	0.50011	2 x 4 = 8	0.5000017
3	0.5000017	2 x 6 = 12	0.50000001
Shooting	0.50000001	18	0.5

The tolerance used here was 0.1D-10 as a stopping criterion. The example is a very sensitive case.

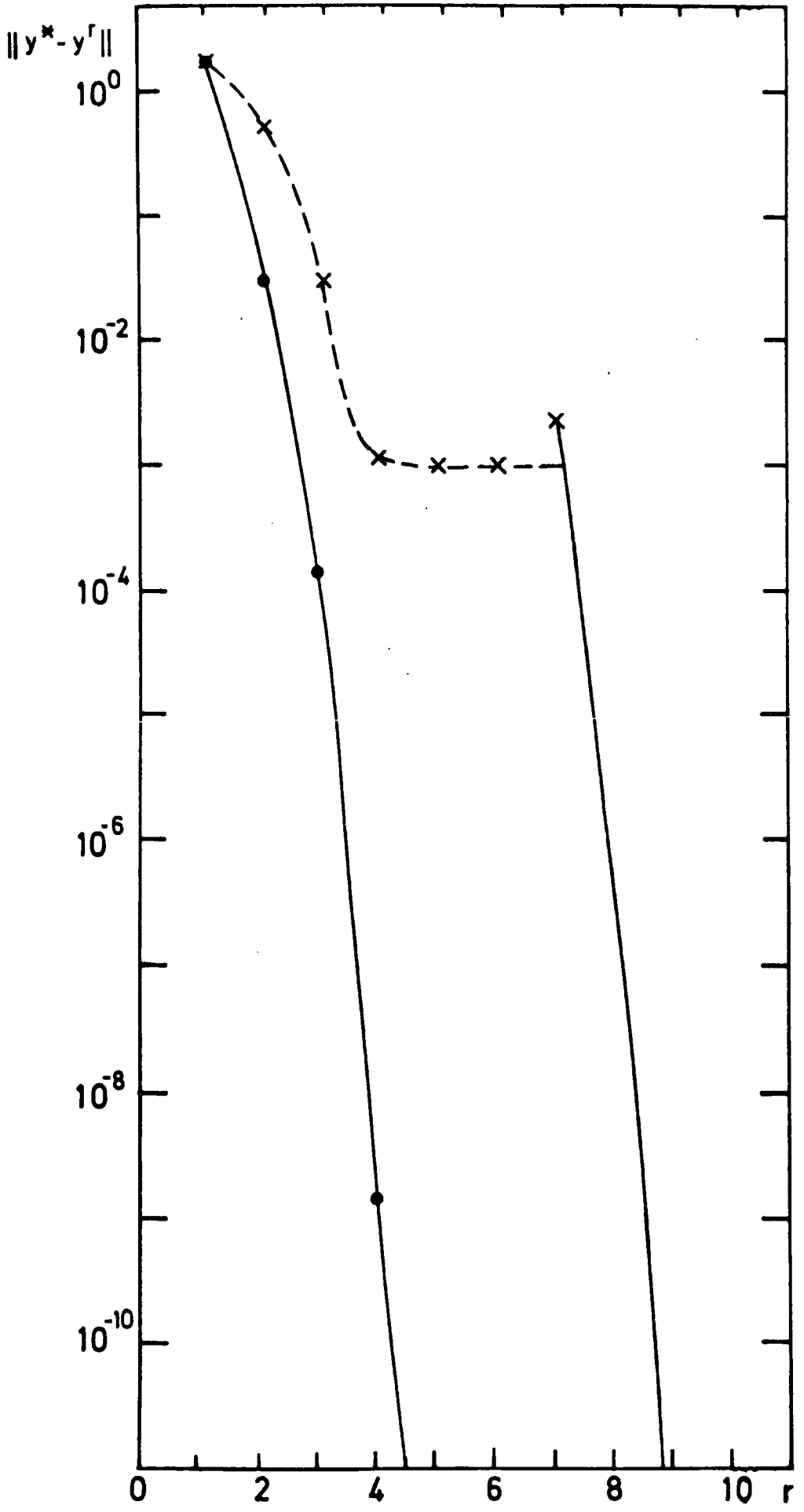
For future work a study of the most economical way of using this continuation technique could be carried out using practical results and relative convergence rates.

