Mixed Collocation Methods for $y'' = f(x, y)$

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A thesis presented for the
degree of Doctor of Philosophy
at the University of Durham

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July 9, 1999

Abstract

The second-order initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = z_0$$

which does not contain the first derivative explicitly and where the solution is oscillatory has been of great interest for many years. Our aim is to construct numerical methods which are tuned to act efficiently on strongly oscillating functions. The frequencies involved determine the oscillatory character of the function and as the frequencies approach zero, the classical methods are obtained. The exponential-fitting tool has become increasingly popular as it is specially tailored for oscillating functions. Many classes of methods have been used with exponential-fitting and this will be discussed in more detail in the thesis.

Collocation methods are considered for which the basis functions are combinations of polynomial and trigonometric terms. The resulting methods can be regarded as Runge-Kutta-Nyström methods with steplength dependent coefficients. We show how order conditions may be obtained, investigate the stability and other properties of particular methods and present some numerical results.

Declaration

The work of chapters 5, 6 and 7 are entirely my own. Chapter 4 contains work undertaken by my supervisor and myself and in particular, sections 4.2.1, 4.2.2 and 4.2.3 are my own.

Statement of Copyright

Acknowledgement

First of all I would like to thank my supervisor, Dr. John Coleman, for all his help and support throughout the three years. Also to Dr. James Blowey, Dr. Clare Woodward, Josephine Coleman, Dr. Alan Craig and Dr. Cheryl Carey for their encouragement and advice and the Engineering Physical Science Research Council whose funding made it possible.

I am very grateful to my parents, my parents-in-law and to the rest of my family for all their support and faith in me. Thanks to Amanda Winn for being there to moan and groan at, to laugh with and for being a great friend. Many thanks also to the following:

To Medina Ablikim, Andrew Pocklington, John Campbell and Rick Coles for keeping me sane; to Rosemary, Laurence and Fred, and Amjid and Jo for constantly keeping in touch; Jan for always putting a smile on my face; Stuart for being a great e-mail friend; to the many friends I have made here including Hilary Davies, Alan Rayfield, Stephen Langdon, Patrick Dorey, John Bolton and Mandy Musgrave to name but a few; to Alima Laguna for helping me to consume vast amounts of coffee; and to the maths 5-a-side team, the womens Gradstaff team and the members of the Graduate Society Football Club for some great games of football.

Finally to my husband Moncef, whose love, encouragement, support (and constant nagging) has enabled me to reach so far.

In memory of Floriane,
her inspiration was unending.

Contents

Chapter 1

Introduction

Over recent years there has been considerable interest in solving initial-value problems of the form

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = z_0 \tag{1.1}$$

for the special class of second-order ordinary differential equations in which the first derivative does not appear explicitly and where $f(x, y)$ is as smooth as we please.

Equations of the type (1.1) are called *special* differential equations [35] and occur frequently. The radial Schrödinger equation

$$y''(x) = \left\{ \frac{l(l+1)}{x^2} + W(x) - E \right\} y(x)$$

is an example of this type of differential equation (1.1) where l is a non-negative integer, $W(x)$ is a potential function and E is a constant. Other examples include the twenty-seven equations describing the motion of the nine planets of our solar system.

As the emphasis in this thesis is on problems which have oscillatory solutions, we consider using a basis of functions other than polynomials. When one considers initial-value problems where the solution is oscillatory, it is advantageous to use information about the ordinary differential equation. One incentive for using a basis of functions other than polynomials is the fact that as every oscillation has to be followed when integrating a highly oscillatory ordinary differential equation, then a large amount of computer time is required and the rounding error accumulates for small step sizes. Methods based on polynomial functions are not so reliable in that case. The following work is related to collocation based Runge-Kutta-Nyström methods with steplength dependent coefficients. An important property of the new formulae is that they reduce to the classical methods when the involved frequencies tend to zero. Collocation simplifies the order conditions and stability analysis for Runge-Kutta-Nyström methods.

In chapter 2, the three main classes of numerical methods are discussed, one-step methods, linear multistep methods and hybrid methods. There has been a vast amount of work on polynomial based methods and how they have been adapted to problem (1.1) to take into account the oscillatory solution. A survey of this work is given and also a description of order, stability and concepts such as dispersion and periodicity.

In chapter 3 numerical methods are considered which have been fitted to exponential functions. Gautschi [28] appears to have been the first to use a basis of functions other than polynomials and introduced the idea of *trigonometric order* for linear multistep methods. Again, a survey on exponentially-fitted methods is given along with stability and order conditions.

Gautschi [28] used only trigonometric functions in his work but we consider a basis of both polynomial and trigonometric functions for the mixed collocation methods in chapter 4. The derivation of the mixed collocation methods is described and also the order conditions with the requirements on the collocation points for the maximum possible order.

In chapter 5 the stability of the mixed collocation methods is discussed, and plots of the stability regions are included for different values of the collocation points. We also show why we require the collocation points to be symmetric. Two new mixed collocation methods are described in chapter 6, the first is exact for a combination of the product of polynomial and trigonometric functions, and the second method is exact for two frequencies.

Chapter 7 is devoted to numerical results and is divided into one-dimensional and two-dimensional problems, all of which have oscillatory solutions and results are presented from other authors work for a comparison with the mixed collocation methods. Conclusions and further areas of research are given in chapter 8.

Chapter 2

Polynomial Based Numerical Methods

There has been an increasing development of numerical integration formulae for solving the initial-value problem (1.1) which has an oscillatory solution. The two main classes of numerical methods for solving problems of the form (1.1) are one-step methods and linear multistep methods. Also included are the most recent class of numerical methods known as hybrid methods which combine features of both one-step and multistep methods. We discuss order and stability of these methods and also the influence of concepts such as periodicity, P-stability and dispersion.

2.1 Linear Multistep Methods

Over the years many multistep methods have been produced which work without the first derivatives to integrate problems of the form (1.1). As we are not interested in the values of the first derivatives, we consider direct methods instead of producing systems of first-order.

A one-step method is a method which in each step uses information from a single step, namely the beginning of the step. We define y_n as the approximation to the value of the exact solution $y(x_n)$ at the grid point x_n. One main question is the size of the quantity $e_n = y(x_n) - y_n$ which is called the *discretization error*. The value of y_{n+1} can be found only if the value of y_n is known and we do not need to know information from the previous steps $y_{n-1}, y_{n-2}, \ldots$. A multistep method uses values from more than one preceding step, so the explicit knowledge of y_n is required as well as $y_{n-1}, y_{n-2}, \ldots$. For a k-step method, we require the values of $y_n, y_{n-1}, \ldots, y_{n+1-k}$

to evaluate y_{n+1}.

To derive a class of linear multistep methods for second-order differential equations, we start at the identity

$$y(x+\gamma h) - y(x) = \gamma h y'(x) + \int_x^{x+\gamma h} (x+\gamma h - r) f(r, y(r))\, dr$$

which may also be regarded as a form of Taylor's formula with a remainder term.

Replace γ by $-\gamma$,

$$y(x-\gamma h) - y(x) = -\gamma h y'(x) + \int_x^{x-\gamma h} (x-\gamma h - r) f(r, y(r))\, dr$$

and add together to eliminate the first derivative $y'(x)$

$$y(x+\gamma h) - 2y(x) + y(x-\gamma h) = \int_x^{x+\gamma h} (x+\gamma h - r) f(r, y(r))\, dr + \int_x^{x-\gamma h} (x-\gamma h - t) f(t, y(t))\, dt.$$

Replace t with $2x-r$ in the second integral on the right hand side of the equation to give

$$\int_x^{x-\gamma h} (x-\gamma h - t)\, f(t, y(t))\, dt = -\int_x^{x+\gamma h} (-x-\gamma h + r)\, f(2x-r)\, dr$$

and thus

$$y(x+\gamma h) - 2y(x) + y(x-\gamma h) = \int_x^{x+\gamma h} (x+\gamma h - r)[f(r) + f(2x-r)]\, dr \quad (2.1)$$

where the second argument of f has been temporarily suppressed.

Different multistep methods are now obtained by choosing appropriate values of x and γ, and by replacing $f(r, y(r))$ and $f(2x-r, y(2x-r))$ by a polynomial interpolating at previous step points. The Störmer-Cowell family of linear multistep methods was developed by applying finite difference quadrature formulae to equation (2.1).

Störmer's explicit multistep methods are given by

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \sum_{m=0}^{q} \sigma_m \nabla^m f_n \quad (2.2)$$

where $\nabla^{j+1} f_n = \nabla^j f_n - \nabla^j f_{n-1}$ are the backward differences and

$$\begin{aligned}\sigma_m &= \frac{(-1)^m}{h^2}\int_{x_n}^{x_{n+1}}(x_{n+1}-x)\left\{\binom{-s}{m}+\binom{s}{m}\right\}dx, \quad s=\frac{x-x_n}{h}\\ &= (-1)^m\int_0^1(1-s)\left\{\binom{-s}{m}+\binom{s}{m}\right\}ds\end{aligned}$$

and Cowell's methods by

$$y_n - 2y_{n-1} + y_{n-2} = h^2\sum_{m=0}^{q}\sigma_m^*\nabla^m f_n \tag{2.3}$$

where

$$\begin{aligned}\sigma_m^* &= \frac{(-1)^m}{h^2}\int_{x_{n-1}}^{x_n}(x_n-x)\left\{\binom{-s}{m}+\binom{s+2}{m}\right\}dx, \quad s=\frac{x-x_n}{h}\\ &= (-1)^m\int_{-1}^{0}(-s)\left\{\binom{-s}{m}+\binom{s+2}{m}\right\}ds\end{aligned}$$

and $f_n = f(x_n, y_n)$.

In 1907, Störmer's method (2.2) was used for extensive numerical calculations concerning the Aurora Borealis [32]. For $q = 0$ and $q = 1$, (2.2) reduces to the simple explicit method

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f_n \tag{2.4}$$

and the left hand side of this equation can be regarded as a second-order difference approximation for $f(x, y(x))$.

In 1910, Cowell and Crommelin studied the motion of Halley's Comet. For $q = 1$, Cowell's method (2.3) reduces to the explicit method (2.4) and for $q = 2$ and $q = 3$, (2.3) reduces to the frequently used implicit method

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}\left\{f_{n+1} + 10f_n + f_{n-1}\right\}$$

which is attributed to Numerov. Cowell's methods are implicit for $q \geq 2$.

The general form of a linear k-step method for the problem (1.1) is written as

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h^2 \sum_{i=0}^{k} \beta_i f_{n+i} \tag{2.5}$$

where $f_{n+p} = f(x_{n+p}, y_{n+p})$ with $x_n = x_0 + nh$, y_n denotes the numerical approximation to the exact solution of the differential equation being considered at the point x_n, and h is the steplength.

The α_i and β_i of (2.5) are constants subject to the conditions

$$\alpha_k = 1 \text{ and } |\alpha_0| + |\beta_0| > 0.$$

The first arises from the fact that both sides of the linear multistep method could be multiplied by the same constant and we want to try and avoid this arbitrariness. The second condition prevents both α_0 and β_0 both being zero. For example, consider the 2-step method

$$y_{n+2} - y_{n+1} + \alpha_0 y_n = h(f_{n+1} + \beta_0 f_n).$$

If $\alpha_0 = 0$ and $\beta_0 = 0$, then the method is a 1-step method and not 2-step as required.

If $\beta_k = 0$, then the method (2.5) is explicit and implicit if $\beta_k \neq 0$.

Definition 2.1 *The* **shift operator** *E is defined by $Eu_n = u_{n+1}$ for any sequence $\{u_n\}$.*

The linear multistep method (2.5) can be written in terms of the shift operator E

$$\rho(E)y_n = h^2\sigma(E)f_n \tag{2.6}$$

where the first and second characteristic polynomials are given respectively by

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^i \text{ and } \sigma(\xi) = \sum_{i=0}^{k} \beta_i \xi^i.$$

We shall refer to the linear multistep method as (ρ, σ).

The linear multistep methods remain popular and have been extensively used over the years. Many authors have derived linear multistep methods by choosing the coefficients α_i and β_i by satisfying certain order and stability criteria which will be discussed in a later section.

2.2 One-Step Methods

In this section we consider Runge-Kutta methods for first-order differential equations, and Runge-Kutta-Nyström, polynomial collocation and hybrid methods for second-order differential equations.

2.2.1 Runge-Kutta Methods

An s-stage Runge-Kutta method for the first-order initial value problem

$$y' = f(x,y), \quad y(x_0) = y_0$$

is defined by

$$y_{n+1} = y_n + h\sum_{i=1}^{s} d_i k_i, \quad k_i = f\left(x_n + c_i h, y_n + h\sum_{j=1}^{s} Q_{ij}k_j\right), \quad i = 1, \dots, s, \qquad (2.7)$$

where $x_n = x_0 + nh$ and y_n is an approximation for $y(x_n)$. We shall always assume that the following (the *row-sum condition*) holds:

$$c_i = \sum_{j=1}^{s} Q_{ij}, \quad i = 1, 2, \dots, s.$$

The constant coefficients c_i, d_i and Q_{ij} can be displayed in the following form, known as a **Butcher Array**

$$\begin{array}{c|c} \mathbf{c} & \mathbf{Q} \\ \hline & \mathbf{d}^{\mathrm{T}} \end{array}$$

where $\mathbf{c}$ and $\mathbf{d}$ are s-dimensional column vectors and $\mathbf{Q}$ is an $s \times s$ matrix where

$$\mathbf{c} = [c_1, c_2, \dots, c_s]^T, \quad \mathbf{d} = [d_1, d_2, \dots, d_s]^T \text{ and } \mathbf{Q} = [Q_{ij}].$$

The method is *explicit* if the matrix $\mathbf{Q}$ is strictly lower triangular. If $Q_{ij} = 0$ for $i < j$ and at least one element on the diagonal is not zero, i.e. $Q_{ii} \neq 0$, then we have a *diagonally implicit* Runge-Kutta method (DIRK). If $Q_{ij} = 0$ for $i < j$ and all the diagonal elements are equal, then the method is *singly diagonally implicit* (SDIRK). For any other case, the method is *implicit*.

We define the local truncation error T_{n+1} of (2.7) at x_{n+1} to be the residual when y_{n+1} is replaced by $y(x_{n+1})$ and y_n by $y(x_n)$; that is,

$$T_{n+1} = y(x_{n+1}) - y(x_n) - h\sum_{i=1}^{s} d_i f\left(x_n + c_i h, y(x_n) + h\sum_{j=1}^{s} Q_{ij}k_j\right)$$

and

$$k_i = f(x_n + c_i h, y(x_n) + h\sum_{j=1}^{s} Q_{ij}k_j), \quad i = 1, \ldots, s.$$

Definition 2.2 *If p is the largest integer such that $T_{n+1} = O(h^{p+1})$, we say that the Runge-Kutta method has* **order** *p.*

A necessary and sufficient condition for a general Runge-Kutta method to be *consistent* [46] is

$$\sum_{i=1}^{s} d_i = 1$$

and this is assumed throughout the thesis. The idea behind the process of embedding is to derive explicit Runge-Kutta methods of orders p and $p+1$ such that they have the same set of function values k_i. Then the formulae contains the numerical approximation y_{n+1}, and a second approximation $\hat{y}_{n+1}$. In terms of the Butcher array,

$$\begin{array}{c|c} \mathbf{c} & \mathbf{Q} \\ \hline & \mathbf{d}^T \\ & \hat{\mathbf{d}}^T \\ \hline & \mathbf{E}^T \end{array}$$

this means that the method defined by $\mathbf{c}$, $\mathbf{Q}$ and $\mathbf{d}$ has order p, and the method defined by $\mathbf{c}$, $\mathbf{Q}$ and $\hat{\mathbf{d}}$ has order $p+1$. An estimate of the local truncation error is the difference between the numerical approximation y_{n+1} generated by the first method and the second approximation $\hat{y}_{n+1}$ by the latter method. The vector $\mathbf{E}^T = [E_1, E_2, \ldots, E_s]$ is $\hat{\mathbf{d}}^T - \mathbf{d}^T$ and so the error estimate is given by $h\sum_{i=1}^{s} E_i k_i$. One advantage of embedded methods is that the error estimate can be used as a basis for monitoring steplength. These types of methods will not be considered in this thesis.

2.2.2 Runge-Kutta-Nyström Methods

The second-order initial value problem

$$y'' = f(x, y(x), y'(x)), \quad y(x_0) = y_0, \quad y'(x_0) = z_0$$

can be split into a pair of coupled first-order equations

$$\begin{pmatrix} y \\ z \end{pmatrix}' = \begin{pmatrix} z \\ f(x, y(x), z(x)) \end{pmatrix}, \quad y(x_0) = y_0, \quad z(x_0) = z_0. \tag{2.8}$$

If we apply an s-stage Runge-Kutta method for first-order differential equations to this problem, we obtain

$$y_{n+1} = y_n + h\sum_{i=1}^{s} d_i K_i, \quad z_{n+1} = z_n + h\sum_{i=1}^{s} d_i L_i,$$

$$K_i = z_n + h\sum_{j=1}^{s} Q_{ij} L_j,$$

$$L_i = f\left(x_n + c_i h, y_n + h\sum_{j=1}^{s} Q_{ij} K_j, z_n + h\sum_{j=1}^{s} Q_{ij} L_j\right), \quad i = 1, \ldots, s,$$

where y_n is an approximation for $y(x_n)$ and z_n is an approximation for $y'(x_n)$. Because of the interest in problem (1.1) in which the first derivative does not appear explicitly, then (2.8) becomes

$$\begin{pmatrix} y \\ z \end{pmatrix}' = \begin{pmatrix} z \\ f(x, y(x)) \end{pmatrix}, \quad y(x_0) = y_0, \quad z(x_0) = z_0 \tag{2.9}$$

and applying the Runge-Kutta method to (2.9), we obtain

$$y_{n+1} = y_n + h\sum_{i=1}^{s} d_i K_i, \quad z_{n+1} = z_n + h\sum_{i=1}^{s} d_i L_i,$$

$$K_i = z_n + h\sum_{j=1}^{s} Q_{ij} L_j, \quad L_i = f\left(x_n + c_i h, y_n + h\sum_{j=1}^{s} Q_{ij} K_j\right), \quad i = 1, \ldots, s.$$

Inserting K_i into the rest of the formulae, we can eliminate K_i to find the s-stage

Runge-Kutta-Nyström formulae

$$\left.\begin{aligned} y_{n+1} &= y_n + hz_n + h^2 \sum_{i=1}^{s} b_i L_i, \\ z_{n+1} &= z_n + h \sum_{i=1}^{s} d_i L_i, \\ L_i &= f\left(x_n + c_i h, y_n + c_i h z_n + h^2 \sum_{j=1}^{s} a_{ij} L_j\right), \quad i = 1, \ldots, s \end{aligned}\right\} \tag{2.10}$$

where the constants b_i and a_{ij} are given by

$$b_i = \sum_{k=1}^{s} d_k Q_{ki}, \quad a_{ij} = \sum_{k=1}^{s} Q_{ik} Q_{kj}. \tag{2.11}$$

The Butcher Array for a Runge-Kutta-Nyström method (2.10) with coefficients given by (2.11) is

$$\begin{array}{c|c} \mathbf{c} & \mathbf{Q^2} \\ \hline & \\ & \mathbf{d^T Q} \\ & \mathbf{d^T} \end{array}$$

Nyström was the first to consider methods of the form (2.10) for the problem (1.1) in which the coefficients do not necessarily satisfy (2.11) and do not involve the reduction to a system of first-order equations. These are known as *direct* methods compared to the *indirect* approach of applying a Runge-Kutta method to a system of first-order equations. The Butcher Array for a Runge-Kutta-Nyström method with $\mathbf{A} = [a_{ij}]$ is

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \\ & \mathbf{b^T} \\ & \mathbf{d^T} \end{array}$$

If we eliminate L_i from (2.10) we obtain the general s-stage Runge-Kutta-Nyström method

$$\left.\begin{aligned} y_{n+1} &= y_n + hz_n + h^2 \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \\ z_{n+1} &= z_n + h \sum_{i=1}^{s} d_i f(x_n + c_i h, Y_i), \\ Y_i &= y_n + c_i h z_n + h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, \ldots, s. \end{aligned}\right\} \qquad (2.12)$$

where y_n is an approximation for $y(x_n)$ and z_n approximates $y'(x_n)$.

When the generating Runge-Kutta method has s implicit stages and is of order p, (c.f. Definition 2.2), then the Runge-Kutta-Nyström method (2.12) also does. Also, the Runge-Kutta-Nyström method is *explicit* if the $s \times s$ matrix $\mathbf{A}$ is strictly lower triangular. A *diagonally implicit* Runge-Kutta-Nyström method (DIRKN) is where the matrix $\mathbf{A}$ is lower triangular and at least one diagonal element is non-zero, whilst for a *singly diagonally implicit* method (SDIRKN), all the diagonal elements are equal. For any other case the method is *implicit*.

2.2.3 Polynomial Collocation Methods

A one-step collocation method for the initial-value problem (1.1) proceeds by approximating the solution on the interval $[x_n, x_{n+1}]$ by a polynomial which satisfies the differential equation at a number of specified collocation points $x_{n+c_i} = x_n + c_i h$ for $i = 1, \ldots, s$. We define $\{c_i\}_{i=1}^{s}$ to be a set of distinct real numbers which are typically taken to be on the interval $[0, 1]$. Let $u(x)$ be the polynomial of degree $s + 1$ defined by

$$u(x_n) = y_n, \quad u'(x_n) = z_n,$$

$$u''(x_n + c_i h) = f(x_n + c_i h, u(x_n + c_i h)), \quad i = 1, \ldots, s.$$

Van der Houwen et al [79] considered both indirect and direct approaches for polynomial based collocation methods and the theory for collocation methods for first-order equations can be applied to indirect collocation methods. We consider an indirect collocation method which is generated by applying a Runge-Kutta collocation method to the first-order system of differential equations (2.9). Following Van der Houwen et al [79], if we let the Runge-Kutta method (2.7) be a collocation method based on the s distinct collocation points $x_n + c_i h$, $i = 1, \ldots, s$ then

$$Q_{ij} = \int_0^{c_i} l_j(t)\, dt, \quad d_i = \int_0^1 l_i(t)\, dt, \quad i, j = 1, \ldots, s$$

where $l_j(t)$ are the Lagrange polynomials

$$l_j(t) = \prod_{k \neq j}^{s} \frac{(t - c_k)}{(c_j - c_k)}, \quad j = 1, \ldots, s.$$

With $f_{n+c_i} := f(x_n + c_i h, y_{n+c_i})$, then we may write

$$u''(x_n + th) = \sum_{i=1}^{s} l_i(t) f_{n+c_i}$$

and integrating twice with respect to t and substituting the initial conditions we obtain

$$u'(x_n + h) = z_n + h \sum_{i=1}^{s} \left\{ \int_0^1 l_i(t)\, \mathrm{d}t \right\} f_{n+c_i},$$

$$u(x_n + h) = y_n + hz_n + h^2 \sum_{j=1}^{s} \left\{ \int_0^1 \int_0^{\xi} l_j(t)\, \mathrm{d}t\, \mathrm{d}\xi \right\} f_{n+c_j}$$

and

$$u(x_n + c_i h) = y_n + c_i h z_n + h^2 \sum_{j=1}^{s} \left\{ \int_0^{c_i} \int_0^{\xi} l_j(t)\, \mathrm{d}t\, \mathrm{d}\xi \right\} f_{n+c_j}$$

$$\text{for } i = 1, \ldots, s.$$

Therefore the coefficients for the Runge-Kutta-Nyström method are given by

$$a_{ij} = \int_0^{c_i} \int_0^{\xi} l_j(t)\, \mathrm{d}t\, \mathrm{d}\xi = \int_0^{c_i} \int_t^{c_i} l_j(t)\, \mathrm{d}\xi\, \mathrm{d}t = \int_0^{c_i} (c_i - t) l_j(t)\, \mathrm{d}t,$$

$$b_i = \int_0^1 \int_0^{\xi} l_j(t)\, \mathrm{d}t\, \mathrm{d}\xi = \int_0^1 \int_t^1 l_j(t)\, \mathrm{d}\xi\, \mathrm{d}t = \int_0^1 (1 - t) l_j(t)\, \mathrm{d}t,$$

$$\text{for } i, j = 1, \ldots, s.$$

A direct way of deriving the polynomial collocation method is to consider approximating the solution $y(x)$ of problem (1.1) on the interval $[x_n, x_{n+1}]$ by a function $u(x)$ of the form

$$u(x) = \sum_{i=0}^{s+1} r_i (x - x_n)^i.$$

If we use a collocation method based on the s distinct collocation points

$$x_{n+c_i} = x_n + c_i h \quad \text{for} \quad i = 1, \ldots, s$$

where $0 \le c_1 < c_2 < \ldots < c_s \le 1$ then the collocation conditions are

$$u''(x_n + c_i h) = f(x_n + c_i h, u(x_n + c_i h)), \; i = 1, \ldots, s.$$

Differentiate the function $u(x)$ twice with respect to x

$$\left.\begin{aligned} u(x) &= \sum_{i=0}^{s+1} r_i (x - x_n)^i \\ u'(x) &= \sum_{i=0}^{s+1} i r_i (x - x_n)^{i-1} \\ u''(x) &= \sum_{i=0}^{s+1} i(i-1) r_i (x - x_n)^{i-2}. \end{aligned}\right\} \tag{2.13}$$

Then the initial conditions are

$$u(x_n) = y_n = r_0, \quad u'(x_n) = z_n = r_1,$$

where y_n and z_n are approximations for $y(x_n)$ and $y'(x_n)$ respectively, and from the collocation conditions

$$f(x_n + c_i h, u(x_n + c_i h)) = 2r_2 + \sum_{j=3}^{s+1} j(j-1) r_j (c_i h)^{j-2}, \quad i = 1, \ldots, s.$$

If we take y_{n+1}, z_{n+1} and y_{n+c_i} as approximations for $y(x_{n+1})$, $y'(x_{n+1})$ and $y(x_{n+c_i})$ respectively, then substituting $x = x_n + h$ into $u(x)$ and $u'(x)$, and $x = x_n + c_i h$ into $u(x)$ from (2.13) with the initial and collocation conditions, we obtain the formulae

$$\left.\begin{aligned} y_{n+1} &= y_n + h z_n + \sum_{i=2}^{s+1} r_i h^i, \\ z_{n+1} &= z_n + \sum_{i=2}^{s+1} i r_i h^{i-1}, \\ y_{n+c_i} &= y_n + c_i h z_n + \sum_{j=2}^{s+1} r_j (c_i h)^j, \quad i = 1, \ldots, s. \end{aligned}\right\} \tag{2.14}$$

Example 1 - One collocation point ($s = 1$)
For convenience, let $f_{n+c} = f(x_n + ch, u(x_n + ch))$. Then,

$$u''(x_n + ch) = 2r_2 = f_{n+c},$$

and substituting $r_2 = \frac{1}{2}f_{n+c}$ into (2.14) with $s = 1$ we obtain the formulae

$$\left.\begin{aligned} y_{n+1} &= y_n + hz_n + r_2h^2 = y_n + hz_n + \frac{h^2}{2}f_{n+c}, \\ z_{n+1} &= z_n + 2r_2h = z_n + hf_{n+c}, \\ y_{n+c} &= y_n + chz_n + r_2(ch)^2 = y_n + chz_n + \frac{c^2h^2}{2}f_{n+c}. \end{aligned}\right\} \quad (2.15)$$

Example 2 - Two collocation points ($s = 2$)
Define $f_{n+c_1} = f(x_n + c_1h, u(x_n + c_1h))$ and $f_{n+c_2} = f(x_n + c_2h, u(x_n + c_2h))$. The collocation conditions give

$$u''(x_n + c_1h) = f_{n+c_1} = 2r_2 + 6r_3c_1h$$
$$u''(x_n + c_2h) = f_{n+c_2} = 2r_2 + 6r_3c_2h$$

from which

$$r_2 = \frac{c_2f_{n+c_1} - c_1f_{n+c_2}}{2(c_2 - c_1)}, \quad r_3 = \frac{f_{n+c_2} - f_{n+c_1}}{6h(c_2 - c_1)}.$$

The formulae for the polynomial collocation method with two collocation points $x_n + c_1h$ and $x_n + c_2h$ are

$$\left.\begin{aligned} y_{n+1} &= y_n + hz_n + \frac{h^2}{6(c_2 - c_1)}\{(3c_2 - 1)f_{n+c_1} + (1 - 3c_1)f_{n+c_2}\}, \\ z_{n+1} &= z_n + \frac{h}{2(c_2 - c_1)}\{(2c_2 - 1)f_{n+c_1} + (1 - 2c_1)f_{n+c_2}\}, \\ y_{n+c_1} &= y_n + c_1hz_n + \frac{c_1^2h^2}{6(c_2 - c_1)}\{(3c_2 - c_1)f_{n+c_1} - 2c_1f_{n+c_2}\}, \\ y_{n+c_2} &= y_n + c_2hz_n + \frac{c_2^2h^2}{6(c_2 - c_1)}\{2c_2f_{n+c_1} + (c_2 - 3c_1)f_{n+c_2}\}. \end{aligned}\right\} \quad (2.16)$$

With $c_1 = 0$ and $c_2 = 1$,

$$\begin{aligned} y_{n+1} &= y_n + hz_n + \frac{h^2}{6}\left\{2f_n + f_{n+1}\right\}, \\ z_{n+1} &= z_n + \frac{h}{2}\left\{f_n + f_{n+1}\right\}. \end{aligned}$$

Example 3 - Three collocation points ($s = 3$)

Again let $f_{n+c_1} = f(x_n + c_1 h, u(x_n + c_1 h))$, $f_{n+c_2} = f(x_n + c_2 h, u(x_n + c_2 h))$ and $f_{n+c_3} = f(x_n + c_3 h, u(x_n + c_3 h))$.

The formulae for the polynomial collocation method with three collocation points $x_n + c_1 h$, $x_n + c_2 h$ and $x_n + c_3 h$ are

$$\left.\begin{aligned} y_{n+1} &= y_n + hz_n + h^2\left\{b_1 f_{n+c_1} + b_2 f_{n+c_2} + b_3 f_{n+c_3}\right\}, \\ z_{n+1} &= z_n + h\left\{d_1 f_{n+c_1} + d_2 f_{n+c_2} + d_3 f_{n+c_3}\right\}, \\ y_{n+c_i} &= y_n + c_i hz_n + h^2\left\{a_{i1} f_{n+c_1} + a_{i2} f_{n+c_2} + a_{i3} f_{n+c_3}\right\} \\ &\qquad \text{for } i = 1, 2, 3 \end{aligned}\right\} \tag{2.17}$$

where

$$b_1 = \frac{1 - 2c_2 - 2c_3 + 6c_2c_3}{12\mathcal{BA}}, \quad b_2 = \frac{1 - 2c_3 - 2c_1 + 6c_3c_1}{12\mathcal{AC}},$$

$$b_3 = -\frac{1 - 2c_1 - 2c_2 + 6c_1c_2}{12\mathcal{BC}}, \quad d_1 = \frac{2 - 3c_2 - 3c_3 + 6c_2c_3}{6\mathcal{BA}},$$

$$d_2 = \frac{2 - 3c_3 - 3c_1 + 6c_3c_1}{6\mathcal{AC}}, \quad d_3 = -\frac{2 - 3c_1 - 3c_2 + 6c_1c_2}{6\mathcal{BC}},$$

$$a_{11} = \frac{c_1^2(c_1^2 - 2c_3c_1 + 6c_2c_3 - 2c_1c_2)}{12\mathcal{BA}}, \quad a_{12} = \frac{c_1^3(4c_3 - c_1)}{12\mathcal{AC}}, \quad a_{13} = \frac{-c_1^3(4c_2 - c_1)}{12\mathcal{BC}},$$

$$a_{21} = \frac{c_2^3(4c_3 - c_2)}{12\mathcal{BA}}, \quad a_{22} = \frac{c_2^2(6c_3c_1 - 2c_1c_2 + c_2^2 - 2c_2c_3)}{12\mathcal{AC}}, \quad a_{23} = \frac{-c_2^3(4c_1 - c_2)}{12\mathcal{BC}},$$

$$a_{31} = \frac{c_3^3(4c_2 - c_3)}{12\mathcal{B}\mathcal{A}}, \quad a_{32} = \frac{c_3^3(4c_1 - c_3)}{12\mathcal{A}\mathcal{C}}, \quad a_{33} = \frac{-c_3^2(6c_1c_2 - 2c_3c_1 + c_3^2 - 2c_2c_3)}{12\mathcal{B}\mathcal{C}}$$

and $\mathcal{A} = c_2 - c_1$, $\mathcal{B} = c_3 - c_1$ and $\mathcal{C} = c_2 - c_3$.

In the case of multiple collocation points, i.e. points that are equivalent, this leads to multiderivative methods. Let D be a partition of $[0, 1]$ given by

$$D : 0 \leq c_1 \leq c_2 \leq \ldots \leq c_s \leq 1,$$

and let q_i for $1 \leq i \leq s$ be non-negative integers. Define $M = s + \sum_{i=1}^{s} q_i$. The collocation solution of (1.1) is a polynomial, $u(x)$, of degree at most $M + 1$ defined by

$$u(x_n) = y_n, \quad u'(x_n) = z_n,$$

$$u^{2+i}(x_n + c_j h) = \frac{d^i f(x_n + c_j h, u(x_n + c_j h))}{dx^i}, \quad j = 1, \ldots, s, \quad 0 \leq i \leq q_j.$$

Kramarz [45] showed that if we use symmetric collocation points, that is $c_j + c_{s+1-j} = 1, \quad j = 1, 2, \ldots, N$, where $N = s/2$ for even s and $N = (s+1)/2$ for odd s, then the method has an interval of periodicity, (c.f. Definition 2.11). Also, as we shall show in chapter 5, when symmetric collocation nodes are used in the one, two and three-point mixed collocation methods, the criteria are satisfied for the methods to have an interval of periodicity. Distinct collocation points only will be considered throughout the rest of this thesis.

The Panovsky-Richardson methods [52] are derived in a similar way to the Störmer-Cowell methods. From equation (2.1), a new variable t is introduced by the relation

$$r = x_n + \frac{h}{2}(1 + t)$$

and setting $x = x_n$ for $n = 0, 1, 2, ..$, then (2.1) becomes

$$y(x + \gamma h) - 2y(x) + y(x - \gamma h) = \frac{h^2}{4} \int_{-1}^{2\gamma - 1} (2\gamma - 1 - t) \left[f(x_{n+}) + f(x_{n-}) \right] dt$$

where

$$f(x_{n\pm}) = f\left(x_n \pm \frac{h}{2}(1 + t), y\left(x_n \pm \frac{h}{2}(1 + t) \right) \right).$$

The Panovsky-Richardson methods are then found by replacing f by interpolating polynomials based on off-step points which are the extrema of a Chebyshev polynomial [21]. Coleman and Booth showed that the methods are equivalent to collocation based Runge-Kutta-Nyström methods.

2.3 Hybrid methods

Hybrid methods have become a popular class of numerical methods due to the fact that desirable properties such as P-stability and unconditional stability (terms to be defined later in this chapter) restrict the algebraic order (or order of accuracy) of linear multistep methods to at most two. Many authors have shown that if off-step points or higher-order derivatives are used to modify a linear multistep method, then higher algebraic order can be achieved. Concepts such as P-stability and periodicity can then be used to modify the methods so that they sometimes solve problems of the form (1.1) more accurately than other classical linear multistep methods such as the family of Störmer-Cowell methods.

In 1955, an explicit method was introduced by De Vogelaere which was one-step but also used off-step values and became a popular alternative to Numerov's method. This method became known as a hybrid method and a new class of numerical methods was created. One reason for the interest in using linear multistep methods with off-step points for the problem $y'' = f(x, y)$ is because there is no need to refer to y' in these methods. An example of a hybrid method is the linear 2-step implicit formulae of Cash [3]

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \sum_{i=0}^{k} \delta_i \left\{ f_{n+\alpha_i} + f_{n-\alpha_i} \right\} + h^2 \gamma f_n \tag{2.18}$$

where $\alpha_0 = 1$, $f_{n\pm\alpha_j} = f(x_n \pm \alpha_j h, y_{n\pm\alpha_j})$ and the quantities $y_{n\pm\alpha_i}$ are approximated by an expression involving the values y_{n+1}, y_n and y_{n-1} only. Cash's family of methods has been used by many authors for various values of k, and with $k = 1$ we obtain the popular form

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left\{ \delta_0 (f_{n+1} + f_{n-1}) + \gamma f_n + \delta_1 (f_{n+\alpha_1} + f_{n-\alpha_1}) \right\} \tag{2.19}$$

where

$$y_{n\pm\alpha_1} = A_\pm y_{n+1} + B_\pm y_n + C_\pm y_{n-1} + h^2 \left(s_\pm f_{n+1} + t_\pm f_n + u_\pm f_{n-1} \right).$$

An alternative approach to deriving hybrid methods is by replacing one or more of the function values with an implicit or explicit stage in a linear multistep method. We will discuss hybrid methods in more detail in section 2.5.4.

2.4 Order

2.4.1 Linear Multistep Methods

To find the order conditions for the linear multistep methods (2.5), we first define the linear functional

$$\mathcal{L}[y(x);h] = \sum_{i=0}^{k} \alpha_i y(x+ih) - h^2 \sum_{i=0}^{k} \beta_i y''(x+ih). \tag{2.20}$$

Assuming that $y(x)$ is as differentiable as we choose, we form a Taylor expansion about a suitable value of x and express the residual as a power series in h. Thus,

$$\mathcal{L}[y(x);h] = \sum_{i=0}^{k} \alpha_i \left\{ y(x) + ih\,y'(x) + \frac{i^2h^2}{2!}y''(x) + \frac{i^3h^3}{3!}y^{(3)}(x) + \frac{i^4h^4}{4!}y^{(4)}(x) + \ldots \right\}$$

$$-h^2 \sum_{i=0}^{k} \beta_i \left\{ y''(x) + ih\,y^{(3)}(x) + \frac{i^2h^2}{2!}y^{(4)}(x) + \ldots \right\}$$

$$\begin{aligned}
&= \sum_{i=0}^{k} \alpha_i\, y(x) + h \sum_{i=0}^{k} i\alpha_i\, y'(x) + h^2 \sum_{i=0}^{k} \left\{ \frac{i^2\alpha_i}{2!} - \beta_i \right\} y''(x) \\
&\quad + h^3 \sum_{i=0}^{k} \left\{ \frac{i^3\alpha_i}{3!} - i\beta_i \right\} y^{(3)}(x) + h^4 \sum_{i=0}^{k} \left\{ \frac{i^4\alpha_i}{4!} - \frac{i^2\beta_i}{2!} \right\} y^{(4)}(x) + \ldots \\
&= C_0\, y(x) + C_1\, h\, y'(x) + C_2\, h^2\, y''(x) + C_3\, h^3\, y^{(3)}(x) \\
&\qquad + C_4\, h^4\, y^{(4)}(x) + \ldots + C_r\, h^r\, y^{(r)}(x) + \ldots
\end{aligned}$$

with

$$C_0 = \sum_{i=0}^{k} \alpha_i = \rho(1), \quad C_1 = \sum_{i=0}^{k} i\alpha_i = \rho'(1)$$

and

$$C_q = \sum_{i=0}^{k} \left\{ \frac{i^q}{q!}\alpha_i - \frac{i^{q-2}}{(q-2)!}\beta_i \right\}, \quad q = 2, 3, \ldots$$

The following definition is taken from Hairer et al [32].

Definition 2.3 *A linear multistep method* (2.5) *and the associated linear operator* (2.20) *are said to be of* **order** p *if* $C_0 = C_1 = \ldots = C_{p+1} = 0$ *and* $C_{p+2} \neq 0$.

The *error constant* is given by

$$C = \frac{C_{p+2}}{\beta_0 + \beta_1 + \ldots + \beta_k}$$

and the *principle local truncation error* at the point x_n is

$$PLTE = C_{p+2}\, h^{p+2}\, y^{(p+2)}(x_n).$$

If we require the method to be consistent, that is of at least order 1, then C_0, C_1 and C_2 must all be equal to zero, and in terms of the characteristic polynomials we have

$$\rho(1) = 0, \;\; \rho'(1) = 0 \;\text{ and }\; \rho''(1) = 2\sigma(1).$$

2.4.2 Runge-Kutta-Nyström Methods

The local truncation error of a Runge-Kutta-Nyström method is the extent to which the exact solution fails to satisfy the difference equations which define the method.

The following definition is taken from Van der Houwen et al [79]

Definition 2.4 *Let* Y_i *denote the vector with components* $y(x_n + c_i h)$ *with* y *the locally exact solution of* (1.1) *satisfying* $y(x_n) = y_n$ *and* $y'(x_n) = z_n$, *and suppose that the local errors are given by*

$$T_{n+1} = y(x_{n+1}) - y_{n+1} = O(h^{p_1+1}), \;\; T'_{n+1} = y'(x_{n+1}) - z_{n+1} = O(h^{p_2+1}),$$

$$Y_i - y_n - c_i h z_n - h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) = O(h^{p_3+1}),$$

then the **order** p *and the* **stage order** r *are respectively defined by*

$$p = \min\{p_1, p_2\}, \;\; r = \min\{p_1, p_2, p_3\}.$$

From the Runge-Kutta-Nyström method (2.12),

$$y_{n+c_i} = y_n + c_i h z_n + h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, y_{n+c_j}) \approx y(x_n + c_i h), \quad i = 1, \ldots, s$$

and

$$z_{n+1} = z_n + h \sum_{i=1}^{s} d_i f(x_n + c_i h, y_{n+c_i}) \approx y'(x_n + h).$$

Using the exact values of the solution and its derivative at x_n,

$$\begin{aligned} y(x_n + c_i h) - y(x_n) - c_i h y'(x_n) - h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) \\ = h^2 \left\{ \frac{c_i^2}{2} - \sum_{j=1}^{s} a_{ij} \right\} y''(x_n) + O(h^3) \end{aligned}$$

and

$$y'(x_n + h) - y'(x_n) - h \sum_{i=1}^{s} d_i f(x_n + c_i h, Y_i) = h \left\{ 1 - \sum_{i=1}^{s} d_i \right\} y''(x_n) + O(h^2).$$

Therefore, if we require that the method is consistent, i.e. has order at least one, then

$$\sum_{i=1}^{s} d_i = 1$$

and we assume the row-sum condition,

$$\sum_{j=1}^{s} a_{ij} = \frac{c_i^2}{2}, \quad i = 1, \ldots, s.$$

The maximum attainable order of an s-stage Runge-Kutta-Nyström method is $2s$.

To find the order conditions for a Runge-Kutta or Runge-Kutta-Nyström method, the work soon becomes complicated using a bare-hands Taylor series expansion because $f(x, y)$ is evaluated at off-step points and so we have to obtain the series expansion of a function of two variables. Butcher's tree theory is a very useful approach for finding the order conditions and greatly reduces the amount of work. Lambert [46] and Hairer et al [32] describe how the order conditions for Runge-Kutta methods can be found by using Butcher's tree approach. The work was extended to Nyström methods by Hairer and Wanner [33] and Hairer [29]. The order conditions for the Runge-Kutta-Nyström method were obtained from the work by Hairer and

Wanner [34] and will be adapted for methods with steplength dependent coefficients in section 3.4.2.

2.4.3 Polynomial Collocation Methods

Collocation based Runge-Kutta-Nyström methods are very useful because they have a high stage order. Van der Houwen et al [79] showed that an s-stage polynomial collocation method given by (2.14) has order at least s for all sets of distinct collocation nodes c_i. They showed that the order can be raised to as much as $2s$ for a suitable choice of the collocation parameters (known as superconvergence). Using the Alexseev-Gröbner Theorem, an s-stage polynomial collocation method can have order $s+q$ if

$$\int_0^1 \xi^{j-1}\prod_{i=1}^{s}(\xi - c_i)d\xi = 0, \quad \text{for } j = 1,\ldots,q.$$

The following table shows the order and the maximum attainable order with the collocation nodes for the one, two and three-point polynomial collocation methods.

Method	Stages	Default Order	Maximum Order	:	Collocation Nodes
(2.15)	1	1	2	:	$\frac{1}{2}$
(2.16)	2	2	4	:	$\frac{3-\sqrt{3}}{6}$ and $\frac{3+\sqrt{3}}{6}$
(2.17)	3	3	6	:	$\frac{5-\sqrt{15}}{10}$, $\frac{1}{2}$ and $\frac{5+\sqrt{15}}{10}$

Since the polynomial collocation methods may be written as Runge-Kutta-Nyström methods, then the theory for the algebraic order of Runge-Kutta-Nyström methods may be applied to polynomial collocation.

2.5 Stability, Periodicity and Dispersion

If we are interested in solving orbit problems, it is natural to ask how a particular numerical method would behave in the very simple case of uniform motion in a circular orbit, described by the test equation $y'' = -w^2 y$, i.e. we want the numerical solutions to mimic the behaviour of the solutions of the test equation.

2.5.1 Linear Multistep Methods

On applying the linear multistep method (2.5) to the test equation $y'' = -w^2 y$, we obtain the difference equation

$$\sum_{j=0}^{k} \left\{ \alpha_j + \nu^2 \beta_j \right\} y_{n+j} = 0, \quad \nu = wh$$

and the solution is determined by the roots ξ_s, assumed distinct, of the *stability or characteristic equation*

$$\Omega(\xi, \nu^2) := \sum_{j=0}^{k} \left\{ \alpha_j + \nu^2 \beta_j \right\} \xi^j = \rho(\xi) + \nu^2 \sigma(\xi) = 0. \tag{2.21}$$

Two of the roots, ξ_1 and ξ_2, say, tend to 1 as $\nu \to 0$ and are known as the principal roots of $\Omega(\xi, \nu^2)$, and ξ_s for $s \geq 3$, if any, are the spurious roots.

A popular way of analysing the stability of linear multistep methods is by using the Routh-Hurwitz criterion [46]. The transformation $\xi \to z$ where $\xi, z \in C$ is made where

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

with $z \neq 1$ and the roots z_1 and z_2 of the stability equation (2.21) now lie in the left-half plane (the unit circle $|\xi| = 1$ is mapped onto the imaginary axis $\operatorname{Re} z = 0$ and the unit disc $|\xi| < 1$ is mapped onto the left half-plane $\operatorname{Re} z < 0$). Let the polynomial $P(z)$ be defined by

$$P(z) := (1-z)^k \times \Omega\left(\frac{1+z}{1-z}, \nu^2\right) = a_0 z^k + a_1 z^{k-1} + \ldots + a_k. \tag{2.22}$$

For the linear multistep method to be absolutely stable, we require the roots ξ_s of the stability polynomial $\Omega(\xi, \nu^2)$ to have modulus less or equal to 1. Therefore, with $k = 2$ for example, we have $|\xi| \leq 1$ if a_0, a_1 and a_2 are positive. For $k \geq 3$, extra conditions are required to satisfy the criteria (c.f. Lambert [46]).