Conclusion

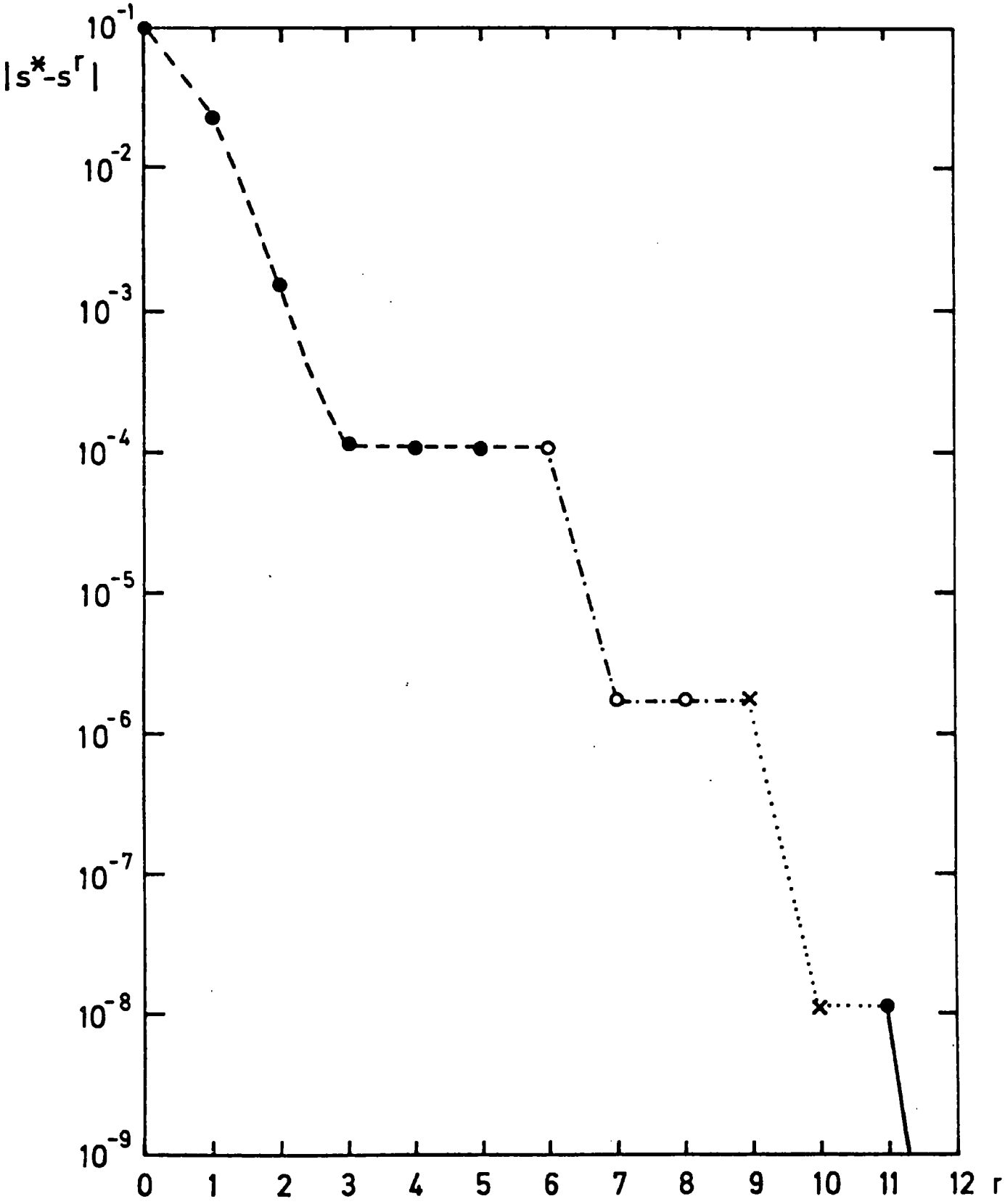
Using series of fixed order we obtain starting values in non-linear boundary value problems for use in normal (Newton) shooting methods. This approach can work when Newton shooting fails, and is more efficient; it is dependent on the interval length.



Graph (7)



Graph (8)



Graph (9)

Appendix A

Order of Accuracy of s_m-Linear Case

In this appendix we find explicit expressions for $s_m - s^*$ using various types of polynomials of order m applied to the linear two-point boundary value problem

$$\left.\begin{aligned} y' &= z \\ z' &= \phi(x) + \psi(x)\, y + \chi(x)\, z \\ y(0) &= \alpha \quad , \quad y(h) = \beta \end{aligned}\right\} \qquad \cdots\cdots\cdots\cdots (1)$$

The exact solution of this, expanded in powers of h, corresponds to $z(0) = s^*$ where

$$s^* = \frac{\beta-\alpha}{h} - \frac{\beta-\alpha}{2}\chi_0 + h\left\{\frac{\beta-\alpha}{12}\chi_0^2 - \frac{\beta-\alpha}{6}\chi_0' - \frac{\beta\psi_0+\phi_0}{6} - \frac{\alpha\psi_0+\phi_0}{3}\right\}$$

$$+ h^2\left\{-\frac{(\beta-\alpha)}{24}\chi_0'' + \frac{(\beta-\alpha)}{24}\chi_0\chi_0' - \frac{\beta}{12}(\psi_0' - \psi_0\chi_0) - \frac{\alpha}{12}\psi_0' + \frac{1}{12}\phi_0\chi_0 - \frac{\phi_0'}{6}\right\}$$

$$+ h^3\left\{-\frac{(\beta-\alpha)}{720}\left(6\chi_0''' - 6\chi_0\chi_0'' - 6\chi_0^2\chi_0' - 2\chi_0'^2 + \chi_0^4 + 18\psi_0'' - 30\psi_0'\chi_0\right.\right.$$

$$\left.\left. - 16\psi_0\chi_0' - 14\psi_0^2 + 8\psi_0\chi_0^2\right) + \left(\frac{\alpha\psi_0+\phi_0}{24}\right)\psi_0 + \left(\frac{\alpha\psi_0'+\phi_0'}{24}\right)\chi_0 - \left(\frac{\alpha\psi_0''+\phi_0''}{24}\right)\right\} + \cdots\cdots$$

(i) Using the cubic two-point series TP_3

Assume $z(0) = s_0$, $z(h) = s_1$ and form the cubic two-point series

$$\hat{y} = A_0 + A_1 x + A_2 x(x-h) + A_3 x^2(x-h) \qquad \cdots\cdots\cdots (2)$$

$$\left.\begin{aligned} A_0 &= \alpha \\ A_1 &= \frac{1}{h}(\beta-\alpha) \\ A_2 &= \frac{1}{h^2}(\beta-\alpha-hs_0) \\ A_3 &= \frac{1}{h^3}[h(s_0+s_1) - 2\beta + 2\alpha] \end{aligned}\right\} \qquad \cdots\cdots\cdots\cdots\cdots (3)$$

Find s_0 and s_1 such that

$$y''(0) = P(0, \alpha, s_0) \quad , \quad y''(h) = P(h, \beta, s_1) \qquad \cdots\cdots\cdots (4)$$

i.e. $$s_0\left(\frac{4}{h} + \chi_0\right) + s_1\left(\frac{2}{h}\right) + \alpha\left(\frac{6}{h^2} + \psi_0\right) - \beta\left(\frac{6}{h^2}\right) + \phi_0 = 0 \qquad \cdots (5)$$

$$s_0\left(\frac{2}{h}\right) + s_1\left(\frac{4}{h} - \chi_h\right) + \alpha\left(\frac{6}{h^2}\right) - \beta\left(\frac{6}{h^2} + \psi_h\right) - \phi_h = 0 \qquad \cdots (6)$$

where $\phi_h = \phi(h)$ and $\phi_0 = \phi(0)$ and similarly for ψ and χ.