The following definition is taken from Hairer et al [32].

Definition 2.5 *The linear multistep method* (ρ, σ) *given by the characteristic polynomials* (2.21) *is said to be* **zero-stable** *if all the roots of* $\rho(\xi)$ *lie on or within the unit disc* $\{z \in C : |z| \leq 1\}$*, and any roots that lie on the unit circle* $\{z \in C : |z| = 1\}$ *have multiplicity at most 2.*

If a linear multistep method (ρ, σ),

(i) has no common factors in $\rho(\xi)$ and $\sigma(\xi)$,

(ii) is consistent, i.e. the order is at least one and

(iii) the method (ρ, σ) is zero-stable,

then the linear multistep method is convergent and the polynomial $\rho(\xi)$ has two roots $\xi_1 = \xi_2 = 1$, c.f. [35, 47].

Definition 2.6 *A linear multistep method* (2.5) *is* **absolutely stable** *for a given value of* ν *if, for that* ν*, all the roots* ξ_s *of equation* (2.21) *satisfy* $|\xi_s| \leq 1$*, and any roots on the unit circle are simple. If the method is absolutely stable for all* $\nu > 0$*, then the method is called* **unconditionally stable** [25].

Dahlquist [25] showed that the order of an unconditionally stable linear multistep method cannot exceed 2 and that it must be implicit. For a second-order implicit linear multistep method to be unconditionally stable, then all the solutions of the characteristic equation (2.21) must be bounded when applied to the test equation $y'' = -w^2 y$ for any value of the steplength h, or alternatively, the roots ξ_s of $\Omega(\xi, \nu^2)$ must not be outside the unit circle for any real ν.

Lambert and Watson [47] found that when Numerov's method was applied to the test equation $y'' = -w^2 y$, for relatively small steplengths h, the numerical solution stays on the orbit, taking into account the accumulation of rounding error. When a Störmer-Cowell method with stepnumber greater than two was applied, then the computed numerical solution spiralled inwards. This phenomenon was called "orbital instability" by Stiefel and Bettis [67]. Ideally, we would want the numerical solution of an integration method to remain periodic for all x with a period close to the true one. Lambert and Watson [47] appear to be the first to introduce the idea of an **interval of periodicity**.

The following definitions are taken from their work [47].

Definition 2.7 *A method has an interval of periodicity* $(0, \nu_0^2)$ *if, for all* $\nu^2 \in (0, \nu_0^2)$*, the roots* ξ_s *of* (2.21) *satisfy*

$$\xi_1 = \exp\{i\theta(\nu)\}, \quad \xi_2 = \exp\{-i\theta(\nu)\}, \quad |\xi_s| \leq 1, \quad s \geq 3$$

where $\theta(\nu)$ *is real.*

Many authors have used the notation $(0, \nu_0^2)$ for an interval of periodicity and this form shall be used for the polynomial based methods in this thesis.

Definition 2.8 *A method is said to be* **P-stable** *if its interval of periodicity is* $(0, \infty)$.

Many numerical methods, when applied to the test equation $y'' = -w^2 y$, give a characteristic equation of the form

$$\xi^2 - 2R_{nm}(\nu^2)\xi + 1 = 0 \tag{2.23}$$

where ν is real and $R_{nm}(\nu^2)$ is a rational function with numerator of degree n and denominator of degree m in ν^2. $R_{nm}(\nu^2)$ is called the *stability function* of the numerical method. Thus, the **primary interval of periodicity** of a method which has a stability equation (2.23) is the largest interval $(0, \beta^2)$ such that $|R_{nm}(\nu^2)| < 1$ for $0 < \nu^2 < \beta^2$. If when β is finite, $|R_{nm}(\nu^2)| < 1$ also for $\gamma^2 < \nu^2 < \delta^2$ where $\gamma^2 > \beta^2$, then the interval (γ^2, δ^2) is a **secondary interval of periodicity**. If $|R_{nm}(\nu^2)| < 1$ for all $\nu^2 > 0$, then the linear 2-step method is P-stable and the stability function $R_{nm}(\nu^2)$ is said to be P-acceptable, [17]. P-stability implies unconditional stability but not the other way around because P-stability requires that the principal roots of the stability polynomial $\Omega(\xi, \nu^2)$ lie on the unit circle whilst for unconditional stability they can lie in the unit disc. For linear multistep methods, the stability equation (2.23) is only obtained when we have 2 steps, that is $k = 2$.

Lambert and Watson [47] showed that a symmetric linear multistep method (ρ, σ) which has no double roots on the unit circle other than the principal roots, has a non vanishing interval of periodicity. They gave examples of 2, 4 and 6-step methods which contained intervals of periodicity and also a 2-step P-stable second-order linear multistep method. Lambert and Watson showed by numerical results that a symmetric 4-step 6th order method which has an interval of periodicity is far superior to a 5-step 6th order Störmer-Cowell method when solving oscillatory problems. Jeltsch [44] studied the stability and criteria for a linear multistep method to have an interval of periodicity. Chawla [8] considered modifying Numerov's method by making the method explicit and found that the resulting method has a larger interval of periodicity. Ixaru and Rizea [38] developed a family of 4-step 6th order methods to integrate problems such as (1.1) and they considered the stability and implementation of the methods.

The two-step implicit method of Cowell (Numerov's method)

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(f_{n+1} + 10f_n + f_{n-1})$$

where $f_{n+j} = f(x_{n+j}, y_{n+j})$, has stability function

$$R_{11}(\nu^2) = \frac{12 - 5\nu^2}{12 + \nu^2}$$

when applied to the test equation $y'' = -w^2 y$ and an interval of periodicity $(0, 6)$. Therefore Cowell's method is not P-stable as it has a finite interval of periodicity. Störmer-Cowell methods with stepnumber greater than two do not have an interval of periodicity. The main purpose of the paper by Stiefel and Bettis [67] was to adapt the coefficients of Cowell's method so that the numerical solution remained on the circular orbit. This was one motivation for fitting functions other than polynomials.

When the numerical solution of the test equation $y'' = -w^2 y$ remains on the circular orbit, the difference between the numerical solution and the exact solution is called the *dispersion*. It is also known as the phase difference, phase-lag error or frequency distortion.

Definition 2.9 *For any method corresponding to the characteristic equation* (2.23), *the quantity*

$$\phi(\nu) = \nu - \cos^{-1}\left[R_{nm}(\nu^2)\right]$$

is called the **dispersion**. *If* $\phi(\nu) = O(\nu^{q+1})$ *as* $\nu \to 0$, *the* **order of dispersion** *is* q.

We can rewrite the above equation for $\phi(\nu)$ as

$$\cos\nu - R_{nm}(\nu^2) = c\nu^{q+2} + O(\nu^{q+4})$$

and thus the order of dispersion can be seen as the order of accuracy of $R_{nm}(\nu^2)$ as an approximation for $\cos\nu$. Coleman [18] has shown that for linear multistep methods, the order of dispersion is equal to the algebraic order and for Runge-Kutta-Nyström methods and hybrid methods, the order of dispersion is greater or equal to the algebraic order.

Methods which have more than two steps have also been proposed [76, 43] and when they are applied to the test equation $y'' = -w^2 y$, a characteristic polynomial of degree k is obtained and the coefficients depend on ν^2. Jain et al [43] used the Routh-Hurwitz transformation to modify the coefficients of the 6th order implicit method of Lambert and Watson [47] and produced a 4-step 6th order P-stable method. Van der Houwen and Sommeijer [76] constructed 4th and 6th order predictor-corrector methods with phase errors up to order 10.

2.5.2 Runge-Kutta-Nyström Methods

The Runge-Kutta-Nyström method (2.12) in vector form is given by

$$\begin{aligned} y_{n+1} &= y_n + hz_n + h^2\mathbf{b}^T\mathbf{f}(\mathbf{e}x_n + \mathbf{c}h, \mathbf{y_{n+c}}) \\ z_{n+1} &= z_n + h\mathbf{d}^T\mathbf{f}(\mathbf{e}x_n + \mathbf{c}h, \mathbf{y_{n+c}}) \\ \mathbf{y_{n+c}} &= \mathbf{e}y_n + \mathbf{c}hz_n + h^2A\mathbf{f}(\mathbf{e}x_n + \mathbf{c}h, \mathbf{y_{n+c}}) \end{aligned}$$

where $\mathbf{e}$ is an $s-$dimensional vector with unit entries. Applying this method to the test equation $y'' = -w^2 y$ with $\nu = wh$ gives

$$\begin{aligned} y_{n+1} &= y_n + hz_n - \nu^2\mathbf{b}^T\mathbf{y_{n+c}} \\ z_{n+1} &= z_n - hw^2\mathbf{d}^T\mathbf{y_{n+c}} \\ \mathbf{y_{n+c}} &= \mathbf{e}y_n + \mathbf{c}hz_n - \nu^2A\mathbf{y_{n+c}}. \end{aligned}$$

Then rearranging the last equation,

$$\mathbf{y_{n+c}} = (I + \nu^2A)^{-1}(\mathbf{e}y_n + \mathbf{c}hz_n)$$

and substituting $\mathbf{y_{n+c}}$ into y_{n+1} gives

$$\begin{aligned} y_{n+1} &= y_n + hz_n - \nu^2\mathbf{b}^T(I + \nu^2A)^{-1}(\mathbf{e}y_n + \mathbf{c}hz_n) \\ &= \left\{1 - \nu^2\mathbf{b}^T(I + \nu^2A)^{-1}\mathbf{e}\right\}y_n + \left\{1 - \nu^2\mathbf{b}^T(I + \nu^2A)^{-1}\mathbf{c}\right\}hz_n. \end{aligned}$$

Similarly substituting $\mathbf{y_{n+c}}$ into hz_{n+1} gives

$$\begin{aligned} hz_{n+1} &= hz_n - \nu^2\mathbf{d}^T(I + \nu^2A)^{-1}(\mathbf{e}y_n + \mathbf{c}hz_n) \\ &= -\nu^2\mathbf{d}^T(I + \nu^2A)^{-1}\mathbf{e}y_n + \left\{1 - \nu^2\mathbf{d}^T(I + \nu^2A)^{-1}\mathbf{c}\right\}hz_n. \end{aligned}$$

We can write this in matrix form as

$$\begin{pmatrix} y_{n+1} \\ hz_{n+1} \end{pmatrix} = M(\nu^2) \begin{pmatrix} y_n \\ hz_n \end{pmatrix}$$

where

$$M(\nu^2) = \begin{pmatrix} 1 - \nu^2 \mathbf{b}^T (I + \nu^2 A)^{-1} \mathbf{e} & 1 - \nu^2 \mathbf{b}^T (I + \nu^2 A)^{-1} \mathbf{c} \\ -\nu^2 \mathbf{d}^T (I + \nu^2 A)^{-1} \mathbf{e} & 1 - \nu^2 \mathbf{d}^T (I + \nu^2 A)^{-1} \mathbf{c} \end{pmatrix}. \tag{2.24}$$

The eigenvalues $\xi(\nu)$ of the amplification matrix $M(\nu^2)$ are the roots of the characteristic equation [79]

$$\xi^2 - 2R_{nm}(\nu^2)\xi + P(\nu^2) = 0, \tag{2.25}$$

where

$$R_{nm}(\nu^2) = \frac{1}{2}\text{trace } M(\nu^2) \text{ and } P(\nu^2) = \det M(\nu^2)$$

are rational functions of ν^2.

Definition 2.10 *A Runge-Kutta-Nyström method* (2.12) *is* **absolutely stable** *for a given value of ν if, for that ν, the roots ξ_s of equation* (2.25) *satisfy* $|\xi_s| \leq 1$, $s = 1, 2$. *If the method is absolutely stable for all $\nu > 0$, then the method is called* **unconditionally stable**.

Hairer [30] showed that an implicit s-stage Runge-Kutta-Nyström method found by applying an implicit Runge-Kutta method based on Gauss-quadrature (c.f. Lambert [46]) to the first order differential system (2.9), has order $2s$ and is unconditionally stable. He also developed a tenth order explicit Runge-Kutta-Nyström method [31] in which only 11 stages are required. If the problem (1.1) is transformed into a system of first-order differential equations and then, for example, a Runge-Kutta method is applied, a minimum of 17 stages are needed. Chawla and Sharma [16] studied the stability properties of explicit Nyström methods and specifically 4th order explicit methods with 4 stages.

Definition 2.11 *A Runge-Kutta-Nyström method has an interval of periodicity* $(0, \nu_0^2)$ *if, for all* $\nu^2 \in (0, \nu_0^2)$, *the roots ξ_s of* (2.25) *satisfy*

$$\xi_1 = \exp\{i\theta(\nu)\} \text{ and } \xi_2 = \exp\{-i\theta(\nu)\},$$

where $\theta(\nu)$ is real.

If $\xi_1 = \exp\{i\theta\}$ and $\xi_2 = \exp\{-i\theta\}$, then

$$(\xi - \xi_1)(\xi - \xi_2) = \xi^2 - \xi(\xi_1 + \xi_2) + \xi_1\xi_2 = \xi^2 - 2\cos\theta\,\xi + 1.$$

Thus, for an interval of periodicity we require $P(\nu^2) = 1$.

When the characteristic equation is of the form (2.25), the following definition by Van der Houwen and Sommeijer [78] may be applied:

Definition 2.12 *The* **phase-error** *or* **dispersion** *of an RKN method with s-stages is defined by*

$$\phi(\nu) = \nu - \cos^{-1}\left[\frac{R_{nm}(\nu^2)}{\sqrt{P(\nu^2)}}\right]$$

assuming that $M(\nu^2)$ has complex conjugate eigenvalues for sufficiently small values of ν. Then, a Runge-Kutta-Nyström method has **order of dispersion** *q if $\phi(\nu) = O(h^{q+1})$ as $\nu \to 0$.*

Simos et al [65] derived a 4-stage 4th order Runge-Kutta-Nyström method with phase-lag of order 8 and found that the method is more accurate than conventional Runge-Kutta-Nyström methods when applied to problems with oscillatory solutions. Van der Houwen and Sommeijer [78] considered modifying diagonally implicit Runge-Kutta-Nyström methods because of the fact that they are self-starting and are easier to implement than fully implicit Runge-Kutta-Nyström methods. They created 2-stage and 3-stage methods with phase-lag of order up to 10 but with relatively low algebraic orders. When the methods were tested on linear problems with oscillatory solutions, they found that the results were considerably better than conventional DIRKN methods. For nonlinear problems and large stepsizes, the low algebraic order affects the accuracy of the methods despite the high dispersive order and the methods are comparable only to the standard DIRKN methods. Sharp et al [59] further investigated the work of [78] and studied families of DIRKN methods with algebraic orders 3 and 4.

Sideridis and Simos [60] studied the phase-lag of embedded Runge-Kutta methods where they derived a 3rd order explicit Runge-Kutta method with order of dispersion 6, and a 4th order method with order of dispersion 4. They showed that it is not possible to have a 5-stage 4th order explicit Runge-Kutta method with order of dispersion 6 because the coefficients have to be complex in order to satisfy all the requirements. Dormand et al [27] considered families of embedded explicit Runge-Kutta-Nyström formulae for problem (1.1).

2.5.3 Polynomial Collocation

One reason for the interest in polynomial collocation methods is because when the method is applied to the test equation $y'' = -w^2y$, we obtain a characteristic equation of the form (2.23) when symmetric collocation points are used. As mentioned earlier, Kramarz [45] showed that a symmetric collocation method has an interval of periodicity but was unable to find any P-stable collocation methods. Coleman [19] was able to prove that no symmetric collocation method can be P-stable. Because the polynomial collocation methods may be regarded as Runge-Kutta-Nyström methods, the stability theory for section 2.5.2 can be applied to polynomial collocation methods.

Stability for one collocation point

When we substitute the coefficients $b_1 = 1/2$, $d_1 = 1$ and $a_{11} = c^2/2$ for the one-point polynomial collocation method (2.15) into the amplification matrix $M(\nu^2)$, equation (2.24), we obtain

$$M_{11} = \frac{2 + c^2\nu^2 - \nu^2}{2 + c^2\nu^2}, \quad M_{12} = \frac{2 + c^2\nu^2 - c\nu^2}{2 + c^2\nu^2},$$

$$M_{21} = -\frac{2\nu^2}{2 + c^2\nu^2}, \quad M_{22} = \frac{2 + c^2\nu^2 - 2c\nu^2}{2 + c^2\nu^2}.$$

Therefore the characteristic equation is given by

$$\xi^2 - 2R_{11}(\nu^2)\xi + P(\nu^2) = 0 \tag{2.26}$$

where the stability function is

$$R_{11}(\nu^2) = \frac{4 + (2c^2 - 2c - 1)\nu^2}{2(2 + c^2\nu^2)}$$

and

$$P(\nu^2) = \frac{2 + (c-1)^2\nu^2}{2 + c^2\nu^2}.$$

For an interval of periodicity, we require $P(\nu^2) = 1$, and thus

$$P(\nu^2) = \frac{2 + (c-1)^2\nu^2}{2 + c^2\nu^2} = 1 \quad \Rightarrow \quad c = \frac{1}{2}.$$

Example : $c = 1/2$
With the collocation point $c = 1/2$, the characteristic equation is given by

$$\xi^2 - 2\left\{\frac{8 - 3\nu^2}{8 + \nu^2}\right\}\xi + 1 = 0.$$

The one-point polynomial collocation method (2.15) is stable if $|R_{11}(\nu^2)| \leq 1$. Thus,

$$\left|\frac{8 - 3\nu^2}{8 + \nu^2}\right| \leq 1$$

from which

$$8 - 3\nu^2 \leq 8 + \nu^2 \quad \Rightarrow \nu^2 \geq 0$$

and

$$-8 + 3\nu^2 \leq 8 + \nu^2 \quad \Rightarrow \nu^2 \leq 8.$$

Therefore the one-point polynomial collocation method has an interval of periodicity $(0, 8)$. Also, the order of dispersion of the method is 2 as

$$\phi(\nu) = \nu - \cos^{-1}\left[R_{11}(\nu^2)\right] = \frac{\nu^3}{48} - \frac{7}{2560}\nu^5 + O(\nu^7).$$

Example : $c = 0$
With the collocation point $c = 0$, the characteristic equation (2.26) is given by

$$\xi^2 - 2\left\{\frac{4 - \nu^2}{4}\right\}\xi + \frac{2 + \nu^2}{2} = 0.$$

Because $(2+\nu^2)/2 > 1$ except when $\nu = 0$, then the one-point polynomial collocation method with $c = 0$ is stable when $\nu = 0$ and unstable everywhere else. (We require the modulus of the roots ξ of the characteristic equation to be less or equal to 1. As $P(\nu^2)$ is the product of the roots, at least one of the roots is greater than 1 in this case).

Example : $c = 1$

The characteristic equation (2.26) with the collocation point $c = 1$ is

$$\xi^2 - \left\{\frac{4-\nu^2}{2+\nu^2}\right\}\xi + \frac{2}{2+\nu^2} = 0.$$

The roots are given by

$$\xi_\pm = \frac{4-\nu^2 \pm \sqrt{\nu^4 - 16\nu^2}}{2[2+\nu^2]}.$$

Using the Routh-Hurwitz approach, substituting $\xi = (1+z)/(1-z)$ into the characteristic equation, multiplying by $(1-z)^2$ and collecting in terms of z, the polynomial $P(z)$ becomes

$$P(z) = a_0 z^2 + a_1 z + a_2 = \frac{8z^2}{2+\nu^2} + \frac{2\nu^2 z}{2+\nu^2} + \frac{2\nu^2}{2+\nu^2}.$$

As the coefficients a_0, a_1 and a_2 are positive for all ν, then the modulus of the roots ξ_1 and ξ_2 of the characteristic equation are less or equal to 1 and the method is unconditionally stable.

Stability for two collocation points

The characteristic equation for the two-point polynomial collocation method (2.16) when applied to the test equation $y'' = -w^2 y$ is given by

$$\xi^2 - 2R_{22}(\nu^2)\xi + P(\nu^2) = 0$$

where the stability function is

$$R_{22}(\nu^2) = \frac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4}{1 + \beta_1\nu^2 + \beta_2\nu^4}$$

with

$$\alpha_0 = 1, \quad \alpha_1 = \frac{1}{6}(c_1^2 + c_2^2 - 2c_1c_2 - 3)$$

$$\alpha_2 = \frac{1}{24}(-c_2^2 + 2c_1^2c_2^2 - 2c_1c_2^2 + 2c_1c_2 + c_1 + c_2 - 2c_1^2c_2 - c_1^2)$$

$$\beta_1 = \frac{1}{6}(c_1 - c_2)^2, \quad \beta_2 = \frac{1}{12}c_1^2c_2^2$$

and

$$P(\nu^2) = \frac{\gamma_0 + \gamma_1\nu^2 + \gamma_2\nu^4}{1 + \delta_1\nu^2 + \delta_2\nu^4}$$

with

$$\gamma_0 = 1, \ \ \gamma_1 = \frac{1}{6}(c_1 - c_2)^2$$

$$\gamma_2 = \frac{1}{12}(c_1 - 1)^2(c_2 - 1)^2, \ \ \delta_1 = \frac{1}{6}(c_1 - c_2)^2, \ \ \delta_2 = \frac{1}{12}c_1^2c_2^2.$$

When $P(\nu^2) = 1$, the criteria for the polynomial collocation method to have an interval of periodicity are satisfied. Thus,

$$P(\nu^2) = 1 \ \ \Rightarrow \ \ (\gamma_0 - 1) + \nu^2(\gamma_1 - \delta_1) + \nu^4(\gamma_2 - \delta_2) = 0$$

and as $\gamma_0 = 1$ and $\gamma_1 = \delta_1$, then we look for values of c_1 and c_2 such that $\gamma_2 - \delta_2 = 0$,

$$\Rightarrow \ \ c_2^2(1 - 2c_1) - 2c_2(1 - c_1)^2 + (1 - c_1)^2 = 0$$

which is satisfied when

$$c_2 = \frac{1 - c_1}{1 - 2c_1} \ \text{ or } \ 1 - c_1.$$

When $c_1 = 1/2$, then the first expression is undefined and the second gives $c_2 = 1/2$. As we are only interested in distinct collocation nodes, we take the symmetric points $c_2 = 1 - c_1$, and the requirements are satisfied for the method to have an interval of periodicity.

Example : $c_1 = 0$ and $c_2 = 1$.
The characteristic equation is given by

$$\xi^2 - 2\left\{\frac{6 - 2\nu^2}{6 + \nu^2}\right\}\xi + 1 = 0$$

and the method has an interval of periodicity $(0, 12)$. The order of dispersion of the method is 2 as

$$\phi(\nu) = \nu - \cos^{-1}\left[R_{11}(\nu^2)\right] = \frac{\nu^3}{24} - \frac{3}{640}\nu^5 + O(\nu^7).$$

Example : $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$.
The characteristic equation is given by

$$\xi^2 - 2\left\{\frac{432 - 192\nu^2 + 7\nu^4}{432 + 24\nu^2 + \nu^4}\right\}\xi + 1 = 0$$

and the method has a primary interval of periodicity $(0, 9)$ and a secondary interval of periodicity $(12, 36)$. The order of dispersion of the method is 4 as

$$\phi(\nu) = \nu - \cos^{-1}\left[R_{22}(\nu^2)\right] = \frac{\nu^5}{4320} - \frac{\nu^7}{54432} + O(\nu^9).$$

Stability for three collocation points

The characteristic equation for the three-point polynomial collocation method (2.17) when applied to the test equation $y'' = -w^2 y$ is given by

$$\xi^2 - 2R_{33}(\nu^2)\xi + P(\nu^2) = 0$$

where

$$R_{33}(\nu^2) = \frac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4 + \alpha_3\nu^6}{1 + \beta_1\nu^2 + \beta_2\nu^4 + \beta_3\nu^6}$$

with

$$\alpha_0 = 1, \quad \alpha_1 = \frac{1}{12}[c_1^2 - (c_2+c_3)c_1 - c_2c_3 + c_2^2 + c_3^2 - 6],$$

$$\alpha_2 = \frac{1}{144}[2(c_2^2 + c_3^2 - 3 - 2c_2c_3)c_1^2 + 4(1 - c_2c_3^2 - c_2^2c_3 + 3c_2c_3)c_1$$
$$+3 + 4c_2 + 4c_3 + 2c_2^2c_3^2 - 6c_2^2 - 6c_3^2],$$

$$\alpha_3 = \frac{1}{288}\left\{[(2c_3^2 - 1 - 2c_3)c_2^2 + (1 + 2c_3 - 2c_3^2)c_2 - c_3(c_3-1)]c_1(c_1-1)\right.$$
$$\left.-c_2c_3(c_3-1)(c_2-1)\right\},$$

$$\beta_1 = \frac{1}{12}[c_1^2 - (c_2+c_3)c_1 + c_2^2 + c_3^2 - c_2c_3],$$

$$\beta_2 = \frac{1}{72}[(c_2-c_3)^2c_1^2 - 2c_2c_3(c_2+c_3)c_1 + c_2^2c_3^2], \quad \beta_3 = \frac{1}{144}c_1^2c_2^2c_3^2,$$

and

$$P = \frac{\gamma_0 + \gamma_1\nu^2 + \gamma_2\nu^4 + \gamma_3\nu^6}{1 + \delta_1\nu^2 + \delta_2\nu^4 + \delta_3\nu^6}$$

where

$$\gamma_0 = 1, \ \ \gamma_1 = \frac{1}{12}(c_1^2 + c_2^2 + c_3^2 - c_2c_3 - c_2c_1 - c_1c_3),$$

$$\gamma_2 = \frac{1}{72}[(c_2 - c_3)^2c_1^2 + (-6c_3 + 12c_2c_3 + 4 - 6c_2 - 2c_2^2c_3 - 2c_2c_3^2)c_1 \\ -6c_2c_3 + 4(c_2 + c_3) + c_2^2c_3^2 - 3],$$

$$\gamma_3 = \frac{1}{144}(c_3 - 1)^2(c_2 - 1)^2(c_1 - 1)^2,$$

$$\delta_1 = \frac{1}{12}(c_1^2 + c_2^2 + c_3^2 - c_2c_3 - c_2c_1 - c_1c_3),$$

$$\delta_2 = \frac{1}{72}[(c_2 - c_3)^2c_1^2 - 2c_2c_3(c_2 + c_3)c_1 + c_2^2c_3^2], \ \ \delta_3 = \frac{1}{144}c_1^2c_2^2c_3^2.$$

It is easily checked that the three-point polynomial collocation method has an interval of periodicity when symmetric collocation points are chosen, i.e. $c_1 = 1 - c_3$ and $c_2 = \frac{1}{2}$.

Example : $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$.
The stability function is a rational function with numerator and denominator of degree 2 in ν^2. The characteristic equation is given by

$$\xi^2 - 2\left\{\frac{288 - 126\nu^2 + 4\nu^4}{288 + 18\nu^2 + \nu^4}\right\}\xi + 1 = 0$$

and the method has two intervals of periodicity $(0, 48/5)$ and $(12, 48)$. The order of dispersion of the method is 4 as

$$\phi(\nu) = \nu - \cos^{-1}\left[R_{22}(\nu^2)\right] = \frac{1}{1920}\nu^5 - \frac{11}{387072}\nu^7 + O(\nu^9).$$

Example : $c_1 = (5 - \sqrt{15})/10$, $c_2 = 1/2$ and $c_3 = (5 + \sqrt{15})/10$.
The stability function is of the form $R_{33}(\nu^2)$, that is the numerator and denominator are cubics in ν^2. The characteristic equation is given by

$$\xi^2 - 2\left\{\frac{57600 - 26640\nu^2 + 1368\nu^4 - 13\nu^6}{57600 + 2160\nu^2 + 48\nu^4 + \nu^6}\right\}\xi + 1 = 0$$

and the method has a primary interval of periodicity $(0, 240/7)$ and a secondary interval of periodicity $(60, 2(27 + \sqrt{489}))$. The order of dispersion of the method is

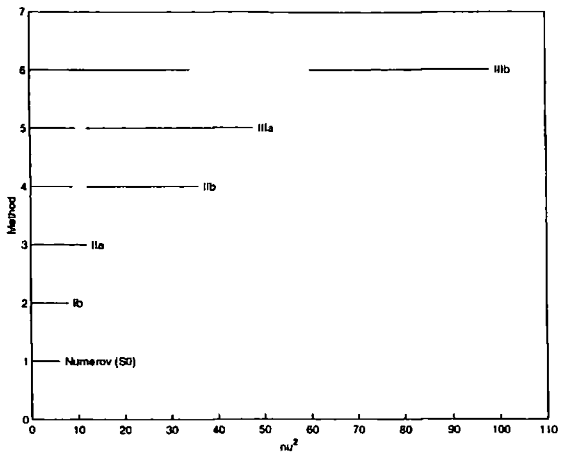

Figure 2.1: Periodicity intervals for the polynomial collocation methods

6 as

$$\phi(\nu) = \nu - \cos^{-1}\left[R_{33}(\nu^2)\right] = \frac{1}{806400}\nu^7 - \frac{1}{16588800}\nu^9 + O(\nu^{11}).$$

In figure 2.1, the intervals of periodicity are given. Method S_0 is Numerov's 4th order method whilst the polynomial collocation methods are listed below:

Method	Stage Number	Algebraic Order	Collocation Parameters
Ib	1	2	1/2
IIa	2	2	0 and 1
IIb	2	4	$(3-\sqrt{3})/6$ and $(3+\sqrt{3})/6$
$IIIa$	3	4	0, 1/2 and 1
$IIIb$	3	6	$(5-\sqrt{15})/10$, 1/2 and $(5+\sqrt{15})/10$

2.5.4 Hybrid Methods

As mentioned in section 2.3, the interest in hybrid methods came about as an answer to the order-barrier problem that a P-stable or unconditionally stable linear multistep method can have at most algebraic order 2, [25]. Cash [3] derived families of hybrid methods with properties such as P-stability and periodicity and imposed symmetry conditions on his methods. He constructed a 2-step 4th order implicit P-stable symmetric method and two 6th order methods, one P-stable and the other with an interval of periodicity (0,26). The main problem with the methods of Cash is the high cost to implement them; the 6th order P-stable method needs 5 function evaluations per iteration at each step.

All of the 2-step hybrid methods have a characteristic equation of the form

$$\xi^2 - 2R_{nm}(\nu^2)\xi + 1 = 0$$

and so the stability theory of the two previous sections can be applied. Coleman [17] showed that the hybrid method (2.18) of Cash [3] and Chawla [6] with $k = 1$ has a stability function of the form

$$R_{22}(\nu^2) = \frac{1 + \alpha_1\nu^2 + \alpha_2\nu^4}{1 + \beta_1\nu^2 + \beta_2\nu^4}$$

where the coefficients $\alpha_1, \alpha_2, \beta_1$ and β_2 are determined by the coefficients of (2.18). Coleman also considered stability functions of the form $R_{33}(\nu^2)$.

There has been a lot of literature on hybrid methods and the desire to modify them so they are suitable for solving (1.1) when the solution is oscillatory [2, 4, 7, 9, 11, 12, 13, 14, 15, 24, 43]. Chawla [6] noted that if a general $2p$-step (algebraic order $2p$) symmetric method is unconditionally stable, then it is also P-stable. He also describes a family of 4th order 2-step methods which possess a non vanishing interval of periodicity. Costabile and Costabile [24] derived a symmetric 2-step 4th order P-stable method which only needs 2 function evaluations per step and which is a special case of Cash's method. Authors who took the approach of modifying the free parameters in the hybrid method by Cash (2.19) include [4, 6, 24, 14, 68, 69].

Chawla [9] developed an explicit hybrid method which was a modification of Numerov's method. The main aim of the paper by Chawla and Neta [11] was to reduce the amount of work needed to implement Cash's hybrid methods (2.18) and they began a characterisation of the family of 4th order P-stable hybrid methods which was completed by Coleman [17]. Chawla et al [10] considered 2-step hybrid methods and derived a family of 4th and 6th order P-stable methods. They showed that the methods are *efficient*. By this they mean that the number of function-evaluations per step is reduced due to a choice of the free parameters of the method. Cash [4], Chawla and Neta [11], and Thomas [69, 70] considered efficient methods.

Some authors have modified their hybrid methods to use the idea of phase-lag to improve their methods as well as insuring that they are P-stable or that they have as large an interval of periodicity as possible [3, 13, 15, 68]. Chawla et al [15] started with a modification of Numerov's method

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}\left\{f_{n+1} + 10\bar{\bar{f}}_n + f_{n-1}\right\}$$

where

$$\bar{y}_n = y_n - \alpha h^2(f_{n+1} - 2f_n + f_{n-1}), \quad \bar{f}_n = f(t_n, \bar{y}_n)$$

$$\bar{\bar{y}}_n = \bar{y}_n - \beta h^2(f_{n+1} - 2\bar{f}_n + f_{n-1}), \quad \bar{\bar{f}}_n = f(t_n, \bar{\bar{y}}_n)$$

and the parameters α and β are free to be chosen to suit the phase-lag requirements. For an interval of periodicity, the modulus of the roots of the stability polynomial are of the form $\xi_{1,2} = \exp\{\pm i\theta(\nu)\}$ where $\theta(\nu)$ is real. Then, the phase-lag $\mathcal{P}(\nu)$, is the leading coefficient in the expansion of $|\{\theta(\nu) - \nu\}/\nu|$. Chawla et al found that for

$$\alpha + \beta = \frac{1}{200} \text{ and } \alpha\beta < -\frac{1}{10800}\left\{\frac{13}{18} + \sqrt{\frac{1331}{1620}}\right\},$$

the modified Numerov method was P-stable, of algebraic order 4 and phase-lag order 6. Anantha Krishnaiah [2] used the Maclaurin series of $\tan^{-1} x$ to find an expression for the phase-lag and obtained a family of 2-step P-stable methods of order 2 and a 6th order 2-step P-stable method with phase-lag of order 6. Twizell and Khaliq [74] and Twizell [73] investigated multiderivative methods, the latter using the same technique as Krishnaiah to find the expression for the phase-lag. This proves to be a clumsy way to do it and most authors use the expansion of $|\{\theta(\nu) - \nu\}/\nu|$ to find the phase-lag $\mathcal{P}(\nu)$. The methods of Chawla and Rao [14] were based on Cash's methods with particular choices of the parameters and they developed an explicit 2-step 6th order method with phase-lag of order 8. Thomas [68, 70] considered the phase-lag of 4th and 6th order P-stable hybrid methods and in the latter paper, reduced the number of function evaluations per iteration for a 6th order P-stable hybrid method to three.

Chapter 3

Exponentially-fitted Methods

In this chapter, we consider exponentially-fitted methods, that is numerical methods for the problem (1.1) which are exact for the particular differential equation $y'' = -k^2 y$ with initial conditions $y(x_0) = y_0$ and $y'(x_0) = z_0$, and which reproduce the exponentials $\exp(\pm ikx)$ exactly, taking into account the accumulation of rounding error.

The term 'mixed interpolation' appears to have been first introduced by De Meyer et al [49]. Polynomial interpolation is widely used, for example, to derive multistep methods or collocation methods for ordinary differential equations. Because of the interest in solving problems with oscillatory solutions, De Meyer et al adapted the interpolation approach to include functions other than polynomials. They considered approximating a function $f(x)$ by a combination of trigonometric and polynomial functions, i.e.

$$f_n(x) = a\cos(kx) + b\sin(kx) + \sum_{i=0}^{n-1} c_i x^i, \quad n \geq 2$$

and required the function $f_n(x)$ to interpolate $f(x)$ at $n+1$ equally spaced points. Then, there exists unique coefficients a, b and c_i, $i = 0, \ldots, n-1$ although the function is undefined for certain values of k. The theory was developed in a more general way by the authors Chakrabarti and Hamsapriye [5]. The trigonometric functions $\cos(kx)$ and $\sin(kx)$ are replaced by the two functions $U_1(kx)$ and $U_2(kx)$ which represent two linearly independent solutions of a general second-order linear ordinary differential equation for some $k > 0$.

Coleman [20] also considered the general approach of approximating $f(x)$ by the function

$$f_n(x) = aC(x) + bS(x) + \sum_{i=0}^{n-2} c_i x^i,$$

and considered existence and uniqueness of the function when $f_n(x_j) = f(x_j)$ for $j = 0, 1, \ldots, n$ where x_j are arbitrarily chosen distinct nodes. Coleman derived Lagrangian and Newtonian formulae for the interpolant and he used the first approach to find the mixed collocation methods [22] whilst the latter approach is used in this thesis.

3.1 Linear Multistep Methods

Consider the linear k-step method

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j y''_{n+j}$$

where α_j and β_j are constants. The linear operator L is defined by

$$L[y(x); h] = \sum_{j=0}^{k} \alpha_j y(x + jh) - h^2 \sum_{j=0}^{k} \beta_j y''(x + jh).$$

For polynomial based multistep methods, we would find α_j and β_j, $j = 0, 1, .., k$ such that the operator L integrates exactly polynomials up to a sufficient order. If the coefficients α_j and β_j are allowed to depend upon the steplength h, then they can be obtained such that the operator L integrates exactly functions of the form $\exp(\pm\mu x)$, as well as polynomials. This approach is known as *exponential-fitting.* If μ is real, the method is suited, for example, to integrate the Schrödinger equation which has an exponentially decaying solution. If μ is imaginary, i.e. $\mu = i\phi$, then the method is suited to solving problems with oscillatory solutions and the methods are exact for $\cos(\phi x)$ and $\sin(\phi x)$. Our interest lies in the latter case.

Gautschi [28] first derived the concept of *trigonometric order* for linear multistep methods.

Definition 3.1 *A functional L is of* **trigonometric order** *p, relative to period T, if it annihilates all trigonometric polynomials of order $\leq p$ with period T.*

A suitable value for the period T has to be chosen to implement the methods.

Gautschi's methods are exact if the solution of the differential equation is oscillatory with constant period (or frequency). He only considered using trigonometric functions but since then, there has been considerable interest in combinations of polynomial and trigonometric functions. Stiefel and Bettis [67] considered both types of functions and modified Cowell's equations. Jain [41] modified the Stiefel-Bettis method so it could be applied to nonlinear problems where $y'' = f(x, y, y')$. Lyche [48] developed the work of Gautschi and considered steplength dependent coefficients for linear multistep methods. He derived a 4th order 2-step method and as the frequencies approach zero, Simpson's method is recovered. Lyche also developed consistency and stability requirements for exponentially-fitted multistep methods but as mentioned in Ixaru and Rizea [37], the stability theory only applies to multistep methods which have steplength dependent coefficients for β_j but with α_j constant.

Before the introduction of exponentially-fitted methods, one of the most popular methods for solving problems with oscillatory solutions was Numerov's method because of its large interval of periodicity. Many authors including [37, 56, 72] take the approach of modifying Numerov's method so that it is exact for polynomial and trigonometric functions. As the fitted frequencies tend to zero, then the methods reduce to Numerov's method. Raptis and Allison [56] found that their methods were more efficient than Numerov's method for solving the Schrödinger equation and they also had the advantage that it integrates exactly $\exp(\pm\mu x)$. The authors [37, 54] derived methods which are exact for certain combinations of products of polynomial and trigonometric functions, i.e. $x^m \sin(kx)$, $x^m \cos(kx)$. Ixaru and Rizea showed that their methods gave more accurate results for the Schrödinger equation using a combination of the functions. They developed stability theory for multistep methods with steplength dependent coefficients.

Many 2-step and 4-step exponentially-fitted methods have been produced, some specifically for the solution of the Schrödinger equation [36, 37, 54, 55, 56, 57, 61, 63, 64, 66, 72]. Simos [63] derived a family of 4-step exponentially-fitted methods starting from the formulae of Henrici [35]

$$y_{n+2} + a_0(y_{n+1} + y_{n-1}) + y_{n-2} = h^2\left[\beta_0(y''_{n+2} + y''_{n-2}) + \beta_1(y''_{n+1} + y''_{n-1}) + \beta_2 y''_n\right]$$

and obtained the coefficients so that the method is exact for a combination of polynomial and trigonometric functions. As for other exponentially-fitted methods, an estimate of the frequency parameter is required. In a later paper by Simos [64], he derived a family of 4-step exponentially-fitted predictor-corrector methods. Thomas et al [72] produced 2-step predictor-corrector methods but they required the methods to integrate as many combinations of polynomial and trigonometric functions as possible. They also looked at the stability of the methods but only when the fitted frequency of the method is the same as the frequency of the test equation. This does not give an accurate analysis of the stability of the methods because the stability definitions they used were designed for methods with constant coefficients. This was also the case by the authors Jain et al [42]. They concluded that their method is P-stable, but this is only when the test frequency and the fitted frequency are the same. Coleman and Ixaru [23] investigated the stability of multistep and hybrid methods with steplength dependent coefficients. Whilst they were mainly concerned with 2-step methods, Ixaru et al [39] considered the stability analysis for 4-step exponentially-fitted methods. The authors Raptis and Cash [57] considered fitting Bessel and Neumann functions to 2-step and 4-step methods respectively. The only drawback of the methods is that the coefficients must be calculated at every step.

3.2 One-step Methods

So far, most of the exponentially-fitted methods that have been produced are linear multistep methods or hybrid methods. The mixed collocation methods that shall be derived in chapter 4 will be exponentially-fitted and also can be written as a Runge-Kutta-Nyström method with steplength dependent coefficients.

3.2.1 Trigonometric Order

Paternoster [53] and Ozawa [51] both adapted the definition for trigonometric order for linear multistep methods and applied it to Runge-Kutta-Nyström methods.

Definition 3.2 *An s-stage Runge-Kutta-Nyström method is said to be of* **trigonometric order** *r relative to the frequency k, if the linear operators given by*

$$\left.\begin{aligned}
\mathcal{L}_1[y] &= y(x+h) - y(x) - hy'(x) - h^2 \sum_{i=1}^{s} b_i f(x + c_i h, Y_i) \\
\mathcal{L}_2[y] &= y'(x+h) - y'(x) - h \sum_{i=1}^{s} d_i f(x + c_i h, Y_i) \\
\mathcal{L}[y] &= y(x+c_i h) - y(x) - c_i hy'(x) - h^2 \sum_{j=1}^{s} a_{ij} f(x + c_j h, Y_j), \\
\text{where}\quad Y_i &= y(x) + c_i hy'(x) + h^2 \sum_{j=1}^{s} a_{ij} f(x + c_j h, Y_j) \\
&\qquad \text{for } i = 1, \ldots, s
\end{aligned}\right\} \quad (3.1)$$

annihilate the functions $y(x) = \cos(pkx)$ *and* $y(x) = \sin(pkx)$ *for* $p = 1, \ldots, r$ *and are not annihilated by* $y(x) = \cos[(r+1)kx]$ *or* $y(x) = \sin[(r+1)kx]$.

Thus, if we require the Runge-Kutta-Nyström method to be of trigonometric order r, for $p = 1, \ldots, r$ then

$$\sum_{i=1}^{s} b_i \cos(p\theta c_i) = \frac{1-\cos(p\theta)}{p^2\theta^2}, \quad \sum_{i=1}^{s} b_i \sin(p\theta c_i) = \frac{p\theta - \sin(p\theta)}{p^2\theta^2},$$

$$\sum_{i=1}^{s} d_i \cos(p\theta c_i) = \frac{\sin(p\theta)}{p\theta}, \quad \sum_{i=1}^{s} d_i \sin(p\theta c_i) = \frac{1-\cos(p\theta)}{p\theta}$$

and

$$\left.\begin{aligned}
\sum_{j=1}^{s} a_{ij} \cos(p\theta c_j) &= \frac{1-\cos(p\theta c_i)}{p^2\theta^2} \\
\sum_{j=1}^{s} a_{ij} \sin(p\theta c_j) &= \frac{p\theta c_i - \sin(p\theta c_i)}{p^2\theta^2}
\end{aligned}\right\} \text{ for } i = 1, \ldots, s.$$

We will show in chapter 4 that for arbitrary c_1 and c_2, the 2-stage Runge-Kutta-Nyström method of trigonometric order 1 (which we shall denote as TRKN1) is the 2-point mixed collocation method. The method derived by Paternoster [53] is a 2nd order TRKN1 method or the two-point mixed collocation method with $c_1 = 1/4$ and $c_2 = 3/4$.

Theorem 1 *For $s \geq 2$, an s-stage Runge-Kutta-Nyström method of trigonometric order 1 has $s^2 - 4$ free parameters.*

Proof: For the coefficients b_i and d_i there are 2 equations in s unknowns respectively, thus each leaving $s - 2$ free parameters. For the coefficients a_{ij} where $i = 1, \ldots, s$ there are again 2 equations in s unknowns for each i and so there are $s \times (s-2)$ free parameters remaining. Thus, we have

$$(s-2) + (s-2) + s \times (s-2) = s^2 - 4 \text{ free parameters.} \blacksquare$$

The method constructed by Ozawa [51] is a 4-stage 4th order implicit TRKN1 method and depending on the choice of the coefficient b_4, the method has order of dispersion 4 or 6. Ozawa showed the improved accuracy of the method with the higher order of dispersion especially when only an estimate of the frequency is available. Ozawa stated that in order to construct an implicit 4th order Runge-Kutta-Nyström method of trigonometric order 1, then it is necessary to have a minimum of 4 stages because of his choice of conditions on the coefficients. In fact, for 2 stages with the coefficients b_i, d_i and a_{ij} above, $r = 1$, and the points $c_1 = (3 - \sqrt{3})/6$ and $c_2 = (3 + \sqrt{3})/6$, we have a TRKN1 method with algebraic order 4. In Appendix A, the coefficients for a 4th order 3-stage TRKN1 method are presented which satisfy Ozawa's order conditions.

3.3 Hybrid Methods

Simos [64] and Thomas et al [72] considered modifying predictor-corrector methods so that they are exponentially-fitted, the former looked at 4-step methods and the latter, Numerov-type methods. This lead to the work by Thomas and Simos [71] in which they included off-step points for the 2-step predictor-corrector methods and developed five methods which integrate exactly functions of the form $[1, x, .., x^m, \exp(\pm ikx), ..., x^p \exp(\pm ikx)]$ with $m = 9$ and $p = 0$, $m = 7$ and $p = 1$, $m = 5$ and $p = 2$, $m = 3$ and $p = 3$, and $m = 1$ and $p = 4$. They showed that because their methods integrate exactly more exponential functions than the authors [64] and [72] and other exponentially-fitted Numerov-type methods, their methods are more accurate when solving the Schrödinger equation. Again, the stability analysis is based on the fact that the fitted frequency of the method and the test equation are the same, i.e. they applied the stability theory for methods with constant coefficients. The authors did study the stability for a range of values for the fitted frequency and deduced that the methods are almost P-stable.