The solution (s_0, s_1) is obtainable as long as

$$\frac{12}{h^2} - \frac{4}{h}(\chi_h - \chi_0) - \chi_0\chi_h \neq 0$$

i.e. $$12 - 4h(\chi_h - \chi_0) - h^2\chi_0\chi_h \neq 0$$

So expansion provides a limiting length via

$$12 - 4h(h\chi_0' + \cdots) - h^2\chi_0^2 \geq 0$$

i.e. $$h \leq \sqrt{\frac{12}{4\chi_0' + \chi_0^2}}$$

Solving for s_0 we get

$$s_0 = \frac{\beta-\alpha}{h} - \frac{\beta-\alpha}{2}\chi_0 - h\left\{\frac{(\beta-\alpha)}{6}\chi_0' - \frac{(\beta-\alpha)}{12}\chi_0^2 + \frac{\alpha\psi_0 + \phi_0}{3} + \frac{\beta\psi_0 + \phi_0}{6}\right\}$$

$$- h^2\left\{\frac{(\beta-\alpha)}{12}\chi_0'' + \frac{(\beta-\alpha)}{12}\chi_0\chi_0' + \frac{\beta\psi_0' + \phi_0'}{6} + \frac{(\beta-\alpha)}{24}\chi_0^3 - \frac{\chi_0}{12}(\alpha\psi_0 + \phi_0)\right\}$$

$$+ \cdots\cdots$$

and

$$s^* - s_0 = \left(\frac{\beta-\alpha}{24}\right)h^2\left\{\chi_0'' + 3\chi_0\chi_0' + 2\psi_0' + 2\psi_0\chi_0 + \chi_0^3\right\} + \cdots$$

Since $\beta - \alpha = O(h)$, this gives $s^* - s_0 = O(h^3)$ in accordance with the general result obtained in 4.3.3.

(ii) Using Taylor series of order 3

$$\hat{y}(x,s) = \alpha + xs + \frac{x^2}{2}(\phi_0 + \psi_0\alpha + \chi_0 s) + \frac{x^3}{6} DP(0,\alpha,s)$$

if $s^{(3)}$ is such that $\hat{y}(h, s^{(3)}) = \beta$, then

$$s^{(3)} = \left(\frac{\beta-\alpha}{h}\right) - \left(\frac{\beta-\alpha}{2}\right)\chi_0 + h\left\{\left(\frac{\beta-\alpha}{12}\right)(\chi_0^2 - 2\chi_0' - 2\psi_0) - \frac{\alpha\psi_0 + \phi_0}{2}\right\}$$

$$+ h^2\left\{\left(\frac{\beta-\alpha}{24}\right)(\chi_0^3 + 4\chi_0\chi_0' + 4\chi_0\psi_0) + \frac{\chi_0}{4}(\alpha\psi_0 + \phi_0)\right.$$

$$\left. - \frac{1}{6}\left[(\alpha\psi_0' + \phi_0') + \chi_0(\alpha\psi_0 + \phi_0)\right]\right\} + \ldots\ldots$$

and

$$s^* - s^{(3)} = -h^2\left(\frac{\beta-\alpha}{24}\right)(\chi_0'' + 3\chi_0\chi_0' + 2\psi_0' + 2\psi_0\chi_0 + \chi_0^3) + \ldots\ldots$$

i.e. the same error as with TP_3 but with the opposite sign.

(iii) $TLL_{2,2}$

With $\hat{y}$, a Taylor series of order 2, used in 3 terms of Lie series, the order of $\bar{y}$ is 4, and if $s^{(4)}$ is such that

$$\bar{y}(h, s^{(4)}) = \beta$$

then

$$s^* - s^{(4)} = -\frac{\beta-\alpha}{720}\left\{12\psi_0\chi_0' + 12\psi_0\chi_0^2 + 6\chi_0'^2 + 10\chi_0'\chi_0^2 + 6\psi_0^2 + 11\chi_0^4\right\} h^3 + \ldots$$

which is of order h^4.