3.4 Order

3.4.1 Linear Multistep Methods

We define the linear functional for the multistep method by

$$\mathcal{L}[y(x);h] = \sum_{j=0}^{k} \alpha_j(h)y(x+jh) - h^2 \sum_{j=0}^{k} \beta_j(h)y''(x+jh) \tag{3.2}$$

where we assume $y(x)$ is as differentiable as we please and the coefficients α_i and β_i depend on the steplength h. Let

$$\begin{aligned}\alpha_i &= \alpha_i^{(0)} + h\alpha_i^{(1)} + h^2\alpha_i^{(2)} + \dots \\ \beta_i &= \beta_i^{(0)} + h\beta_i^{(1)} + h^2\beta_i^{(2)} + \dots.\end{aligned}$$

Then

$$\mathcal{L}[y(x);h] = C_0' + C_1'h + C_2'h^2 + \dots + C_r'h^r + \dots$$

where

$$C_0' = \sum_{i=0}^{k} \alpha_i^{(0)} y(x), \quad C_1' = \sum_{i=0}^{k} \left\{ \alpha_i^{(1)} y(x) + i\alpha_i^{(0)} y'(x) \right\},$$

and for $r = 2, 3, \dots$,

$$C_r' = \sum_{i=0}^{k} \left\{ \alpha_i^{(r)} y(x) + \sum_{j=1}^{r} \left[\frac{i^j\, \alpha_i^{(r-j)}}{j!} y^{(j)}(x) \right] - \sum_{j=2}^{r} \left[\frac{i^{j-2}\, \beta_i^{(r-j)}}{(j-2)!} y^{(j)}(x) \right] \right\}.$$

Definition 3.3 *A linear multistep method* (2.5) *and the associated linear operator* (3.2) *with coefficients α_j and β_j dependent on the steplength h, are said to be of* **order p** *if $C_0' = C_1' = .. = C_{p+1}' = 0$ and $C_{p+2}' \neq 0$.*

Therefore, for **order 1** we require

$$C_0' = 0 \;\Rightarrow\; \sum_{i=0}^{k} \alpha_i^{(0)} = 0,$$

$$C_1' = 0 \;\Rightarrow\; \sum_{i=0}^{k}\alpha_i^{(1)} = 0,\; \sum_{i=0}^{k} i\alpha_i^{(0)} = 0,$$

and

$$C_2' = 0 \;\Rightarrow\; \sum_{i=0}^{k}\alpha_i^{(2)} = 0,\; \sum_{i=0}^{k} i\alpha_i^{(1)} = 0,\; \sum_{i=0}^{k}\left[\frac{i^2}{2}\alpha_i^{(0)} - \beta_i^{(0)}\right] = 0.$$

3.4.2 Runge-Kutta-Nyström Methods

First, we expand the coefficients of the Runge-Kutta-Nyström method about $h = 0$ and let

$$\begin{aligned} b_i(h) &= b_i^{(0)} + hb_i^{(1)} + h^2 b_i^{(2)} + \dots \\ d_i(h) &= d_i^{(0)} + hd_i^{(1)} + h^2 d_i^{(2)} + \dots \\ a_{ij}(h) &= a_{ij}^{(0)} + ha_{ij}^{(1)} + h^2 a_{ij}^{(2)} + \dots \end{aligned}$$

The difference operators for the Runge-Kutta-Nyström method are defined by

$$\begin{aligned} \mathcal{L}[y] &= y(x_n + c_i h) - y(x_n) - c_i h y'(x_n) - h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), \\ \mathcal{L}_1[y] &= y(x_n + h) - y(x_n) - hy'(x_n) - h^2 \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i) \\ \mathcal{L}_2[y] &= y'(x_n + h) - y'(x_n) - h\sum_{i=1}^{s} d_i f(x_n + c_i h, Y_i). \end{aligned}$$

Here, a bare-hands Taylor series approach is used to expand the difference operators $\mathcal{L}_1[y]$, $\mathcal{L}_2[y]$ and $\mathcal{L}[y]$ but the work soon becomes very complicated if higher powers of the steplength h are required, even though we are only dealing with a single equation. A different technique for finding the higher order conditions will be studied later on in this section.

First, expand

$$\begin{aligned} \mathcal{L}[y] &= y(x_n + c_i h) - Y_i \\ &= y(x_n + c_i h) - y(x_n) - c_i h y'(x_n) - h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) \\ &= \frac{c_i^2}{2} h^2 y''(x_n) + \frac{c_i^3}{6} h^3 y^{(3)}(x_n) + \frac{c_i^4}{24} h^4 y^{(4)}(x_n) - h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) + .. \\ &= h^2 \delta_i \end{aligned}$$

where δ_i is finite as $h \to 0$, and so

$$Y_i = y(x_n + c_i h) - \mathcal{L}[y] = y(x_n + c_i h) - h^2 \delta_i.$$

If we substitute Y_j into $f(x_n + c_j h, Y_j)$ and expand about $x_n + c_j h$, then $\mathcal{L}[y]$ becomes

$$\mathcal{L}[y] = h^2 \left(\frac{c_i^2}{2} - \sum_{j=1}^{s} a_{ij} \right) y''(x_n) + h^3 \left(\frac{c_i^3}{6} - \sum_{j=1}^{s} a_{ij} c_j \right) y^{(3)}(x_n)$$
$$+ h^4 \left\{ \left(\frac{c_i^4}{24} - \sum_{j=1}^{s} \frac{a_{ij} c_j^2}{2} \right) y^{(4)}(x_n) \right.$$
$$\left. + \sum_{j=1}^{s} a_{ij} \left(\frac{c_j^2}{2} - \sum_{k=1}^{s} a_{jk} \right) y''(x_n) f_y(x_n + c_j h, y(x_n + c_j h)) \right\} + O(h^5).$$

Using the expansion for a_{ij} and setting $f_y(x_n + c_j h, y(x_n + c_j h)) = f_y(c_j)$, then

$$\mathcal{L}[y] = h^2 \left(\frac{c_i^2}{2} - \sum_{j=1}^{s} a_{ij}^{(0)} \right) y''(x_n) + h^3 \left\{ \left(\frac{c_i^3}{6} - \sum_{j=1}^{s} a_{ij}^{(0)} c_j \right) y^{(3)}(x_n) - \sum_{j=1}^{s} a_{ij}^{(1)} y''(x_n) \right\}$$
$$+ h^4 \left\{ \left(\frac{c_i^4}{24} - \sum_{j=1}^{s} \frac{a_{ij}^{(0)} c_j^2}{2} \right) y^{(4)}(x_n) - \sum_{j=1}^{s} a_{ij}^{(2)} y''(x_n) - \sum_{j=1}^{s} a_{ij}^{(1)} c_j y^{(3)}(x_n) \right.$$
$$\left. + \sum_{j=1}^{s} a_{ij}^{(0)} \left(\frac{c_j^2}{2} - \sum_{k=1}^{s} a_{jk}^{(0)} \right) y''(x_n) f_y(c_j) \right\} + O(h^5) = h^2 \delta_i.$$

Therefore

$$f(x_n + c_i h, Y_i) = y''(x_n) + c_i h y'''(x_n) + h^2 \left\{ \frac{c_i^2}{2} y^{(4)}(x_n) - \left(\frac{c_i^2}{2} - \sum_{j=1}^{s} a_{ij}^{(0)} \right) y''(x_n) f_y(c_i) \right\}$$
$$+ h^3 \left\{ \frac{c_i^3}{6} y^{(5)}(x_n) - f_y(c_i) \left[\left(\frac{c_i^3}{6} - \sum_{j=1}^{s} a_{ij}^{(0)} c_j \right) y^{(3)}(x_n) - \sum_{j=1}^{s} a_{ij}^{(1)} y''(x_n) \right] \right\}$$
$$+ h^4 \left\{ \frac{c_i^4}{24} y^{(6)}(x_n) - f_y(c_i) \left[\left(\frac{c_i^4}{24} - \sum_{j=1}^{s} \frac{a_{ij}^{(0)} c_j^2}{2} \right) y^{(4)}(x_n) - \sum_{j=1}^{s} a_{ij}^{(2)} y''(x_n) \right. \right.$$
$$\left. - \sum_{j=1}^{s} a_{ij}^{(1)} c_j y^{(3)}(x_n) + \sum_{j=1}^{s} a_{ij}^{(0)} \left(\frac{c_j^2}{2} - \sum_{k=1}^{s} a_{jk}^{(0)} \right) y''(x_n) f_y(c_j) \right]$$

$$+\frac{1}{2}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s}a_{ij}^{(0)}\right)^2 f_{yy}(c_i)y''(x_n)^2\Bigg\}+O(h^5).$$

We need to expand $f_y(x_n+c_ih, y(x_n+c_ih))$. With $\mathcal{F}(h)=f_y(x_n+c_ih, y(x_n+c_ih))$,

$$\mathcal{F}(h)=\mathcal{F}(0)+h\mathcal{F}'(0)+\frac{h^2}{2}\mathcal{F}''(0)+O(h^3)$$

where

$$\mathcal{F}(0)=f_y(x_n,y(x_n)),\quad \mathcal{F}'(0)=c_i\left\{y'(x_n)f_{yy}(x_n,y(x_n))+f_{yx}(x_n,y(x_n))\right\},$$

$$\mathcal{F}''(0)=c_i^2\left\{f_{yxx}(x_n,y(x_n))+2y'(x_n)f_{yyx}(x_n,y(x_n))\right.$$
$$\left.+y''(x_n)f_{yy}(x_n,y(x_n))+y'(x_n)^2f_{yyy}(x_n,y(x_n))\right\}.$$

For convenience in notation, let $f=f(x_n,y(x_n))$, $f_y=\dfrac{\partial f(x_n,y(x_n))}{\partial y}$, etc., then

$$\mathcal{L}_1[y]=h^2\left(\frac{1}{2}-\sum_{i=1}^{s}b_i^{(0)}\right)y''(x_n)$$

$$+\quad h^3\left\{\left(\frac{1}{6}-\sum_{i=1}^{s}b_i^{(0)}c_i\right)y^{(3)}(x_n)-\sum_{i=1}^{s}b_i^{(1)}y''(x_n)\right\}$$

$$+\quad h^4\left\{\left(\frac{1}{24}-\sum_{i=1}^{s}\frac{b_i^{(0)}c_i^2}{2}\right)y^{(4)}(x_n)-\sum_{i=1}^{s}b_i^{(2)}y''(x_n)-\sum_{i=1}^{s}b_i^{(1)}c_iy^{(3)}(x_n)\right.$$
$$\left.+\sum_{i=1}^{s}b_i^{(0)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s}a_{ij}^{(0)}\right)y''(x_n)f_y\right\}$$

$$+\quad h^5\left\{\left(\frac{1}{120}-\sum_{i=1}^{s}\frac{b_i^{(0)}c_i^3}{6}\right)y^{(5)}(x_n)-\sum_{i=1}^{s}b_i^{(3)}y''(x_n)-\sum_{i=1}^{s}b_i^{(2)}c_iy^{(3)}(x_n)\right.$$
$$-\sum_{i=1}^{s}\frac{b_i^{(1)}c_i^2}{2}y^{(4)}(x_n)+\sum_{i=1}^{s}\left[b_i^{(1)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s}a_{ij}^{(0)}\right)-\sum_{j=1}^{s}b_i^{(0)}a_{ij}^{(1)}\right]y''(x_n)f_y$$

$$+\sum_{i=1}^{s} b_i^{(0)}\left(\frac{c_i^3}{6}-\sum_{j=1}^{s} a_{ij}^{(0)}c_j\right) y^{(3)}(x_n)f_y+\sum_{i=1}^{s} b_i^{(0)}c_i\left(\frac{c_i^2}{2}-\sum_{j=1}^{s} a_{ij}^{(0)}\right) y''(x_n)f_{xy}$$

$$+\sum_{i=1}^{s} b_i^{(0)}c_i\left(\frac{c_i^2}{2}-\sum_{j=1}^{s} a_{ij}^{(0)}\right) y'(x_n)y''(x_n)f_{yy}\Bigg\}+O(h^6)$$

and

$$\mathcal{L}_2[y] = h\left(1-\sum_{i=1}^{s} d_i^{(0)}\right)y''(x_n)+h^2\left\{\left(\frac{1}{2}-\sum_{i=1}^{s} d_i^{(0)}c_i\right)y^{(3)}(x_n)-\sum_{i=1}^{s} d_i^{(1)}y''(x_n)\right\}$$

$$+ h^3\Bigg\{\left(\frac{1}{6}-\sum_{i=1}^{s}\frac{d_i^{(0)}c_i^2}{2}\right)y^{(4)}(x_n)-\sum_{i=1}^{s} d_i^{(2)}y''(x_n)-\sum_{i=1}^{s} d_i^{(1)}c_iy^{(3)}(x_n)$$

$$+\sum_{i=1}^{s} d_i^{(0)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s} a_{ij}^{(0)}\right)y''(x_n)f_y\Bigg\}$$

$$+ h^4\Bigg\{\left(\frac{1}{24}-\sum_{i=1}^{s}\frac{d_i^{(0)}c_i^3}{6}\right)y^{(5)}(x_n)-\sum_{i=1}^{s} d_i^{(3)}y''(x_n)-\sum_{i=1}^{s} d_i^{(2)}c_iy^{(3)}(x_n)$$

$$-\sum_{i=1}^{s}\frac{d_i^{(1)}c_i^2}{2}y^{(4)}(x_n)+\sum_{i=1}^{s}\left[d_i^{(1)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s} a_{ij}^{(0)}\right)-\sum_{j=1}^{s} d_i^{(0)}a_{ij}^{(1)}\right]y''(x_n)f_y$$

$$+\sum_{i=1}^{s} d_i^{(0)}\left(\frac{c_i^3}{6}-\sum_{j=1}^{s} a_{ij}^{(0)}c_j\right)y^{(3)}(x_n)f_y$$

$$+\sum_{i=1}^{s} d_i^{(0)}c_i\left(\frac{c_i^2}{2}-\sum_{j=1}^{s} a_{ij}^{(0)}\right)y''(x_n)\left[y'(x_n)f_{yy}+f_{xy}\right]\Bigg\}$$

$$+ h^5\Bigg\{\left(\frac{1}{120}-\sum_{i=1}^{s}\frac{d_i^{(0)}c_i^4}{24}\right)y^{(6)}(x_n)-\sum_{i=1}^{s} d_i^{(4)}y''(x_n)-\sum_{i=1}^{s} d_i^{(3)}c_iy^{(3)}(x_n)$$

$$-\sum_{i=1}^{s}\frac{d_i^{(2)}c_i^2}{2}y^{(4)}(x_n)-\sum_{i=1}^{s}\frac{d_i^{(1)}c_i^3}{6}y^{(5)}(x_n)$$

$$+\sum_{i=1}^{s}\left[d_i^{(2)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s} a_{ij}^{(0)}\right)-\sum_{j=1}^{s} d_i^{(0)}a_{ij}^{(2)}-\sum_{j=1}^{s} d_i^{(1)}a_{ij}^{(1)}\right]y''(x_n)f_y$$

$$+\sum_{i=1}^{s}\left[d_i^{(1)}\left(\frac{c_i^3}{6}-\sum_{j=1}^{s}a_{ij}^{(0)}c_j\right)-\sum_{j=1}^{s}d_i^{(0)}a_{ij}^{(1)}c_j\right]y^{(3)}(x_n)f_y$$

$$+\sum_{i=1}^{s}d_i^{(0)}\left(\frac{c_i^4}{24}-\sum_{j=1}^{s}\frac{a_{ij}^{(0)}c_j^2}{2}\right)y^{(4)}(x_n)f_y$$

$$+\sum_{i=1}^{s}\sum_{j=1}^{s}d_i^{(0)}a_{ij}^{(0)}\left(\frac{c_j^2}{2}-\sum_{k=1}^{s}a_{jk}^{(0)}\right)y''(x_n)f_y^2$$

$$+\frac{1}{2}\sum_{i=1}^{s}d_i^{(0)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s}a_{ij}^{(0)}\right)^2 y''(x_n)^2 f_{yy}$$

$$+\sum_{i=1}^{s}c_i\left[d_i^{(1)}\left(\frac{c_i^2}{2}-\sum_{j=1}^{s}a_{ij}^{(0)}\right)-\sum_{j=1}^{s}d_i^{(0)}a_{ij}^{(1)}\right]y''(x_n)\left[y'(x_n)f_{yy}+f_{xy}\right]$$

$$+\sum_{i=1}^{s}d_i^{(0)}c_i\left(\frac{c_i^3}{6}-\sum_{j=1}^{s}a_{ij}^{(0)}c_j\right)y'''(x_n)\left[y'(x_n)f_{yy}+f_{xy}\right]$$

$$+\frac{1}{2}\sum_{i=1}^{s}d_i^{(0)}c_i^2\left(\frac{c_i^2}{2}-\sum_{j=1}^{s}a_{ij}^{(0)}\right)y''(x_n)\left[f_{yxx}+2y'(x_n)f_{yyx}+y'(x_n)^2f_{yyy}\right]\Bigg\}+O(h^6).$$

From Definition 2.4 the order conditions are as follows: (The order 6 conditions were obtained using Butcher's tree approach which is described at the end of this section).

The Order Conditions

Order 1:

$$1.)\sum_{i=1}^{s}d_i^{(0)}=1.$$

Order 2:

$$2.)\sum_{i=1}^{s}d_i^{(0)}c_i=\frac{1}{2},\quad 3.)\sum_{i=1}^{s}d_i^{(1)}=0,\quad 4.)\sum_{i=1}^{s}b_i^{(0)}=\frac{1}{2}.$$

Order 3:

$$5.)\sum_{i=1}^{s}d_i^{(0)}c_i^2=\frac{1}{3},\quad 6.)\sum_{i=1}^{s}d_i^{(1)}c_i=0,\quad 7.)\sum_{i=1}^{s}d_i^{(2)}=0,$$

$$8.)\sum_{i=1}^{s}\sum_{j=1}^{s}d_i^{(0)}a_{ij}^{(0)}=\frac{1}{6},\quad 9.)\sum_{i=1}^{s}b_i^{(0)}c_i=\frac{1}{6},\quad 10.)\sum_{i=1}^{s}b_i^{(1)}=0.$$

Order 4:

$$11.)\sum_{i=1}^{s} d_i^{(0)} c_i^3 = \frac{1}{4},\quad 12.)\sum_{i=1}^{s} d_i^{(1)} c_i^2 = 0,\quad 13.)\sum_{i=1}^{s} d_i^{(2)} c_i = 0,\quad 14.)\sum_{i=1}^{s} d_i^{(3)} = 0,$$

$$15.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{d_i^{(1)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(1)}\right\} = 0,\quad 16.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j = \frac{1}{24},$$

$$17.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i = \frac{1}{8},\quad 18.)\sum_{i=1}^{s} b_i^{(0)} c_i^2 = \frac{1}{12},$$

$$19.)\sum_{i=1}^{s} b_i^{(2)} = 0,\quad 20.)\sum_{i=1}^{s} b_i^{(1)} c_i = 0,\quad 21.)\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} = \frac{1}{24}.$$

Order 5:

$$22.)\sum_{i=1}^{s} d_i^{(0)} c_i^4 = \frac{1}{5},\quad 23.)\sum_{i=1}^{s} d_i^{(1)} c_i^3 = 0,\quad 24.)\sum_{i=1}^{s} d_i^{(2)} c_i^2 = 0,\quad 25.)\sum_{i=1}^{s} d_i^{(3)} c_i = 0,$$

$$26.)\sum_{i=1}^{s} d_i^{(4)} = 0,\quad 27.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{d_i^{(2)} a_{ij}^{(0)} + d_i^{(1)} a_{ij}^{(1)} + d_i^{(0)} a_{ij}^{(2)}\right\} = 0,$$

$$28.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{d_i^{(1)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(1)}\right\} c_j = 0,\quad 29.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j^2 = \frac{1}{60},$$

$$30.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} = \frac{1}{120},\quad 31.)\sum_{i=1}^{s} d_i^{(0)}\left(\sum_{j=1}^{s} a_{ij}^{(0)}\right)^2 = \frac{1}{20},$$

$$32.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{d_i^{(1)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(1)}\right\} c_i = 0,\quad 33.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i c_j = \frac{1}{30},$$

$$34.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^2 = \frac{1}{10},\quad 35.)\sum_{i=1}^{s} b_i^{(0)} c_i^3 = \frac{1}{20},\quad 36.)\sum_{i=1}^{s} b_i^{(1)} c_i^2 = 0,$$

$$37.)\ \sum_{i=1}^{s} b_i^{(2)} c_i = 0,\quad 38.)\ \sum_{i=1}^{s} b_i^{(3)} = 0,\quad 39.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ b_i^{(1)} a_{ij}^{(0)} + b_i^{(0)} a_{ij}^{(1)} \right\} = 0,$$

$$40.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_j = \frac{1}{120},\quad 41.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_i = \frac{1}{40}.$$

Order 6:

$$42.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^5 = \frac{1}{6},\quad 43.)\ \sum_{i=1}^{s} d_i^{(1)} c_i^4 = 0,\quad 44.)\ \sum_{i=1}^{s} d_i^{(2)} c_i^3 = 0,$$

$$45.)\ \sum_{i=1}^{s} d_i^{(3)} c_i^2 = 0,\quad 46.)\ \sum_{i=1}^{s} d_i^{(4)} c_i = 0,\quad 47.)\ \sum_{i=1}^{s} d_i^{(5)} = 0,$$

$$48.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(3)} a_{ij}^{(0)} + d_i^{(2)} a_{ij}^{(1)} + d_i^{(1)} a_{ij}^{(2)} + d_i^{(0)} a_{ij}^{(3)} \right\} = 0,$$

$$49.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(2)} a_{ij}^{(0)} + d_i^{(1)} a_{ij}^{(1)} + d_i^{(0)} a_{ij}^{(2)} \right\} c_i = 0,$$

$$50.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(2)} a_{ij}^{(0)} + d_i^{(1)} a_{ij}^{(1)} + d_i^{(0)} a_{ij}^{(2)} \right\} c_j = 0,$$

$$51.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(1)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(1)} \right\} c_i^2 = 0,$$

$$52.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(1)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(1)} \right\} c_j^2 = 0,\quad 53.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(1)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(1)} \right\} c_i c_j = 0,$$

$$54.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^3 = \frac{1}{12},\quad 55.)\ \sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} c_i = \frac{1}{144},$$

$$56.)\ \sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{ik}^{(0)} c_k = \frac{1}{72}, \quad 57.)\ \sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} c_j = \frac{1}{240},$$

$$58.)\ \sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} c_k = \frac{1}{720}, \quad 59.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j^3 = \frac{1}{120},$$

$$60.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i c_j^2 = \frac{1}{72}, \quad 61.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^2 c_j = \frac{1}{36},$$

$$62.)\ \sum_{i=1}^{s} d_i^{(0)} c_i \left(\sum_{j=1}^{s} a_{ij}^{(0)}\right)^2 = \frac{1}{24}, \quad 63.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(1)} \left(a_{ij}^{(0)}\right)^2 + 2 d_i^{(0)} a_{ij}^{(1)} a_{ij}^{(0)} \right\} = 0,$$

$$64.)\ \sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} \left\{ d_i^{(1)} a_{ij}^{(0)} a_{jk}^{(0)} + d_i^{(0)} a_{ij}^{(1)} a_{jk}^{(0)} + d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(1)} \right\} = 0,$$

$$65.)\ \sum_{i=1}^{s} b_i^{(0)} c_i^4 = \frac{1}{30}, \quad 66.)\ \sum_{i=1}^{s} b_i^{(1)} c_i^3 = 0, \quad 67.)\ \sum_{i=1}^{s} b_i^{(2)} c_i^2 = 0, \quad 68.)\ \sum_{i=1}^{s} b_i^{(3)} c_i = 0,$$

$$69.)\ \sum_{i=1}^{s} b_i^{(4)} = 0, \quad 70.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ b_i^{(2)} a_{ij}^{(0)} + b_i^{(1)} a_{ij}^{(1)} + b_i^{(0)} a_{ij}^{(2)} \right\} = 0,$$

$$71.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ b_i^{(1)} a_{ij}^{(0)} + b_i^{(0)} a_{ij}^{(1)} \right\} c_i = 0, \quad 72.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ b_i^{(1)} a_{ij}^{(0)} + b_i^{(0)} a_{ij}^{(1)} \right\} c_j = 0,$$

$$73.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_i^2 = \frac{1}{60}, \quad 74.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_i c_j = \frac{1}{180},$$

$$75.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_j^2 = \frac{1}{360}, \quad 76.)\ \sum_{i=1}^{s} b_i^{(0)} \left(\sum_{j=1}^{s} a_{ij}^{(0)}\right)^2 = \frac{1}{120},$$

$$77.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} b_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} = \frac{1}{720}.$$

The order conditions can be applied to any Runge-Kutta-Nyström method with steplength dependent coefficients and they reduce to those for the Runge-Kutta-Nyström method with constant coefficients if we retain $b_i^{(0)}$, $d_i^{(0)}$ and $a_{ij}^{(0)}$ and set the rest of the coefficients to zero.

Butcher's tree approach

It is possible to identify the order conditions for methods with relatively few stages using a bare-hands Taylor series approach. As we have seen, the work soon becomes difficult and this approach is unsuitable for most methods due to the complexity and number of the computations involved. The order conditions for order 6 were found using Butcher's tree based approach [46, 32, 34] which although usually used for Runge-Kutta and Runge-Kutta-Nyström methods with constant coefficients, is easily extended to apply to Runge-Kutta-Nyström methods with steplength dependent coefficients.

The Runge-Kutta-Nyström method with constant coefficients is of at least **order** 1 when

$$\sum_{i=1}^{s} d_i = 1,$$

and for **order** 2, in addition to the above we require

$$\sum_{i=1}^{s} d_i c_i = \frac{1}{2} \text{ and } \sum_{i=1}^{s} b_i = \frac{1}{2}.$$

First, let the coefficients depend on the steplength and define

$$\begin{aligned} b_i(h) &= b_i^{(0)} + h b_i^{(1)} + h^2 b_i^{(2)} + \dots \\ d_i(h) &= d_i^{(0)} + h d_i^{(1)} + h^2 d_i^{(2)} + \dots \\ a_{ij}(h) &= a_{ij}^{(0)} + h a_{ij}^{(1)} + h^2 a_{ij}^{(2)} + \dots \end{aligned}$$

Following Coleman [22] and using the notation of Dormand et al [27], an alternative way of writing the local truncation error of a Runge-Kutta-Nyström method is

$$t_{n+1} = y(x_{n+1}) - y_{n+1} = \sum_{i=2}^{N} h^i \left(\sum_{j=1}^{\eta_i} \tau_j^{(i)} F_j^{(i)} \right) + O(h^{N+1})$$

where we make the usual localising assumption. The terms τ are made up of combinations of the coefficients b_i, d_i and a_{ij}, and each of the expressions $F^{(i)}$ is an elementary differential. A similar expression can be found for the error in the approximation for the first derivative,

$$t'_{n+1} = y'(x_{n+1}) - z_{n+1} = \sum_{i=2}^{N} h^{i-1} \left(\sum_{j=1}^{\eta_i} \tau_j^{(i)'} F_j^{(i)} \right) + O(h^{N+1}).$$

When we consider steplength dependent coefficients for a Runge-Kutta-Nyström method, all that is required is to expand the τ expressions in terms of the steplength h. As the $F_j^{(i)}$ are independent then the appropriate expressions can be collected in terms of the steplength. The method is then of order at least p if $t_{n+1} = O(h^{p+1})$ and $t'_{n+1} = O(h^{p+1})$.

Thus, the order conditions for a Runge-Kutta-Nyström method with steplength dependent coefficients are,

for **order** at least 1,

$$\sum_{i=1}^{s} d_i^{(0)} = 1,$$

and for **order** at least 2 along with the above condition,

$$\sum_{i=1}^{s} d_i^{(1)} = 0, \quad \sum_{i=1}^{s} d_i^{(0)} c_i = \frac{1}{2} \quad \text{and} \quad \sum_{i=1}^{s} b_i^{(0)} = \frac{1}{2}.$$

The conditions involving only coefficients which have a superscript 0 are the order conditions for the Runge-Kutta-Nyström method with constant coefficients.

3.5 Stability Analysis

Stability analysis becomes more complicated for exponential-fitted methods as there are now three parameters h, k and w to consider. The stability analysis is based on the test equation $y'' = -w^2 y$ for problems which have oscillatory solutions. As before, k is the fitted frequency of the mixed collocation method and specifies a pair of functions $\exp(\pm ikx)$ which the numerical method will integrate exactly. The steplength is h, and w, which is real, determines the relevant frequency in the test equation $y'' = -w^2 y$.

For many numerical methods and the mixed collocation methods of this thesis, when they are applied to the test equation $y'' = -w^2 y$, the characteristic equation is of the form

$$\xi^2 - 2R_{nm}(\nu^2;\theta)\xi + P(\nu^2;\theta) = 0$$

where $\theta = kh$ and $\nu = wh$. When $P(\nu^2;\theta) = 1$, the question posed by Coleman and Ixaru [23] is:

For a given method (i.e. a given k), what restriction, if any, must be placed on the steplength h to ensure that the condition $|R_{nm}(\nu^2;\theta)| < 1$ is satisfied?

The following definition is taken from the work by Coleman and Ixaru [23]:

Definition 3.4 *A* **region of stability** *is a region of the $\nu - \theta$ plane, throughout which $|R_{nm}(\nu^2;\theta)| < 1$. Any closed curve defined by $|R_{nm}(\nu^2;\theta)| = 1$ is a* **stability boundary**.

Definition 3.5 *For an exponential-fitting method with the stability function given by $R_{nm}(\nu^2;\theta)$, where $\nu = wh$ and $\theta = kh$, and w and k are given, the* **primary interval of periodicity** *is the largest interval $(0, h_0)$ such that $|R_{nm}(\nu^2;\theta)| < 1$ for all steplengths $h \in (0, h_0)$. If, when h_0 is finite, $|R_{nm}(\nu^2;\theta)| < 1$ also for $\gamma < h < \delta$, where $\gamma > h_0$, then the interval (γ, δ) is a* **secondary interval of periodicity** [23].

Alternatively, an exponential-fitting method with the stability function $R_{nm}(\nu^2;\theta)$ has an interval of periodicity $(0, \beta^2)$ if the roots ξ_i of

$$\xi^2 - 2R_{nm}(\nu^2;\theta)\xi + 1 = 0 \qquad (3.3)$$

satisfy

$$\xi_1 = \exp\{i\theta(\nu)\}, \quad \xi_2 = \exp\{-i\theta(\nu)\}.$$

When $|R_{nm}(\nu^2;\theta)| < 1$, the roots of the equation (3.3) are distinct and lie on the unit circle.

When $|R_{nm}(\nu^2;\theta)| > 1$, the method is unstable since the corresponding difference equation has an unbounded solution.

Note that for a polynomial based method the notation for an interval of periodicity used by many authors is $(0, \nu_0^2)$ (c.f. Definitions (2.7) and (2.11)), whilst for exponentially-fitted methods it is $(0, h_0)$. As $k \to 0$, the periodicity interval for the corresponding polynomial based method is easily found from the interval of periodicity for the exponentially-fitted method.

Definition 3.6 *A family of exponential-fitting methods with the stability function given by $R_{nm}(\nu^2; \theta)$ is* **P-stable** *if, for each value of k, the inequality $|R_{nm}(\nu^2; \theta)| < 1$ holds for all values of w and for all steplengths h, except possibly for a discrete set of exceptional values of h determined by the chosen value of k.*

As an example, Coleman and Ixaru [23] developed a P-stable method satisfying Definition 3.6. The 2-step exponentially-fitted method is

$$y_{n+1} - 2y_n + y_{n-1} = h^2[\beta_1(f_{n+1} + f_{n-1}) - 2\alpha_1 f_n]$$

where

$$\beta_1 = \frac{1 - \cos\theta + \gamma\theta^2}{\theta^2(1 + \cos\theta)}, \quad \alpha_1 = \gamma - \beta_1, \quad \gamma \geq 0$$

and it is undefined when $\theta = (2n-1)\pi$, but $R_{11}(\nu^2; \theta) \to 1$ as $\theta \to (2n-1)\pi$.

A method corresponding to a given value of the parameter k must solve the test equation $y'' = -w^2 y$ exactly, in the absence of rounding error, when $k = w$, i.e. $\theta = \nu$. Since all solutions of the test equation satisfy

$$y(x_{n+2}) - 2(\cos\nu)y(x_{n+1}) + y(x_n) = 0,$$

the stability function may be regarded as a rational approximation for $\cos\nu$.

Chapter 4

The Mixed Collocation Method

In this chapter, we derive the mixed collocation methods which are exact for the problem

$$y'' = -k^2 y, \;\; y(x_0) = y_0, \;\; y'(x_0) = z_0$$

where k is a constant. It will be shown that the mixed collocation methods may be regarded as Runge-Kutta-Nyström methods with steplength dependent coefficients and a study of the order conditions is given.

Consider approximating the solution $y(x)$ on the interval $[x_n, x_{n+1}]$ by a function $u(x)$ of the form

$$u(x) = a \cos\, k(x - x_n) + b \sin\, k(x - x_n) + \sum_{i=0}^{s-1} r_i (x - x_n)^i.$$

The choice of the functions cos $k(x - x_n)$ and sin $k(x - x_n)$ is that they are the two linearly independent solutions of the second-order differential operator

$$L = \frac{d^2}{dx^2} + k^2.$$

If we use a collocation method based on the s distinct collocation points

$$x_{n+c_j} = x_n + c_j h, \;\; j = 1, \ldots, s$$

where $0 \le c_1 < c_2 < \ldots < c_s \le 1$ then the collocation conditions are

$$u''(x_n + c_j h) = f(x_n + c_j h, u(x_n + c_j h)), \;\; j = 1, \ldots, s.$$

Differentiating the collocating function $u(x)$ with respect to x,

$$\left.\begin{aligned} u(x) &= a\cos kt + b\sin kt + \sum_{i=0}^{s-1} r_i t^i \\ u'(x) &= -ak\sin kt + bk\cos kt + \sum_{i=0}^{s-1} i r_i t^{(i-1)} \\ u''(x) &= -ak^2\cos kt - bk^2\sin kt + \sum_{i=0}^{s-1} i(i-1) r_i t^{(i-2)} \end{aligned}\right\} \quad (4.1)$$

where $t = x - x_n$ and applying the initial and collocation conditions we obtain

$$\left.\begin{aligned} u(x_n) = y_n \quad &\Rightarrow \quad y_n = a + r_0 \\ u'(x_n) = z_n \quad &\Rightarrow \quad \begin{cases} z_n = bk, & s = 1 \\ z_n = bk + r_1, & s \geq 2 \end{cases} \\ u''(x_n + c_j h) \quad &= \quad -ak^2\cos(\theta c_j) - bk^2\sin(\theta c_j) + \sum_{i=2}^{s-1} i(i-1) r_i (c_j h)^{(i-2)} \\ &\qquad j = 1, \ldots, s \end{aligned}\right\} \quad (4.2)$$

with $\theta = kh$.

4.1 Construction

4.1.1 One Collocation Point

Consider the function

$$u(x) = a\cos[k(x - x_n)] + b\sin[k(x - x_n)] + r_0.$$

A one-point mixed collocation method is defined by

$$\begin{aligned} y_{n+1} &= a\cos\theta + b\sin\theta + r_0 \\ z_{n+1} &= -ak\sin\theta + bk\cos\theta \\ y_{n+c} &= a\cos(\theta c) + b\sin(\theta c) + r_0 \end{aligned}$$

where $\theta = kh$, and y_{n+1}, z_{n+1} and y_{n+c} are approximations for the exact solutions $y(x_n + h)$, $y'(x_n + h)$ and $y(x_n + ch)$ respectively.

From the initial and collocation conditions (4.2) for $s = 1$,

$$r_0 = y_n - a,\ b = z_n/k,\ -ak^2\cos(\theta c) - bk^2\sin(\theta c) = f(x_n + ch, u(x_n + ch)).$$

The latter equation can be easily solved to give

$$a = -h^2\left\{\frac{f(x_n + ch, u(x_n + ch)) + z_n k\sin(\theta c)}{\theta^2\cos(\theta c)}\right\}$$

which is undefined if $\theta = 0$ or $\cos(\theta c) = 0$. Thus the formulae for a one-point mixed collocation method with collocation node $x_n + ch$ are

$$\begin{aligned} y_{n+1} &= y_n + hz_n\frac{\sin\theta}{\theta} + h^2(1-\cos\theta)\left\{\frac{f(x_n + ch, Y) + z_n k\sin(\theta c)}{\theta^2\cos(\theta c)}\right\}, \\ z_{n+1} &= z_n\cos\theta + h\sin\theta\left\{\frac{f(x_n + ch, Y) + z_n k\sin(\theta c)}{\theta\cos(\theta c)}\right\}, \\ Y &= y_n + hz_n\frac{\sin(\theta c)}{\theta} + h^2(1-\cos(\theta c))\left\{\frac{f(x_n + ch, Y) + z_n k\sin(\theta c)}{\theta^2\cos(\theta c)}\right\} \end{aligned}$$

where $Y = y_{n+c}$.

This can be rewritten as

$$\left.\begin{aligned} y_{n+1} &= y_n + hz_n\left\{\frac{\sin[\theta(1-c)] + \sin(\theta c)}{\theta\cos(\theta c)}\right\} + h^2\frac{(1-\cos\theta)}{\theta^2\cos(\theta c)}f_{n+c}, \\ z_{n+1} &= z_n\frac{\cos[\theta(1-c)]}{\cos(\theta c)} + h\frac{\sin\theta}{\theta\cos(\theta c)}f_{n+c}, \\ Y &= y_n + hz_n\frac{\sin(\theta c)}{\theta\cos(\theta c)} + h^2\frac{(1-\cos(\theta c))}{\theta^2\cos(\theta c)}f_{n+c} \end{aligned}\right\} \qquad (4.3)$$

where $f_{n+c} = f(x_n + ch, Y)$.

Note that when $\theta\cos(\theta c) = 0$ the method is undefined. Also, the coefficients of method (4.3) are even functions of θ.

As $k \to 0$ the mixed collocation method (4.3) reduces to

$$\begin{aligned} y_{n+1} &= y_n + hz_n + \frac{h^2}{2}f_{n+c}, \\ z_{n+1} &= z_n + hf_{n+c}, \end{aligned}$$

$$Y = y_n + chz_n + \frac{c^2h^2}{2} f_{n+c},$$

which is the one-point polynomial collocation method (2.15). The mixed collocation method (4.3) cannot be written as a Runge-Kutta-Nyström method except in the limit as $k \to 0$. We will see that this is only the case for the one-point mixed collocation method.

Example : $c = 0$
Substituting $c = 0$ into (4.3)

$$y_{n+1} = y_n + hz_n \frac{\sin\theta}{\theta} + h^2 \frac{(1-\cos\theta)}{\theta^2} f(x_n, y_n), \qquad (4.4)$$

$$z_{n+1} = z_n \cos\theta + h \frac{\sin\theta}{\theta} f(x_n, y_n). \qquad (4.5)$$

For convenience in notation let $f_{n+j} = f(x_{n+j}, y_{n+j})$. Then from (4.4) with the subscript increased by 1, we may write y_{n+2} as

$$y_{n+2} = y_{n+1} + hz_{n+1} \frac{\sin\theta}{\theta} + h^2 \frac{(1-\cos\theta)}{\theta^2} f_{n+1},$$

and if we substitute (4.5) into y_{n+2} then

$$\begin{aligned} y_{n+2} &= y_{n+1} + h\frac{\sin\theta}{\theta}\left\{ z_n\cos\theta + h\frac{\sin\theta}{\theta} f_n \right\} + h^2\frac{(1-\cos\theta)}{\theta^2} f_{n+1}, \\ &= y_{n+1} + h\frac{\sin\theta\cos\theta}{\theta} z_n + h^2\frac{\sin^2\theta}{\theta^2} f_n + h^2\left\{\frac{1-\cos\theta}{\theta^2}\right\} f_{n+1}. \end{aligned}$$

Substituting for z_n from (4.4) gives

$$y_{n+2} = y_{n+1} + \cos\theta\left\{ y_{n+1} - y_n - h^2\frac{(1-\cos\theta)}{\theta^2} f_n \right\} + h^2\frac{\sin^2\theta}{\theta^2} f_n + h^2\frac{(1-\cos\theta)}{\theta^2} f_{n+1}$$

and this can be rewritten in two-step form as

$$y_{n+2} - (1+\cos\theta)y_{n+1} + \cos\theta y_n = h^2\frac{(1-\cos\theta)}{\theta^2}\left\{ f_{n+1} + f_n \right\}.$$

Example : $c = 1$

Substituting $c = 1$ into (4.3) gives

$$\begin{aligned} y_{n+1} &= y_n + hz_n\frac{\sin\theta}{\theta\cos\theta} + h^2\frac{(1-\cos\theta)}{\theta^2\cos\theta}f_{n+1}, \\ z_{n+1} &= \frac{z_n}{\cos\theta} + h\frac{\sin\theta}{\theta\cos\theta}f_{n+1}, \end{aligned}$$

which can be written in two-step form as

$$\cos\theta\, y_{n+2} - (1+\cos\theta)y_{n+1} + y_n = h^2\frac{(1-\cos\theta)}{\theta^2}\left\{f_{n+1} + f_{n+2}\right\}.$$

Example : $c = 1/2$

Substituting $c = 1/2$ into (4.3) gives

$$\begin{aligned} y_{n+1} &= y_n + hz_n\frac{2\sin\frac{\theta}{2}}{\theta\cos\frac{\theta}{2}} + h^2\frac{(1-\cos\theta)}{\theta^2\cos\frac{\theta}{2}}f_{n+1/2}, \\ z_{n+1} &= z_n + h\frac{\sin\theta}{\theta\cos\frac{\theta}{2}}f_{n+1/2}, \\ y_{n+\frac{1}{2}} &= y_n + hz_n\frac{\sin\frac{\theta}{2}}{\theta\cos\frac{\theta}{2}} + h^2\frac{(1-\cos\frac{\theta}{2})}{\theta^2\cos\frac{\theta}{2}}f_{n+1/2}. \end{aligned}$$

4.1.2 Two or More Collocation Points

First we define $F(c_j) = f(x_n + c_jh, u(x_n + c_jh))$ for $j = 1, \ldots, s$.

For $s \geq 2$, from the initial and collocation conditions (4.2), we obtain a system of $s+2$ equations in $s+2$ unknowns of the form $\mathrm{A}\mathbf{x} = \mathbf{b}$ where

$$A = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & \ldots & 0 \\ 0 & k & 0 & 1 & 0 & 0 & \ldots & 0 \\ -k^2\cos(\theta c_1) & -k^2\sin(\theta c_1) & 0 & 0 & 2 & 6c_1h & \ldots & g(s)(c_1h)^{s-3} \\ -k^2\cos(\theta c_2) & -k^2\sin(\theta c_2) & 0 & 0 & 2 & 6c_2h & \ldots & g(s)(c_2h)^{s-3} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ -k^2\cos(\theta c_s) & -k^2\sin(\theta c_s) & 0 & 0 & 2 & 6c_sh & \ldots & g(s)(c_sh)^{s-3} \end{pmatrix},$$

$$\mathbf{x} = \begin{pmatrix} a \\ b \\ r_0 \\ r_1 \\ \cdots \\ r_{s-1} \end{pmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} y_n \\ z_n \\ F(c_1) \\ F(c_2) \\ \cdots \\ F(c_s) \end{pmatrix}$$

where $\theta = kh$ and we define $g(s) = (s-1)(s-2)$. If the matrix A is non-singular, then it is possible to find a, b and $\{r_i\}$, $i = 0, \ldots, s-1$.

First, reduce the determinant of A to an $s \times s$ determinant:

$$\det A = \begin{vmatrix} -k^2\cos(\theta c_1) & -k^2\sin(\theta c_1) & 2 & 6c_1h & \ldots & (s-1)(s-2)(c_1h)^{s-3} \\ -k^2\cos(\theta c_2) & -k^2\sin(\theta c_2) & 2 & 6c_2h & \ldots & (s-1)(s-2)(c_2h)^{s-3} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -k^2\cos(\theta c_s) & -k^2\sin(\theta c_s) & 2 & 6c_sh & \ldots & (s-1)(s-2)(c_sh)^{s-3} \end{vmatrix}$$

$$\begin{aligned} &= k^4 \,.\, 2 \,.\, 6h \,.\, 12h^2 \,.\, 20h^3 \ldots (s-1) \,.\, (s-2) \,.\, h^{s-3} \times (\det B) \\ &= k^4\,(s-1)!\,(s-2)!\,h \,.\, h^2 \,.\, h^3 \ldots h^{s-3} \times (\det B) \\ &= k^4\,(s-1)!\,(s-2)!\,h^{(s-2)(s-3)/2} \times (\det B) \end{aligned}$$

where

$$B = \begin{pmatrix} \cos(\theta c_1) & \sin(\theta c_1) & 1 & c_1 & c_1^2 & \ldots & c_1^{s-3} \\ \cos(\theta c_2) & \sin(\theta c_2) & 1 & c_2 & c_2^2 & \ldots & c_2^{s-3} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cos(\theta c_s) & \sin(\theta c_s) & 1 & c_s & c_s^2 & \ldots & c_s^{s-3} \end{pmatrix}. \tag{4.6}$$

The determinant of B is evaluated using the technique applied to the Vandermonde determinant. First, multiply the third column of det B by the leading terms of the first and second columns and subtract the modified column from columns one and two respectively. For columns 4 to s, multiply each preceding column by the leading term of column 4 and subtract this from the columns respectively from which the determinant of B is given by

$$\begin{vmatrix} 0 & 0 & 1 & 0 & 0 & \dots & 0 \\ \cos(\theta c_2)-\cos(\theta c_1) & \sin(\theta c_2)-\sin(\theta c_1) & 1 & W_{2,1} & c_2 W_{2,1} & \dots & c_2^{s-4} W_{2,1} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \cos(\theta c_s)-\cos(\theta c_1) & \sin(\theta c_s)-\sin(\theta c_1) & 1 & W_{s,1} & c_s W_{s,1} & \dots & c_s^{s-4} W_{s,1} \end{vmatrix}$$

where $W_{p,1} = c_p - c_1$.

The determinant of B can be reduced to an $(s-1)\times(s-1)$ determinant and we divide the i-th row by $(c_i - c_1)$, thus we have

$$(c_2-c_1)\dots(c_s-c_1)\begin{vmatrix} \dfrac{\cos(\theta c_2)-\cos(\theta c_1)}{(c_2-c_1)} & \dfrac{\sin(\theta c_2)-\sin(\theta c_1)}{(c_2-c_1)} & 1 & c_2 & \dots & c_2^{s-4} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dfrac{\cos(\theta c_s)-\cos(\theta c_1)}{(c_s-c_1)} & \dfrac{\sin(\theta c_s)-\sin(\theta c_1)}{(c_s-c_1)} & 1 & c_s & \dots & c_s^{s-4} \end{vmatrix}.$$

Definition 4.1 *Let $R(c_j)$ be a function evaluated at q distinct points $\{c_i\}_{i=1}^{q}$. Then, we define the* **divided differences** *$R[c_1, c_2, \dots, c_j]$, $j = 1, 2, \dots, q$ recursively by*

$$R[c_j] := R(c_j), \quad R[c_1, c_2, \dots, c_j] := \frac{R[c_2, c_3, \dots, c_j] - R[c_1, c_2, \dots, c_{j-1}]}{c_j - c_1}.$$

If we define $\bar{p}(x) = \cos(\theta x)$, $\bar{q}(x) = \sin(\theta x)$ and $F(c_j) = f(x_n + c_j h, u(x_n + c_j h))$ for $j = 1, 2, \dots, s$ then

$$\bar{p}[c_1, c_2, \dots, c_j] = \frac{\bar{p}[c_2, c_3, \dots, c_j] - \bar{p}[c_1, c_2, \dots, c_{j-1}]}{c_j - c_1},$$
$$\bar{q}[c_1, c_2, \dots, c_j] = \frac{\bar{q}[c_2, c_3, \dots, c_j] - \bar{q}[c_1, c_2, \dots, c_{j-1}]}{c_j - c_1},$$
$$F[c_1, c_2, \dots, c_j] = \frac{F[c_2, c_3, \dots, c_j] - F[c_1, c_2, \dots, c_{j-1}]}{c_j - c_1}.$$

Thus

$$\det B = \prod_{i=2}^{s}(c_i - c_1)\begin{vmatrix} \bar{p}[c_1,c_2] & \bar{q}[c_1,c_2] & 1 & c_2 & \dots & c_2^{s-4} \\ \bar{p}[c_1,c_3] & \bar{q}[c_1,c_3] & 1 & c_3 & \dots & c_3^{s-4} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \bar{p}[c_1,c_s] & \bar{q}[c_1,c_s] & 1 & c_s & \dots & c_s^{s-4} \end{vmatrix}.$$

Repeating the above process, the determinant of B is

$$\prod_{i=2}^{s}(c_i - c_1)\prod_{i=3}^{s}(c_i - c_2)\ldots\prod_{i=s-1}^{s}(c_i - c_{s-2})\begin{vmatrix} \bar{p}[c_1,\ldots,c_{s-2},c_{s-1}] & \bar{q}[c_1,\ldots,c_{s-2},c_{s-1}] \\ \bar{p}[c_1,\ldots,c_{s-2},c_s] & \bar{q}[c_1,\ldots,c_{s-2},c_s] \end{vmatrix}.$$

As

$$\begin{vmatrix} \bar{p}[c_1,\ldots,c_{s-2},c_{s-1}] & \bar{q}[c_1,\ldots,c_{s-2},c_{s-1}] \\ \bar{p}[c_1,\ldots,c_{s-2},c_s] & \bar{q}[c_1,\ldots,c_{s-2},c_s] \end{vmatrix}$$

$$= (c_s - c_{s-1})\begin{vmatrix} \bar{p}[c_1,\ldots,c_{s-2},c_{s-1}] & \bar{q}[c_1,\ldots,c_{s-2},c_{s-1}] \\ \bar{p}[c_1,\ldots,c_{s-1},c_s] & \bar{q}[c_1,\ldots,c_{s-1},c_s] \end{vmatrix}$$

then the determinant of B is

$$\det B = \prod_{i>k}^{s}(c_i - c_k) \times D \tag{4.7}$$

where

$$D = \bar{p}[c_1,\ldots,c_{s-2},c_{s-1}]\,\bar{q}[c_1,\ldots,c_{s-1},c_s] - \bar{p}[c_1,\ldots,c_{s-1},c_s]\,\bar{q}[c_1,\ldots,c_{s-2},c_{s-1}]. \tag{4.8}$$

An alternative way of writing the determinant is by using the formula

$$\bar{p}[c_{s-q},c_{s+1-q},\ldots,c_{s-1},c_s] = \sum_{j=0}^{q}\left\{\frac{\bar{p}(c_{s-j})}{\prod\limits_{i=0,i\neq j}^{q}(c_{s-j} - c_{s-i})}\right\},\ q = 0,1,\ldots$$

and so substituting into det B for $\bar{p}(x)$ and $\bar{q}(x)$

$$\det B = \prod_{i>k}^{s}(c_i - c_k) \times \sum_{j=0}^{s-1}\sum_{l=0}^{s-2}\left\{\frac{\bar{q}(c_{s-j})\bar{p}(c_{s-1-l}) - \bar{p}(c_{s-j})\bar{q}(c_{s-1-l})}{\prod\limits_{q=0,q\neq j}^{s-1}(c_{s-j} - c_{s-q})\prod\limits_{p=0,p\neq l}^{s-2}(c_{s-1-l} - c_{s-1-p})}\right\}.$$

As

$$\bar{q}(c_a)\bar{p}(c_b) - \bar{p}(c_a)\bar{q}(c_b) = \sin(\theta c_a)\cos(\theta c_b) - \cos(\theta c_a)\sin(\theta c_b) = \sin[\theta(c_a - c_b)],$$

then,

$$\det B = \prod_{i>k}^{s}(c_i - c_k) \times \sum_{j=0}^{s-1}\sum_{l=0}^{s-2}\left\{\frac{\sin[\theta(c_{s-j} - c_{s-1-l})]}{\prod_{q=0,q\neq j}^{s-1}(c_{s-j} - c_{s-q}) \prod_{p=0,p\neq l}^{s-2}(c_{s-1-l} - c_{s-1-p})}\right\}. \quad (4.9)$$

Thus the determinant of A is given by

$$\det A = k^4\,(s-1)!\,(s-2)!\,h^{(s-2)(s-3)/2} \times \prod_{i>k}^{s}(c_i - c_k) \times$$

$$\sum_{j=0}^{s-1}\sum_{l=0}^{s-2}\left\{\frac{\sin[\theta(c_{s-j} - c_{s-1-l})]}{\prod_{q=0,q\neq j}^{s-1}(c_{s-j} - c_{s-q}) \prod_{p=0,p\neq l}^{s-2}(c_{s-1-l} - c_{s-1-p})}\right\} \text{ for } s \geq 2. \quad (4.10)$$

In particular, with $s = 2$, this gives

$$\det A = k^4 \sin\theta(c_2 - c_1)$$

and A is singular if $\theta(c_2 - c_1) = n\pi$, where n is integer. Therefore distinct collocation points do not guarantee a unique solution.

We now require the coefficients a, b and r_i, $i = 0, \ldots, s-1$. As r_0 and r_1 can be found from the initial conditions, we only need to find a, b and r_i, $i = 2, \ldots, s-1$. Therefore, the system of equations $A\mathbf{x} = \mathbf{b}$ may be written as an $s \times s$ system of equations $T'\mathbf{x}' = \mathbf{t}'$ where

$$T' = \begin{pmatrix} -k^2\cos(\theta c_1) & -k^2\sin(\theta c_1) & 2 & 6c_1h & \ldots & (s-1)(s-2)(c_1h)^{s-3} \\ -k^2\cos(\theta c_2) & -k^2\sin(\theta c_2) & 2 & 6c_2h & \ldots & (s-1)(s-2)(c_2h)^{s-3} \\ -k^2\cos(\theta c_3) & -k^2\sin(\theta c_3) & 2 & 6c_3h & \ldots & (s-1)(s-2)(c_3h)^{s-3} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ -k^2\cos(\theta c_s) & -k^2\sin(\theta c_s) & 2 & 6c_sh & \ldots & (s-1)(s-2)(c_sh)^{s-3} \end{pmatrix},$$

$$\mathbf{x}' = \begin{pmatrix} a \\ b \\ r_2 \\ \cdots \\ r_{s-1} \end{pmatrix} \text{ and } \mathbf{t}' = \begin{pmatrix} F(c_1) \\ F(c_2) \\ F(c_3) \\ \cdots \\ F(c_s) \end{pmatrix}.$$

Define $\bar{p}_{1,2,..,j} = \bar{p}[c_1, c_2, \ldots, c_j]$, $\bar{q}_{1,2,..,j} = \bar{q}[c_1, c_2, \ldots, c_j]$ and similarly $F_{1,2,..,j} = F[c_1, c_2, \ldots, c_j]$.

We use linear combinations of the rows with the formula

$$\text{row } k \rightarrow \frac{\text{row } k - \text{row } j}{c_k - c_j}, \quad j = 1, \ldots, s-1, \quad k = j+1, \ldots, s$$

and divided differences to find the coefficients a, b and r_i, $i = 2, \ldots, s-1$. For $j = 1$,

$$\text{row } k \rightarrow \frac{\text{row } k - \text{row } 1}{c_k - c_1}, \quad k = 2, \ldots, s$$

and therefore the matrix T' is replaced by

$$\begin{pmatrix} -k^2\bar{p}(c_1) & -k^2\bar{q}(c_1) & 2 & 6c_1h & 12c_1^2h^2 & \cdots & g(s)(c_1h)^{s-3} \\ -k^2\bar{p}_{1,2} & -k^2\bar{q}_{1,2} & 0 & 6h & 12h^2(c_1+c_2) & \cdots & g(s)h^{s-3}\frac{(c_2^{s-3} - c_1^{s-3})}{(c_2 - c_1)} \\ -k^2\bar{p}_{1,3} & -k^2\bar{q}_{1,3} & 0 & 6h & 12h^2(c_1+c_3) & \cdots & g(s)h^{s-3}\frac{(c_3^{s-3} - c_1^{s-3})}{(c_3 - c_1)} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \\ -k^2\bar{p}_{1,s} & -k^2\bar{q}_{1,s} & 0 & 6h & 12h^2(c_1+c_s) & \cdots & g(s)h^{s-3}\frac{(c_s^{s-3} - c_1^{s-3})}{(c_s - c_1)} \end{pmatrix}$$

where $g(s) = (s-1)(s-2)$ and the column vector $\mathbf{t}'$ is replaced by

$$[F(c_1), F[c_1, c_2], F[c_1, c_3], \ldots, F[c_1, c_s]]^T.$$

Let $B_j(x) = x^j$. If we repeat the above process a new system of equations $T\mathbf{x}' = \mathbf{t}$

is obtained where the matrix T is

$$\begin{pmatrix} -k^2\bar{p}_1 & -k^2\bar{q}_1 & 2 & 6c_1h & 12c_1^2h^2 & \dots & g(s)(c_1h)^{s-3} \\ -k^2\bar{p}_{1,2} & -k^2\bar{q}_{1,2} & 0 & 6h & 12h^2(c_1+c_2) & \dots & g(s)h^{s-3}B_{s-3}[c_1,c_2] \\ -k^2\bar{p}_{1,2,3} & -k^2\bar{q}_{1,2,3} & 0 & 0 & 12h^2 & \dots & g(s)h^{s-3}B_{s-3}[c_1,c_2,c_3] \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ -k^2\bar{p}_{1,2,..,s-2} & -k^2\bar{q}_{1,2,..,s-2} & 0 & 0 & 0 & \dots & g(s)h^{s-3} \\ -k^2\bar{p}_{1,2,..,s-1} & -k^2\bar{q}_{1,2,..,s-1} & 0 & 0 & 0 & \dots & 0 \\ -k^2\bar{p}_{1,2,..,s} & -k^2\bar{q}_{1,2,..,s} & 0 & 0 & 0 & \dots & 0 \end{pmatrix}$$

with

$$\mathbf{x}' = \begin{pmatrix} a \\ b \\ r_2 \\ \dots \\ r_{s-3} \\ r_{s-2} \\ r_{s-1} \end{pmatrix} \quad \text{and} \quad \mathbf{t} = \begin{pmatrix} F_1 \\ F_{1,2} \\ F_{1,2,3} \\ \dots \\ F_{1,2,..,s-2} \\ F_{1,2,..,s-1} \\ F_{1,2,..,s} \end{pmatrix}.$$

The determinant of T is

$$\det T = 2\,.\,6h\,.\,12h^2\dots(s-1)\,.\,(s-2)\,.\,h^{s-3}\,k^4\times D = k^4\,(s-1)!\,(s-2)!\,h^{(s-2)(s-3)/2}\times D$$

where D is given by (4.8).

Let $T_{p,k}$ be the minor of the element in the (p,k) position in the coefficient matrix T and using Cramer's Rule

$$a = \frac{1}{\det T}\sum_{p=1}^{s}(-1)^{p-1}T_{p,1}F[c_1,\dots,c_p], \tag{4.11}$$

$$b = \frac{1}{\det T}\sum_{p=1}^{s}(-1)^{p}T_{p,2}F[c_1,\dots,c_p], \tag{4.12}$$

and

$$r_i = \frac{1}{\det T}\sum_{p=1}^{s}(-1)^{p+i-1}T_{p,1+i}F[c_1,\dots,c_p], \quad i=2,\dots,s-1. \tag{4.13}$$

Alternatively, if we leave the matrix A (given at the start of section 4.1.2) as an $(s+2)\times(s+2)$ matrix and use the same technique to find the coefficients, then we obtain the coefficients a and b in the form

$$\begin{aligned} a &= -\frac{1}{k^2}\left\{\frac{F[c_1,c_2,\ldots,c_{s-1}]\bar{q}[c_1,c_2,\ldots,c_s]-F[c_1,c_2,\ldots,c_s]\bar{q}[c_1,c_2,\ldots,c_{s-1}]}{\bar{p}[c_1,c_2,\ldots,c_{s-1}]\bar{q}[c_1,c_2,\ldots,c_s]-\bar{p}[c_1,c_2,\ldots,c_s]\bar{q}[c_1,c_2,\ldots,c_{s-1}]}\right\} \\ &= -\frac{1}{k^2 D}\left\{F[c_1,c_2,\ldots,c_{s-1}]\bar{q}[c_1,c_2,\ldots,c_s]-F[c_1,c_2,\ldots,c_s]\bar{q}[c_1,c_2,\ldots,c_{s-1}]\right\} \end{aligned}$$

and

$$\begin{aligned} b &= -\frac{1}{k^2}\left\{\frac{F[c_1,c_2,\ldots,c_s]\bar{p}[c_1,c_2,\ldots,c_{s-1}]-F[c_1,c_2,\ldots,c_{s-1}]\bar{p}[c_1,c_2,\ldots,c_s]}{\bar{p}[c_1,c_2,\ldots,c_{s-1}]\bar{q}[c_1,c_2,\ldots,c_s]-\bar{p}[c_1,c_2,\ldots,c_s]\bar{q}[c_1,c_2,\ldots,c_{s-1}]}\right\} \\ &= -\frac{1}{k^2 D}\left\{F[c_1,c_2,\ldots,c_s]\bar{p}[c_1,c_2,\ldots,c_{s-1}]-F[c_1,c_2,\ldots,c_{s-1}]\bar{p}[c_1,c_2,\ldots,c_s]\right\}. \end{aligned}$$

Therefore, substituting the conditions (4.2) and the coefficients (4.11), (4.12) and (4.13) into $u(x)$, equation (4.1), we have

$$\begin{aligned} u(x) &= a\cos k(x-x_n)+b\sin k(x-x_n)+\sum_{i=0}^{s-1} r_i(x-x_n)^i \\ &= a\cos k(x-x_n)+b\sin k(x-x_n)+r_0+(x-x_n)r_1+\sum_{i=2}^{s-1} r_i(x-x_n)^i \\ &= y_n+(x-x_n)z_n+\frac{1}{\det T}\sum_{p=1}^{s}\Big\{(-1)^{p-1}T_{p,1}[\cos k(x-x_n)-1]+ \end{aligned}$$

$$(-1)^p T_{p,2}[\sin k(x-x_n)-k(x-x_n)]+\sum_{i=2}^{s-1}(-1)^{p+i-1}T_{p,1+i}(x-x_n)^i\Big\}F[c_1,\ldots,c_p].$$

Thus, the last equation may be written as

$$u(x)=y_n+(x-x_n)z_n+\frac{1}{\det T}\left\{\sum_{p=1}^{s}T_p(x)F[c_1,\ldots,c_p]\right\} \tag{4.14}$$

where $T_p(x)$ is the determinant obtained by replacing the p^{th} row of $\det T$ by

$$\Big[\cos k(x-x_n)-1,\ \sin k(x-x_n)-k(x-x_n),\ (x-x_n)^2,\ \ldots,\ (x-x_n)^{s-1}\Big].$$

Similarly,

$$u'(x) = -ak\sin k(x-x_n)+bk\cos k(x-x_n)+\sum_{i=0}^{s-1} ir_i(x-x_n)^{i-1}$$

$$= -ak\sin k(x-x_n) + bk\cos k(x-x_n) + r_1 + \sum_{i=2}^{s-1} i r_i (x-x_n)^{i-1}$$

$$= z_n + \frac{1}{\det T}\sum_{p=1}^{s}\Big\{-(-1)^{p-1}T_{p,1}k\sin k(x-x_n) +$$

$$(-1)^p\,k\,T_{p,2}[\cos k(x-x_n)-1] + \sum_{i=2}^{s-1}(-1)^{p+i-1}T_{p,1+i}\,i(x-x_n)^{i-1}\Big\}\,F[c_1,\ldots,c_p].$$

Therefore

$$u'(x) = z_n + \frac{1}{\det T}\left\{\sum_{p=1}^{s} T'_p(x)F[c_1,\ldots,c_p]\right\} \tag{4.15}$$

where $T'_p(x)$ is the determinant obtained by replacing the p^{th} row of $\det T$ by

$$\left[-k\sin k(x-x_n),\ k\cos k(x-x_n)-k,\ 2(x-x_n),\ \ldots,\ (s-1)(x-x_n)^{s-2}\right].$$

Example

With $s = 2$,

$$u(x) = y_n + (x-x_n)z_n + \frac{1}{\det T}\{T_1(x)F[c_1] + T_2(x)F[c_1,c_2]\}$$

where

$$\begin{aligned} T_1(x) &= \begin{vmatrix} \cos k(x-x_n)-1 & \sin k(x-x_n)-k(x-x_n) \\ -k^2\bar{p}[c_1,c_2] & -k^2\bar{q}[c_1,c_2] \end{vmatrix} \\ &= \left\{\frac{k^2}{c_2-c_1}\right\}\{\sin[k(x-x_n)-\theta c_2] - \sin[k(x-x_n)-\theta c_1] \\ &\qquad -k(x-x_n)[\cos(\theta c_2)-\cos(\theta c_1)] + \sin(\theta c_2) - \sin(\theta c_1)\} \end{aligned}$$

and

$$\begin{aligned} T_2(x) &= \begin{vmatrix} -k^2\bar{p}(c_1) & -k^2\bar{q}(c_1) \\ \cos k(x-x_n)-1 & \sin k(x-x_n)-k(x-x_n) \end{vmatrix} \\ &= k^2\{-\sin[k(x-x_n)-\theta c_1] + k(x-x_n)\cos(\theta c_1) - \sin(\theta c_1)\} \end{aligned}$$

with

$$\det T = \frac{k^4\sin[\theta(c_2-c_1)]}{c_2-c_1}.$$

Therefore,

$$u(x) = y_n + (x - x_n)z_n + \frac{h^2}{\theta^2 \sin[\theta(c_2 - c_1)]} \{\mathcal{P}_1 F(c_1) - \mathcal{P}_2 F(c_2)\}$$

where

$$\mathcal{P}_1 = \sin[k(x - x_n) - \theta c_2] + \sin(\theta c_2) - k(x - x_n)\cos(\theta c_2),$$

$$\mathcal{P}_2 = \sin[k(x - x_n) - \theta c_1] + \sin(\theta c_1) - k(x - x_n)\cos(\theta c_1).$$

Let y_{n+1}, z_{n+1} and y_{n+c_i} be approximations for $y(x_n + h)$, $y'(x_n + h)$ and $y(x_n + c_i h)$ respectively, then

$$\begin{aligned} y_{n+1} &= y_n + hz_n + h^2 \left\{ \left[\frac{\sin[\theta(1 - c_2)] + \sin(\theta c_2) - \theta\cos(\theta c_2)}{\theta^2 \sin[\theta(c_2 - c_1)]} \right] f_{n+c_1} \right. \\ & \qquad \left. - \left[\frac{\sin[\theta(1 - c_1)] + \sin(\theta c_1) - \theta\cos(\theta c_1)}{\theta^2 \sin[\theta(c_2 - c_1)]} \right] f_{n+c_2} \right\}. \end{aligned}$$

$$\begin{aligned} z_{n+1} &= z_n + h \left\{ \left[\frac{\cos[\theta(c_2 - 1)] - \cos(\theta c_2)}{\theta \sin[\theta(c_2 - c_1)]} \right] f_{n+c_1} \right. \\ & \qquad \left. + \left[\frac{\cos(\theta c_1) - \cos[\theta(c_1 - 1)]}{\theta \sin[\theta(c_2 - c_1)]} \right] f_{n+c_2} \right\}. \end{aligned}$$

$$\begin{aligned} y_{n+c_i} &= y_n + c_i h z_n + h^2 \left\{ \left[\frac{\sin[\theta(c_i - c_2)] + \sin(\theta c_2) - \theta c_i \cos(\theta c_2)}{\theta^2 \sin[\theta(c_2 - c_1)]} \right] f_{n+c_1} \right. \\ & \qquad \left. - \left[\frac{\sin[\theta(c_i - c_1)] + \sin(\theta c_1) - \theta c_i \cos(\theta c_1)}{\theta^2 \sin[\theta(c_2 - c_1)]} \right] f_{n+c_2} \right\}, \quad i = 1, 2 \end{aligned}$$

where $f_{n+c_1} = f(x_{n+c_1}, y_{n+c_1})$ and $f_{n+c_2} = f(x_{n+c_2}, y_{n+c_2})$.

Thus, the two-point mixed collocation method may be written as a Runge-Kutta-Nyström method with steplength dependent coefficients. In general, the s-point mixed collocation method is given by

$$\left.\begin{array}{rcl} y_{n+1} & = & y_n + hz_n + \dfrac{1}{\det T}\left\{\displaystyle\sum_{p=1}^{s} T_p(x_n+h)F[c_1,c_2,\ldots,c_p]\right\} \\ z_{n+1} & = & z_n + \dfrac{1}{\det T}\left\{\displaystyle\sum_{p=1}^{s} T_p'(x_n+h)F[c_1,c_2,\ldots,c_p]\right\} \\ y_{n+c_j} & = & y_n + c_jhz_n + \dfrac{1}{\det T}\left\{\displaystyle\sum_{p=1}^{s} T_p(x_n+c_jh)F[c_1,c_2,\ldots,c_p]\right\} \\ & & \qquad\qquad \text{for } j=1,\ldots,s \end{array}\right\} \quad (4.16)$$

where $T_p(x_n+h)$, $T_p'(x_n+h)$ and $T_p(x_n+c_jh)$ are the determinants obtained by replacing the p-th row of det T by

$$[\cos\theta - 1, \sin\theta - \theta, h^2, \ldots, h^{s-1}],$$

$$[-k\sin\theta, k(\cos\theta - 1), 2h, \ldots, (s-1)h^{s-2}]$$

and

$$[\cos(\theta c_j) - 1, \sin(\theta c_j) - \theta c_j, (c_jh)^2, \ldots, (c_jh)^{s-1}]$$

respectively, where $\theta = kh$.

An alternative approach

Because the coefficients a, b and r_i, equations (4.11), (4.12) and (4.13) respectively, are in terms of divided differences for $f(x,y)$ at the collocation points, it is difficult to see whether the mixed collocation methods can be written as a Runge-Kutta-Nyström method (2.12) for arbitrary s. Coleman [20] considered interpolation methods using a function of the form $aC(x) + bS(x) + \sum_{i=0}^{n-2} \alpha_i x^i$, where C and S are given functions for arbitrarily chosen distinct nodes and he derived both Lagrangian and Newtonian formulae. Coleman showed in [22] that it is possible to write the mixed collocation methods as a Runge-Kutta-Nyström method with steplength dependent coefficients. The following is a brief description of his work in deriving the coefficients of the mixed collocation method.

Consider approximating the solution $y(x)$ by a function $u(x)$ of the form

$$u(x) = a\cos\, k(x - x_n) + b\sin\, k(x - x_n) + \sum_{i=0}^{s-1} r_i (x - x_n)^i$$

but introduce a new variable $t = (x - x_n)/h$. The function $u(x)$ becomes

$$u(x_n + th) = a\cos\theta t + b\sin\theta t + \sum_{i=0}^{s-1} r_i h^i t^i.$$

Observe that $u''(x)$ is a function which combines a polynomial of degree $s-3$ and two trigonometric functions. Also $u''(x)$ interpolates the s data points $[x_n + c_i h, u''(x_n + c_i h)]$, for $i = 1, 2, .., s$. Therefore in terms of t, for two or more collocation points (i.e. $s \geq 2$), the approximation for the second derivative can be expressed as

$$u''(x_n + th) = \sum_{i=1}^{s} L_i(t)\, f_{n+c_i}, \tag{4.17}$$

where $f_{n+c_i} = f(x_n + c_i h, u(x_n + c_i h))$ and the canonical function $L_i(t)$ is given by

$$L_i(t) = \mathcal{A}^{(i)} \cos(\theta t) + \mathcal{B}^{(i)} \sin(\theta t) + \sum_{j=0}^{s-3} \mathcal{R}_j^{(i)} t^j, \quad i = 1, 2, \ldots, s.$$

The canonical function $L_i(t)$ satisfies the interpolation conditions

$$L_i(c_j) = \delta_{ij}, \quad \text{for } \; i, j = 1, 2, \ldots, s.$$

Substituting the collocation points into $L_i(t)$, a system of $s \times s$ equations is obtained which we denote $B\mathbf{x} = \mathbf{l}$. Matrix B is given by (4.6) and $\mathbf{x}$ and $\mathbf{l}$ are s-dimensional column vectors given by

$$\mathbf{x} = \begin{pmatrix} \mathcal{A}^{(i)} \\ \mathcal{B}^{(i)} \\ \mathcal{R}_0^{(i)} \\ \mathcal{R}_1^{(i)} \\ \cdots \\ \mathcal{R}_{s-3}^{(i)} \end{pmatrix} \quad \text{and} \quad \mathbf{l} = \begin{pmatrix} L_i(c_1) \\ L_i(c_2) \\ L_i(c_3) \\ L_i(c_4) \\ \cdots \\ L_i(c_s) \end{pmatrix},$$

i.e. $\mathbf{l}$ is the unit vector with 1 as its i-th component and zero everywhere else.

Using Cramer's Rule to find the coefficients $\mathcal{A}^{(i)}$, $\mathcal{B}^{(i)}$ and $\mathcal{R}_j^{(i)}$, the canonical function $L_i(t)$ may be written as

$$L_i(t) = \frac{B_i(t)}{\det B}$$

where $B_i(t)$ is the determinant obtained when the i-th row of det B is replaced by

$$[\cos(\theta t), \sin(\theta t), 1, t, \ldots, t^{s-3}].$$

Returning to (4.17), integrate with respect to t

$$u'(x_n + th) = z_n + h \sum_{i=1}^{s} \alpha_i(t) f_{n+c_i} \tag{4.18}$$

where

$$\alpha_i(t) = \int_0^t L_i(\tau)\, d\tau.$$

Integrating (4.18) with respect to t, we obtain

$$u(x_n + th) = y_n + hz_n + h^2 \sum_{i=1}^{s} \beta_i(t) f_{n+c_i},$$

where

$$\beta_i(t) = \int_0^t \alpha_i(\tau)\, d\tau = \int_0^t \int_0^\tau L_i(\sigma)\, d\sigma\, d\tau = \int_0^t (t-\tau) L_i(\tau)\, d\tau.$$

Thus, the mixed collocation method may be written as an implicit s-stage Runge-Kutta-Nyström method (2.12) with coefficients

$$b_i = \beta_i(1), \quad d_i = \alpha_i(1) \text{ and } a_{ij} = \beta_j(c_i).$$

As only one row of det B depends on t, then we can integrate to give

$$\alpha_i(t) = \frac{B_i^{(1)}(t)}{\det B} \quad \text{and} \quad \beta_i(t) = \frac{B_i^{(2)}(t)}{\det B},$$

where $B_i^{(1)}(t)$ and $B_i^{(2)}(t)$ are the determinants obtained when the i-th row of det B is replaced by

$$\left[\frac{\sin(\theta t)}{\theta}, \frac{1-\cos(\theta t)}{\theta}, t, \frac{t^2}{2}, \ldots, \frac{t^{s-2}}{s-2}\right]$$

and

$$\left[\frac{1-\cos(\theta t)}{\theta^2}, \frac{\theta t-\sin(\theta t)}{\theta^2}, \frac{t^2}{2}, \frac{t^3}{6}, \ldots, \frac{t^{s-1}}{(s-1)(s-2)}\right]$$

respectively.

Coleman showed that by replacing θ by $-\theta$ in det B, $B_i(t)$, $B_i^{(1)}(t)$ and $B_i^{(2)}(t)$, then the determinants are multiplied by (-1) and thus the quotients $\alpha_i(t)$ and $\beta_i(t)$ are even functions of θ and so the coefficients of the mixed collocation method are even functions of θ.

4.1.3 Mixed Collocation Method for $s = 2$ and $s = 3$

Two Collocation Points $(s = 2)$

Define $f_{n+c_i} = f(x_n + c_i h, Y_i)$ for $i = 1, \ldots, s$. The formulae for the two-point mixed collocation method with collocation nodes $x_n + c_1 h$ and $x_n + c_2 h$ are

$$\left.\begin{aligned}
y_{n+1} &= y_n + hz_n + h^2\left\{\frac{\sin[\theta(c_2-1)] + \theta\cos(\theta c_2) - \sin(\theta c_2)}{\theta^2 \sin[\theta(c_1-c_2)]} f_{n+c_1}\right. \\
&\qquad \left. - \frac{\sin[\theta(c_1-1)] + \theta\cos(\theta c_1) - \sin(\theta c_1)}{\theta^2 \sin[\theta(c_1-c_2)]} f_{n+c_2}\right\}, \\
z_{n+1} &= z_n + h\left\{\frac{\cos(\theta c_2) - \cos[\theta(c_2-1)]}{\theta \sin[\theta(c_1-c_2)]} f_{n+c_1}\right. \\
&\qquad \left. + \frac{\cos[\theta(c_1-1)] - \cos(\theta c_1)}{\theta \sin[\theta(c_1-c_2)]} f_{n+c_2}\right\}, \\
Y_1 &= y_n + c_1 hz_n + h^2\left\{\frac{\sin[\theta(c_2-c_1)] + \theta c_1\cos(\theta c_2) - \sin(\theta c_2)}{\theta^2 \sin[\theta(c_1-c_2)]} f_{n+c_1}\right. \\
&\qquad \left. + \frac{\sin(\theta c_1) - \theta c_1\cos(\theta c_1)}{\theta^2 \sin[\theta(c_1-c_2)]} f_{n+c_2}\right\}, \\
Y_2 &= y_n + c_2 hz_n + h^2\left\{\frac{\theta c_2\cos(\theta c_2) - \sin(\theta c_2)}{\theta^2 \sin[\theta(c_1-c_2)]} f_{n+c_1}\right. \\
&\qquad \left. - \frac{\sin[\theta(c_1-c_2)] + \theta c_2\cos(\theta c_1) - \sin(\theta c_1)}{\theta^2 \sin[\theta(c_1-c_2)]} f_{n+c_2}\right\}
\end{aligned}\right\} \quad (4.19)$$

where $\theta^2 \sin[\theta(c_1 - c_2)] \neq 0$.

As $k \to 0$ the formulae become

$$\begin{aligned}
y_{n+1} &= y_n + hz_n + \frac{h^2}{6(c_2-c_1)}\left\{(3c_2-1)f_{n+c_1} + (1-3c_1)f_{n+c_2}\right\}, \\
z_{n+1} &= z_n + \frac{h}{2(c_2-c_1)}\left\{(2c_2-1)f_{n+c_1} + (1-2c_1)f_{n+c_2}\right\},
\end{aligned}$$

$$
\begin{aligned}
Y_1 &= y_n + c_1 h z_n + h^2 \left\{ \frac{c_1^2(3c_2 - c_1)}{6(c_2 - c_1)} f_{n+c_1} - \frac{c_1^3}{3(c_2 - c_1)} f_{n+c_2} \right\}, \\
Y_2 &= y_n + c_2 h z_n + h^2 \left\{ \frac{c_2^3}{3(c_2 - c_1)} f_{n+c_1} + \frac{c_2^2(c_2 - 3c_1)}{6(c_2 - c_1)} f_{n+c_2} \right\},
\end{aligned}
$$

which is the polynomial collocation method (2.16) for two collocation points.

Example : $c_1 = 0, \ c_2 = 1$

Substituting $c_1 = 0, \ c_2 = 1$ in (4.19) gives

$$
\begin{aligned}
y_{n+1} &= y_n + h z_n + h^2 \left\{ \frac{\{\sin\theta - \theta\cos\theta\}}{\theta^2 \sin\theta} f_n + \frac{\{\theta - \sin\theta\}}{\theta^2 \sin\theta} f_{n+1} \right\}, \\
z_{n+1} &= z_n + h \left(\frac{1 - \cos\theta}{\theta \sin\theta} \right) \{f_n + f_{n+1}\}
\end{aligned}
$$

and from (4.10)

$$
\det A = k^4 \sin\theta
$$

which is non-zero for $\theta \neq n\pi$, n integer. Thus the method is undefined when $\theta = n\pi$.

In the limit as $k \to 0$, the mixed collocation method for $c_1 = 0$ and $c_2 = 1$ reduces to

$$
\begin{aligned}
y_{n+1} &= y_n + h z_n + \frac{h^2}{6} \{2f_n + f_{n+1}\}, \\
z_{n+1} &= z_n + \frac{h}{2} \{f_n + f_{n+1}\}.
\end{aligned}
$$

If we compare the two-point collocation method (4.19) with the Runge-Kutta-Nyström method (2.12), then the coefficients are

$$
\begin{aligned}
b_1 &= \frac{\sin[\theta(1 - c_2)] - \theta\cos(\theta c_2) + \sin(\theta c_2)}{\theta^2 \sin[\theta(c_2 - c_1)]}, \\
b_2 &= -\frac{\sin[\theta(1 - c_1)] - \theta\cos(\theta c_1) + \sin(\theta c_1)}{\theta^2 \sin[\theta(c_2 - c_1)]}, \\
d_1 &= \frac{-\cos(\theta c_2) + \cos[\theta(c_2 - 1)]}{\theta \sin[\theta(c_2 - c_1)]}, \\
d_2 &= \frac{-\cos[\theta(c_1 - 1)] + \cos(\theta c_1)}{\theta \sin[\theta(c_2 - c_1)]}, \\
a_{11} &= \frac{\sin[\theta(c_1 - c_2)] - \theta c_1 \cos(\theta c_2) + \sin(\theta c_2)}{\theta^2 \sin[\theta(c_2 - c_1)]},
\end{aligned}
$$

$$
\begin{aligned}
a_{12} &= -\frac{\sin(\theta c_1) - \theta c_1 \cos(\theta c_1)}{\theta^2 \sin[\theta(c_2 - c_1)]}, \\
a_{21} &= \frac{-\theta c_2 \cos(\theta c_2) + \sin(\theta c_2)}{\theta^2 \sin[\theta(c_2 - c_1)]}, \\
a_{22} &= -\frac{\sin[\theta(c_2 - c_1)] - \theta c_2 \cos(\theta c_1) + \sin(\theta c_1)}{\theta^2 \sin[\theta(c_2 - c_1)]}.
\end{aligned}
$$

It is easily verified that these coefficients are even functions of θ.

Three Collocation Points ($s = 3$)

The general formula for the three-point mixed collocation method is

$$
\begin{aligned}
y_{n+1} &= y_n + h z_n + h^2 \left\{ b_1 f_{n+c_1} + b_2 f_{n+c_2} + b_3 f_{n+c_3} \right\}, \\
z_{n+1} &= z_n + h \left\{ d_1 f_{n+c_1} + d_2 f_{n+c_2} + d_3 f_{n+c_3} \right\},
\end{aligned}
$$

and

$$
Y_i = y_n + c_i h z_n + h^2 \left\{ a_{i1} f_{n+c_1} + a_{i2} f_{n+c_2} + a_{i3} f_{n+c_3} \right\} \quad \text{for } i = 1, 2, 3
$$

where

$$
\begin{aligned}
b_1 &= \frac{\theta^2 \sin[\theta(c_3 - c_2)] + 2\mathcal{Q}[c_3 - 1, c_2 - 1] - 2\mathcal{Q}[c_3, c_2] + 2\theta \mathcal{P}[c_3, c_2]}{2\theta^2 \mathcal{E}}, \\
b_2 &= \frac{\theta^2 \sin[\theta(c_1 - c_3)] + 2\mathcal{Q}[c_1 - 1, c_3 - 1] - 2\mathcal{Q}[c_1, c_3] + 2\theta \mathcal{P}[c_1, c_3]}{2\theta^2 \mathcal{E}}, \\
b_3 &= \frac{\theta^2 \sin[\theta(c_2 - c_1)] + 2\mathcal{Q}[c_2 - 1, c_1 - 1] - 2\mathcal{Q}[c_2, c_1] + 2\theta \mathcal{P}[c_2, c_1]}{2\theta^2 \mathcal{E}},
\end{aligned}
$$

$$
\begin{aligned}
d_1 &= \frac{\theta \sin[\theta(c_3 - c_2)] - P[c_3 - 1, c_2 - 1] + P[c_3, c_2]}{\theta \mathcal{E}}, \\
d_2 &= \frac{\theta \sin[\theta(c_1 - c_3)] - P[c_1 - 1, c_3 - 1] + P[c_1, c_3]}{\theta \mathcal{E}}, \\
d_3 &= \frac{\theta \sin[\theta(c_2 - c_1)] - P[c_2 - 1, c_1 - 1] + P[c_2, c_1]}{\theta \mathcal{E}},
\end{aligned}
$$

and

$$\begin{aligned}
a_{i1} &= \frac{c_i^2\theta^2 \sin[\theta(c_3 - c_2)] + 2Q[c_3 - c_i, c_2 - c_i] - 2Q[c_3, c_2] + 2\theta c_i P[c_3, c_2]}{2\theta^2\, \mathcal{E}}, \\
a_{i2} &= \frac{c_i^2\theta^2 \sin[\theta(c_1 - c_3)] + 2Q[c_1 - c_i, c_3 - c_i] - 2Q[c_1, c_3] + 2\theta c_i P[c_1, c_3]}{2\theta^2\, \mathcal{E}}, \\
a_{i3} &= \frac{c_i^2\theta^2 \sin[\theta(c_2 - c_1)] + 2Q[c_2 - c_i, c_1 - c_i] - 2Q[c_2, c_1] + 2\theta c_i P[c_2, c_1]}{2\theta^2\, \mathcal{E}},
\end{aligned}$$

with

$$\mathcal{P}[x,y] = \cos(\theta x) - \cos(\theta y), \quad \mathcal{Q}[x,y] = \sin(\theta x) - \sin(\theta y),$$

and

$$\begin{aligned}
\mathcal{E} &= \sin[\theta(c_3 - c_2)] + \sin[\theta(c_1 - c_3)] + \sin[\theta(c_2 - c_1)] \\
&= 4 \sin\left[\theta\left(\frac{c_3 - c_2}{2}\right)\right] \sin\left[\theta\left(\frac{c_1 - c_3}{2}\right)\right] \sin\left[\theta\left(\frac{c_2 - c_1}{2}\right)\right]
\end{aligned}$$

where we require $\mathcal{E} \neq 0$. As $k \to 0$, the three-point mixed collocation method reduces to the polynomial collocation method (2.17).

Example

With $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$

$$\begin{aligned}
y_{n+1} &= y_n + hz_n + h^2 \left\{b_1 f_n + b_2 f_{n+1/2} + b_3 f_{n+1}\right\}, \\
z_{n+1} &= z_n + h \left\{d_1 f_n + d_2 f_{n+1/2} + d_3 f_{n+1}\right\},
\end{aligned}$$

and

$$y_{n+1/2} = y_n + \frac{h}{2} z_n + h^2 \left\{a_{21} f_n + a_{22} f_{n+1/2} + a_{23} f_{n+1}\right\}$$

where

$$b_1 = \frac{\theta^2 \sin(\theta/2) + 4\sin(\theta/2) - 2\sin\theta + 2\theta\cos\theta - 2\theta\cos(\theta/2)}{2\theta^2\{2\sin(\theta/2) - \sin\theta\}},$$

$$b_2 = \frac{2 - \theta\sin\theta - 2\cos\theta}{2\theta\{2\sin(\theta/2) - \sin\theta\}},$$

$$b_3 = \frac{\theta^2 \sin(\theta/2) + 2\sin\theta - 4\sin(\theta/2) + 2\theta\cos(\theta/2) - 2\theta}{2\theta^2\{2\sin(\theta/2) - \sin\theta\}},$$

$$d_1 = \frac{\theta\sin(\theta/2) + \cos\theta - 1}{\theta\{2\sin(\theta/2) - \sin\theta\}}, \quad d_2 = \frac{2 - \theta\sin\theta - 2\cos\theta}{\theta\{2\sin(\theta/2) - \sin\theta\}},$$

$$d_3 = \frac{\theta\sin(\theta/2)+\cos\theta-1}{\theta\{2\sin(\theta/2)-\sin\theta\}},$$

and

$$a_{21} = \frac{(\theta^2+16)\sin(\theta/2)-8\sin\theta+4\theta\cos\theta-4\theta\cos(\theta/2)}{8\theta^2\{2\sin(\theta/2)-\sin\theta\}},$$

$$a_{22} = -\frac{\theta^2\sin\theta+16\sin(\theta/2)-8\sin\theta-4\theta+4\theta\cos\theta}{8\theta^2\{2\sin(\theta/2)-\sin\theta\}},$$

$$a_{23} = \frac{\theta\sin(\theta/2)+4\cos(\theta/2)-4}{8\theta\{2\sin(\theta/2)-\sin\theta\}}.$$

The determinant of A is

$$\det A = 4k^4\sin(\theta/2) - 2k^4\sin\theta = 4k^4\sin(\theta/2)\{1-\cos(\theta/2)\}$$

which is zero when $\theta = 2n\pi$, where n is a non-negative integer. So the method is undefined when $\theta = 2n\pi$.

Row-sum condition for the mixed collocation method

From the Runge-Kutta-Nyström method, (2.12)

$$Y_i^{RKN} = y_n + c_i h z_n + h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) \approx y(x_n + c_i h), \quad i = 1, \ldots, s.$$

The row-sum condition is a customary condition to impose on Runge-Kutta-Nyström methods and ensures that the stage order is at least 2. Therefore we set $y'' = f(x,y) = 1$ and thus $f(x_n + c_i h, Y_i) = 1$, for $i = 1, \ldots, s$. Using the exact values of the solution and its first derivative at x_n,

$$Y_i^{RKN} = y(x_n) + c_i h y'(x_n) + h^2 \sum_{j=1}^{s} a_{ij}. \tag{4.20}$$

For the mixed collocation method (4.14)

$$u(x) = y_n + (x - x_n) z_n + \frac{1}{\det T}\left\{\sum_{p=1}^{s} T_p(x) F[c_1, c_2, \ldots, c_p]\right\}.$$

Substituting $x = x_n + c_i h$, where $u(x_n + c_i h) = Y_i = y_{n+c_i} \approx y(x_n + c_i h)$, then

$$Y_i^{MC} = y_n + c_i h z_n + \frac{1}{\det T}\left\{\sum_{p=1}^{s} T_p(x_n + c_i h) F[c_1, \ldots, c_p]\right\} \approx y(x_n + c_i h) \quad (4.21)$$

for $i = 1, \ldots, s$.

Using exact values,

$$Y_i^{MC} = y(x_n) + c_i h y'(x_n) + \frac{1}{\det T}\left\{\sum_{p=1}^{s} T_p(x_n + c_i h) F[c_1, \ldots, c_p]\right\}. \quad (4.22)$$

We want to compare Y_i^{MC} (4.22) with the expression for Y_i^{RKN} (4.20) for the Runge-Kutta-Nyström method. As $f(x,y) = y'' = 1$, then $F[c_i] = f(x_n + c_i h, u(x_n + c_i h)) = 1$ for $i = 1, \ldots, s$, and expanding the divided differences we obtain

$$F[c_i] = 1 \text{ for } i = 1, \ldots, s, \quad F[c_1, c_2] = \frac{F[c_1] - F[c_2]}{c_1 - c_2} = 0$$

and hence $F[c_1, \ldots, c_p] = 0$, for $p = 2, \ldots, s$. Therefore (4.22) becomes

$$Y_i^{MC} = y(x_n) + c_i h y'(x_n) + \frac{T_1(x_n + c_i h)}{\det T}. \quad (4.23)$$

Now, $T_1(x_n + c_i h)$ is given by

$$\begin{vmatrix} \cos(\theta c_i) - 1 & \sin(\theta c_i) - \theta c_i & c_i^2 h^2 & c_i^3 h^3 & \ldots & (c_i h)^{s-1} \\ -k^2 \bar{p}_{1,2} & -k^2 \bar{q}_{1,2} & 0 & 6h & \ldots & g(s) h^{s-3} B_{s-3}[c_1, c_2] \\ -k^2 \bar{p}_{1,2,3} & -k^2 \bar{q}_{1,2,3} & 0 & 0 & \ldots & g(s) h^{s-3} B_{s-3}[c_1, c_2, c_3] \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ -k^2 \bar{p}_{1,2,..,s-2} & -k^2 \bar{q}_{1,2,..,s-2} & 0 & 0 & \ldots & g(s) h^{s-3} \\ -k^2 \bar{p}_{1,2,..,s-1} & -k^2 \bar{q}_{1,2,..,s-1} & 0 & 0 & \ldots & 0 \\ -k^2 \bar{p}_{1,2,..,s} & -k^2 \bar{q}_{1,2,..,s} & 0 & 0 & \ldots & 0 \end{vmatrix},$$

where $g(s) = (s-1)(s-2)$. For $s \geq 3$, the determinant may be reduced to

$$c_i^2 h^2 \begin{vmatrix} -k^2\bar{p}_{1,2} & -k^2\bar{q}_{1,2} & 6h & \dots & g(s)h^{s-3}B_{s-3}[c_1,c_2] \\ -k^2\bar{p}_{1,2,3} & -k^2\bar{q}_{1,2,3} & 0 & \dots & g(s)h^{s-3}B_{s-3}[c_1,c_2,c_3] \\ \dots & \dots & \dots & \dots & \dots \\ -k^2\bar{p}_{1,2,..,s-2} & -k^2\bar{q}_{1,2,..,s-2} & 0 & \dots & g(s)h^{s-3} \\ -k^2\bar{p}_{1,2,..,s-1} & -k^2\bar{q}_{1,2,..,s-1} & 0 & \dots & 0 \\ -k^2\bar{p}_{1,2,..,s} & -k^2\bar{q}_{1,2,..,s} & 0 & \dots & 0 \end{vmatrix},$$

and this can be reduced again until we obtain

$$\begin{aligned} T_1(x_n + c_i h) &= k^4 \,.\, c_i^2 h^2 \,.\, 6h \,.\, 12h^2 \,.\, (s-1) \,.\, (s-2) \,.\, h^{(s-3)} \times D \\ &= \frac{c_i^2 h^2}{2} k^4 \,(s-1)!\,(s-2)!\, h^{(s-2)(s-3)/2} \times D \end{aligned},$$

where D is given by

$$D = \bar{p}[c_1,\dots,c_{s-2},c_{s-1}]\,\bar{q}[c_1,\dots,c_{s-1},c_s] - \bar{p}[c_1,\dots,c_{s-1},c_s]\,\bar{q}[c_1,\dots,c_{s-2},c_{s-1}].$$

As $T_1(x_n + c_i h)$ can not be written in the above form for $s = 1$ or 2, we will look at these cases separately.