Appendix B

Explicit Conditions for Convergence to s_m

Consider the non-linear boundary value problem

$$\left.\begin{aligned} y' &= z \\ z' &= f(x,y,z) \\ y(0) &= \alpha\,, \quad y(1) = \beta \end{aligned}\right\} \qquad \ldots\ldots \quad (1)$$

(i) TL_3

Assume $z(0) = s_0$

then $\hat{y}(x,s_0) = \alpha + x s_0 + \frac{x^2}{2} f(0,\alpha,s_0) + \frac{x^3}{6}\left(f_x + f_y s_0 + f_z f_0\right)_{0,\alpha,s_0}$

$$\hat{y}(1,s_0) = \alpha + s_0 + \frac{1}{2} f(0,\alpha,s_0) + \frac{1}{6}\left(f_x + f_y s_0 + f_z f_0\right)_{0,\alpha,s_0}$$

For the correction equation

$$\hat{p}(x,s_0) = x + \frac{x^2}{2} f_z(0,\alpha,s_0) + \frac{x^3}{6}\left(f_{xz} + f_{yz} z + f_{zz} f + f_y + f_z^2\right)_{0,\alpha,s_0}$$

$$\hat{p}(1,s_0) = 1 + \frac{1}{2} f_z(0,\alpha,s_0) + \frac{1}{6}\left(f_{xz} + f_{yz} z + f_{zz} f + f_y + f_z^2\right)_{0,\alpha,s_0}$$

The iterative process used is

$$s_1 = s_0 - \frac{1}{\hat{p}(1,s_0)}\left[\hat{y}(1,s_0) - \beta\right] = G(s_0)$$

and so since

$$\frac{d\hat{y}(1,s_0)}{ds_0} = \hat{p}(1,s_0)$$

$$G'(s_0) = \frac{1}{\left[\hat{p}(1,s_0)\right]^2}\left\{\frac{1}{2} f_{zz} + \frac{1}{6}\left(f_{xzz} + f_{yzz} s_0 + f_{yz} + f_{zzz} f + 3 f_z f_{zz} + f_{yz}\right)\right\}\left(\hat{y}(1,s_0) - \beta\right)$$

For convergence $|G'(s_0)| < 1$, *in some neighbourhood of* s^*

$$\left|\left(\hat{y}(1,s_0) - \beta\right) \times \frac{1}{\left[\hat{p}(1,s_0)\right]^2}\left(\frac{1}{2} f_{zz} + \frac{1}{6}\left(f_{xzz} + f_{yzz} s_0 + 2 f_{yz} + f_{zzz} f + 3 f_z f_{zz}\right)\right)\right| < 1$$

and the rate of convergence will depend on $|G'(s_0)|$.

(ii) $\underline{TLL_{2,2}}$

For the same non-linear boundary value problem, let

$$\hat{y}(x,s_0) = \alpha + xs_0 + \frac{x^2}{2} f(0,\alpha,s_0)$$

$$\hat{z}(x,s_0) = s_0 + x f(0,\alpha,s_0)$$

then $$\bar{y}(x,s_0) = \alpha + xs_0 + \frac{x^2}{2} f(0,\alpha,s_0) + \int_0^x \frac{(x-t)^2}{2} (f_x + f_y z + f_z f)_{t,\hat{y},\hat{z}} \, dt$$

For the correction equation

$$\hat{p}(x,s_0) = x + \frac{x^2}{2} f_z(0,\alpha,s_0)$$

$$\hat{Q}(x,s_0) = 1 + x f_z(0,\alpha,s_0)$$

$$\bar{p}(x,s_0) = x + \frac{x^2}{2} f_z(0,\alpha,s_0) + \int_0^x \frac{(x-t)^2}{2} [(f_{xy} + f_{yy} z + f_{yz} f)\hat{p}$$

$$+ (f_{xz} + f_{yz} z + f_{zz} f)\hat{Q} + f_y \hat{Q} + f_z (f_y \hat{p} + f_z \hat{Q})]_{t,\bar{y},\bar{z}} \, dt$$

$$s_1 = s_0 - \frac{1}{\bar{p}(1,s_0)} [\bar{y}(1,s_0) - \beta] = G(s_0)$$

and so since $$\frac{d\bar{y}(1,s_0)}{ds_0} = \bar{p}(1,s_0)$$

$$\frac{dG}{ds_0} = \frac{\bar{p}'(1,s_0)}{[\bar{p}(1,s_0)]^2} (\bar{y}(1,s_0) - \beta)$$

Again for convergence $$\left| \frac{dG}{ds_0} \right| < 1$$

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