So, for 3 or more collocation points, i.e. $s \geq 3$, we have

$$T_1(x_n + c_i h) = \frac{c_i^2 h^2}{2} k^4 \,(s-1)!\,(s-2)!\, h^{(s-2)(s-3)/2} \times D$$

where

$$\det T = k^4 \,(s-1)!\,(s-2)!\, h^{(s-2)(s-3)/2} \times D$$

and from equation (4.23)

$$Y_i^{MC} = y(x_n) + c_i h y'(x_n) + \frac{c_i^2}{2} h^2.$$

When this equation is compared to (4.20), we obtain the row-sum condition

$$\sum_{j=1}^{s} a_{ij} = \frac{c_i^2}{2}, \quad i = 1,\dots,s, \quad s \geq 3.$$

For the one-point mixed collocation method (4.3), the equation for Y is

$$Y = y_n + h\frac{\sin(\theta c)}{\theta\cos(\theta c)}z_n + h^2\left\{\frac{1-\cos(\theta c)}{\theta^2\cos(\theta c)}\right\}f_{n+c}$$

and clearly does not satisfy the row-sum condition, but in the limit as $k \to 0$,

$$Y \to y_n + chz_n + \frac{c^2h^2}{2}f_{n+c}$$

and so the corresponding polynomial collocation method satisfies the row-sum condition.

For the two-point mixed collocation method (4.19),

$$\begin{aligned}\frac{T_1(x_n+c_ih)}{\det T} &= h^2\left\{\frac{[\cos(\theta c_2)-\cos(\theta c_1)][\sin(\theta c_i)-\theta c_i]}{\theta^2\sin[\theta(c_2-c_1)]}\right.\\ &\qquad\left.-\frac{[\cos(\theta c_i)-1][\sin(\theta c_2)-\sin(\theta c_1)]}{\theta^2\sin[\theta(c_2-c_1)]}\right\}\\ &\neq \frac{c_i^2h^2}{2},\quad i=1,2.\end{aligned}$$

Therefore, for two collocation points, the mixed collocation method does not satisfy the row-sum condition. Again, as $k \to 0$,

$$Y_i \to y_n + c_ihz_n + \frac{c_i^2h^2}{2},\quad \text{for } i=1,2$$

and so the row-sum condition is satisfied for the corresponding two-point polynomial collocation method (2.16).

We conclude that the row-sum condition applies only to 3 or more collocation points ($s \geq 3$) for the mixed collocation method (4.16). When the row-sum condition is imposed, the stage-order is at least two and the number of steplength dependent order conditions is reduced.

Trigonometric Order

Following Definition 3.2 in Chapter 3, for a mixed collocation method to be of trigonometric order 1, we require that the linear operators of the method are annihilated by the functions $y(x) = \cos(kx)$ and $\sin(kx)$. The collocating function is of the form

$$u(x) = a\cos\, k(x - x_n) + b\sin\, k(x - x_n) + \sum_{i=0}^{s-1} r_i(x - x_n)^i. \tag{4.24}$$

It is only necessary to see that if the collocating function satisfies (3.1), i.e.

$$u(x_n + c_jh) = \cos\, k(x_n + c_jh) \;\text{ for }\; j = 1, \ldots, s \;\text{ when }\; y(x) = \cos(kx),$$

and similarly

$$u(x_n + c_jh) = \sin\, k(x_n + c_jh) \;\text{ for }\; j = 1, \ldots, s \;\text{ when }\; y(x) = \sin(kx),$$

then the mixed collocation methods are of trigonometric order 1.

Let $y(x) = \cos(kx)$, then $f(x, y) = y''(x) = -k^2y(x)$ where the general solution is

$$y(x) = A\cos(kx) + B\sin(kx).$$

Also the initial conditions and collocation conditions are $u(x_n) = y_n$, $u'(x_n) = z_n$ and

$$u''(x_n + c_jh) = -k^2u(x_n + c_jh), \quad j = 1, .., s.$$

As the collocating function is of the form (4.24), then the coefficients a, b and r_i can be found so that $u(x) = y(x)$. Similar results are found when substituting $y(x) = \sin(kx)$. Also, by the straight substitution of $y(x) = \cos(kx)$ and $\sin(kx)$ into the formulae for the mixed collocation methods, it is easily verified that the methods are of trigonometric order 1.

Theorem 2 *Every 2-stage Runge-Kutta-Nyström method which is of trigonometric order 1 is a 2-stage mixed collocation method.*

Proof: From Definition 3.2, for a 2-stage Runge-Kutta-Nyström method to be of trigonometric order 1, we have two equations in two unknowns for the coefficients b_i and d_i respectively, and for the coefficients a_{ij}, there are four equations in four unknowns and the coefficients are precisely those of the 2-stage mixed collocation method (4.19). ∎

4.2 Order

4.2.1 One Collocation Point

To find the order for a one-point mixed collocation method, we introduce the idea of using the residual as a measure of the accuracy of the method. We form a Taylor expansion about some suitable value of x and express the residual as a power series in h.

Using the exact values $y(x_n + h)$, $y'(x_n + h)$ and $y(x_n + ch)$ the *difference operators* for the one-point mixed collocation method (4.3) are defined by

$$\begin{aligned}
L[y] &= y(x_n + ch) - y(x_n) - hy'(x_n)\left\{\frac{\sin(\theta c)}{\theta\cos(\theta c)}\right\} - h^2\left\{\frac{1-\cos(\theta c)}{\theta^2\cos(\theta c)}\right\} f_{n+c}, \\
L_1[y] &= y(x_n + h) - y(x_n) - hy'(x_n)\left\{\frac{\sin[\theta(1-c)] + \sin(\theta c)}{\theta\cos(\theta c)}\right\} \\
&\qquad - h^2\left\{\frac{1-\cos\theta}{\theta^2\cos(\theta c)}\right\} f_{n+c} \\
L_2[y] &= y'(x_n + h) - y'(x_n)\left\{\frac{\cos[\theta(1-c)]}{\cos(\theta c)}\right\} - h\left\{\frac{\sin\theta}{\theta\cos(\theta c)}\right\} f_{n+c},
\end{aligned}$$

where $f_{n+c} = f(x_n + ch, Y)$ and

$$Y = y(x_n) + hy'(x_n)\frac{\sin(\theta c)}{\theta\cos(\theta c)} + h^2\frac{\{1-\cos(\theta c)\}}{\theta^2\cos(\theta c)} f(x_n + ch, Y).$$

Expand the trigonometric functions about $h = 0$ to give

$$\begin{aligned}
L[y] &= y(x_n + ch) - y(x_n) - hy'(x_n)\left\{c + \frac{c^3\theta^2}{3} + \ldots\right\} \\
&\qquad - \left\{\frac{c^2h^2}{2} + \ldots\right\} f(x_n + ch, Y) \\
&= \frac{c^2h^2}{2}\{y''(x_n) - f(x_n + ch, Y)\} + \frac{c^3h^3}{6}\left\{y^{(3)}(x_n) - 2k^2y'(x_n)\right\} + O(h^4) \\
&= h^2\beta
\end{aligned}$$

where β is finite as $h \to 0$.

Therefore

$$Y = y(x_n + ch) - L[y] = y(x_n + ch) - h^2\beta,$$

from which

$$\begin{aligned} f(x_n + ch, Y) &= f(x_n + ch, y(x_n + ch) - h^2\beta) \\ &= f(x_n + ch, y(x_n + ch)) - h^2\beta f_y(x_n + ch, y(x_n + ch)) + O(h^4) \\ &= y''(x_n + ch) - h^2\beta f_y(x_n + ch, y(x_n + ch)) + O(h^4). \end{aligned}$$

We need to expand $f_y(x_n + ch, y(x_n + ch))$. Let $\mathcal{F}(h) = f_y(x_n + ch, y(x_n + ch))$, then using a Taylor expansion about $h = 0$

$$\mathcal{F}(h) = \mathcal{F}(0) + h\mathcal{F}'(0) + O(h^2)$$

where

$$\mathcal{F}(0) = f_y(x_n, y(x_n)), \quad \mathcal{F}'(0) = c\left\{y'(x_n)f_{yy}(x_n, y(x_n)) + f_{yx}(x_n, y(x_n))\right\}.$$

Substituting back into $f(x_n + ch, Y)$,

$$f(x_n + ch, Y) = y''(x_n) + chy^{(3)}(x_n) + \frac{c^2h^2}{2}y^{(4)}(x_n)$$

$$+\frac{c^3h^3}{6}\left\{y^{(5)}(x_n) + 2f_y(x_n, y(x_n))\left[y^{(3)}(x_n) + k^2y'(x_n)\right]\right\} + O(h^4).$$

The functional $L_1[y]$ is given by

$$L_1[y] = y(x_n + h) - y(x_n) - hy'(x_n) - \left\{\frac{k^2h^3}{6}(3c - 1) + \dots\right\}y'(x_n)$$

$$-\left\{\frac{h^2}{2} + h^4k^2\left(\frac{c^2}{4} - \frac{1}{24}\right) + \dots\right\}\left\{y''(x_n) + chy^{(3)}(x_n) + \frac{c^2h^2}{2}y^{(4)}(x_n) + \dots\right\}$$

$$= \frac{h^3}{6}(1 - 3c)\left\{y^{(3)}(x_n) + k^2y'(x_n)\right\} + \frac{h^4}{24}(1 - 6c^2)\left\{y^{(4)}(x_n) + k^2y''(x_n)\right\} + O(h^5),$$

and similarly for $L_2[y]$

$$L_2[y] = y'(x_n + h) - \left\{1 + k^2h^2\left(c - \frac{1}{2}\right) + \dots\right\}y'(x_n)$$

$$-\left\{h + k^2h^3\left(\frac{c^2}{2} - \frac{1}{6}\right) + \ldots\right\} f(x_n + ch, Y)$$

$$= \frac{h^2}{2}(1-2c)\left\{y^{(3)}(x_n) + k^2y'(x_n)\right\} + \frac{h^3}{6}(1-3c^2)\left\{y^{(4)}(x_n) + k^2y''(x_n)\right\} + O(h^4).$$

Thus

$$\begin{array}{rrcl} \text{if } c \neq \frac{1}{2}, & L_1[y] & = & O(h^3) \text{ or higher,} \\ & L_2[y] & = & O(h^2) \quad \Rightarrow \textbf{Order 1}. \\ \text{If } c = \frac{1}{2}, & L_1[y] & = & O(h^3), \\ & L_2[y] & = & O(h^3) \quad \Rightarrow \textbf{Order 2}. \end{array}$$

And so the highest possible order for the one-point mixed collocation method is 2 when $c = \frac{1}{2}$.

4.2.2 Two or More Collocation Points

It was shown in section 4.1.2 that every mixed collocation method (4.16) for two or more collocation points can be written as a Runge-Kutta-Nyström method (2.12) where the coefficients b_i, d_i and a_{ij} are functions of the steplength h and the fitted frequency k. We expand the coefficients about $h = 0$ and define

$$\begin{aligned} b_i(h) &= b_i^{(0)} + hb_i^{(1)} + h^2b_i^{(2)} + \ldots \\ d_i(h) &= d_i^{(0)} + hd_i^{(1)} + h^2d_i^{(2)} + \ldots \\ a_{ij}(h) &= a_{ij}^{(0)} + ha_{ij}^{(1)} + h^2a_{ij}^{(2)} + \ldots \end{aligned}$$

Then we can apply the order conditions in section 3.4.2. Because the coefficients of the mixed collocation method are even functions of θ, then any conditions which contain a coefficient with an odd integer for the superscript can be eliminated. Up to and including order 6, there are 50 order conditions for the mixed collocation method for two or more collocation nodes. When the row-sum condition is imposed for $s \geq 3$, a further 18 conditions are eliminated leaving 32 conditions to be satisfied for orders 1-6.

Order Conditions for Mixed Collocation Methods with $s \geq 2$

Order 1:

$$1.)\ \sum_{i=1}^{s} d_i^{(0)} = 1.$$

Order 2:

$$2.)\ \sum_{i=1}^{s} d_i^{(0)} c_i = \frac{1}{2}, \quad 4.)\ \sum_{i=1}^{s} b_i^{(0)} = \frac{1}{2}.$$

Order 3:

$$5.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^2 = \frac{1}{3}, \quad 7.)\ \sum_{i=1}^{s} d_i^{(2)} = 0, \quad 8.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} = \frac{1}{6}, \quad 9.)\ \sum_{i=1}^{s} b_i^{(0)} c_i = \frac{1}{6}.$$

Order 4:

$$11.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^3 = \frac{1}{4}, \quad 13.)\ \sum_{i=1}^{s} d_i^{(2)} c_i = 0,$$

$$16.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j = \frac{1}{24}, \quad 17.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i = \frac{1}{8},$$

$$18.)\ \sum_{i=1}^{s} b_i^{(0)} c_i^2 = \frac{1}{12}, \quad 19.)\ \sum_{i=1}^{s} b_i^{(2)} = 0, \quad 21.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} = \frac{1}{24}.$$

Order 5:

$$22.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^4 = \frac{1}{5}, \quad 24.)\ \sum_{i=1}^{s} d_i^{(2)} c_i^2 = 0, \quad 26.)\ \sum_{i=1}^{s} d_i^{(4)} = 0,$$

$$27.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} \left\{ d_i^{(2)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(2)} \right\} = 0, \quad 29.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j^2 = \frac{1}{60},$$

$$30.)\ \sum_{i=1}^{s} \sum_{j=1}^{s} \sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} = \frac{1}{120}, \quad 31.)\ \sum_{i=1}^{s} d_i^{(0)} \left(\sum_{j=1}^{s} a_{ij}^{(0)} \right)^2 = \frac{1}{20},$$

$$33.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i c_j = \frac{1}{30},\quad 34.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^2 = \frac{1}{10},\quad 35.)\sum_{i=1}^{s} b_i^{(0)} c_i^3 = \frac{1}{20},$$

$$37.)\sum_{i=1}^{s} b_i^{(2)} c_i = 0,\quad 40.)\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_j = \frac{1}{120},\quad 41.)\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_i = \frac{1}{40}.$$

Order 6:

$$42.)\sum_{i=1}^{s} d_i^{(0)} c_i^5 = \frac{1}{6},\quad 44.)\sum_{i=1}^{s} d_i^{(2)} c_i^3 = 0,\quad 46.)\sum_{i=1}^{s} d_i^{(4)} c_i = 0,$$

$$49.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{d_i^{(2)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(2)}\right\} c_i = 0,\quad 50.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{d_i^{(2)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(2)}\right\} c_j = 0,$$

$$54.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^3 = \frac{1}{12},\quad 55.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} c_i = \frac{1}{144},$$

$$56.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{ik}^{(0)} c_k = \frac{1}{72},\quad 57.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} c_j = \frac{1}{240},$$

$$58.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} c_k = \frac{1}{720},\quad 59.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j^3 = \frac{1}{120},$$

$$60.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i c_j^2 = \frac{1}{72},\quad 61.)\sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^2 c_j = \frac{1}{36},$$

$$62.)\sum_{i=1}^{s} d_i^{(0)} c_i \left(\sum_{j=1}^{s} a_{ij}^{(0)}\right)^2 = \frac{1}{24},\quad 65.)\sum_{i=1}^{s} b_i^{(0)} c_i^4 = \frac{1}{30},\quad 67.)\sum_{i=1}^{s} b_i^{(2)} c_i^2 = 0,$$

$$69.)\sum_{i=1}^{s} b_i^{(4)} = 0, \quad 70.)\sum_{i=1}^{s}\sum_{j=1}^{s}\left\{b_i^{(2)}a_{ij}^{(0)} + b_i^{(0)}a_{ij}^{(2)}\right\} = 0, \quad 73.)\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)}a_{ij}^{(0)}c_i^2 = \frac{1}{60},$$

$$74.)\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)}a_{ij}^{(0)}c_ic_j = \frac{1}{180}, \quad 75.)\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)}a_{ij}^{(0)}c_j^2 = \frac{1}{360},$$

$$76.)\sum_{i=1}^{s} b_i^{(0)}\left(\sum_{j=1}^{s} a_{ij}^{(0)}\right)^2 = \frac{1}{120}, \quad 77.)\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} b_i^{(0)}a_{ij}^{(0)}a_{jk}^{(0)} = \frac{1}{720}.$$

For one collocation point, we require $c \neq \frac{1}{2}$ for **order 1** and $c = \frac{1}{2}$ for **order 2**, the highest possible order. Therefore, from the order conditions for **order 1**, we require $d_1^{(0)} = 1$ and for **order 2** we require $d_1^{(0)}c = \frac{1}{2}$ and $b_1^{(0)} = \frac{1}{2}$.

Thus, when $c \neq \frac{1}{2}$,

$$d_1^{(0)} = 1 \text{ but } d_1^{(0)}c \neq \frac{1}{2}$$

and so **order 2** is not satisfied. When $c = \frac{1}{2}$

$$d_1^{(0)} = 1 \quad \Rightarrow \textbf{ order 1}, \quad d_1^{(0)}c = \frac{1}{2} \text{ and } b_1^{(0)} = \frac{1}{2},$$

so we have **order 2**. In conclusion, the order conditions in section 4.2.2 are valid for one collocation point for the mixed collocation method.

We know that as the frequency $k \to 0$, the mixed collocation methods reduce to the corresponding polynomial collocation methods. As the set of order conditions for the polynomial collocation methods are included in those for the mixed collocation methods, then we have the following property [22]:

Property 2 *The order of an s-point mixed collocation method does not exceed that of the corresponding polynomial collocation method, and in particular, does not exceed 2s.*

The evidence so far suggests that the order of a mixed collocation method is the same as the corresponding polynomial collocation method but we have not yet found a proof.

4.2.3 Examples

Order Conditions for Two Collocation Points

Using the order conditions of section 4.2.2 it is possible to find the values of the collocation nodes so that the highest attainable order is reached for the mixed collocation method. As b_i, d_i and a_{ij} are even functions, when the expressions are expanded about $h = 0$, the coefficients of the odd powers of h are zero. Maple was used to carry out the expansions.

$$\begin{aligned}
b_1 &= b_1^{(0)} + h^2 b_1^{(2)} + h^4 b_1^{(4)} + \dots \\
&= \frac{3c_2 - 1}{6(c_2 - c_1)} + h^2k^2\left\{\frac{20c_2^2 - 15c_2 + 3 + 30c_2c_1^2 + 20c_1c_2 - 60c_1c_2^2 - 10c_1^2}{360(c_2 - c_1)}\right\} + \dots \\
b_2 &= b_2^{(0)} + h^2 b_2^{(2)} + h^4 b_2^{(4)} + \dots \\
&= \frac{1 - 3c_1}{6(c_2 - c_1)} - h^2k^2\left\{\frac{20c_1^2 - 15c_1 + 3 + 30c_1c_2^2 + 20c_1c_2 - 60c_2c_1^2 - 10c_2^2}{360(c_2 - c_1)}\right\} + \dots \\
d_1 &= d_1^{(0)} + h^2 d_1^{(2)} + h^4 d_1^{(4)} + \dots \\
&= \frac{2c_2 - 1}{2(c_2 - c_1)} + h^2k^2\left\{\frac{4c_2^2 - 4c_2 + 1 + 4c_2c_1^2 + 4c_1c_2 - 8c_1c_2^2 - 2c_1^2}{24(c_2 - c_1)}\right\} + \dots \\
d_2 &= d_2^{(0)} + h^2 d_2^{(2)} + h^4 d_2^{(4)} + \dots \\
&= \frac{1 - 2c_1}{2(c_2 - c_1)} - h^2k^2\left\{\frac{4c_1^2 - 4c_1 + 1 + 4c_1c_2^2 + 4c_1c_2 - 8c_2c_1^2 - 2c_2^2}{24(c_2 - c_1)}\right\} + \dots \\
a_{11} &= a_{11}^{(0)} + h^2 a_{11}^{(2)} + h^4 a_{11}^{(4)} + \dots \\
&= \frac{c_1^2(3c_2 - c_1)}{6(c_2 - c_1)} - c_1^3h^2k^2\left\{\frac{7c_1^2 - 35c_1c_2 + 40c_2^2}{360(c_2 - c_1)}\right\} + \dots \\
a_{12} &= a_{12}^{(0)} + h^2 a_{12}^{(2)} + h^4 a_{12}^{(4)} + \dots \\
&= -\frac{c_1^3}{3(c_2 - c_1)} - c_1^3h^2k^2\left\{\frac{2c_1^2 - 10c_1c_2 + 5c_2^2}{90(c_2 - c_1)}\right\} + \dots \\
a_{21} &= a_{21}^{(0)} + h^2 a_{21}^{(2)} + h^4 a_{21}^{(4)} + \dots \\
&= \frac{c_2^3}{3(c_2 - c_1)} + c_2^3h^2k^2\left\{\frac{2c_2^2 - 10c_1c_2 + 5c_1^2}{90(c_2 - c_1)}\right\} + \dots \\
a_{22} &= a_{22}^{(0)} + h^2 a_{22}^{(2)} + h^4 a_{22}^{(4)} + \dots \\
&= \frac{c_2^2(c_2 - 3c_1)}{6(c_2 - c_1)} + c_2^3h^2k^2\left\{\frac{40c_1^2 - 35c_1c_2 + 7c_2^2}{360(c_2 - c_1)}\right\} + \dots
\end{aligned}$$

where we assume distinct collocation nodes.

For **order ≥ 1** we require

$$1.)\ d_1^{(0)} + d_2^{(0)} = 1 \Rightarrow \frac{2c_2 - 1}{2(c_2 - c_1)} + \frac{1 - 2c_1}{2(c_2 - c_1)} = 1$$

which is satisfied automatically.

For **order ≥ 2**,

$$2.)\ d_1^{(0)} c_1 + d_2^{(0)} c_2 = \frac{1}{2} \Rightarrow \frac{2c_2 - 1}{2(c_2 - c_1)} c_1 + \frac{1 - 2c_1}{2(c_2 - c_1)} c_2 = \frac{-c_1 + c_2}{2(c_2 - c_1)} = \frac{1}{2}$$

$$4.)\ b_1^{(0)} + b_2^{(0)} = \frac{1}{2} \Rightarrow \frac{3c_2 - 1}{6(c_2 - c_1)} + \frac{1 - 3c_1}{6(c_2 - c_1)} = \frac{1}{2}$$

and again all the order conditions are satisfied automatically.

For **order ≥ 3**,

$$5.)\ d_1^{(0)} c_1^2 + d_2^{(0)} c_2^2 = \frac{1}{3} \Rightarrow \frac{2c_2 - 1}{2(c_2 - c_1)} c_1^2 + \frac{1 - 2c_1}{2(c_2 - c_1)} c_2^2 = \frac{c_1 + c_2 - 2c_1 c_2}{2} = \frac{1}{3},$$

and so we require

$$\Rightarrow 3c_1 + 3c_2 - 6c_1 c_2 = 2,$$

therefore

$$c_1 = \frac{2 - 3c_2}{3 - 6c_2}, \quad c_2 \neq \frac{1}{2}.$$

The rest of the conditions are

$$\begin{aligned} 7.)\ d_1^{(2)} + d_2^{(2)} &= k^2 \left\{ \frac{6(c_2^2 - c_1^2) - 4(c_2 - c_1) - 12c_1 c_2 (c_2 - c_1)}{24(c_2 - c_1)} \right\} \\ &= k^2 \left\{ \frac{3(c_2 + c_1) - 2 - 6c_1 c_2}{12} \right\} \\ &= k^2 \left\{ \frac{3\left\{c_2 + \left(\frac{2-3c_2}{3-6c_2}\right)\right\} - 2 - 6\left(\frac{2-3c_2}{3-6c_2}\right) c_2}{12} \right\} = 0, \end{aligned}$$

$$\begin{aligned} 8.)\ d_1^{(0)}\left(a_{11}^{(0)} + a_{12}^{(0)}\right) + d_2^{(0)}\left(a_{21}^{(0)} + a_{22}^{(0)}\right) &= \frac{c_1^2(2c_2 - 1) + c_2^2(1 - 2c_1)}{4(c_2 - c_1)} \\ &= \frac{c_1 + c_2 - 2c_1 c_2}{4} \\ &= \frac{\left(\frac{2-3c_2}{3-6c_2}\right) + c_2 - 2\left(\frac{2-3c_2}{3-6c_2}\right) c_2}{4} \end{aligned}$$

$$= \frac{2-4c_2}{4(3-6c_2)} = \frac{1}{6},$$

$$9.)\ b_1^{(0)}c_1 + b_2^{(0)}c_2 = \frac{1}{6} \Rightarrow \frac{3c_2-1}{6(c_2-c_1)}c_1 + \frac{1-3c_1}{6(c_2-c_1)}c_2 = \frac{1}{6},$$

which are satisfied when $c_1 = \dfrac{2-3c_2}{3-6c_2}$.

Thus, with $c_1 = \dfrac{2-3c_2}{3-6c_2}$ we have order greater or equal to 3.

For **order $\geq$ 4** we require,

$$11.)\ d_1^{(0)}c_1^3 + d_2^{(0)}c_2^3 = \frac{1}{4}$$

where

$$\begin{aligned} d_1^{(0)}c_1^3 + d_2^{(0)}c_2^3 &= \frac{2c_2-1}{2(c_2-c_1)}c_1^3 + \frac{1-2c_1}{2(c_2-c_1)}c_2^3 \\ &= \frac{2c_2c_1^3 - c_1^3 + c_2^3 - 2c_1c_2^3}{2(c_2-c_1)} \\ &= \frac{2c_1c_2(c_1^2-c_2^2) + (c_2-c_1)(c_2^2+c_1c_2+c_1^2)}{2(c_2-c_1)} \\ &= \frac{-2c_1c_2(c_1+c_2) + c_2^2 + c_1c_2 + c_1^2}{2} = \frac{1}{4}, \end{aligned}$$

$$\Rightarrow -4c_1c_2(c_1+c_2) + 2c_2^2 + 2c_1c_2 + 2c_1^2 = 1.$$

Therefore substituting $c_1 = (2-3c_2)/(3-6c_2)$ into the above equation gives

$$\frac{2}{9}\left\{\frac{3c_2^2+6c_2-2}{2c_2-1}\right\} = 1,$$

$$\Rightarrow\ c_1 = \frac{3-\sqrt{3}}{6} \text{ and } c_2 = \frac{3+\sqrt{3}}{6} \text{ which are the Gauss nodes.}$$

The order conditions 13.), 16.), 18.) and 19.) are satisfied when $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$ and so the two-point mixed collocation method is of order at least 4.

For **order ≥ 5** we require,

$$22.)\ d_1^{(0)}c_1^4 + d_2^{(0)}c_2^4 = \frac{1}{5}$$

$$\begin{aligned}
\text{but } d_1^{(0)}c_1^4 + d_2^{(0)}c_2^4 &= \frac{2c_2-1}{2(c_2-c_1)}c_1^4 + \frac{1-2c_1}{2(c_2-c_1)}c_2^4 \\
&= \frac{1}{2}\left(\frac{3-\sqrt{3}}{6}\right)^4 + \frac{1}{2}\left(\frac{3+\sqrt{3}}{6}\right)^4 \\
&= \frac{7}{36} \neq \frac{1}{5}.
\end{aligned}$$

Thus, for the particular values $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$, the order conditions are satisfied for **order 4** but not for **order 5**. Therefore the two-point mixed collocation method has **order 3** when $c_1 = (2-3c_2)/(3-6c_2)$, $(c_2 \neq 1/2)$, and **order 4** when c_1 and c_2 are the Gauss nodes. Otherwise the method has **order 2**.

When the collocation points are symmetric, i.e. $c_1 + c_2 = 1$, then the order is at least 2 and the nodes $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$ give the highest order of 4.

Order Conditions for Three Collocation Points

As the three-point mixed collocation method may be written as a Runge-Kutta-Nyström method, the order conditions of section 4.2.2 can be applied. Using Maple, the conditions for **orders 1, 2** and **3** are satisfied for all values of c_1, c_2 and c_3.

For **order 4**, all the conditions are satisfied iff

$$c_1 = \frac{1}{2}\left(\frac{6c_2c_3 - 4(c_2+c_3)+3}{6c_2c_3 - 3(c_2+c_3)+2}\right).$$

For **order 5**, all the conditions are satisfied iff

$$c_1 = \frac{1}{2}\left(\frac{6c_2c_3 - 4(c_2+c_3)+3}{6c_2c_3 - 3(c_2+c_3)+2}\right),$$

and

$$c_2 = \frac{30c_3^2 - 32c_3 + 6 \pm \sqrt{(300c_3^4 - 600c_3^3 + 384c_3^2 - 84c_3 + 6)}}{60c_3^2 - 60c_3 + 10}.$$

For **order 6**, we require

$$c_1 = \frac{5-\sqrt{15}}{10}, \; c_2 = \frac{1}{2}, \; c_3 = \frac{5+\sqrt{15}}{10}.$$

If the symmetric collocation points, $c_1 + c_3 = 1$ and $c_2 = 1/2$ are substituted into the order conditions, we have order at least 4, which is one order more than the default order. The highest order of 6 is obtained when $c_1 = (5-\sqrt{15})/10$, $c_2 = 1/2$ and $c_3 = (5+\sqrt{15})/10$.

Chapter 5

Stability Analysis

In this chapter, we consider the stability of the one, two and three-point mixed collocation methods. Coleman and Ixaru [23] were concerned with the stability analysis of exponentially-fitted multistep methods, but the theory can be easily applied to the mixed collocation methods which we shall regard as Runge-Kutta-Nyström methods with steplength dependent coefficients. The definitions for stability and for concepts such as periodicity for exponentially-fitted methods are presented in chapter 3.

5.1 Stability Concepts

When the mixed collocation method (4.16) is applied to the test equation $y'' = -w^2 y$ we obtain the recurrence relation

$$y_{n+2} - S(\nu^2;\theta)y_{n+1} + P(\nu^2;\theta)y_n = 0.$$

We look for solutions of the characteristic equation

$$\xi^2 - 2R_{nm}(\nu^2;\theta)\xi + P(\nu^2;\theta) = 0$$

where R_{nm} is a rational function of ν^2 expressible as

$$R_{nm}(\nu^2;\theta) = \frac{\alpha_0 + \sum\limits_{k=1}^{n} \alpha_k \nu^{2k}}{1 + \sum\limits_{k=1}^{m} \beta_k \nu^{2k}} \tag{5.1}$$

where $\nu = wh$, and the coefficients α_k and β_k are dependent on the steplength h.

$R_{nm}(\nu^2;\theta)$ is called the **stability function** of a corresponding mixed collocation method. Note that the subscript n for the stability function and in the recurrence relation are not the same.

If the characteristic equation is of the form

$$\xi^2 - 2R_{nm}(\nu^2;\theta)\xi + 1 = 0$$

then we can apply Definition 3.4.

Example : $n = m = 1$
Assuming $P(\nu^2;\theta) = 1$, from Definition 3.4, the stability boundary for $R_{11}(\nu^2;\theta)$ is given by

$$|R_{11}(\nu^2;\theta)| = \left|\frac{\alpha_0 + \alpha_1\nu^2}{1 + \beta_1\nu^2}\right| = 1.$$

For $R_{11}(\nu^2;\theta) = 1$ we have $\alpha_0 + \alpha_1\nu^2 = 1 + \beta_1\nu^2$ from which

$$\nu = \pm\left\{\frac{1 - \alpha_0}{\alpha_1 - \beta_1}\right\}^{1/2}$$

or

$$\alpha_0 - 1 = 0 \text{ and } \alpha_1 - \beta_1 = 0.$$

For $R_{11}(\nu^2;\theta) = -1$ we obtain $\alpha_0 + \alpha_1\nu^2 = -1 - \beta_1\nu^2$ from which

$$\nu = \pm\left\{\frac{-1 - \alpha_0}{\alpha_1 + \beta_1}\right\}^{1/2}$$

or

$$\alpha_0 + 1 = 0 \text{ and } \alpha_1 + \beta_1 = 0.$$

Thus the stability boundaries are

$$\nu = \nu_{\pm}(\theta) = \left\{-\left(\frac{\alpha_0 \pm 1}{\alpha_1 \pm \beta_1}\right)\right\}^{1/2} \tag{5.2}$$

and the lines corresponding to any values of θ for which

$$\alpha_0(\theta) \pm 1 = 0 = \alpha_1(\theta) \pm \beta_1(\theta). \tag{5.3}$$

We also need to consider any values of θ for which the coefficients α_i and β_i are undefined.

5.1.1 One Collocation Point

The formulae for the one-point mixed collocation method is

$$\begin{aligned} y_{n+1} &= y_n + hA_1 z_n + h^2 A_2 f_{n+c} \\ z_{n+1} &= A_3 z_n + hA_4 f_{n+c} \\ y_{n+c} &= y_n + hA_5 z_n + h^2 A_6 f_{n+c} \end{aligned}$$

where

$$A_1 = \frac{\sin[\theta(1-c)] + \sin(\theta c)}{\theta \cos(\theta c)}, \quad A_2 = \frac{1-\cos\theta}{\theta^2 \cos(\theta c)}, \quad A_3 = \frac{\cos[\theta(1-c)]}{\cos(\theta c)},$$

$$A_4 = \frac{\sin\theta}{\theta\cos(\theta c)}, \quad A_5 = \frac{\sin(\theta c)}{\theta\cos(\theta c)}, \quad A_6 = \frac{1-\cos(\theta c)}{\theta^2\cos(\theta c)}$$

and $\theta = kh$. The method is undefined when $\theta = 0$ or $\cos(\theta c) = 0$.

Applying the method to the test equation $y'' = -w^2 y$ and setting $\nu = wh$ gives

$$\begin{aligned} y_{n+1} &= y_n + hA_1 z_n - \nu^2 A_2 y_{n+c}, \\ hz_{n+1} &= A_3 hz_n - \nu^2 A_4 y_{n+c}, \\ y_{n+c} &= y_n + hA_5 z_n - \nu^2 A_6 y_{n+c} \end{aligned}$$

and we make y_{n+c} the subject of the last equation

$$y_{n+c} = \frac{y_n + hA_5 z_n}{1+\nu^2 A_6}.$$

Substituting y_{n+c} into y_{n+1} and rearranging gives

$$\begin{aligned} y_{n+1} &= y_n\left(\frac{1+\nu^2(A_6 - A_2)}{1+\nu^2 A_6}\right) + hz_n\left(\frac{A_1 + \nu^2(A_1A_6 - A_2A_5)}{1+\nu^2 A_6}\right) \\ &= D_1 y_n + D_2 hz_n. \end{aligned}$$

Similarly substituting y_{n+c} into hz_{n+1},

$$\begin{aligned} hz_{n+1} &= \left(\frac{-\nu^2 A_4}{1+\nu^2 A_6}\right) y_n + hz_n \left(\frac{A_3+\nu^2(A_3A_6 - A_4A_5)}{1+\nu^2 A_6}\right) \\ &= D_3 y_n + D_4 hz_n. \end{aligned}$$

Therefore,

$$y_{n+1} = D_1 y_n + hD_2 z_n \quad (5.4)$$

$$hz_{n+1} = D_3 y_n + hD_4 z_n. \quad (5.5)$$

Rewrite (5.4) as

$$y_{n+2} = D_1 y_{n+1} + hD_2 z_{n+1}$$

and substitute (5.5) for z_{n+1} into the last equation to give

$$\begin{aligned} y_{n+2} &= D_1 y_{n+1} + D_2 D_3 y_n + D_2 D_4 hz_n \\ &= D_1 y_{n+1} + D_2 D_3 y_n + D_4(y_{n+1} - D_1 y_n). \end{aligned}$$

Therefore the recurrence relation is

$$y_{n+2} - (D_1 + D_4) y_{n+1} + (D_1 D_4 - D_2 D_3) y_n = 0.$$

We look for the solution of the characteristic equation

$$\xi^2 - (D_1 + D_4)\xi + (D_1 D_4 - D_2 D_3) = 0.$$

Substituting the values for D_i and A_i and rearranging gives

$$D_1 + D_4 = \frac{\theta^2(\cos(\theta c) + \cos[\theta(1-c)]) + \nu^2(2\cos\theta - \cos(\theta c) - \cos[\theta(1-c)])}{\theta^2 \cos(\theta c) + \nu^2(1 - \cos(\theta c))}$$

and

$$D_1 D_4 - D_2 D_3 = \frac{\theta^2 \cos[\theta(1-c)] + \nu^2(1 - \cos[\theta(1-c)])}{\theta^2 \cos(\theta c) + \nu^2(1 - \cos(\theta c))}.$$

Thus the characteristic equation for the one-point mixed collocation method is

$$\xi^2 - \left\{\frac{\theta^2(\cos(\theta c) + \cos[\theta(1-c)]) + \nu^2(2\cos\theta - \cos(\theta c) - \cos[\theta(1-c)])}{\theta^2 \cos(\theta c) + \nu^2[1 - \cos(\theta c)]}\right\}\xi$$

$$+\frac{\theta^2\cos[\theta(1-c)]+\nu^2(1-\cos[\theta(1-c)])}{\theta^2\cos(\theta c)+\nu^2[1-\cos(\theta c)]}=0. \quad (5.6)$$

For an interval of periodicity we require

$$P(\nu^2;\theta)=\frac{\theta^2\cos[\theta(1-c)]+\nu^2(1-\cos[\theta(1-c)])}{\theta^2\cos(\theta c)+\nu^2[1-\cos(\theta c)]}=1$$

$$\begin{aligned}\Rightarrow \theta^2\cos[\theta(1-c)]+\nu^2(1-\cos[\theta(1-c)]) &= \theta^2\cos(\theta c)+\nu^2[1-\cos(\theta c)]\\ \Rightarrow \nu^2(\cos(\theta c)-\cos[\theta(1-c)]) &= \theta^2(\cos(\theta c)-\cos[\theta(1-c)])\end{aligned}$$

from which either $\nu^2=\theta^2 \Rightarrow \nu=\theta$ or $\cos(\theta c)-\cos[\theta(1-c)]=0$. Thus as

$$\cos(\theta c)-\cos[\theta(1-c)]=2\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}(1-2c)\right)$$

then the most suitable value for which $\cos(\theta c)-\cos[\theta(1-c)]$ is zero is when $c=1/2$ and checking, this value of the collocation point satisfies $P(\nu^2;\theta)=1$.

Therefore, when $c=1/2$, the characteristic equation (5.6) is

$$\xi^2-2R_{11}(\nu^2;\theta)\xi+1=0$$

where $R_{11}(\nu^2;\theta)$ is the stability function given by

$$R_{11}(\nu^2;\theta)=\frac{\theta^2\cos(\theta/2)+\nu^2\{\cos\theta-\cos(\theta/2)\}}{\theta^2\cos(\theta/2)+\nu^2\{1-\cos(\theta/2)\}}.$$

For $\theta^2\cos(\theta/2)\neq 0 \Rightarrow \theta\neq(2n+1)\pi$ where n is a non-negative integer, we can rewrite $R_{11}(\nu^2;\theta)$ as

$$R_{11}(\nu^2;\theta)=\frac{1+\nu^2\left\{\dfrac{\cos\theta-\cos(\theta/2)}{\theta^2\cos(\theta/2)}\right\}}{1+\nu^2\left\{\dfrac{1-\cos(\theta/2)}{\theta^2\cos(\theta/2)}\right\}}$$

where the coefficients of the stability function are

$$\alpha_0=1,\quad \alpha_1=\frac{\cos\theta-\cos(\theta/2)}{\theta^2\cos(\theta/2)},\quad \beta_1=\frac{1-\cos(\theta/2)}{\theta^2\cos(\theta/2)}.$$

The stability boundary is given by $|R_{11}(\nu^2;\theta)| = 1$ by definition and so from (5.2) the stability curves are

$$\nu = \nu_\pm(\theta) = \left\{-\left(\frac{1 \pm 1}{\cos\theta - \cos(\theta/2) \pm (1 - \cos(\theta/2))}\right)\theta^2\cos(\theta/2)\right\}^{1/2}.$$

Therefore

$$\nu_+(\theta) = \left\{\frac{2\theta^2\cos(\theta/2)}{2\cos(\theta/2) - 2\cos^2(\theta/2)}\right\}^{1/2} = \left\{\frac{\theta^2}{1 - \cos(\theta/2)}\right\}^{1/2}$$

and

$$\nu_-(\theta) = 0.$$

Also, as $\alpha_0 = 1$, we look at the stability boundaries given by the lines corresponding to any values of θ for which $\alpha_1 - \beta_1 = 0$. Thus from (5.3),

$$\alpha_0 - 1 = 1 - 1 = 0 \quad \text{and} \quad \alpha_1 - \beta_1 = \frac{\cos\theta - 1}{\theta^2\cos(\theta/2)},$$

and $\alpha_1 - \beta_1 = 0$ when $\cos\theta = 1 \;\Rightarrow\; \theta = 2n\pi$, where n is a non-negative integer. The curves

$$\nu_+(\theta) = \left\{\frac{\theta^2}{1 - \cos(\theta/2)}\right\}^{1/2}$$

are undefined when $1 - \cos(\theta/2) = 0 \;\Rightarrow\; \theta = 4n\pi$, where n is a non-negative integer.

Summarising, the stability boundaries for the one-point mixed collocation method with $c = 1/2$ are the axis $\nu_-(\theta) = 0$, the curves

$$\nu_+(\theta) = \frac{\theta}{\sqrt{(1 - \cos(\theta/2))}}$$

and the lines $\theta = 2n\pi$ where n is a non-negative integer. The method is undefined when $\theta = (2n+1)\pi$, i.e. any odd multiples of π.

Since all solutions of the test equation $y'' = -w^2 y$ satisfy

$$y(x_{n+2}) - 2(\cos\nu)\, y(x_{n+1}) + y(x_n) = 0,$$

the stability function $R_{nm}(\nu^2;\theta)$ can be regarded as a rational approximation for

$\cos\nu$. Therefore, when $\theta = \nu$,

$$R_{11}(\nu^2;\nu) = \frac{\nu^2\cos(\nu/2) + \nu^2\{\cos\nu - \cos(\nu/2)\}}{\nu^2\cos(\nu/2) + \nu^2\{1 - \cos(\nu/2)\}} = \cos\nu.$$

In the limit as $\theta \to n\pi$, for positive integers n,

$$R_{11}(\nu^2;n\pi) \to \frac{n^2\pi^2\cos(n\pi/2) + \nu^2\{(-1)^n - \cos(n\pi/2)\}}{n^2\pi^2\cos(n\pi/2) + \nu^2\{1 - \cos(n\pi/2)\}}$$

and for n odd, where the coefficients α_1 and β_1 are undefined, the stability function is

$$R_{11}(\nu^2;n\pi) \to \frac{0 + \nu^2\{-1 - 0\}}{0 + \nu^2\{1 - 0\}} = -1,$$

and for n even,

$$R_{11}(\nu^2;n\pi) \to \frac{n^2\pi^2\cos(n\pi/2) + \nu^2\{1 - \cos(n\pi/2)\}}{n^2\pi^2\cos(n\pi/2) + \nu^2\{1 - \cos(n\pi/2)\}} = 1.$$

One ratio which is very important in the stability analysis of mixed collocation methods is the quantity $r = \theta/\nu = k/w$. For any given value of r, intervals of periodicity correspond to the values of the steplength h for which the line $\theta = r\nu$ lies in a stability region of the $\nu - \theta$ plane. When $r = 1$ then $k = w$, and so the exponentially-fitted method solves the test equation exactly and the method must be stable. Therefore the line $r = 1$ can only pass through stable regions.

Substituting $\theta = r\nu$ into the stability function,

$$R_{11}(\nu^2;\theta) = \frac{\theta^2\cos(\theta/2) + \nu^2\{\cos\theta - \cos(\theta/2)\}}{\theta^2\cos(\theta/2) + \nu^2\{1 - \cos(\theta/2)\}} = \frac{(r^2-1)\cos(\theta/2) + \cos\theta}{(r^2-1)\cos(\theta/2) + 1}.$$

Here and in subsequent figures, the stability region is shaded and the line $r = 1$ is shown. The stability region for one collocation point with $c = 1/2$ is given in figure 5.1. The curves $\nu = \nu_+(\theta)$ are asymptotic to lines of constant θ corresponding to the zeros of $\alpha_1 + \beta_1$, which are $\theta = 4n\pi$ for non-negative integers n. Since $\lim_{\theta\to 0}\ \nu_+(\theta) = 2\sqrt{2}$, the interval of periodicity for $r < 1$ is $(0, h_0)$, where h_0 increases from $2\sqrt{2}/w$ when $r = 0$, (corresponding to the interval of periodicity for the polynomial collocation method in section 2.5.3), to π/w when $r = 1$, for fixed w. For $r > 1$, the primary interval of periodicity is $(0, \pi/k)$.

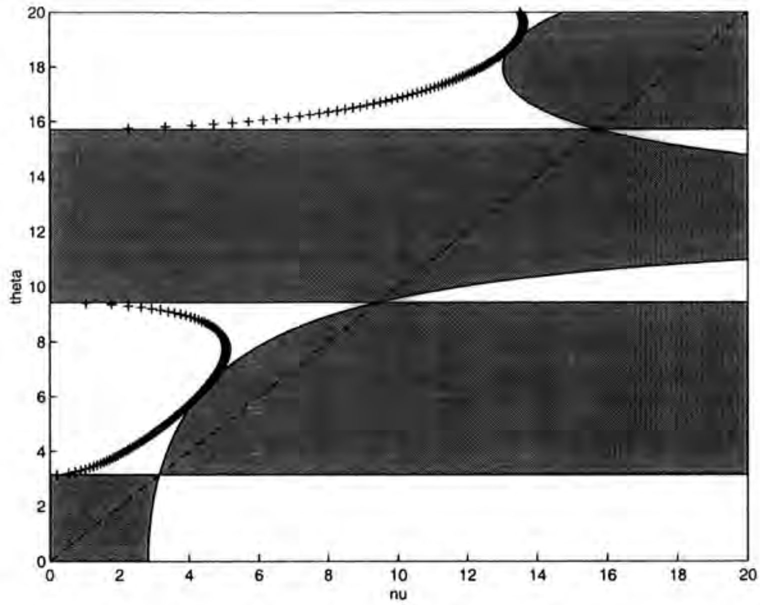

Figure 5.1: $\nu - \theta$ plot for one collocation point : c = 1/2

A number of 'apparent' inconsistencies occur on the lines $\theta = 2(2n+1)\pi$. If $\nu_+(\theta)$ is substituted into the stability function, then

$$R_{11}(\nu_+^2;\theta) = \frac{\theta^2\cos(\theta/2) + \left\{\dfrac{\theta^2}{1-\cos(\theta/2)}\right\}[\cos\theta - \cos(\theta/2)]}{\theta^2\cos(\theta/2) + \left\{\dfrac{\theta^2}{1-\cos(\theta/2)}\right\}[1-\cos(\theta/2)]} = -1.$$

Hence along the curves $\nu_+(\theta)$, we have $R_{11}(\nu_+^2;\theta) = -1$. The problem is that on the lines $\theta = 2(2n+1)\pi$ we have $R_{11}(\nu^2;\theta) = 1$, yet the lines intersect the stability curves $\nu_+(\theta)$ on which $R_{11}(\nu_+^2;\theta) = -1$. The reason for this is the stability function is undefined at the points where the lines and curves intersect. The denominator of the stability function is equal to zero when

$$\theta^2\cos(\theta/2) + \nu^2[1-\cos(\theta/2)] = 0$$

$$\Rightarrow \quad \nu = \bar{\nu}(\theta) = \sqrt{\frac{\theta^2\cos(\theta/2)}{\cos(\theta/2)-1}}$$

and the curves $\bar{\nu}(\theta)$ are given by crosses (+) in figure 5.1. The curves $\bar{\nu}(\theta)$ where

$R_{11}(\nu^2, \theta)$ is undefined meet the stability curves $\nu_+(\theta)$ when

$$\sqrt{\frac{\theta^2 \cos(\theta/2)}{\cos(\theta/2) - 1}} = \sqrt{\frac{\theta^2}{1 - \cos(\theta/2)}}$$

$$\Rightarrow \quad \cos(\theta/2) + 1 = 0$$

i.e. when $\theta = 2(2n+1)\pi$ which agrees with the figure.

We now investigate what happens as $\theta \to n\pi$. For n even, the lines are the stability boundaries, and for n odd, the coefficients of the method are undefined. Let $\theta = n\pi + \epsilon$, where ϵ is small. For n even, let $n = 2m$, and for n odd, let $n = 2m+1$ where m and n are non-negative integers.

Case i.) n **even**
For $n = 2m$, $\theta = 2m\pi + \epsilon$ and as

$$\cos\theta = \cos(2m\pi + \epsilon) = \cos\epsilon \quad \text{and} \quad \cos(\theta/2) = \cos\left(\frac{2m\pi + \epsilon}{2}\right) = (-1)^m \cos(\epsilon/2),$$

then

$$\begin{aligned} R_{11}(\nu^2;\theta) &= \frac{(r^2-1)(-1)^m \cos(\epsilon/2) + \cos\epsilon}{(r^2-1)(-1)^m \cos(\epsilon/2) + 1} \\ &= \frac{\left[(r^2-1)(-1)^m\left\{1 - \frac{\epsilon^2}{8}\right\} + 1 - \frac{\epsilon^2}{2} + ..\right]}{\left[1 + (r^2-1)(-1)^m\left\{1 - \frac{\epsilon^2}{8} + ..\right\}\right]} \\ &= 1 - \frac{\epsilon^2}{2}\frac{1}{[(-1)^m(r^2-1)+1]} + O(\epsilon^4) \end{aligned}$$

As $\epsilon \to 0$, $R_{11}(\nu^2;\theta) \to 1$.

For even m, i.e. $\theta = 4\pi, 8\pi, 12\pi, \ldots$ we have

$$R_{11}(\nu^2;\theta) = 1 - \frac{\epsilon^2}{2r^2} + O(\epsilon^4)$$

and $|R_{11}(\nu^2;\theta)| \leq 1$ for small ϵ, i.e. we have a stable region either side of the line $\theta = 2m\pi$ and these do not affect the stability regions.

For odd m, i.e. $\theta = 2\pi, 6\pi, 10\pi, \ldots$ we have

$$R_{11}(\nu^2;\theta) = 1 - \frac{\epsilon^2}{2(2-r^2)} + O(\epsilon^4).$$

Since $\frac{1}{2(2-r^2)}$ is negative when $r > \sqrt{2}$, then $|R_{11}(\nu^2;\theta)| > 1$ for small values of ϵ and we have an unstable region. For $r < \sqrt{2}$, $|R_{11}(\nu^2;\theta)| < 1$ and therefore we have a stable region.

Case ii.) n odd

For $n = 2m+1$, we have $\theta = (2m+1)\pi + \epsilon$ and as

$$\cos\theta = \cos((2m+1)\pi + \epsilon) = -\cos\epsilon,$$

$$\cos(\theta/2) = \cos\left(\frac{(2m+1)\pi + \epsilon}{2}\right) = (-1)^{m+1}\sin(\epsilon/2),$$

then

$$\begin{aligned}
R_{11}(\nu^2;\theta) &= \frac{(r^2-1)(-1)^{m+1}\sin(\epsilon/2) - \cos\epsilon}{(r^2-1)(-1)^{m+1}\sin(\epsilon/2) + 1} \\
&= \frac{(r^2-1)(-1)^{m+1}\left\{\frac{\epsilon}{2} + O(\epsilon^2)\right\} - 1}{1 + (r^2-1)(-1)^{m+1}\left\{\frac{\epsilon}{2} + O(\epsilon^2)\right\}} \\
&= \left[-1 + \frac{\epsilon}{2}(r^2-1)(-1)^{m+1}\right]\left[1 - \frac{\epsilon}{2}(r^2-1)(-1)^{m+1}\right] + O(\epsilon^2) \\
&= -1 + (r^2-1)(-1)^{m+1}\epsilon + O(\epsilon^2).
\end{aligned}$$

So, $R_{11}(\nu^2;\theta) \to -1$ as $\epsilon \to 0$.

For m even, i.e. $\theta = \pi, 5\pi, 9\pi, \ldots$ we have

$$R_{11}(\nu^2;\theta) = -1 - (r^2-1)\epsilon + O(\epsilon^2)$$

and as ϵ increases from negative to positive values, $|R_{11}(\nu^2;\theta)|$ increases or decreases through 1 for r greater than or less than 1 respectively.

For m odd, i.e. $\theta = 3\pi, 7\pi, 11\pi, \ldots$, we have

$$R_{11}(\nu^2;\theta) = -1 + (r^2-1)\epsilon + O(\epsilon^2)$$

and as ϵ increases from negative to positive values, $|R_{11}(\nu^2;\theta)|$ increases or decreases through 1 for r less than or greater than 1 respectively.

We know that as $k \to 0$, the mixed collocation methods reduce to the classical polynomial collocation methods described in section 2.2.3. As mentioned previously, the interval of periodicity for the polynomial collocation methods is given by $(0, \nu_0^2)$, Definition 2.11, whilst for exponentially-fitted methods, it is of the form $(0, h_0)$, Definition 3.5. From section 2.5.3, the stability function for the polynomial collocation method with $c = 1/2$ is

$$R_{11}^{PC}(\nu^2) = \frac{8 - 3\nu^2}{8 + \nu^2}.$$

For the one-point mixed collocation method with $c = 1/2$, the stability function is

$$R_{11}^{MC}(\nu^2;\theta) = \frac{\theta^2\cos(\theta/2) + \nu^2(\cos\theta - \cos(\theta/2))}{\theta^2\cos(\theta/2) + \nu^2(1 - \cos(\theta/2))}.$$

As $k \to 0$,

$$R_{11}^{MC}(\nu^2;\theta) \to \frac{1 - 3\nu^2/8}{1 + \nu^2/8} = \frac{8 - 3\nu^2}{8 + \nu^2}$$

as required.

Stability for one collocation point $c = 0$

If we substitute $c = 0$ into (5.6), the stability equation is

$$\xi^2 - \left\{\frac{\theta^2[1 + \cos\theta] + \nu^2[\cos\theta - 1]}{\theta^2}\right\}\xi + \frac{\theta^2\cos\theta + \nu^2[1 - \cos\theta]}{\theta^2} = 0.$$

As $P(\nu^2;\theta) \neq 1$, except for the exact case when $\nu = \theta$, we look for where the roots ξ_s of the stability equation satisfy $|\xi_s| \leq 1$, and any roots on the unit circle are simple. Thus, if the modulus of the roots are less than or equal to 1, then the modulus of the product of the roots must be less than or equal to 1, i.e. $|\xi_1.\xi_2| \leq 1$. Therefore,

$$\left|\frac{\theta^2\cos\theta + \nu^2[1 - \cos\theta]}{\theta^2}\right| \leq 1$$

$$\Rightarrow \quad \theta^2\cos\theta + \nu^2[1 - \cos\theta] \leq \theta^2 \quad \Rightarrow \quad \nu^2 \leq \theta^2 \quad \text{i.e.} \quad \nu \leq \theta,$$

and

$$-\theta^2\cos\theta - \nu^2[1 - \cos\theta] \leq \theta^2 \quad \Rightarrow \quad \nu^2 \geq \frac{\theta^2[\cos\theta + 1]}{\cos\theta - 1} \quad \text{for } \theta \neq 2n\pi.$$

As the right hand side of the latter inequality is less than zero for all θ, then the inequality is satisfied for all θ. Thus, the method is unstable when $\nu > \theta$, i.e. $w > k$.

When $\nu = \theta$, the stability equation becomes

$$\xi^2 - 2\cos\theta\,\xi + 1 = 0$$

and as the modulus of the roots $\xi_\pm$ are equal to 1, then the method is stable.

We now use the Routh-Hurwitz approach. Substituting $\xi = \frac{1+z}{1-z}$ $(z \neq 1)$ into the characteristic equation and multiplying by $(1-z)^2$, we have

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

where

$$a_0 = 2(\cos\theta + 1), \quad a_1 = \frac{2(\theta^2 - \nu^2)(1-\cos\theta)}{\theta^2} \quad \text{and} \quad a_2 = \frac{2(1-\cos\theta)\nu^2}{\theta^2}.$$

The method is stable if the coefficients a_0, a_1 and a_2 are greater or equal to 0. Thus,

$$\begin{aligned} a_0 \geq 0 &\Rightarrow \cos\theta + 1 \geq 0, \\ a_1 \geq 0 &\Rightarrow 1 - \cos\theta \geq 0 \text{ and } \nu \leq \theta, \\ a_2 \geq 0 &\Rightarrow 1 - \cos\theta \geq 0. \end{aligned} \tag{5.7}$$

As $1 - \cos\theta \geq 0$ and $\cos\theta + 1 \geq 0$ for all θ, then the one-point mixed collocation method with $c = 0$ is stable if $\nu \leq \theta$.

Stability for one collocation point $c = 1$

Substituting $c = 1$ into (5.6), the stability equation is given by

$$\xi^2 - \left\{\frac{\theta^2[1+\cos\theta] + \nu^2[\cos\theta - 1]}{\theta^2\cos\theta + \nu^2[1-\cos\theta]}\right\}\xi + \frac{\theta^2}{\theta^2\cos\theta + \nu^2[1-\cos\theta]} = 0.$$

The roots of the stability equation are

$$\begin{aligned} \xi_\pm = -\frac{1}{2}\Bigg\{ & \frac{(\cos\theta - 1)\nu^2 + \theta^2(\cos\theta + 1)}{[(\cos\theta - 1)\nu^2 - \theta^2\cos\theta]} \\ & \pm \frac{\sqrt{(\cos\theta - 1)[(\cos\theta - 1)(\theta^4 + \nu^4) + 2\theta^2(\cos\theta + 3)\nu^2]}}{[(\cos\theta - 1)\nu^2 - \theta^2\cos\theta]}\Bigg\}. \end{aligned}$$

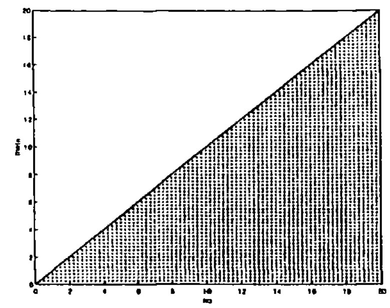

Figure 5.2: Stability regions for the one-point mixed collocation method : c = 1

Again, as $P(\nu^2;\theta) \neq 1$, except for the exact case when $\nu = \theta$, we look for where the modulus of the product of the roots are less than or equal to 1. Thus,,

$$\left|\frac{\theta^2}{\theta^2\cos\theta + \nu^2[1-\cos\theta]}\right| \leq 1$$

$$\Rightarrow \quad \theta^2\cos\theta + \nu^2[1-\cos\theta] \geq \theta^2 \quad \Rightarrow \quad \theta^2 \leq \nu^2 \quad \text{i.e.} \quad \theta \leq \nu,$$

and

$$\theta^2\cos\theta + \nu^2[1-\cos\theta] \geq -\theta^2 \quad \Rightarrow \quad \nu^2 \geq \frac{\theta^2[\cos\theta + 1]}{\cos\theta - 1}$$

and as the last inequality is satisfied because the right hand side is less than zero for all θ, then the method is unstable when $\nu < \theta$, i.e. $w < k$.

Again, when $\nu = \theta$,

$$\xi_{\pm} = \frac{\theta^2\cos\theta \pm \sqrt{-\theta^4\sin^2\theta}}{\theta^2} = \cos\theta \pm i\sin\theta.$$

Therefore, the modulus of the roots $\xi_{\pm}$ are equal to 1 and so the method is stable when $\nu = \theta$.

For $\nu \geq \theta$, one approach is to substitute particular values for ν and θ into the stability equation above and solve for ξ to see whether the method is stable ($|\xi_s| \leq 1$). In figure 5.2, a dot is a stable point for where both $|\xi_+|$ and $|\xi_-|$ are less or equal to 1 for particular values of ν and θ.

As we can see from figure 5.2, all the points satisfy $\nu \geq \theta$ and so the one-point mixed collocation method with $c = 1$ is stable when $\nu \geq \theta$.

Two or more collocation points ($s \geq 2$)

If we apply the mixed collocation methods to the test equation $y'' = -w^2 y$ and rearrange, we obtain

$$\begin{pmatrix} y_{n+1} \\ hz_{n+1} \end{pmatrix} = M(\nu^2;\theta) \begin{pmatrix} y_n \\ hz_n \end{pmatrix}$$

where

$$M(\nu^2;\theta) = \begin{pmatrix} 1 - \nu^2 \mathbf{b}^T(I+\nu^2 A)^{-1}\mathbf{e} & 1 - \nu^2 \mathbf{b}^T(I+\nu^2 A)^{-1}\mathbf{c} \\ -\nu^2 \mathbf{d}^T(I+\nu^2 A)^{-1}\mathbf{e} & 1 - \nu^2 \mathbf{d}^T(I+\nu^2 A)^{-1}\mathbf{c} \end{pmatrix} \tag{5.8}$$

and the coefficients b_i, d_i and a_{ij} depend on the steplength h.

A characteristic equation of the form

$$\xi^2 - 2R_{nm}(\nu^2;\theta)\xi + P(\nu^2;\theta) = 0$$

is obtained where

$$R_{nm}(\nu^2;\theta) = \frac{1}{2}\,\text{trace}\ M(\nu^2;\theta) \quad \text{and} \quad P(\nu^2;\theta) = \det\ M(\nu^2;\theta)$$

and we can apply the stability theory for exponentially-fitted methods in chapter 3.

5.1.2 Two Collocation Points

Using Maple, the characteristic equation for two collocation points is

$$\xi^2 - 2R_{22}(\nu^2;\theta)\xi + P(\nu^2;\theta) = 0$$

where the stability function is

$$R_{22}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4}{1 + \beta_1\nu^2 + \beta_2\nu^4} \tag{5.9}$$

with

$$\begin{aligned} \alpha_0 &= 1, \\ \alpha_1 &= \{\theta[\mathcal{P}\cos(\theta c_2) - \mathcal{Q}\cos(\theta c_1) + c_2\cos(\theta\mathcal{P}) - c_1\cos(\theta\mathcal{Q})] \end{aligned}$$

$$\begin{aligned}
&\quad + \sin(\theta c_2) - \sin(\theta c_1) - \sin(\theta \mathcal{Q}) + \sin(\theta \mathcal{P}) - 4\mathcal{E}\} / (2\theta^2 \mathcal{E}), \\
\alpha_2 &= \{\theta[c_1 \cos(\theta \mathcal{Q}) - c_2 \cos(\theta \mathcal{P}) + \mathcal{Q}\cos(\theta c_1) - \mathcal{P}\cos(\theta c_2) + 2(c_2 - c_1)\cos\theta] \\
&\quad + 2\mathcal{E} + \sin(\theta \mathcal{Q}) - \sin(\theta \mathcal{P}) + \sin(\theta c_1) - \sin(\theta c_2)\} / (2\theta^4 \mathcal{E}), \\
\beta_1 &= \frac{\sin(\theta c_2) - \sin(\theta c_1) + \theta[c_2 \cos(\theta c_1) - c_1 \cos(\theta c_2)] - 2\mathcal{E}}{\theta^2 \mathcal{E}}, \\
\beta_2 &= \frac{\sin(\theta c_1) - \sin(\theta c_2) + \theta[c_2 - c_1 + c_1 \cos(\theta c_2) - c_2 \cos(\theta c_1)] + \mathcal{E}}{\theta^4 \mathcal{E}},
\end{aligned}$$

and $P(\nu^2;\theta)$ is given by

$$P(\nu^2;\theta) = \frac{\rho_0 + \rho_1 \nu^2 + \rho_2 \nu^4}{1 + \sigma_1 \nu^2 + \sigma_2 \nu^4} \tag{5.10}$$

with

$$\begin{aligned}
\rho_0 &= 1, \\
\rho_1 &= \frac{-\sin(\theta \mathcal{Q}) + \sin(\theta \mathcal{P}) + \theta[\mathcal{P}\cos(\theta \mathcal{Q}) - \mathcal{Q}\cos(\theta \mathcal{P})] - 2\mathcal{E}}{\theta^2 \mathcal{E}}, \\
\rho_2 &= \frac{-\sin(\theta \mathcal{P}) + \sin(\theta \mathcal{Q}) + \theta[c_2 - c_1 + \mathcal{Q}\cos(\theta \mathcal{P}) - \mathcal{P}\cos(\theta \mathcal{Q})] + \mathcal{E}}{\theta^4 \mathcal{E}}, \\
\sigma_1 &= \frac{\sin(\theta c_2) - \sin(\theta c_1) + \theta[c_2 \cos(\theta c_1) - c_1 \cos(\theta c_2)] - 2\mathcal{E}}{\theta^2 \mathcal{E}}, \\
\sigma_2 &= \frac{\sin(\theta c_1) - \sin(\theta c_2) + \theta[c_2 - c_1 + c_1 \cos(\theta c_2) - c_2 \cos(\theta c_1)] + \mathcal{E}}{\theta^4 \mathcal{E}}
\end{aligned}$$

where

$$\mathcal{E} = \sin[\theta(c_2 - c_1)], \quad \mathcal{P} = 1 - c_1 \quad \text{and} \quad \mathcal{Q} = 1 - c_2.$$

As the collocation nodes are distinct, we require $\theta(c_2 - c_1) \neq n\pi$ where n is a non-negative integer, for $R_{22}(\nu^2;\theta)$ and $P(\nu^2;\theta)$ to be defined.

For an interval of periodicity we require $P(\nu^2;\theta) = 1$. The series expansion of $P(\nu^2;\theta)$ about $h = 0$ is

$$P(\nu^2;\theta) = 1 + \frac{1}{12}(c_2 + c_1 - 1)(2c_1c_2 - c_1 - c_2 + 1)(k^2 - w^2)w^2h^4$$

$$+\frac{1}{720}(c_2 + c_1 - 1)(k^2 - w^2)(14k^2c_1^3c_2 - 7k^2c_1^3 + 19k^2c_1^2c_2 - 40k^2c_2^2c_1^2$$

$$+3k^2c_1^2 + 14k^2c_1c_2^3 + 8k^2c_1 - 34k^2c_1c_2 + 19k^2c_1c_2^2 + 8k^2c_2 - 4k^2 - 7k^2c_2^3$$

$$+3k^2c_2^2 + 40w^2c_1^2c_2^2 - 20w^2c_1^3c_2 + 10w^2c_1^3 - 20w^2c_1c_2^3 + 10w^2c_2^3 - 10w^2c_2^2$$

$$-10w^2c_1c_2^2 + 20w^2c_1c_2 - 10w^2c_1^2 - 10w^2c_1^2c_2)w^2h^6 + O(h^7).$$

If we take the collocation nodes to be symmetric, i.e. $c_1 + c_2 = 1$, then substituting the nodes back into the exact form for $P(\nu^2;\theta)$, we obtain $P(\nu^2;\theta) = 1$. Therefore, for example, if we set $c_1 = 0$ and $c_2 = 1$, then $P(\nu^2;\theta) = 1$ and the stability function is of the form $R_{11}(\nu^2;\theta)$, that is the numerator and denominator are linear in ν^2. The mixed collocation method has order 2 for these particular values of the collocation nodes.

When $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$, then $P(\nu^2;\theta) = 1$ and we also obtain the highest possible algebraic order 4. Therefore, the pattern emerging appears to be that for a mixed collocation method to have an interval of periodicity, we require the collocation nodes to be symmetric. As yet, we have been unable to prove this for the general case.

Example: $c_1 = 0$ and $c_2 = 1$
For $c_1 = 0$ and $c_2 = 1$, the characteristic equation is $\xi^2 - 2R_{11}(\nu^2;\theta)\xi + 1 = 0$ where

$$R_{11}(\nu^2;\theta) = \frac{\theta^2\sin\theta + \nu^2(\theta\cos\theta - \sin\theta)}{\theta^2\sin\theta + \nu^2(\theta - \sin\theta)} = \frac{1 + \nu^2\left\{\dfrac{\theta\cos\theta - \sin\theta}{\theta^2\sin\theta}\right\}}{1 + \nu^2\left\{\dfrac{\theta - \sin\theta}{\theta^2\sin\theta}\right\}}$$

for $\theta^2\sin\theta \neq 0$.
The coefficients in (5.1) are

$$\alpha_0 = 1, \quad \alpha_1 = \frac{\theta\cos\theta - \sin\theta}{\theta^2\sin\theta}, \quad \beta_1 = \frac{\theta - \sin\theta}{\theta^2\sin\theta}$$

and α_1 and β_1 are undefined when $\theta^2\sin\theta = 0$, that is when $\theta = n\pi$ where n is a non-negative integer.

The stability boundaries are given by (5.2) and so

$$\nu = \nu_\pm(\theta) = \left\{-\left(\frac{1\pm 1}{\theta\cos\theta - \sin\theta \pm (\theta - \sin\theta)}\right)\theta^2\sin\theta\right\}^{1/2}$$

which are rearranged to give

$$\nu_+(\theta) = \left\{ \frac{2\theta^2 \sin\theta}{2\sin\theta - \theta(\cos\theta + 1)} \right\}^{1/2} \quad \text{and} \quad \nu_-(\theta) = 0.$$

From (5.3), as $\alpha_0 = 1$, we need to find values of θ for which $\alpha_1 - \beta_1 = 0$. From the coefficients α_1 and β_1,

$$\alpha_1 - \beta_1 = \theta\frac{(\cos\theta - 1)}{\theta^2 \sin\theta} = \frac{-2\sin^2(\theta/2)}{2\theta \sin(\theta/2)\cos(\theta/2)} = \frac{-\tan(\theta/2)}{\theta},$$

and so $\alpha_1 - \beta_1 = 0$ when $\theta = 2n\pi$ where n is a non-negative integer.

When $\theta = \nu$,

$$R_{11}(\nu^2; \nu) = \frac{\nu^2 \sin\nu + \nu^2(\nu\cos\nu - \sin\nu)}{\nu^2 \sin\nu + \nu^2(\nu - \sin\nu)} = \cos\nu.$$

For $\theta = n\pi$,

$$R_{11}(\nu^2; n\pi) = \frac{n^2\pi^2 \sin(n\pi) + \nu^2\{n\pi\cos(n\pi) - \sin(n\pi)\}}{n^2\pi^2 \sin(n\pi) + \nu^2\{n\pi - \sin(n\pi)\}} = \cos(n\pi) = (-1)^n,$$

so for n even, $R_{11}(\nu^2; n\pi) = 1$ and for n odd, $R_{11}(\nu^2; n\pi) = -1$.

In figure 5.3, the stability region is shaded. The curves $\nu = \nu_+(\theta)$ are asymptotic to $\theta = 8.9868$ and $\theta = 15.4505$ which are the zeros of $\alpha_1 + \beta_1$. When $r < 1$, the length of the primary interval of periodicity is $(0, h_0)$ where h_0 decreases from $2\sqrt{3}/w$ when $r = 0$ to π/w as $r \to 1$, for fixed w. There is a succession of secondary intervals for $r > 1$ given by $(2n\pi/k, (2n+1)\pi/k)$, where n is a non-negative integer. The stability function has unit modulus when $\theta = 2n\pi$ and these lines do not affect the stability boundaries. We check that the value of the stability function on the stability curves $\nu_+(\theta)$ agrees with the value on the lines $\theta = (2n+1)\pi$ when the lines and curves touch. Along the curves $\nu_+(\theta)$, $R_{11}(\nu_+^2; \theta) = -1$ and as $R_{11}(\nu^2; (2n+1)\pi) = -1$, then this is satisfied.

With $\theta = r\nu$,

$$R_{11}(\nu^2; \theta) = \frac{(r^2 - 1)\sin\theta + \theta\cos\theta}{(r^2 - 1)\sin\theta + \theta}.$$

To investigate what happens as $\theta \to n\pi$, the values for which the method is unde-

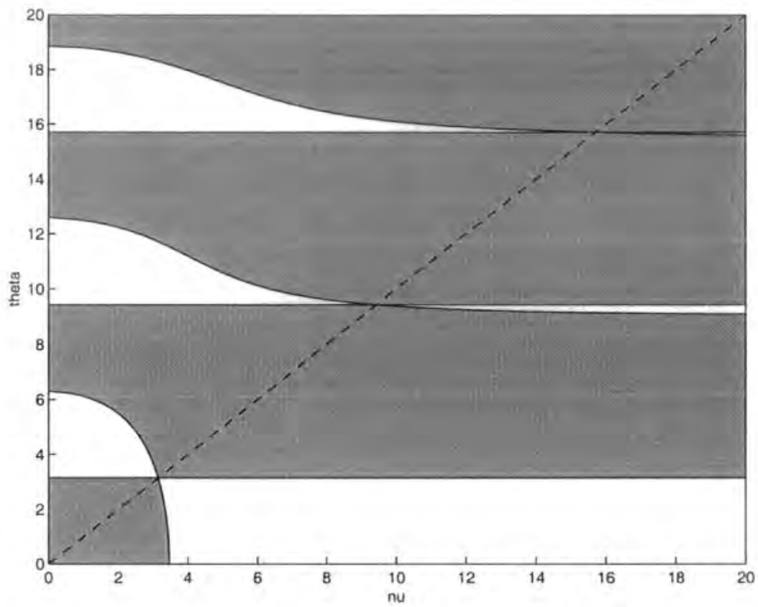

Figure 5.3: $\nu - \theta$ plot for two collocation points : c = 0 and 1

fined, let $\theta = n\pi + \epsilon$ where ϵ is small. Then

$$\sin\theta = \sin(n\pi + \epsilon) = (-1)^n \sin\epsilon \quad \text{and} \quad \cos\theta = \cos(n\pi + \epsilon) = (-1)^n \cos\epsilon.$$

Thus, the stability function becomes

$$\begin{aligned} R_{11}(\nu^2;\theta) &= \frac{(r^2-1)(-1)^n \sin\epsilon + (n\pi+\epsilon)(-1)^n\cos\epsilon}{(r^2-1)(-1)^n\sin\epsilon + n\pi + \epsilon} \\ &= (-1)^n + \frac{\epsilon}{n\pi}(r^2-1)\left[(-1)^n - 1\right] \\ &\quad + \frac{\epsilon^2}{2n^2\pi^2}\left\{2\left[(-1)^n - 1\right](r^2-1)(r^2-2) - (-1)^n n^2\pi^2\right\} \\ &\quad - \frac{\epsilon^3}{6n^3\pi^3}(r^2-1)\left\{6(r^2-2)^2\left[1-(-1)^n\right] + n^2\pi^2\left[(-1)^n - 4\right]\right\} + O(\epsilon^4) \end{aligned}$$

As $\epsilon \to 0$, $R_{11}(\nu^2;\theta) \to (-1)^n$. For n odd,

$$R_{11}(\nu^2;\theta) = -1 - \frac{2\epsilon(r^2-1)}{n\pi} + O(\epsilon^2)$$

and as ϵ increases from negative to positive values, $|R_{11}(\nu^2;\theta)|$ increases or decreases through 1 for r greater than or less than 1 respectively. For n even,

$$R_{11}(\nu^2;\theta) = 1 - \frac{\epsilon^2}{2} + \frac{\epsilon^3(r^2-1)}{2n\pi} + O(\epsilon^4)$$

and as ϵ increases from negative to positive values, $|R_{11}(\nu^2;\theta)| \leq 1$ for all r.

We again check that the mixed collocation method for $s = 2$ reduces to the classical polynomial collocation method. For $s = 2$ with $c_1 = 0$ and $c_2 = 1$, the stability function for the polynomial collocation method is given by

$$R_{11}^{PC}(\nu^2) = \frac{6-2\nu^2}{6+\nu^2}.$$

For the mixed collocation method, the stability function is

$$R_{11}^{MC}(\nu^2;\theta) = \frac{\theta^2\sin\theta + \nu^2(\theta\cos\theta - \sin\theta)}{\theta^2\sin\theta + \nu^2(\theta - \sin\theta)}$$

for $c_1 = 0$ and $c_2 = 1$ and as $k \to 0$,

$$R_{11}^{MC}(\nu^2;\theta) \to \frac{1-\nu^2/3}{1+\nu^2/6} = \frac{6-2\nu^2}{6+\nu^2}.$$

Stability function $R_{22}(\nu^2;\theta)$

With the choice of the end-points of the interval for the two-point mixed collocation method, the stability function is reduced to the form

$$R_{11}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\nu^2}{1+\beta_1\nu^2}.$$

When, for example, $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$, the stability function is of the form (5.9), a quotient of quadratics in ν^2. Assuming symmetric nodes have been chosen, the characteristic equation is given by

$$\xi^2 - 2R_{22}(\nu^2;\theta)\xi + 1 = 0.$$

Then, from Definition 3.4, the stability boundaries of $R_{22}(\nu^2;\theta)$ are

$$|R_{22}(\nu^2;\theta)| = \left|\frac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4}{1+\beta_1\nu^2+\beta_2\nu^4}\right| = 1.$$

For $R_{22}(\nu^2;\theta) = 1$, we have

$$\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4 = 1 + \beta_1\nu^2 + \beta_2\nu^4$$

from which

$$\nu^2 = \frac{-(\alpha_1 - \beta_1) \pm \{(\alpha_1 - \beta_1)^2 - 4(\alpha_2 - \beta_2)(\alpha_0 - 1)\}^{1/2}}{2(\alpha_2 - \beta_2)}$$

for $\alpha_2 \neq \beta_2$ or

$$\alpha_0 - 1 = 0, \quad \alpha_1 - \beta_1 = 0 \text{ and } \alpha_2 - \beta_2 = 0.$$

For $R_{22}(\nu^2;\theta) = -1$,

$$\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4 = -1 - \beta_1\nu^2 - \beta_2\nu^4$$

from which we obtain

$$\nu^2 = \frac{-(\alpha_1 + \beta_1) \pm \{(\alpha_1 + \beta_1)^2 - 4(\alpha_2 + \beta_2)(\alpha_0 + 1)\}^{1/2}}{2(\alpha_2 + \beta_2)}$$

for $\alpha_2 \neq -\beta_2$ or

$$\alpha_0 + 1 = 0, \quad \alpha_1 + \beta_1 = 0 \text{ and } \alpha_2 + \beta_2 = 0.$$

As we are taking $\nu(\theta)$ to be non-negative the stability boundaries are

$$\nu_{\pm}^{(1)}(\theta) = \sqrt{\frac{-(\alpha_1 - \beta_1) \pm \{(\alpha_1 - \beta_1)^2 - 4(\alpha_2 - \beta_2)(\alpha_0 - 1)\}^{1/2}}{2(\alpha_2 - \beta_2)}} \tag{5.11}$$

and

$$\nu_{\pm}^{(2)}(\theta) = \sqrt{\frac{-(\alpha_1 + \beta_1) \pm \{(\alpha_1 + \beta_1)^2 - 4(\alpha_2 + \beta_2)(\alpha_0 + 1)\}^{1/2}}{2(\alpha_2 + \beta_2)}}. \tag{5.12}$$

Therefore the stability boundaries are the curves described by the equations $\nu_{\pm}^{(1)}(\theta)$, $\nu_{\pm}^{(2)}(\theta)$ and the lines corresponding to any values of θ for which

$$\alpha_0 \pm 1 = 0, \quad \alpha_1 \pm \beta_1 = 0 \text{ and } \alpha_2 \pm \beta_2 = 0.$$

We also consider any values of θ for which the method is undefined.

Example: $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$
As mentioned earlier, with $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$, the highest possible order of 4 is obtained for two collocation points. The stability function is given by

$$R_{22}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4}{1+\beta_1\nu^2+\beta_2\nu^4}$$

where

$$\alpha_0 = 1,$$
$$\alpha_1 = \frac{\cos(\theta/2)\{6\mathcal{A}+\sqrt{3}\theta\mathcal{B}\} - 3\theta\mathcal{A}\sin(\theta/2) - 12\mathcal{A}\mathcal{B}}{6\theta^2\mathcal{A}\mathcal{B}},$$
$$\alpha_2 = -\frac{\cos(\theta/2)\{6\mathcal{A}+\sqrt{3}\theta\mathcal{B}\} - 3\theta\mathcal{A}\sin(\theta/2) - 6\mathcal{A}\mathcal{B} - \sqrt{3}\theta\cos\theta}{6\theta^4\mathcal{A}\mathcal{B}},$$
$$\beta_1 = \frac{\cos(\theta/2)\{6\mathcal{A}+\sqrt{3}\theta\mathcal{B}\} + 3\theta\mathcal{A}\sin(\theta/2) - 12\mathcal{A}\mathcal{B}}{6\theta^2\mathcal{A}\mathcal{B}},$$
$$\beta_2 = -\frac{\cos(\theta/2)\{6\mathcal{A}+\sqrt{3}\theta\mathcal{B}\} + 3\theta\mathcal{A}\sin(\theta/2) - 6\mathcal{A}\mathcal{B} - \sqrt{3}\theta}{6\theta^4\mathcal{A}\mathcal{B}}$$

and we define

$$\mathcal{A} = \sin(\theta\sqrt{3}/6) \text{ and } \mathcal{B} = \cos(\theta\sqrt{3}/6).$$

The coefficients are undefined when $\theta = \sqrt{3}n\pi$ where n is a non-negative integer.

Substitute $\alpha_0 = 1$ into (5.11) and (5.12) to find

$$\nu_+^{(1)}(\theta) = 0, \quad \nu_-^{(1)}(\theta) = \sqrt{\frac{-(\alpha_1-\beta_1)}{(\alpha_2-\beta_2)}} \tag{5.13}$$

and

$$\nu_\pm^{(2)}(\theta) = \sqrt{\frac{-(\alpha_1+\beta_1) \pm \{(\alpha_1+\beta_1)^2 - 8(\alpha_2+\beta_2)\}^{1/2}}{2(\alpha_2+\beta_2)}}. \tag{5.14}$$

Substituting α_1, α_2, β_1 and β_2 into (5.13) and (5.14), the stability curves are given by

$$\nu_+^{(1)}(\theta) = 0, \quad \nu_-^{(1)}(\theta) = \left\{\frac{3\theta^2\mathcal{A}}{3\mathcal{A} - \sqrt{3}\sin(\theta/2)}\right\}^{1/2}$$

and

$$\nu_+^{(2)}(\theta) = \left\{ \frac{\theta^2 \mathcal{B}}{\mathcal{B} - \cos(\theta/2)} \right\}^{1/2}, \quad \nu_-^{(2)}(\theta) = \left\{ \frac{6\theta^2 \mathcal{A}}{6\mathcal{A} - \sqrt{3}\theta \cos(\theta/2)} \right\}^{1/2}.$$

We also consider any values of θ for which

$$\alpha_0 - 1 = 0, \;\; \alpha_1 - \beta_1 = 0 \;\text{ and }\; \alpha_2 - \beta_2 = 0.$$

From the coefficients,

$$\alpha_1 - \beta_1 = \frac{-\sin(\theta/2)}{\theta \mathcal{B}},$$

$$\alpha_2 - \beta_2 = \frac{6\mathcal{A}\sin(\theta/2) + \sqrt{3}\cos\theta - \sqrt{3}}{6\theta^3 \mathcal{A}\mathcal{B}}$$

and $\alpha_1 - \beta_1 = 0$ when $\theta = 2n\pi$ where n is a non-negative integer. Also $\alpha_2 - \beta_2 = 0$ when $\theta = 0, 2\pi, 11.7159, 4\pi, 6\pi, 20.3578, \ldots$.

When $\theta = \nu$,

$$R_{22}(\nu^2; \nu) = \frac{1 + \alpha_1 \nu^2 + \alpha_2 \nu^4}{1 + \beta_1 \nu^2 + \beta_2 \nu^4}$$

where the numerator of $R_{22}(\nu^2; \nu)$ is

$$1 - \frac{1}{6\mathcal{A}\mathcal{B}} \left\{ -\cos(\nu/2)(6\mathcal{A} + \sqrt{3}\nu\mathcal{B}) + 3\nu\mathcal{A}\sin(\nu/2) + 12\mathcal{A}\mathcal{B} \right\}$$

$$-\frac{1}{6\mathcal{A}\mathcal{B}} \left\{ \cos(\nu/2)(6\mathcal{A} + \sqrt{3}\nu\mathcal{B}) - 3\nu\mathcal{A}\sin(\nu/2) - 6\mathcal{A}\mathcal{B} - \sqrt{3}\nu\cos\nu \right\} = \frac{\sqrt{3}\nu\cos\nu}{6\mathcal{A}\mathcal{B}}$$

and the denominator is

$$1 - \frac{1}{6\mathcal{A}\mathcal{B}} \left\{ -\cos(\nu/2)(6\mathcal{A} + \sqrt{3}\nu\mathcal{B}) - 3\nu\mathcal{A}\sin(\nu/2) + 12\mathcal{A}\mathcal{B} \right\}$$

$$-\frac{1}{6\mathcal{A}\mathcal{B}} \left\{ \cos(\nu/2)(6\mathcal{A} + \sqrt{3}\nu\mathcal{B}) + 3\nu\mathcal{A}\sin(\nu/2) - 6\mathcal{A}\mathcal{B} - \sqrt{3}\nu \right\} = \frac{\sqrt{3}\nu}{6\mathcal{A}\mathcal{B}}.$$

Therefore, $R_{22}(\nu^2; \nu) = \cos\nu$.

When $\theta = 2n\pi$,

$$\cos(\theta/2) = \cos(n\pi) = (-1)^n, \;\; \sin(\theta/2) = \sin(n\pi) = 0 \;\text{ and }\; \cos\theta = 1,$$

so

$$\alpha_1 = \beta_1 = \frac{-1}{6\theta^2 \mathcal{AB}} \left\{ -(-1)^n (6\mathcal{A} + \sqrt{3}\theta\mathcal{B}) + 12\mathcal{AB} \right\}$$

and

$$\alpha_2 = \beta_2 = \frac{-1}{6\theta^4 \mathcal{AB}} \left\{ (-1)^n (6\mathcal{A} + \sqrt{3}\theta\mathcal{B}) - 6\mathcal{AB} - \sqrt{3}\theta \right\}.$$

Therefore, $R_{22}(\nu^2; 2n\pi) = \dfrac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4}{1 + \beta_1\nu^2 + \beta_2\nu^4} = 1.$

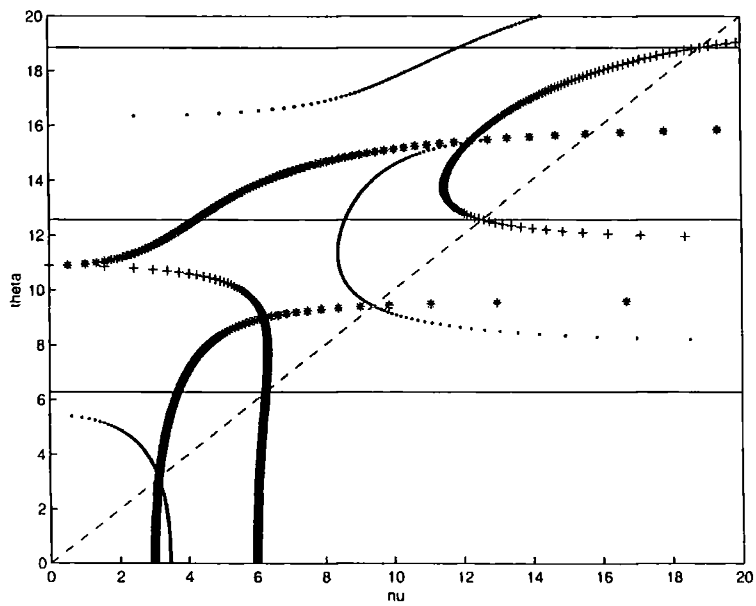

Figure 5.4: $\nu - \theta$ plot for two collocation points : $c = \frac{3-\sqrt{3}}{6}$ and $\frac{3+\sqrt{3}}{6}$

The stability regions are shown in figures 5.4 - 5.7. In figure 5.4, the curves $\nu_-^1(\theta)$ are given by (+), $\nu_+^2(\theta)$ by (.) and $\nu_-^2(\theta)$ by (*). Figures 5.6 and 5.7 are enlargements of sections of figure 5.5. The curves $\nu = \nu_\pm^{(2)}(\theta)$ are asymptotic to lines of constant θ corresponding to the zeros of $\alpha_2 + \beta_2$ of which the first five are $\theta = 0, 7.9668, 9.6709, 15.9335, 16.1400, \ldots$ The curves $\nu = \nu_-^{(1)}(\theta)$ are asymptotic to $\theta = 11.7159$ and $\theta = 20.3578$, which are the zeros of $\alpha_2 - \beta_2$. Since $\lim_{\theta\to 0} \nu_-^{(1)}(\theta) = 6$, $\lim_{\theta\to 0} \nu_+^{(2)}(\theta) = 2\sqrt{3}$ and $\lim_{\theta\to 0} \nu_-^{(2)}(\theta) = 3$, the primary interval of periodicity is $(0, h_0)$ where h_0 increases from $3/w$ when $r = 0$ to π/w when $r = 1$, for fixed w. There is a secondary interval of periodicity given by $(2\sqrt{3}/w, 6/w)$ when $r = 0$ and the length of the interval increases to $(\pi/w, 2\pi/w)$ as $r \to 1$, for fixed w.

A number of 'apparent' inconsistencies take place in figure 5.5. Along the curves $\nu = \nu_-^{(1)}(\theta)$ and the lines $\theta = 2\pi$, 4π and 6π, the value of the stability function is

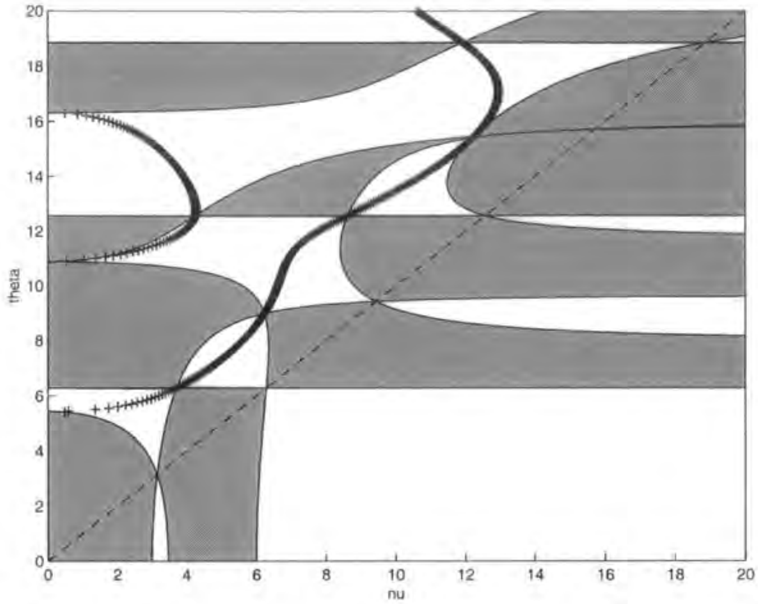

Figure 5.5: $\nu - \theta$ plot for two collocation points : $c = \frac{3-\sqrt{3}}{6}$ and $\frac{3+\sqrt{3}}{6}$

1, whilst along the curves $\nu = \nu_+^{(2)}(\theta)$ and $\nu = \nu_-^{(2)}(\theta)$, the stability function is -1 and the latter curves coincide with $\nu = \nu_-^{(1)}(\theta)$ and the lines $\theta = 2\pi$, 4π and 6π at certain points in the figure. Again, the reason for this is that the stability function is undefined at these points. In figure 5.5, the curves $\bar{\nu}(\theta)$ are plotted (+) which are where the denominator of $R_{22}(\nu^2;\theta)$ is equal to zero and they are given by

$$\nu = \bar{\nu}(\theta) = \left\{ \frac{-\beta_1 \pm \sqrt{\beta_1^2 - 4\beta_2}}{2\beta_2} \right\}^{1/2}$$

for $\beta_2 \neq 0$ where

$$\beta_1 = \frac{\cos(\theta/2)\{6\mathcal{A} + \sqrt{3}\theta\mathcal{B}\} + 3\theta\mathcal{A}\sin(\theta/2) - 12\mathcal{A}\mathcal{B}}{6\theta^2\mathcal{A}\mathcal{B}},$$

$$\beta_2 = -\frac{\cos(\theta/2)\{6\mathcal{A} + \sqrt{3}\theta\mathcal{B}\} + 3\theta\mathcal{A}\sin(\theta/2) - 6\mathcal{A}\mathcal{B} - \sqrt{3}\theta}{6\theta^4\mathcal{A}\mathcal{B}}$$

and as before

$$\mathcal{A} = \sin(\theta\sqrt{3}/6) \text{ and } \mathcal{B} = \cos(\theta\sqrt{3}/6).$$

From figure 5.5, the curves $\bar{\nu}(\theta)$ pass through the points where the inconsistencies arise.

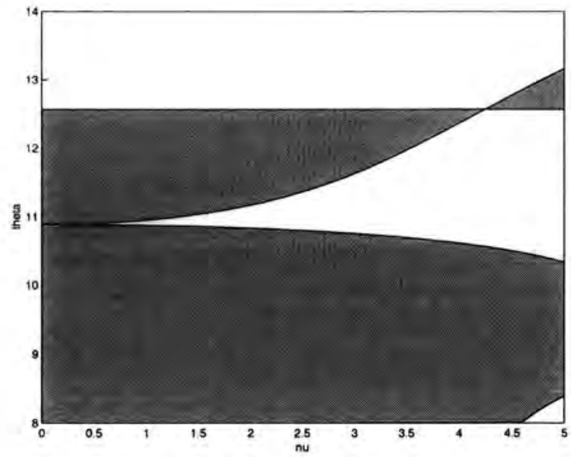

Figure 5.6: $\nu - \theta$ plot for two collocation points : $c = \frac{3-\sqrt{3}}{6}$ and $\frac{3+\sqrt{3}}{6}$

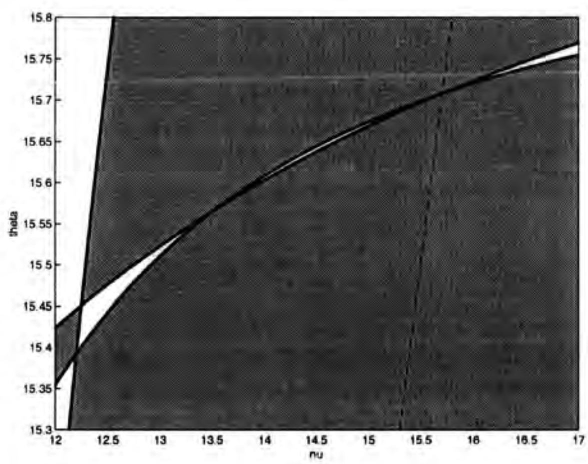

Figure 5.7: $\nu - \theta$ plot for two collocation points : $c = \frac{3-\sqrt{3}}{6}$ and $\frac{3+\sqrt{3}}{6}$

When $\nu = \theta/r$, the stability function becomes

$$R = \frac{\sigma_0 + \sigma_1 r^2 + \sigma_2 r^4}{\omega_0 + \omega_1 r^2 + \omega_2 r^4}$$

where

$$\sigma_0 = 3\,S_1 - 6\,S_2\,C_3 + \sqrt{3}\,\theta\,\cos\theta - \sqrt{3}\,\theta\,C_2\,C_3 + 3\,\theta\,S_2\,S_3,$$

$$\sigma_1 = 6\,S_2\,C_3 - 3\,\theta\,S_2\,S_3 + \sqrt{3}\,\theta\,C_2\,C_3 - 6\,S_1, \quad \sigma_2 = 3\,S_1,$$

$$\omega_0 = \sqrt{3}\,\theta - 3\,\theta\,S_2\,S_3 - \sqrt{3}\,\theta\,C_2\,C_3 + 3\,S_1 - 6\,S_2\,C_3,$$

$$\omega_1 = 3\,\theta\,S_2\,S_3 - 6\,S_1 + \sqrt{3}\,\theta\,C_2\,C_3 + 6\,S_2\,C_3, \quad \omega_2 = 3S_1$$

and

$$S_1 = \sin(\frac{1}{3}\theta\sqrt{3}),\ \ S_2 = \sin(\frac{1}{6}\theta\sqrt{3}),\ \ S_3 = \sin(\frac{1}{2}\theta),$$
$$C_1 = \cos(\frac{1}{3}\theta\sqrt{3}),\ \ C_2 = \cos(\frac{1}{6}\theta\sqrt{3}),\ \ C_3 = \cos(\frac{1}{2}\theta).$$

The coefficients α_1, α_2, β_1 and β_2 are undefined when $\theta = \sqrt{3}n\pi$ and we investigate what happens to the stability function for $\theta = \sqrt{3}\pi$, $2\sqrt{3}\pi$ and $3\sqrt{3}\pi$.

For $\theta = \sqrt{3}\pi$,

$$R_{22}(\nu^2;\theta) = \frac{(2\mathcal{A} - \sqrt{3}\pi\mathcal{B})(r^2-1) + \pi\cos(\sqrt{3}\pi)}{(2\mathcal{A} + \sqrt{3}\pi\mathcal{B})(r^2-1) + \pi}$$

where

$$\mathcal{A} = \cos(\sqrt{3}\pi/2) \text{ and } \mathcal{B} = \sin(\sqrt{3}\pi/2).$$

In figure 5.5, the line $\theta = \sqrt{3}\pi$ crosses the curves $\nu_-^{(1)}(\theta)$ and $\nu_-^{(2)}(\theta)$ at $\nu = 6.2249$ and $\nu = 3.488$ from which $r = 0.8741$ and $r = 1.5600$ respectively.

For $0 < r < 0.8741$, $|R_{22}(\nu^2;\sqrt{3}\pi)| > 1$, for $0.8741 < r < 1.5600$, $|R_{22}(\nu^2;\sqrt{3}\pi)| < 1$ and for $r > 1.5600$, $|R_{22}(\nu^2;\sqrt{3}\pi)| > 1$ which satisfies the stability regions.

For $\theta = 2\sqrt{3}\pi$,

$$R_{22}(\nu^2;\theta) = \frac{-\cos(\sqrt{3}\pi)(r^2-1) + \cos(2\sqrt{3}\pi)}{-\cos(\sqrt{3}\pi)(r^2-1) + 1}$$

and the line $\theta = 2\sqrt{3}\pi$ crosses the curves $\nu_+^{(2)}(\theta)$ at $\nu = 8.4311$ from which $r = 1.2908$.

For $0 < r < 1.2908$, $|R_{22}(\nu^2;2\sqrt{3}\pi)| < 1$ and for $r > 1.2908$, $|R_{22}(\nu^2;2\sqrt{3}\pi)| > 1$ which satisfies the stability regions.

For $\theta = 3\sqrt{3}\pi$,

$$R_{22}(\nu^2;\theta) = \frac{\left[(2\mathcal{A}(3-4\mathcal{A}^2) + 3\sqrt{3}\pi\mathcal{B}(4\mathcal{A}^2-1)\right](r^2-1) + 6\pi\mathcal{A}^2(4\mathcal{A}^2-3)^2 - 3\pi}{\left[(2\mathcal{A}(3-4\mathcal{A}^2) - 3\sqrt{3}\pi\mathcal{B}(4\mathcal{A}^2-1)\right](r^2-1) + 3\pi}$$

where

$$\mathcal{A} = \cos(\sqrt{3}\pi/2) \text{ and } \mathcal{B} = \sin(\sqrt{3}\pi/2).$$

The line $\theta = 3\sqrt{3}\pi$ crosses the curves $\nu_-^{(1)}(\theta)$ at $\nu = 13.1112$ from which we obtain

$r = 1.2451$.

For $0 < r < 1.2451$, $|R_{22}(\nu^2; 3\sqrt{3}\pi)| < 1$ and for $r > 1.2451$, $|R_{22}(\nu^2; 3\sqrt{3}\pi)| > 1$ which again satisfies the stability regions in figure 5.5.

Therefore, the lines $\theta = \sqrt{3}n\pi$, $n = 1, 2$ and 3 do not need to be included in figure 5.5 as they satisfy the stability regions.

To investigate what happens as $\theta \to 2n\pi$, let $\theta = 2n\pi + \epsilon$. We consider separately, $\theta = 2\pi + \epsilon$, $\theta = 4\pi + \epsilon$ and $\theta = 6\pi + \epsilon$.

With $\nu = \theta/r$ and $\theta = 2n\pi + \epsilon$

$$R_{22}(\nu^2; \theta) = 1 - \frac{3\mathcal{Q}_n(-1)^n n\pi(r^2-1)\epsilon}{[(-1)^n\mathcal{P}_n(r^2-1)+1][\sqrt{3}n\pi + 3(-1)^n\mathcal{Q}_n(r^2-1)]} + O(\epsilon^2)$$

where

$$\mathcal{Q}_n = \sin(n\pi/\sqrt{3}) \text{ and } \mathcal{P}_n = \cos(n\pi/\sqrt{3}).$$

Case i) $\theta = 2\pi + \epsilon$.

When $\theta = 2\pi + \epsilon$ is substituted into the stability function $R_{22}(\nu^2; \theta)$ then

$$R_{22}(\nu^2; \theta) = 1 + \frac{3\mathcal{Q}_1\pi(r^2-1)\epsilon}{[\mathcal{P}_1(r^2-1)-1][3\mathcal{Q}_1(r^2-1)-\sqrt{3}\pi]} + O(\epsilon^2).$$

As $\epsilon \to 0$, $R_{22}(\nu^2; \theta) \to 1$.

We look for the values of r for which the coefficient of ϵ is undefined. Therefore,

$$\mathcal{P}_1(r^2-1) - 1 = 0 \;\Rightarrow\; r = \left\{\frac{\mathcal{P}_1+1}{\mathcal{P}_1}\right\}^{1/2} = \sqrt{-3.15596}$$

and

$$3\mathcal{Q}_1(r^2-1) - \sqrt{3}\pi = 0 \;\Rightarrow\; r = \left\{\frac{3\mathcal{Q}_1+\sqrt{3}\pi}{3\mathcal{Q}_1}\right\}^{1/2} = 1.69372.$$

For ϵ small, as ϵ increases from negative to positive values,

i) for $r < 1$, $|R_{22}(\nu^2; \theta)|$ decreases through 1,

ii) for $1 < r < 1.69372$, $|R_{22}(\nu^2; \theta)|$ increases through 1,

iii) for $r > 1.69372$, $|R_{22}(\nu^2; \theta)|$ decreases through 1.

Case ii) $\theta = 4\pi + \epsilon$.

When $\theta = 4\pi + \epsilon$ is substituted into the stability function $R_{22}(\nu^2;\theta)$,

$$R_{22}(\nu^2;\theta) = 1 - \frac{6\mathcal{Q}_2\pi(r^2-1)\epsilon}{[\mathcal{P}_2(r^2-1)+1][2\sqrt{3}\pi + 3\mathcal{Q}_2(r^2-1)]} + O(\epsilon^2).$$

As $\epsilon \to 0$, $R_{22}(\nu^2;\theta) \to 1$.

Again we look for the values of r for which the coefficient of ϵ is undefined. Therefore,

$$\mathcal{P}_2(r^2-1)+1 = 0 \;\Rightarrow\; r = \left\{\frac{\mathcal{P}_2 - 1}{\mathcal{P}_2}\right\}^{1/2} = 1.45978$$

and

$$2\sqrt{3}\pi + 3\mathcal{Q}_2(r^2-1) = 0 \;\Rightarrow\; r = \left\{\frac{3\mathcal{Q}_2 - 2\sqrt{3}\pi}{3\mathcal{Q}_2}\right\}^{1/2} = 2.96078.$$

For ϵ small, as ϵ increases from negative to positive values,

i) for $r < 1$, $|R_{22}(\nu^2;\theta)|$ decreases through 1,

ii) for $1 < r < 1.45978$, $|R_{22}(\nu^2;\theta)|$ increases through 1,

iii) for $1.45978 < r < 2.96078$, $|R_{22}(\nu^2;\theta)|$ decreases through 1,

iv) for $r > 2.96078$, $|R_{22}(\nu^2;\theta)|$ increases through 1.

Case iii) $\theta = 6\pi + \epsilon$.

Finally, substituting $\theta = 6\pi + \epsilon$ into the stability function $R_{22}(\nu^2;\theta)$,

$$R_{22}(\nu^2;\theta) = 1 + \frac{9\pi\mathcal{Q}_3(r^2-1)\epsilon}{[\mathcal{P}_3(r^2-1)-1][3\mathcal{Q}_3(r^2-1) - 3\sqrt{3}\pi]} + O(\epsilon^2).$$

As $\epsilon \to 0$, $R_{22}(\nu^2;\theta) \to 1$.

The coefficient of ϵ is undefined when

$$\mathcal{P}_3(r^2-1)-1 = 0 \;\Rightarrow\; r = \left\{\frac{\mathcal{P}_3 + 1}{\mathcal{P}_3}\right\}^{1/2} = 1.58152$$

and

$$3\mathcal{Q}_3(r^2-1) - 3\sqrt{3}\pi = 0 \;\Rightarrow\; r = \left\{\frac{3\mathcal{Q}_3 + 3\sqrt{3}\pi}{3\mathcal{Q}_3}\right\}^{1/2} = \sqrt{-6.29571}.$$

For ϵ small, as ϵ increases from negative to positive values,

i) for $r < 1$, $|R_{22}(\nu^2;\theta)|$ increases through 1,

ii) for $1 < r < 1.58152$, $|R_{22}(\nu^2;\theta)|$ decreases through 1,

iii) for $r > 1.58152$, $|R_{22}(\nu^2;\theta)|$ increases through 1.

We check that the mixed collocation method for $s = 2$ reduces to the classical polynomial collocation method. For two collocation points with the values $c_1 = (3-\sqrt{3})/6$ and $c_2 = (3+\sqrt{3})/6$, the stability function for the polynomial collocation method is

$$R_{22}^{PC}(\nu^2) = \frac{432 - 192\nu^2 + 7\nu^4}{432 + 24\nu^2 + \nu^4}.$$

For the mixed collocation method, as $k \to 0$,

$$\alpha_0 \to 1, \quad \alpha_1 \to \frac{-4}{9}, \quad \alpha_2 \to \frac{7}{432}, \quad \beta_1 \to \frac{1}{18}, \quad \beta_2 \to \frac{1}{432}$$

and the stability function reduces to

$$R_{22}^{MC}(\nu^2;\theta) \to \frac{1 - \frac{4}{9}\nu^2 + \frac{7}{432}\nu^4}{1 + \frac{1}{18}\nu^2 + \frac{1}{432}\nu^4} = \frac{432 - 192\nu^2 + 7\nu^4}{432 + 24\nu^2 + \nu^4}$$

as required.

5.1.3 Three Collocation Points

As for the one-point and two-point mixed collocation methods, we require $P(\nu^2;\theta) = 1$ for the method to have an interval of periodicity. This is satisfied if symmetric nodes are chosen. i.e. if $c_1 + c_3 = 1$ and $c_2 = 1/2$.

It is possible to obtain a stability function which is a quotient of two cubics in ν^2. For example, if $c_1 = (5 - \sqrt{15})/10$, $c_2 = 1/2$ and $c_3 = (5 + \sqrt{15})/10$, then the stability function is of the form $R_{3,3}(\nu^2;\theta)$ but the algebra is complicated. The best way to see whether the method is stable for a particular problem is to substitute a range of values of ν and θ into the amplification matrix (5.8) and check to see whether the modulus of the roots of the characteristic equation are less or equal to 1. For the rest of this section we consider the stability of the method when the collocation nodes are the end-points $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$.

Example

Substituting $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$ into the formulae for $M(\nu^2;\theta)$, (5.8), the characteristic equation is

$$\xi^2 - 2R_{22}(\nu^2;\theta)\xi + 1 = 0.$$

The stability function is given by

$$R_{22}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\nu^2 + \alpha_2\nu^4}{1 + \beta_1\nu^2 + \beta_2\nu^4} \tag{5.15}$$

where

$$\alpha_0 = 1$$

$$\alpha_1 = \frac{\cos^2(\theta/2)(16+3\theta^2) + \theta^2\cos(\theta/2) + 2\theta\sin\theta - 2\theta^2 - 16}{8\theta^2\sin^2(\theta/2)}$$

$$\alpha_2 = \frac{\sin\theta(3\theta^2+8) + 8\theta\cos(\theta/2) - 4\sin(\theta/2)(\theta^2+4) + \theta^3 - 2\theta\cos^2(\theta/2)(\theta^2+4)}{16\theta^4\sin(\theta/2)(\cos(\theta/2)-1)}$$

$$\beta_1 = \frac{\cos^2(\theta/2)(16-\theta^2) + \theta^2\cos(\theta/2) + 2\theta\sin\theta + 2\theta^2 - 16}{8\theta^2\sin^2(\theta/2)}$$

$$\beta_2 = \frac{\sin\theta(\theta^2-8) + 8\theta\cos(\theta/2)(\cos(\theta/2)-1) + 4\sin(\theta/2)(4-\theta^2) + \theta^3}{-16\theta^4\sin(\theta/2)(\cos(\theta/2)-1)}$$

and the coefficients α_1, β_1, α_2 and β_2 are undefined when $\theta = 2n\pi$ where n is a non-negative integer. The stability function $R_{22}(\nu^2;\theta)$ may also be written as

$$\frac{2\mathcal{A}\sin(\theta/2)\,[2\mathcal{B} - \mathcal{C}\cos(\theta/2)] + 2\nu^2\theta\cos(\theta/2)\,[\mathcal{B}\cos(\theta/2) - 4\mathcal{A}] - \nu^4\theta^3}{-2\mathcal{A}\sin(\theta/2)\,[2\mathcal{D} - \mathcal{E}\cos(\theta/2)] + 8\nu^2\theta\mathcal{A}\cos(\theta/2)\,[\cos(\theta/2)-1] + \nu^4\theta^3} \tag{5.16}$$

with

$$\mathcal{A}(\nu^2;\theta) = (\nu^2-\theta^2), \quad \mathcal{B}(\nu^2;\theta) = (\nu^2\theta^2 + 4\nu^2 - 4\theta^2),$$

$$\mathcal{C}(\nu^2;\theta) = (3\nu^2\theta^2 + 8\nu^2 - 8\theta^2), \quad \mathcal{D}(\nu^2;\theta) = (\nu^2\theta^2 - 4\nu^2 + 4\theta^2),$$

$$\mathcal{E}(\nu^2;\theta) = (\nu^2\theta^2 - 8\nu^2 + 8\theta^2).$$

As $\alpha_0 = 1$, after some simplification

$$\beta_1 - \alpha_1 = \frac{1}{2},$$

$$\alpha_1 + \beta_1 = \frac{\cos^2(\theta/2)\,[\theta^2 + 16] + 2\theta \sin\theta + \theta^2 \cos(\theta/2) - 16}{4\theta^2 \sin^2(\theta/2)},$$

$$\alpha_2 - \beta_2 = \frac{4\sin(\theta/2) - \theta\,[1 + \cos(\theta/2)]}{8\theta^2 \sin(\theta/2)},$$

$$\alpha_2 + \beta_2 = \frac{8\theta\cos(\theta/2)\,[1 - \cos(\theta/2)] + \sin\theta\,[\theta^2 + 8] - 16\sin(\theta/2) - \theta^3\cos^2(\theta/2)}{8\theta^4 \sin(\theta/2)\,[\cos(\theta/2) - 1]}.$$

Therefore, the stability boundaries given by (5.13) and (5.14) are

$$\nu_+^{(1)}(\theta) = 0, \quad \nu_-^{(1)}(\theta) = \sqrt{\frac{4\theta^2 \sin(\theta/2)}{4\sin(\theta/2) - \theta\,[1 + \cos(\theta/2)]}}$$

and

$$\nu_+^{(2)}(\theta) = \left\{\frac{\theta^2 \mathcal{X}_1}{\mathcal{X}}\right\}^{1/2}, \quad \nu_-^{(2)}(\theta) = \left\{\frac{-\theta^2 \mathcal{X}_2}{\mathcal{X}}\right\}^{1/2},$$

where, if we define $p = \cos(\theta/2)$ and $q = \sin(\theta/2)$, then

$$\mathcal{X}_1 = (p-1)\left\{16(p^2-1) + \theta^2 p(p+1) + 2\theta\sin\theta + \theta^2(p^2-1)\sqrt{\mathcal{W}}\right\},$$

$$\mathcal{X}_2 = (p-1)\left\{-16(p^2-1) - \theta^2 p(p+1) - 2\theta\sin\theta + \theta^2(p^2-1)\sqrt{\mathcal{W}}\right\},$$

$$\mathcal{X} = \left\{8(p-1) + \theta^2 p\right\}\left\{2(p^2-1) + \theta p q\right\}$$

and

$$\mathcal{W} = \cos^2(\theta/2)\left\{\frac{\cos(\theta/2)(\theta^2 - 16) + 16 + \theta^2 - 8\theta\sin(\theta/2)}{\theta^2(\cos(\theta/2) - 1)(\cos^2(\theta/2) - 1)}\right\}.$$

When $\theta = \nu$, we have $\mathcal{A} = 0$, $\mathcal{B} = \nu^4$, $\mathcal{C} = 3\nu^4$, $\mathcal{D} = \nu^4$ and $\mathcal{E} = \nu^4$, and from (5.16), the stability function is

$$R_{22}(\nu^2;\nu) = -\left\{\frac{2\nu^7\cos^2(\nu/2) - \nu^7}{-\nu^7}\right\} = \cos\nu.$$

When $\theta = 2n\pi$,

$$R_{22}(\nu^2;\theta) = 1.$$

In figures 5.9 - 5.12, the stability regions are shaded for $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$. In figure 5.8, the stability curves $\nu_-^{(1)}(\theta)$ are given by (+), $\nu_+^{(2)}(\theta)$ by (*) and $\nu_-^{(2)}(\theta)$ by (.). Figures 5.10 - 5.12 are enlargements of sections of 5.9. The curves $\nu = \nu_-^{(1)}(\theta)$ are asymptotic to lines of constant $\theta = 17.9736, \ldots$, corresponding to the zeros of

$\alpha_2 - \beta_2$. Also the curves $\nu = \nu_{\pm}^{(2)}(\theta)$ are asymptotic to the lines θ which are the zeros of $\alpha_2 + \beta_2$ and $\alpha_1 + \beta_1$. The first three zeros of $\alpha_2 + \beta_2$ are $\theta = 0, 9.5851, 15.4505, \ldots$ and for $\alpha_1 + \beta_1$, we have $\theta = 0, 9.8254, 15.6076, \ldots$. As $\theta \to 0$, $\nu_{-}^{(1)}(\theta) \to 4\sqrt{3}$, $\nu_{+}^{(2)}(\theta) \to 2\sqrt{3}$ and $\nu_{-}^{(2)}(\theta) \to \sqrt{48/5}$. For $r < 1$, the primary interval of periodicity is $(0, h_0)$ where $h_0 = \frac{1}{w}\sqrt{\frac{48}{5}}$ when $r = 0$ and increases to π/w as $r \to 1$, for fixed w. There is a second interval of periodicity given by $(2\sqrt{3}/w, 4\sqrt{3}/w)$ when $r = 0$ which increases to $(\pi/w, 2\pi/w)$ as $r \to 1$. The stability function has unit modulus when $\theta = 4n\pi$ and these lines do not affect the stability boundaries.

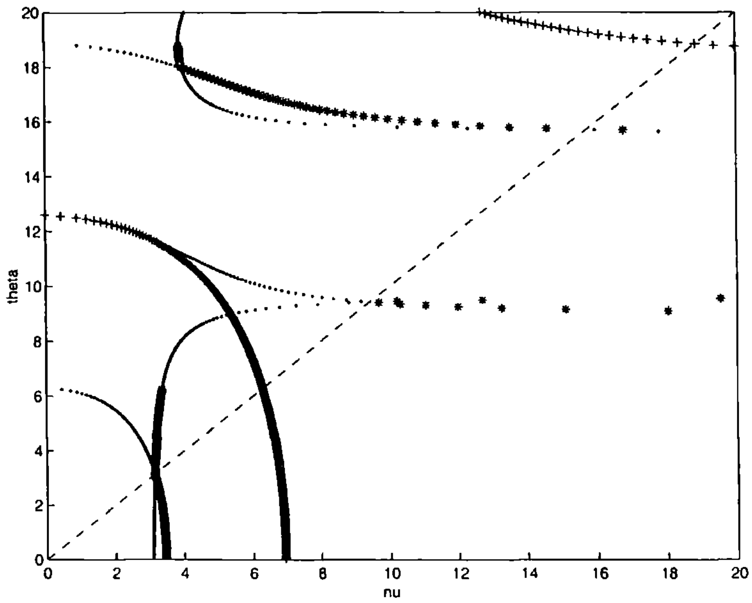

Figure 5.8: $\nu - \theta$ plot for three collocation points : c = 0, 1/2 and 1

Again, a few 'apparent' inconsistencies occur in figure 5.9. There are a number of points where a curve on which the stability function has value 1 intersects another curve or line on which the stability function has value -1. The curves $\nu = \bar{\nu}(\theta)$ given by (+) in figure 5.9 are where $R_{22}(\nu^2; \theta)$ is undefined and these curves touch all the points where the inconsistencies occur.

To investigate what happens as $\theta \to 2n\pi$, the values for which the method is undefined, let $\nu = \theta/r$, $\theta = 2n\pi + \epsilon$. The following calculations were done using Maple. After some simplification, the stability function is

$$R(\theta^2/r^2; 2n\pi + \epsilon) = R_0 + R_1\epsilon + R_2\epsilon^2 + O(\epsilon^3)$$

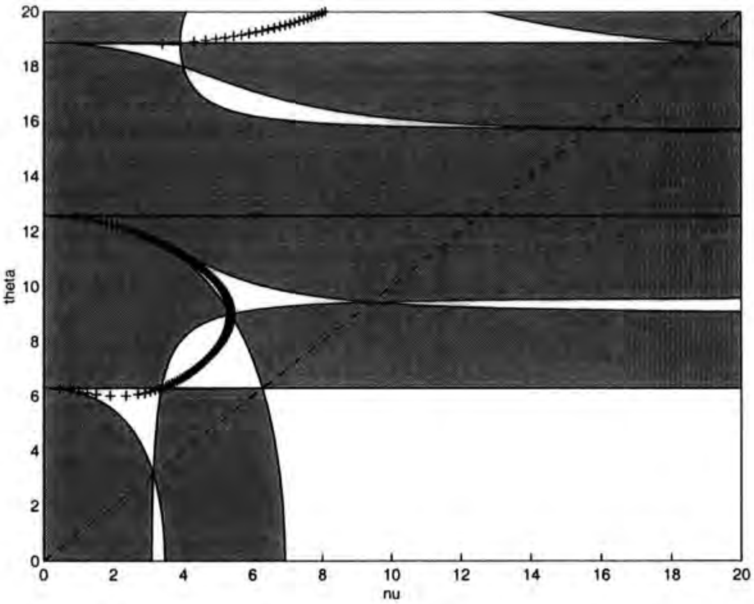

Figure 5.9: $\nu - \theta$ plot for three collocation points : c = 0, 1/2 and 1

where

$$R_0 = 1, \quad R_1 = -2\,\frac{n\pi(r^2-1)\,[(-1)^n - 1]}{n^2\pi^2 + 2(r^2-1)\,[(-1)^n - 1]}$$

and

$$R_2 = -\frac{1}{2}\,\frac{n^4\pi^4 + 6\pi^2(r^2-1)^2\,[(-1)^n-1]n^2 + 8(r^2-2)\,(r^2-1)^2[(-1)^n-1]}{\{n^2\pi^2 + 2(r^2-1)\,[(-1)^n-1]\}^2}.$$

For n even, i.e. $\theta = 4\pi, 8\pi, 12\pi, \ldots$

$$R_{22}(\nu^2;\theta) = 1 - \frac{1}{2}\epsilon^2 + O(\epsilon^4)$$

therefore $|R_{22}(\nu^2;\theta)| < 1$ for all r and ϵ small.

For n odd, i.e. $\theta = 2\pi, 6\pi, 10\pi, \ldots$

$$R_{22}(\nu^2;\theta) = 1 - \left\{\frac{4n\pi(1-r^2)}{4(1-r^2)+n^2\pi^2}\right\}\epsilon + O(\epsilon^2).$$

Now, $4(1-r^2) + n^2\pi^2 = 0$ when $r = (\sqrt{4+n^2\pi^2})/2$. For $n = 1$ or $\theta = 2\pi + \epsilon$, as ϵ increases from negative to positive values,

i.) for $r < 1$, $|R_{22}(\nu^2;\theta)|$ decreases through 1;

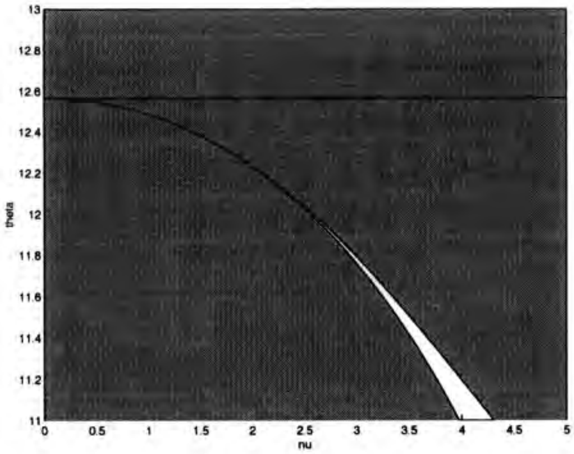

Figure 5.10: $\nu - \theta$ plot for three collocation points : c = 0, 1/2 and 1

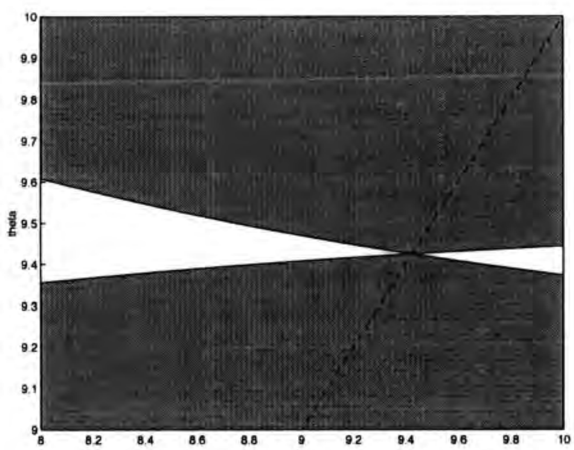

Figure 5.11: $\nu - \theta$ plot for three collocation points : c = 0, 1/2 and 1

ii.) for $1 < r < (\sqrt{4+\pi^2})/2$, $|R_{22}(\nu^2;\theta)|$ increases through 1;

iii.) for $r > (\sqrt{4+\pi^2})/2$, $|R_{22}(\nu^2;\theta)|$ decreases through 1.

For $n = 3$ or $\theta = 6\pi + \epsilon$, we have that as ϵ increases from negative to positive values,

i.) for $r < 1$, $|R_{22}(\nu^2;\theta)|$ decreases through 1;

ii.) for $1 < r < (\sqrt{4+9\pi^2})/2$, $|R_{22}(\nu^2;\theta)|$ increases through 1;

iii.) for $r > (\sqrt{4+9\pi^2})/2$, $|R_{22}(\nu^2;\theta)|$ decreases through 1.

Our final check is that the stability function for the mixed collocation method reduces to the corresponding polynomial collocation method as the fitted frequency

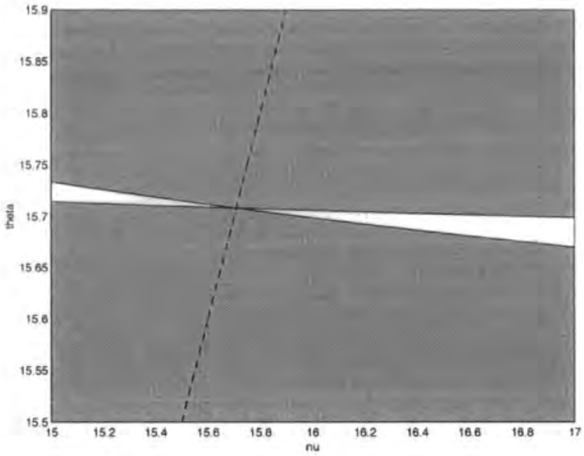

Figure 5.12: $\nu - \theta$ plot for three collocation points : c = 0, 1/2 and 1

$k \to 0$. Thus, as $k \to 0$,

$$\alpha_0 \to 1, \;\; \alpha_1 \to -\frac{7}{16}, \;\; \alpha_2 \to \frac{1}{72}, \;\; \beta_1 \to \frac{1}{16} \text{ and } \beta_2 \to 1288.$$

Therefore

$$R_{22}^{MC}(\nu^2;\theta) \to 2\left\{\frac{144 - 63\nu^2 + 2\nu^4}{288 + 18\nu^2 + \nu^4}\right\}$$

which is the stability function for the corresponding polynomial case.

Chapter 6

Extension of the Mixed Collocation Methods

6.1 Method I

The trigonometric functions $\cos kx$, $\sin kx$ and the monomials $x^i, i = 1, \ldots, s-1$ are the basis functions for the mixed collocation methods. In this section, we study an extension of the mixed collocation methods where the functions $x \cos kx$ and $x \sin kx$ are included in the basis. Ixaru and Rizea [37] showed that when a combination of products of polynomial and trigonometric functions were used in their methods, they obtained more accurate results for the solution of the Schrödinger equation. Another motivation behind doing this is so that we have a method which is exact for problems such as the almost periodic problem studied by Stiefel and Bettis [67]

$$z'' = -z + 0.001e^{ix}, \quad z(0) = 1, \quad z'(0) = 0.9995i, \quad z \in C$$

which has exact solution

$$z(x) = e^{ix}(1 - 0.0005ix).$$

If we set $z = y_1 + iy_2$, then the differential problem can be written in the equivalent form

$$y_1'' = -y_1 + 0.001 \cos x, \quad y_1(0) = 1, \quad y_1'(0) = 0$$

$$y_2'' = -y_2 + 0.001 \sin x, \quad y_2(0) = 0, \quad y_2'(0) = 0.9995$$

with the exact solution given by

$$y_1(x) = \cos x + 0.0005x \sin x \text{ and } y_2(x) = \sin x - 0.0005x \cos x.$$

Therefore, consider approximating the solution $y(x)$ of problem (1.1) on the interval $[x_n, x_{n+1}]$ by a function of the form

$$u(x) = [a_0 + a_1 t]\cos(kt) + [b_0 + b_1 t]\sin(kt) + \sum_{i=0}^{s-3} r_i t^i \tag{6.1}$$

where $t = x - x_n$.

Using a collocation method based on the s distinct collocation points .

$$x_{n+c_j} = x_n + c_j h, \; j = 1, \ldots, s$$

where $0 \leq c_1 < c_2 < \ldots < c_s \leq 1$, then we have the initial and collocation conditions

$$u(x_n) = y_n, \quad u'(x_n) = z_n$$

and

$$u''(x_n + c_j h) = f(x_n + c_j h, u(x_n + c_j h)), \; j = 1, \ldots, s.$$

Differentiate (6.1) with respect to x twice to give

$$\begin{aligned} u'(x) &= [a_1 + kb_0 + kb_1 t]\cos(kt) + [b_1 - ka_0 - ka_1 t]\sin(kt) + \sum_{i=1}^{s-3} i r_i t^{i-1} \\ u''(x) &= k[2b_1 - ka_0 - ka_1 t]\cos(kt) - k[2a_1 + kb_0 + kb_1 t]\sin(kt) + \sum_{i=2}^{s-3} i(i-1) r_i t^{i-2} \end{aligned}$$

where $t = x - x_n$.

Thus, the initial and collocation conditions are

$$y_n = \begin{cases} a_0, & s = 2, \\ a_0 + r_0, & s \geq 3, \end{cases} \qquad z_n = \begin{cases} a_1 + b_0 k, & s = 2 \text{ and } 3, \\ a_1 + b_0 k + r_1, & s \geq 4. \end{cases}$$

and

$$F(c_j) = k\{2b_1 - ka_0 - a_1 \theta c_j\}\cos(\theta c_j)$$

$$-k\left\{2a_1 + kb_0 + b_1\theta c_j\right\}\sin(\theta c_j) + \sum_{i=2}^{s-3} i(i-1)r_i(c_jh)^{i-2}, \quad j = 1,\ldots,s$$

where $F(c_j) = f(x_n + c_jh, u(x_n + c_jh))$ for $j = 1, \ldots, s$ and $\theta = kh$.

For $s \geq 4$, the system of equations can be written in matrix form $\mathcal{A}'\mathbf{x}' = \mathbf{b}'$ where $\mathbf{x}'$ and $\mathbf{b}'$ are $s+2$ dimensional column vectors given by

$$\mathbf{x}' = [a_0, a_1, b_0, b_1, r_0, r_1, \ldots, r_{s-3}]^T,$$

$$\mathbf{b}' = [y_n, z_n, F(c_1), F(c_2), \ldots, F(c_s)]^T$$

and $\mathcal{A}'$ is an $(s+2) \times (s+2)$ matrix given by

$$\mathcal{A}' = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & \ldots & 0 \\ 0 & 1 & k & 0 & 0 & 1 & \ldots & 0 \\ \mathcal{A}'_{3,1} & \mathcal{A}'_{3,2} & \mathcal{A}'_{3,3} & \mathcal{A}'_{3,4} & 0 & 0 & \ldots & \mathcal{A}'_{3,s+2} \\ \mathcal{A}'_{4,1} & \mathcal{A}'_{4,2} & \mathcal{A}'_{4,3} & \mathcal{A}'_{4,4} & 0 & 0 & \ldots & \mathcal{A}'_{4,s+2} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \mathcal{A}'_{s+2,1} & \mathcal{A}'_{s+2,2} & \mathcal{A}'_{s+2,3} & \mathcal{A}'_{s+2,4} & 0 & 0 & \ldots & \mathcal{A}'_{s+2,s+2} \end{pmatrix},$$

where for $j = 1, \ldots, s$

$$\mathcal{A}'_{j+2,1} = -k^2\cos(\theta c_j), \quad \mathcal{A}'_{j+2,2} = -k\theta c_j\cos(\theta c_j) - 2k\sin(\theta c_j),$$

$$\mathcal{A}'_{j+2,3} = -k^2\sin(\theta c_j), \quad \mathcal{A}'_{j+2,4} = -k\theta c_j\sin(\theta c_j) + 2k\cos(\theta c_j)$$

and

$$\mathcal{A}'_{j+2,l+2} = (l-3)(l-4)(c_jh)^{l-5}, \quad j = 1,\ldots,s, \quad l = 3,\ldots,s.$$

One can see that the matrix $\mathcal{A}'$ is slightly more complicated than the matrix A in section 4.1.2. The first four columns involve trigonometric functions and a lot of work is needed to obtain general formulae for this problem when looking at more than two collocation points. The following work is based on a 2-stage method ($s = 2$) and a study of order conditions and stability follows.

Two collocation points $s = 2$

For $s = 2$, we obtain the system of equations $\mathcal{A}'\mathbf{x}' = \mathbf{b}'$ where

$$\mathcal{A}' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & k & 0 \\ \mathcal{A}'_{3,1} & \mathcal{A}'_{3,2} & \mathcal{A}'_{3,3} & \mathcal{A}'_{3,4} \\ \mathcal{A}'_{4,1} & \mathcal{A}'_{4,2} & \mathcal{A}'_{4,3} & \mathcal{A}'_{4,4} \end{pmatrix}$$

$$\mathbf{x}' = [a_0, a_1, b_0, b_1]^T \text{ and } \mathbf{b}' = [y_n, z_n, F(c_1), F(c_2)]^T.$$

Rewriting the initial conditions, the system can be easily solved to find

$$a_0 = y_n, \quad b_0 = \frac{z_n - a_1}{k},$$

$$a_1 = \frac{V_1}{h}y_n + V_2 z_n + hV_3 f_{n+c_1} + hV_4 f_{n+c_2}$$

$$b_1 = \frac{W_1}{h}y_n + W_2 z_n + hW_3 f_{n+c_1} + hW_4 f_{n+c_2}$$

with

$$V_1 = -\theta^2\left\{\frac{\mathcal{Q}\sin(\theta\mathcal{P}) + \mathcal{P}\sin(\theta\mathcal{Q})}{\mathcal{G}}\right\}, \quad V_2 = \left\{\frac{\theta\mathcal{P}[\cos(\theta\mathcal{Q}) - \cos(\theta\mathcal{P})] - 4\sin(\theta\mathcal{P})}{\mathcal{G}}\right\}$$

$$V_3 = -2\left\{\frac{\theta c_2\sin(\theta c_2) - 2\cos(\theta c_2)}{\theta\mathcal{G}}\right\}, \quad V_4 = 2\left\{\frac{\theta c_1\sin(\theta c_1) - 2\cos(\theta c_1)}{\theta\mathcal{G}}\right\}$$

and

$$W_1 = \theta\left\{\frac{2\sin(\theta\mathcal{P}) + \theta\mathcal{P}[\cos(\theta\mathcal{P}) + \cos(\theta\mathcal{Q})]}{\mathcal{G}}\right\}, \quad W_2 = \theta\left\{\frac{\mathcal{P}\sin(\theta\mathcal{Q}) - \mathcal{Q}\sin(\theta\mathcal{P})}{\mathcal{G}}\right\}$$

$$W_3 = 2\left\{\frac{\sin(\theta c_2) + \theta c_2\cos(\theta c_2)}{\theta\mathcal{G}}\right\}, \quad W_4 = -2\left\{\frac{\sin(\theta c_1) + \theta c_1\cos(\theta c_1)}{\theta\mathcal{G}}\right\}$$

where $\mathcal{P} = c_2 - c_1$, $\mathcal{Q} = c_2 + c_1$, $\theta = kh$ and

$$\mathcal{G} = 2[2 + \theta^2 c_1 c_2]\sin(\theta\mathcal{P}) + 3\theta\mathcal{P}\cos(\theta\mathcal{P}) + \theta\mathcal{P}\cos(\theta\mathcal{Q})$$

where $\mathcal{G} \neq 0$.

Let y_{n+1}, z_{n+1} and y_{n+c_j} for $j = 1, 2$ be approximations for the exact solutions $y(x_n + h)$, $y'(x_n + h)$ and $y(x_n + c_j h)$ respectively. Then the two-point collocation method which fits the functions $[\sin kx, \cos kx, x\sin kx, x\cos kx]$ exactly, is given by

$$\left.\begin{aligned} y_{n+1} &= [a_0 + a_1 h]\cos\theta + [b_0 + b_1 h]\sin\theta \\ z_{n+1} &= [a_1 + k(b_0 + b_1 h)]\cos\theta + [b_1 - k(a_0 + a_1 h)]\sin\theta \\ y_{n+c_j} &= [a_0 + a_1 c_j h]\cos(\theta c_j) + [b_0 + b_1 c_j h]\sin(\theta c_j). \end{aligned}\right\} \quad (6.2)$$

The coefficients a_0, a_1, b_0 and b_1 can then be substituted into (6.2) to give the formulae for the two-point method. The method can be written in the form

$$\left.\begin{aligned} y_{n+1} &= \mathcal{A}_1 y_n + \mathcal{A}_2 h z_n + \mathcal{A}_3 h^2 f_{n+c_1} + \mathcal{A}_4 h^2 f_{n+c_2} \\ z_{n+1} &= \frac{\mathcal{B}_1}{h} y_n + \mathcal{B}_2 z_n + \mathcal{B}_3 h f_{n+c_1} + \mathcal{B}_4 h f_{n+c_2} \\ y_{n+c_1} &= \mathcal{P}_1 y_n + \mathcal{P}_2 h z_n + \mathcal{P}_3 h^2 f_{n+c_1} + \mathcal{P}_4 h^2 f_{n+c_2} \\ y_{n+c_2} &= \mathcal{Q}_1 y_n + \mathcal{Q}_2 h z_n + \mathcal{Q}_3 h^2 f_{n+c_1} + \mathcal{Q}_4 h^2 f_{n+c_2} \end{aligned}\right\} \quad (6.3)$$

where $f_{n+c_j} = f(x_n + c_j h, y_{n+c_j})$ and $\mathcal{A}_i$, $\mathcal{B}_i$, $\mathcal{P}_i$ and $\mathcal{Q}_i$ are given in Appendix B.2 for arbitrary c_1 and c_2. Also in Appendix B.2 is a Maple program to find the extended mixed collocation method for s collocation points. We have successfully found the methods for up to 3 stages.

Example : $c_1 = 0$ and $c_2 = 1$

The formulae for the two-point extended mixed collocation method with points $c_1 = 0$ and $c_2 = 1$ can be written in the form (6.3) with $\mathcal{P}_1 = 1$, $\mathcal{P}_2 = \mathcal{P}_3 = \mathcal{P}_4 = 0$ and $\mathcal{Q}_i = \mathcal{A}_i$ for $i = 1, \ldots, 4$. The coefficients are given along with the series expansions about $\theta = 0$.

$$\mathcal{A}_1 = \frac{\theta + \cos\theta\sin\theta}{\mathcal{E}} = 1 + \frac{\theta^4}{24} + \ldots \qquad \mathcal{A}_2 = \frac{2\sin^2\theta}{\theta\mathcal{E}} = 1 + \frac{7\theta^4}{360} + \ldots$$

$$\mathcal{A}_3 = \frac{\theta - \cos\theta\sin\theta}{\theta^2\mathcal{E}} = \frac{1}{3} + \frac{2\theta^2}{45} + \ldots \qquad \mathcal{A}_4 = \frac{\sin\theta - \theta\cos\theta}{\theta^2\mathcal{E}} = \frac{1}{6} + \frac{7\theta^2}{180} + \ldots$$

$$\mathcal{B}_1 = \frac{\theta^3 - \theta\sin^2\theta}{2\mathcal{E}} = \frac{\theta^4}{12} + \ldots \qquad \mathcal{B}_2 = \frac{\theta + \sin\theta\cos\theta}{\mathcal{E}} = 1 + \frac{\theta^4}{24} + \ldots$$

$$\mathcal{B}_3 = \frac{\theta^2 + \sin^2\theta}{2\theta\mathcal{E}} = \frac{1}{2} + \frac{\theta^2}{12} + \dots \qquad \mathcal{B}_4 = \frac{\sin\theta}{\mathcal{E}} = \frac{1}{2} + \frac{\theta^2}{12} + \dots$$

where $\theta = kh$ and $\mathcal{E} = \sin\theta + \theta\cos\theta$.

The method is undefined when $\theta = 0$ or $\sin\theta + \theta\cos\theta = 0$. Substituting the expressions for the expansions of the coefficients back into the method we obtain the following approximations for y_{n+1} and z_{n+1},

$$y_{n+1} \approx \left\{1 + \frac{\theta^4}{24}\right\} y_n + h\left\{1 + \frac{7\theta^4}{360}\right\} z_n + h^2\left\{\frac{1}{3} + \frac{2\theta^2}{45}\right\} f_n + h^2\left\{\frac{1}{6} + \frac{7\theta^2}{180}\right\} f_{n+1}$$

$$z_{n+1} \approx \frac{\theta^4}{12h} y_n + \left\{1 + \frac{\theta^4}{24}\right\} z_n + h\left\{\frac{1}{2} + \frac{\theta^2}{12}\right\} f_n + h\left\{\frac{1}{2} + \frac{\theta^2}{12}\right\} f_{n+1}\ ,$$

and as $k \to 0$, the mixed collocation method reduces to the corresponding polynomial collocation method for 2 collocation points (2.16) with $c_1 = 0$ and $c_2 = 1$.

Example : $c_1 = (3 - \sqrt{3})/6$ **and** $c_2 = (3 + \sqrt{3})/6$
The formulae for the two-point mixed collocation method with collocation nodes $c_1 = (3 - \sqrt{3})/6$ and $c_2 = (3 + \sqrt{3})/6$ are given by (6.3) and the coefficients $\mathcal{A}_i$, $\mathcal{B}_i$, $\mathcal{P}_i$ and $\mathcal{Q}_i$ are listed in Appendix B.2. The coefficients are very complex even for 2-stages when the collocation points are the Gauss nodes.

Using Maple to find the series expansions of the coefficients about $\theta = 0$ the coefficients reduce to

$$\mathcal{A}_1 \to 1,\ \mathcal{A}_2 \to 1,\ \mathcal{A}_3 \to \frac{3+\sqrt{3}}{12},\ \mathcal{A}_4 \to \frac{3-\sqrt{3}}{12},$$

$$\mathcal{B}_1 \to 0,\ \mathcal{B}_2 \to 1,\ \mathcal{B}_3 \to \frac{1}{2},\ \mathcal{B}_4 \to \frac{1}{2},$$

$$\mathcal{P}_1 \to 1,\ \mathcal{P}_2 \to \frac{3-\sqrt{3}}{6},\ \mathcal{P}_3 \to \frac{1}{36},\ \mathcal{P}_4 \to \frac{5-3\sqrt{3}}{36},$$

$$\mathcal{Q}_1 \to 1,\ \mathcal{Q}_2 \to \frac{3+\sqrt{3}}{6},\ \mathcal{Q}_3 \to \frac{5+3\sqrt{3}}{36},\ \mathcal{Q}_4 \to \frac{1}{36},$$

and we obtain the polynomial collocation method (2.16) with Gauss points for the collocation parameters as $k \to 0$.

6.1.1 Order Conditions

Using the idea of the residual with the exact values of the solution and its first derivative at x_n, the difference operators for the mixed collocation method I with two collocation points (6.3) are given by

$$\begin{aligned} L_1[y] &= y(x_n+h) - \mathcal{A}_1 y(x_n) - \mathcal{A}_2 h y'(x_n) \\ &\qquad -h^2[\mathcal{A}_3 f(x_n+c_1h, Y_1) + \mathcal{A}_4 f(x_n+c_2h, Y_2)] \\ L_2[y] &= y'(x_n+h) - \frac{\mathcal{B}_1}{h} y(x_n) - \mathcal{B}_2 y'(x_n) \\ &\qquad -h[\mathcal{B}_3 f(x_n+c_1h, Y_1) + \mathcal{B}_4 f(x_n+c_2h, Y_2)] \end{aligned}$$

where

$$Y_1 = \mathcal{P}_1 y(x_n) + \mathcal{P}_2 h y'(x_n) + \mathcal{P}_3 h^2 f(x_n+c_1h, Y_1) + \mathcal{P}_4 h^2 f(x_n+c_2h, Y_2),$$

$$Y_2 = \mathcal{Q}_1 y(x_n) + \mathcal{Q}_2 h y'(x_n) + \mathcal{Q}_3 h^2 f(x_n+c_1h, Y_1) + \mathcal{Q}_4 h^2 f(x_n+c_2h, Y_2).$$

Substituting the coefficients $\mathcal{A}_i$, $\mathcal{B}_i$, $\mathcal{P}_i$ and $\mathcal{Q}_i$ into the difference operators above and using a Taylor expansion in powers of the steplength h we obtain

$$L_1[y] = \frac{h^4}{24}[1-2c_1-2c_2+6c_1c_2]\left\{f_{xx}+2f_{xy}y'+f_{yy}[y']^2+f_yf+2k^2f+k^4y\right\}$$

$$+\frac{h^5}{360}[3-10c_1^2-10c_2^2-10c_1c_2+30c_1c_2(c_1+c_2)]\left\{f_{xxx}+3f_{xy}f+f_y^2y'+f_{yyy}[y']^3\right.$$
$$\left.+3f_{xyy}[y']^2+3f_{xxy}y'+f_yf_x+3f_{yy}fy'+2k^2(f_yy'+f_x)+k^4y'\right\}+O(h^6)$$

and

$$L_2[y] = \frac{h^3}{12}[2-3c_1-3c_2+6c_1c_2]\left\{f_{xx}+2f_{xy}y'+f_{yy}[y']^2+f_yf+2k^2f+k^4y\right\}$$

$$+\frac{h^4}{24}[1-2c_1^2-2c_2^2-2c_1c_2+4c_1c_2(c_1+c_2)]\left\{f_{xxx}+3f_{xy}f+f_y^2y'+f_{yyy}[y']^3+3f_{xyy}[y']^2\right.$$
$$\left.+3f_{xxy}y'+f_yf_x+3f_{yy}fy'+2k^2(f_yy'+f_x)+k^4y'\right\}+O(h^6)$$

where $y'=y'(x_n)$, $f=f(x_n,y(x_n))$, $f_x=f_x(x_n,y(x_n))$, $f_y=f_y(x_n,y(x_n))$ etc.

For algebraic **order 3**, we require

$$2 - 3c_1 - 3c_2 + 6c_1c_2 = 0 \quad \Rightarrow \quad c_1 = \frac{3c_2 - 2}{6c_2 - 3}, \quad (c_2 \neq 1/2)$$

and for **order 4**, we require

$$c_1 = \frac{3c_2 - 2}{6c_2 - 3} \quad \text{and} \quad 1 - 2c_1 - 2c_2 + 6c_1c_2 = 0$$

from which

$$6c_2^2 - 6c_2 + 1 = 0 \quad \Rightarrow \quad c_2 = \frac{3 \pm \sqrt{3}}{6}.$$

Therefore, as $L_1[y] = O(h^4)$ and $L_2[y] = O(h^3)$ for arbitrary c_1 and c_2, we have a default order of 2. When the collocation points are the Gauss nodes, then $L_1[y] = O(h^5)$ and $L_2[y] = O(h^5)$, and the highest possible order of 4 is obtained.

6.1.2 Stability

Example : $c_1 = 0$ and $c_2 = 1$
Applying the method (6.3) to the test equation $y'' = -w^2 y$ with $\mathcal{P}_1 = 1$, $\mathcal{P}_2 = \mathcal{P}_3 = \mathcal{P}_4 = 0$ and $\mathcal{Q}_i = \mathcal{A}_i$ for $i = 1, \ldots, 4$ we obtain

$$y_{n+1} = \mathcal{A}_1 y_n + \mathcal{A}_2 h z_n - \mathcal{A}_3 \nu^2 y_n - \mathcal{A}_4 \nu^2 y_{n+1} \tag{6.4}$$

$$h z_{n+1} = \mathcal{B}_1 y_n + \mathcal{B}_2 h z_n - \mathcal{B}_3 \nu^2 y_n - \mathcal{B}_4 \nu^2 y_{n+1} \tag{6.5}$$

where $\nu = wh$.

Rewrite equation (6.4) as

$$y_{n+2} = \mathcal{A}_1 y_{n+1} + \mathcal{A}_2 h z_{n+1} - \mathcal{A}_3 \nu^2 y_{n+1} - \mathcal{A}_4 \nu^2 y_{n+2}$$

and then substitute (6.5) for z_{n+1}. We can eliminate z_n using (6.4) to obtain

$$\begin{aligned} &\left\{1 + \nu^2 \mathcal{A}_4\right\} y_{n+2} - \left\{\mathcal{A}_1 + \mathcal{B}_2 - \nu^2(\mathcal{A}_3 + \mathcal{A}_2\mathcal{B}_4 - \mathcal{A}_4\mathcal{B}_2)\right\} y_{n+1} \\ &+ \left\{\mathcal{A}_1\mathcal{B}_2 - \mathcal{A}_2\mathcal{B}_1 + \nu^2(\mathcal{A}_2\mathcal{B}_3 - \mathcal{A}_3\mathcal{B}_2)\right\} y_n = 0. \end{aligned}$$

Therefore the stability equation is given by

$$\xi^2 - 2R_{11}(\nu^2;\theta)\xi + P(\nu^2;\theta) = 0$$

where

$$R_{11}(\nu^2;\theta) = \frac{\mathcal{A}_1 + \mathcal{B}_2 - \nu^2(\mathcal{A}_3 + \mathcal{A}_2\mathcal{B}_4 - \mathcal{A}_4\mathcal{B}_2)}{2[1+\nu^2\mathcal{A}_4]}$$

and

$$P(\nu^2;\theta) = \frac{\mathcal{A}_1\mathcal{B}_2 - \mathcal{A}_2\mathcal{B}_1 + \nu^2(\mathcal{A}_2\mathcal{B}_3 - \mathcal{A}_3\mathcal{B}_2)}{1+\nu^2\mathcal{A}_4}.$$

Substituting the values for $\mathcal{A}_i$ and $\mathcal{B}_i$, for $i = 1, \ldots, 4$ and after some simplification

$$R_{11}(\nu^2;\theta) = \frac{\theta^2(\theta + \sin\theta\cos\theta) + \nu^2(\sin\theta\cos\theta - \theta)}{\theta^2(\sin\theta + \theta\cos\theta) + \nu^2(\sin\theta - \theta\cos\theta)} \quad \text{and} \quad P(\nu^2;\theta) = 1.$$

Thus the requirement for the method to have an interval of periodicity is satisfied. The stability function $R_{11}(\nu^2;\theta)$ may be written as

$$R_{11}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\nu^2}{1+\beta_1\nu^2}$$

where

$$\alpha_0 = \frac{\theta + \sin\theta\cos\theta}{\sin\theta + \theta\cos\theta}, \quad \alpha_1 = \frac{\sin\theta\cos\theta - \theta}{\theta^2(\sin\theta + \theta\cos\theta)} \quad \text{and} \quad \beta_1 = \frac{\sin\theta - \theta\cos\theta}{\theta^2(\sin\theta + \theta\cos\theta)}.$$

When $\theta = \nu$,

$$R_{11}(\nu^2;\nu) = \frac{\nu^3 + \nu^2\sin\nu\cos\nu + \nu^2\sin\nu\cos\nu - \nu^3}{\nu^2\sin\nu + \nu^3\cos\nu + \nu^2\sin\nu - \nu^3\cos\nu} = \cos\nu$$

and when $\theta = n\pi$,

$$R_{11}(\nu^2;n\pi) = \frac{(n\pi)^2(n\pi + 0) + \nu^2(0 - n\pi)}{(n\pi)^2(0 + n\pi(-1)^n) + \nu^2(0 - n\pi(-1)^n)} = (-1)^n.$$

Following Definition 3.4 in chapter 3, the stability boundaries are the curves

$$\nu_+(\theta) = \left\{-\frac{\alpha_0 + 1}{\alpha_1 + \beta_1}\right\}^{1/2} = \theta\left\{\frac{\theta + \sin\theta}{\theta - \sin\theta}\right\}^{1/2},$$

$$\nu_-(\theta) = \left\{-\frac{\alpha_0 - 1}{\alpha_1 - \beta_1}\right\}^{1/2} = \theta\left\{\frac{\theta - \sin\theta}{\theta + \sin\theta}\right\}^{1/2}$$

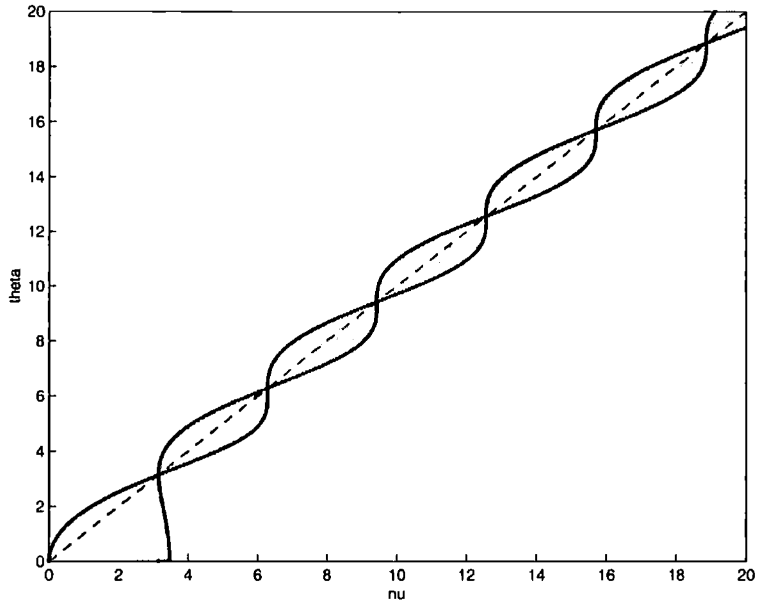

Figure 6.1: $\nu - \theta$ plot for extended mixed collocation method I : $c = 0$ and 1

and the lines corresponding to any values of θ for which

$$\alpha_0 \pm 1 = 0 = \alpha_1 \pm \beta_1.$$

Thus,

$$\alpha_0 + 1 = 0 = \alpha_1 + \beta_1 \quad \Rightarrow \quad \frac{(\theta + \sin\theta)(1 + \cos\theta)}{\sin\theta + \theta\cos\theta} = 0 \text{ and } \frac{(\sin\theta - \theta)(1 + \cos\theta)}{\theta^2(\sin\theta + \theta\cos\theta)} = 0$$

and both of these equations are satisfied when $\theta = (2n + 1)\pi$ where n is a non-negative integer. Also

$$\alpha_0 - 1 = 0 = \alpha_1 - \beta_1 \quad \Rightarrow \quad \frac{(\theta - \sin\theta)(1 - \cos\theta)}{\sin\theta - \theta\cos\theta} = 0 \text{ and } \frac{(\sin\theta + \theta)(1 - \cos\theta)}{\theta^2(\sin\theta + \theta\cos\theta)} = 0$$

and these two equations are satisfied when $\theta = 2n\pi$.

Therefore the stability boundaries are given by the curves

$$\nu_+(\theta) = \theta \left\{ \frac{\theta + \sin\theta}{\theta - \sin\theta} \right\}^{1/2} \text{ and } \nu_-(\theta) = \theta \left\{ \frac{\theta - \sin\theta}{\theta + \sin\theta} \right\}^{1/2}.$$

The lines $\theta = n\pi$ where n is a non-negative integer are also possible boundaries.

The stability regions are shown in figure 6.1. The equations $\nu_+(\theta)$ and $\nu_-(\theta)$ define two continuous oscillating curves which cross at multiples of π and enclose the stability regions between them. When $\theta = n\pi$, the modulus of the stability function is 1 but these lines do not act as stability boundaries. There is an interval of periodicity $(0, h_0)$ where h_0 decreases from $\sqrt{12}/w$ when $r = 0$ to π/w when $r = 1$ for fixed w. When $r > 1$, the periodicity interval decreases from π/k (with k fixed) when $r = 1$ and tends to 0 as r increases. We note that the stability regions are very similar to those of the exponentially-fitted multistep method S_3 which is exact for $[\exp(\pm ikx), x\exp(\pm ikx), x^2\exp(\pm ikx)]$, (c.f. [23]).

The stability function for the mixed collocation method for $s = 2$ with fitted trigonometric functions $[\cos kx, \sin kx, x\cos kx, x\sin kx]$ is given by

$$R_{11}^{MC}(\nu^2;\theta) = \frac{\theta^2(\theta + \sin\theta\cos\theta) + \nu^2(\sin\theta\cos\theta - \theta)}{\theta^2(\sin\theta + \theta\cos\theta) + \nu^2(\sin\theta - \theta\cos\theta)}.$$

As $k \to 0$

$$R_{11}^{MC}(\nu^2;\theta) \to \frac{2 - 2\nu^2/3}{2 + \nu^2/3} = \frac{6 - 2\nu^2}{6 + \nu^2}$$

and this agrees with the stability function for the polynomial collocation method in section 2.5.3 with $c_1 = 0$ and $c_2 = 1$.

Example : $c_1 = (3 - \sqrt{3})/6$ **and** $c_2 = (3 + \sqrt{3})/6$

If we apply the method (6.3) to the test equation $y'' = -w^2 y$, we obtain

$$\begin{aligned}
y_{n+1} &= \mathcal{A}_1\, y_n + \mathcal{A}_2\, h\, z_n - \mathcal{A}_3\, \nu^2\, y_{n+c_1} - \mathcal{A}_4\, \nu^2\, y_{n+c_2} \\
hz_{n+1} &= \mathcal{B}_1\, y_n + \mathcal{B}_2\, h\, z_n - \mathcal{B}_3\, \nu^2\, y_{n+c_1} - \mathcal{B}_4\, \nu^2\, y_{n+c_2} \\
y_{n+c_1} &= \mathcal{P}_1\, y_n + \mathcal{P}_2\, h\, z_n - \mathcal{P}_3\, \nu^2\, y_{n+c_1} - \mathcal{P}_4\, \nu^2\, y_{n+c_2} \\
y_{n+c_2} &= \mathcal{Q}_1\, y_n + \mathcal{Q}_2\, h\, z_n - \mathcal{Q}_3\, \nu^2\, y_{n+c_1} - \mathcal{Q}_4\, \nu^2\, y_{n+c_2}
\end{aligned}$$

where $\nu = wh$. The coefficients are given in Appendix B.2 for arbitrary c_1 and c_2. The method is undefined when either $\theta = 0$ or

$$-\left\{\frac{1}{3}\theta^2 + 4\right\}\sin\left(\frac{\sqrt{3}}{3}\theta\right) - \theta\sqrt{3}\cos\left(\frac{\sqrt{3}}{3}\theta\right) - \frac{\sqrt{3}}{3}\theta\cos\theta = 0$$

$$\Rightarrow \quad \theta = 0, 4.1607, 10.2989, 15.6182, \ldots$$

to 4 decimal places. After some simplification, the characteristic equation is given by

$$\xi^2 - 2R_{22}(\nu^2;\theta)\xi + P(\nu^2;\theta) = 0$$

where the stability function is

$$R_{22}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\,\nu^2 + \alpha_2\,\nu^4}{1 + \beta_1\,\nu^2 + \beta_2\,\nu^4}$$

with

$$\alpha_0 = \frac{1}{2}\left\{\mathcal{B}_2 + \mathcal{A}_1\right\}$$

$$\alpha_1 = \frac{1}{2}\left\{\mathcal{A}_1\,\mathcal{Q}_4 - \mathcal{A}_3\,\mathcal{P}_1 - \mathcal{P}_2\,\mathcal{B}_3 + \mathcal{A}_1\,\mathcal{P}_3 + \mathcal{Q}_4\,\mathcal{B}_2 - \mathcal{A}_4\,\mathcal{Q}_1 + \mathcal{B}_2\,\mathcal{P}_3 - \mathcal{B}_4\,\mathcal{Q}_2\right\}$$

$$\alpha_2 = \frac{1}{2}\left\{\begin{vmatrix} \mathcal{B}_2 & \mathcal{B}_3 & \mathcal{B}_4 \\ \mathcal{P}_2 & \mathcal{P}_3 & \mathcal{P}_4 \\ \mathcal{Q}_2 & \mathcal{Q}_3 & \mathcal{Q}_4 \end{vmatrix} + \begin{vmatrix} \mathcal{A}_1 & \mathcal{A}_3 & \mathcal{A}_4 \\ \mathcal{P}_1 & \mathcal{P}_3 & \mathcal{P}_4 \\ \mathcal{Q}_1 & \mathcal{Q}_3 & \mathcal{Q}_4 \end{vmatrix}\right\}$$

$$\beta_1 = \mathcal{Q}_4 + \mathcal{P}_3,\quad \beta_2 = \mathcal{P}_3\,\mathcal{Q}_4 - \mathcal{P}_4\,\mathcal{Q}_3$$

and

$$P(\nu^2;\theta) = \frac{\rho_0 + \rho_1\,\nu^2 + \rho_2\,\nu^4}{1 + \sigma_1\,\nu^2 + \sigma_2\,\nu^4}$$

with

$$\rho_0 = \mathcal{B}_2\,\mathcal{A}_1 - \mathcal{A}_2\,\mathcal{B}_1$$

$$\rho_1 = \begin{vmatrix} \mathcal{A}_1 & \mathcal{A}_2 & \mathcal{A}_3 \\ \mathcal{B}_1 & \mathcal{B}_2 & \mathcal{B}_3 \\ \mathcal{P}_1 & \mathcal{P}_2 & \mathcal{P}_3 \end{vmatrix} + \begin{vmatrix} \mathcal{A}_1 & \mathcal{A}_2 & \mathcal{A}_4 \\ \mathcal{B}_1 & \mathcal{B}_2 & \mathcal{B}_4 \\ \mathcal{Q}_1 & \mathcal{Q}_2 & \mathcal{Q}_4 \end{vmatrix},\quad \rho_2 = \begin{vmatrix} \mathcal{A}_1 & \mathcal{A}_2 & \mathcal{A}_3 & \mathcal{A}_4 \\ \mathcal{B}_1 & \mathcal{B}_2 & \mathcal{B}_3 & \mathcal{B}_4 \\ \mathcal{P}_1 & \mathcal{P}_2 & \mathcal{P}_3 & \mathcal{P}_4 \\ \mathcal{Q}_1 & \mathcal{Q}_2 & \mathcal{Q}_3 & \mathcal{Q}_4 \end{vmatrix}$$

$$\sigma_1 = \mathcal{Q}_4 + \mathcal{P}_3,\quad \sigma_2 = \mathcal{P}_3\,\mathcal{Q}_4 - \mathcal{P}_4\,\mathcal{Q}_3.$$

As we can see, the expressions are already complicated before the coefficients of the method are substituted. As a result, we were unable to find a general formula for the characteristic equation as there was not enough memory using Maple. Instead, in figure 6.2 a method of trial and error was used to find the stable regions. For each value of ν and θ that was substituted, $P(\nu^2;\theta) = 1$ and so we are only concerned with whether the absolute value of the stability function is less than or equal to 1 to have a stable region.

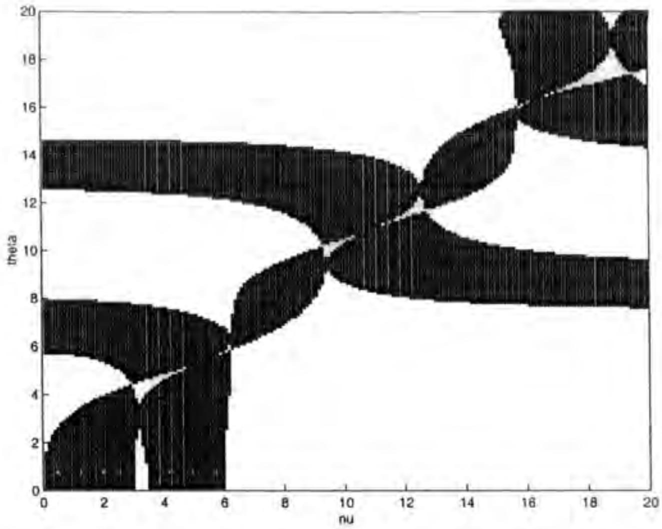

Figure 6.2: $\nu - \theta$ plot for extended MC method I : $c_1 = (3-\sqrt{3})/6$ & $c_2 = (3+\sqrt{3})/6$

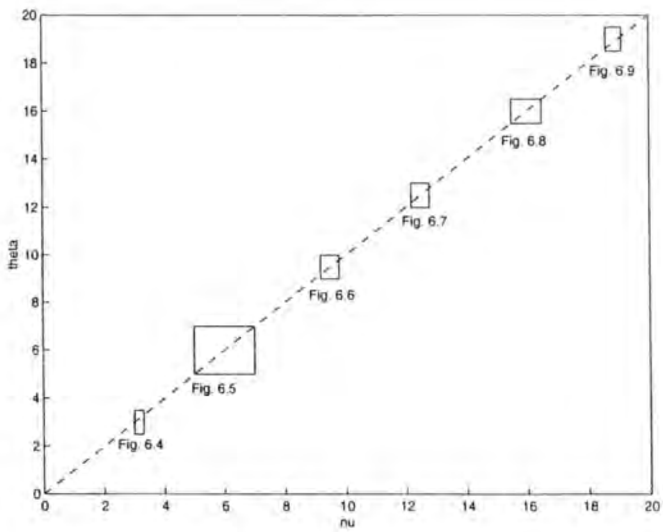

Figure 6.3: Enlargements of sections of figure 6.2

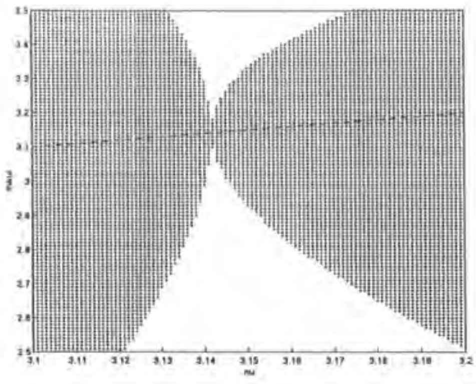

Figure 6.4: $\nu - \theta$ plot for extended MC method I : Gauss nodes

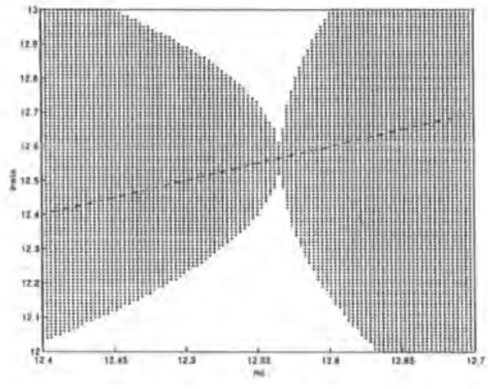

Figure 6.5: $\nu - \theta$ plot for extended MC method I : Gauss nodes

In figure 6.2, a dot refers to a stable region for a particular value of ν and θ. For $r < 1$, the primary interval of periodicity is $(0, h_0)$ where h_0 increases from $3/w$ when $r = 0$ to π/w when $r = 1$, for fixed w. There is a secondary interval of periodicity given by $(2\sqrt{3}/w, 6/w)$ when $r = 0$ and the length of the interval increases to $(\pi/w, 2\pi/w)$ as $r \to 1$. As $k \to 0$, the intervals of periodicity for the two-point polynomial collocation method (2.16) with Gauss nodes are recovered. Also included are figures 6.4 - 6.9 which are enlargements of various sections of figure 6.2. The line $\nu = \theta$ is drawn and we have a stable region along this line for all ν and θ.

As $k \to 0$, then

$$R_{22}^{MC}(\nu^2; \theta) \to \frac{432 - 192\nu^2 + 7\nu^4}{432 + 24\nu^2 + \nu^4}$$

which is the stability function for the 2-stage polynomial collocation method with Gauss points.

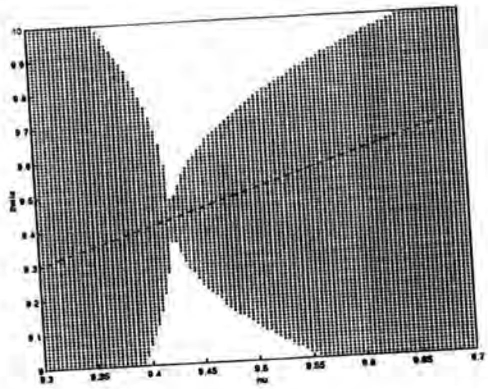

Figure 6.6: $\nu - \theta$ plot for extended MC method I : Gauss nodes

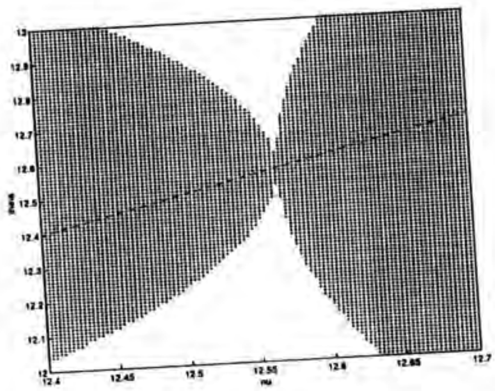

Figure 6.7: $\nu - \theta$ plot for extended MC method I : Gauss nodes

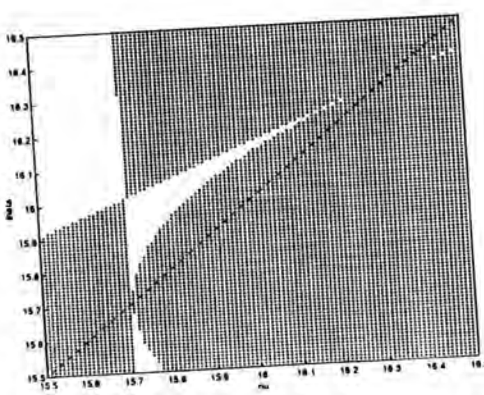

Figure 6.8: $\nu - \theta$ plot for extended MC method I : Gauss nodes

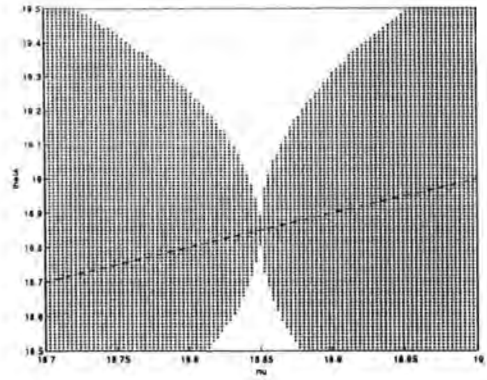

Figure 6.9: $\nu - \theta$ plot for extended MC method I : Gauss nodes

6.2 Method II

An alternative way of forming the basis of functions is by considering more than one frequency. Many problems have theoretical solutions which involve more than one frequency and so it would be useful to derive a mixed collocation method which is exact for two or more frequencies.

Consider the problem of approximating the solution $y(x)$ of the problem (1.1) by a function of the form

$$u(x) = a_0 \cos k_1 t + b_0 \cos k_2 t + a_1 \sin k_1 t + b_1 \sin k_2 t + \sum_{i=0}^{s-3} r_i t^i$$

where $t = x - x_n$, and k_1 and k_2 are the angular frequencies with $k_1 \neq k_2$.

Again, the initial and collocation conditions are given by

$$y(x_n) = y_n, \quad y'(x_n) = z_n$$

and

$$u''(x_n + c_j h) = f(x_n + c_j h, u(x_n + c_j h)), \; j = 1, \ldots, s$$

As with method I, the work becomes complicated and we will concern ourselves with just two collocation points.

Example : $s = 2$

With $s = 2$, $u(x)$ is of the form

$$u(x) = a_0 \cos k_1(x - x_n) + b_0 \cos k_2(x - x_n) + a_1 \sin k_1(x - x_n) + b_1 \sin k_2(x - x_n)$$

and from the initial and collocation conditions, we have

$$a_0 + b_0 = y_n, \quad a_1 k_1 + b_1 k_2 = z_n$$

and

$$f_{n+c_j} = -a_0 k_1^2 \cos(\theta_1 c_j) - b_0 k_2^2 \cos(\theta_2 c_j) - a_1 k_1^2 \sin(\theta_1 c_j) - b_1 k_2^2 \sin(\theta_2 c_j), \quad j = 1, 2$$

where $\theta_1 = k_1 h$, $\theta_2 = k_2 h$ and $f_{n+c_j} = f(x_n + c_j h, y_{n+c_j})$.

(Note that for $s = 3$, the initial conditions give

$$a_0 + b_0 + r_0 = y_n, \quad a_1 k_1 + b_1 k_2 = z_n,$$

and for $s \geq 4$, the initial conditions are

$$a_0 + b_0 + r_0 = y_n, \quad a_1 k_1 + b_1 k_2 + r_1 = z_n.)$$

A system of equations is obtained which is easily solved to give

$$a_0 = y_n - b_0, \quad a_1 = \frac{z_n - b_1 k_2}{k_1},$$

$$b_0 = S_1\, y_n + h\, S_2\, z_n + h^2 \left[S_3\, f_{n+c_1} + S_4\, f_{n+c_2}\right]$$

where

$$S_1 = \theta_1^2 \left\{\theta_2 \sin(\theta_1 c_1 + \theta_2 c_2) + 2\theta_1 \sin[\theta_1(c_1 - c_2)] - \theta_2 \sin(\theta_2 c_1 + \theta_1 c_2) \right.$$
$$\left. -\theta_2 \sin(\theta_2 c_1 - \theta_1 c_2) - \theta_2 \sin(\theta_1 c_1 - \theta_2 c_2)\right\} / G,$$

$$S_2 = -\theta_1 \theta_2 \left\{-\cos(\theta_2\, c_1 + \theta_1 c_2) - \cos(\theta_1 c_1 - \theta_2 c_2) \right.$$
$$\left. +\cos(\theta_1 c_1 + \theta_2\, c_2) + \cos(\theta_2 c_1 - \theta_1 c_2)\right\} / G,$$

$$S_3 = -2\left\{\frac{\theta_1\sin(\theta_1 c_2) - \theta_2\sin(\theta_2 c_2)}{G}\right\}, \quad S_4 = 2\left\{\frac{\theta_1\sin(\theta_1 c_1) - \theta_2\sin(\theta_2 c_1)}{G}\right\},$$

$$\begin{aligned} G = {} & 2\theta_1^3\sin[\theta_1(c_1 - c_2)] - \theta_1^2\theta_2\sin(\theta_1 c_1 - \theta_2 c_2) - \theta_2^2\theta_1\sin(\theta_2 c_1 - \theta_1 c_2) \\ & + \theta_1^2\theta_2\sin(\theta_1 c_1 + \theta_2 c_2) - \theta_2^2\theta_1\sin(\theta_1 c_1 - \theta_2 c_2) + \theta_2^2\theta_1\sin(\theta_2 c_1 + \theta_1 c_2) \\ & + 2\theta_2^3\sin[\theta_2(c_1 - c_2)] - \theta_2^2\theta_1\sin(\theta_1 c_1 + \theta_2 c_2) - \theta_1^2\theta_2\sin(\theta_2 c_1 + \theta_1 c_2) \\ & - \theta_1^2\theta_2\sin(\theta_2 c_1 - \theta_1 c_2) \end{aligned}$$

with $G \neq 0$ and b_1 is given by

$$b_1 = T_1\, y_n + h\, T_2\, z_n + h^2\left[T_3\, f_{n+c_1} + T_4\, f_{n+c_2}\right]$$

where

$$T_1 = \frac{-\cos(\theta_1 c_2)\theta_1^2 S_1 + \cos(\theta_2 c_2)\theta_2^2 S_1 + \cos(\theta_1 c_2)\theta_1^2}{\theta_2[\theta_1\sin(\theta_1 c_2) - \theta_2\sin(\theta_2 c_2)]},$$

$$T_2 = \frac{\theta_1\sin(\theta_1 c_2) + \cos(\theta_2 c_2)\theta_2^2 S_2 - \cos(\theta_1 c_2)\theta_1^2 S_2}{\theta_2[\theta_1\sin(\theta_1 c_2) - \theta_2\sin(\theta_2 c_2)]},$$

$$T_3 = \frac{S_3[\cos(\theta_2 c_2)\theta_2^2 - \cos(\theta_1 c_2)\theta_1^2]}{\theta_2[\theta_1\sin(\theta_1 c_2) - \theta_2\sin(\theta_2 c_2)]},$$

$$T_4 = \frac{1 + \cos(\theta_2 c_2)\theta_2^2 S_4 - \cos(\theta_1 c_2)\theta_1^2 S_4}{\theta_2[\theta_1\sin(\theta_1 c_2) - \theta_2\sin(\theta_2 c_2)]}$$

for $\theta_2[\theta_1\sin(\theta_1 c_2) - \theta_2\sin(\theta_2 c_2)] \neq 0$.

Let y_{n+1}, z_{n+1} and y_{n+c_j} for $j = 1, 2$ be approximations for the exact solutions $y(x_n + h)$, $y'(x_n + h)$ and $y(x_n + c_j h)$ respectively. Then the two-point collocation method which fits the functions $[\sin k_1 x, \cos k_1 x, \sin k_2 x, \cos k_2 x]$ exactly is given by

$$\begin{aligned} y_{n+1} &= a_0\cos\theta_1 + b_0\cos\theta_2 + a_1\sin\theta_1 + b_1\sin\theta_2, \\ z_{n+1} &= -a_0 k_1\sin\theta_1 - b_0 k_2\sin\theta_2 + a_1 k_1\cos\theta_1 + b_1 k_2\cos\theta_2 \end{aligned}$$

and

$$y_{n+c_j} = -a_0 k_1^2\cos(\theta_1 c_j) - b_0 k_2^2\cos(\theta_2 c_j) - a_1 k_1^2\sin(\theta_1 c_j) - b_1 k_2^2\sin(\theta_2 c_j), \; j = 1, 2$$

where $\theta_1 = k_1 h$ and $\theta_2 = k_2 h$. The coefficients a_0, a_1, b_0 and b_1 can then be substituted to find the general form for the two-point mixed collocation method with two frequencies.

Example : $c_1 = 0$ **and** $c_2 = 1$

The two-point two-frequency mixed collocation method is given by

$$\left.\begin{aligned} y_{n+1} &= \mathcal{A}_1 y_n + \mathcal{A}_2 h z_n + \mathcal{A}_3 h^2 f_n + \mathcal{A}_4 h^2 f_{n+1} \\ z_{n+1} &= \frac{\mathcal{B}_1}{h} y_n + \mathcal{B}_2 z_n + \mathcal{B}_3 h f_n + \mathcal{B}_4 h f_{n+1} \end{aligned}\right\} \tag{6.6}$$

where

$$\mathcal{A}_1 = \frac{\theta_2 \cos\theta_1 \sin\theta_2 - \theta_1 \sin\theta_1 \cos\theta_2}{\mathcal{E}}, \quad \mathcal{A}_2 = \frac{\sin\theta_1 \sin\theta_2 [\theta_2^2 - \theta_1^2]}{\theta_1 \theta_2 \mathcal{E}},$$

$$\mathcal{A}_3 = \frac{\theta_1 \cos\theta_1 \sin\theta_2 - \theta_2 \sin\theta_1 \cos\theta_2}{\theta_1 \theta_2 \mathcal{E}}, \quad \mathcal{A}_4 = \frac{\theta_2 \sin\theta_1 - \theta_1 \sin\theta_2}{\theta_1 \theta_2 \mathcal{E}},$$

$$\mathcal{B}_1 = -\theta_1 \theta_2 \frac{\theta_1^2 \sin\theta_1 \sin\theta_2 + \theta_2^2 \sin\theta_1 \sin\theta_2 - 2\theta_1\theta_2 + 2\theta_1\theta_2 \cos\theta_1 \cos\theta_2}{[\theta_2^2 - \theta_1^2]\mathcal{E}},$$

$$\mathcal{B}_2 = \frac{\theta_2 \cos\theta_1 \sin\theta_2 - \theta_1 \sin\theta_1 \cos\theta_2}{\mathcal{E}},$$

$$\mathcal{B}_3 = -\frac{\theta_1^2 \cos\theta_1 \cos\theta_2 + \theta_2^2 \cos\theta_1 \cos\theta_2 - \theta_1^2 - \theta_2^2 + 2\theta_1\theta_2 \sin\theta_1 \sin\theta_2}{[\theta_2^2 - \theta_1^2]\mathcal{E}},$$

$$\mathcal{B}_4 = \frac{\cos\theta_1 - \cos\theta_2}{\mathcal{E}}$$

with $\mathcal{E} = \theta_2 \sin\theta_2 - \theta_1 \sin\theta_1 \neq 0$, and $\theta_1 = k_1 h$ and $\theta_2 = k_2 h$ where k_1 and k_2 are the fitted angular frequencies.

The method is undefined when $\theta_1 = \theta_2$, which implies $k_1 = k_2$, or when θ_1 and θ_2 are multiples of π. As $k_1 \to 0$ and $k_2 \to 0$, we obtain the polynomial collocation method given by (2.16) with $c_1 = 0$ and $c_2 = 1$. As $k_1 \to k_2$, then we obtain method I in the previous section for the collocation points $c_1 = 0$ and $c_2 = 1$.

There is a Maple program in Appendix B.3 to find the two-frequency method for s collocation points.

6.2.1 Order Conditions

Example : $c_1 = 0$ **and** $c_2 = 1$

Using the exact values for the solution and its derivative at x_n, the linear difference operators are defined by

$$\mathcal{L}_1[y] = y(x_n + h) - \mathcal{A}_1 y(x_n) - \mathcal{A}_2 h y'(x_n) - \mathcal{A}_3 h^2 y''(x_n) - \mathcal{A}_4 h^2 f(x_n + h, Y)$$

and

$$\mathcal{L}_2[y] = y'(x_n + h) - \frac{\mathcal{B}_1}{h} y(x_n) - \mathcal{B}_2 y'(x_n) - \mathcal{B}_3 h y''(x_n) - \mathcal{B}_4 h f(x_n + h, Y)$$

where

$$Y = \mathcal{A}_1 y(x_n) + \mathcal{A}_2 h y'(x_n) + \mathcal{A}_3 h^2 y''(x_n) + \mathcal{A}_4 h^2 f(x_n + h, Y).$$

The series expansions in powers of the steplength h of the coefficients in method (6.6) are

$$\mathcal{A}_1 = 1 + \frac{k_1^2 k_2^2}{24} h^4 + \ldots, \qquad \mathcal{A}_2 = 1 + \frac{7 k_1^2 k_2^2}{360} h^4 + \ldots$$

$$\mathcal{A}_3 = \frac{1}{3} + \frac{1}{45}(k_1^2 + k_2^2) h^2 + \frac{1}{7560}(16 k_1^4 + 65 k_1^2 k_2^2 + 16 k_2^4) h^4 + \ldots$$

$$\mathcal{A}_4 = \frac{1}{6} + \frac{7}{360}(k_1^2 + k_2^2) h^2 + \frac{1}{15120}(31 k_1^4 + 80 k_1^2 k_2^2 + 31 k_2^4) h^4 + \ldots$$

$$\mathcal{B}_1 = \frac{k_1^2 k_2^2}{12} h^4 + \ldots, \qquad \mathcal{B}_2 = 1 + \frac{k_1^2 k_2^2}{24} h^4 + \ldots$$

$$\mathcal{B}_3 = \frac{1}{2} + \frac{1}{24}(k_1^2 + k_2^2) h^2 + \frac{1}{720}(3 k_1^4 + 13 k_1^2 k_2^2 + 3 k_2^4) h^4 + \ldots$$

$$\mathcal{B}_4 = \frac{1}{2} + \frac{1}{24}(k_1^2 + k_2^2) h^2 + \frac{1}{720}(3 k_1^4 + 8 k_1^2 k_2^2 + 3 k_2^4) h^4 + \ldots$$

Substituting the coefficients into the difference operators and expanding about $h = 0$, we obtain

$$\mathcal{L}_1[y] = -\frac{h^4}{24}\left\{ f_{xx} + f f_y + 2 f_{xy} y' + f_{yy} [y']^2 + (k_1^2 + k_2^2) f + k_1^2 k_2^2 y \right\} + O(h^5)$$

and

$$\mathcal{L}_2[y] = -\frac{h^3}{12}\left\{f_{xx} + ff_y + 2f_{xy}y' + f_{yy}[y']^2 + (k_1^2 + k_2^2)f + k_1^2k_2^2y\right\} + O(h^3)$$

where $y = y(x_n)$, $f = f(x_n, y(x_n))$, etc.

Therefore, as $\mathcal{L}_1[y] = O(h^4)$ and $\mathcal{L}_2[y] = O(h^3)$, then the two-frequency mixed collocation method (6.6) with collocation points $c_1 = 0$ and $c_2 = 1$ is of order 2.

6.2.2 Stability

The stability analysis of exponentially-fitted methods with more than one frequency is complicated. One approach is to relate the frequencies in a simple way. For example, for two frequencies k_1 and k_2, one could set $k_2 = mk_1$ and apply the stability theory of chapter 3. First, we derive the characteristic equation for the two-frequency method with $c_1 = 0$ and $c_2 = 1$.

Following the work of section 6.1.2 the characteristic equation for the two-frequency method (6.6) is

$$\xi^2 - 2R_{11}(\nu^2; \theta_1, \theta_2)\xi + P(\nu^2; \theta_1, \theta_2) = 0$$

where

$$R_{11}(\nu^2; \theta_1, \theta_2) = \frac{\mathcal{A}_1 + \mathcal{B}_2 - \nu^2(\mathcal{A}_3 + \mathcal{A}_2\mathcal{B}_4 - \mathcal{A}_4\mathcal{B}_2)}{2[1 + \nu^2\mathcal{A}_4]}$$

and

$$P(\nu^2; \theta_1, \theta_2) = \frac{\mathcal{A}_1\mathcal{B}_2 - \mathcal{A}_2\mathcal{B}_1 + \nu^2(\mathcal{A}_2\mathcal{B}_3 - \mathcal{A}_3\mathcal{B}_2)}{1 + \nu^2\mathcal{A}_4}.$$

Substituting the coefficients $\mathcal{A}_i$ and $\mathcal{B}_i$ (6.6) and simplifying, the stability function $R_{11}(\nu^2; \theta_1, \theta_2)$ is given by

$$\frac{\theta_1\theta_2[\theta_2\cos\theta_1\sin\theta_2 - \theta_1\sin\theta_1\cos\theta_2] + \nu^2[\theta_2\cos\theta_2\sin\theta_1 - \theta_1\cos\theta_1\sin\theta_2]}{\theta_1\theta_2[\theta_2\sin\theta_2 - \theta_1\sin\theta_1] + \nu^2[\theta_2\sin\theta_1 - \theta_1\sin\theta_2]}$$

and

$$P(\nu^2; \theta_1, \theta_2) = 1.$$

Thus, the criteria for the method to have an interval of periodicity are satisfied. The method is stable if $|R_{11}(\nu^2; \theta_1, \theta_2)| \leq 1$ and for the numerical examples in chapter 7, this is easily checked by substituting in the particular values of θ_1, θ_2 and ν. As mentioned earlier, we can set one frequency as a multiple of the other, i.e. let

$\theta_2 = m\theta_1$ and with $\theta_1 = \theta$ the stability function becomes

$$R_{11}(\nu^2;\theta) = \frac{(m-1)\sin(\theta(m+1))[\nu^2 + m\theta^2] - (m+1)\sin(\theta(m-1))[\nu^2 - m\theta^2]}{2m\theta^2[m\sin(m\theta) - \sin\theta] + 2\nu^2[m\sin\theta - \sin(m\theta)]}.$$

Example : $m = 2$

The stability function is given by

$$R_{11}(\nu^2;\theta) = \frac{\sin(3\theta)[\nu^2 + 2\theta^2] - 3\sin\theta[\nu^2 - 2\theta^2]}{4\theta^2[2\sin(2\theta) - \sin\theta] + 2\nu^2[2\sin\theta - \sin(2\theta)]}$$

$$= \frac{\theta^2[1 + 2\cos^2\theta] + \nu^2[\cos^2\theta - 1]}{\theta^2[4\cos\theta - 1] + \nu^2[1 - \cos\theta]}.$$

This may be rewritten as

$$R_{11}(\nu^2;\theta) = \frac{\alpha_0 + \alpha_1\nu^2}{1 + \beta_1\nu^2}$$

where

$$\alpha_0 = \frac{2\cos^2\theta + 1}{4\cos\theta - 1}, \quad \alpha_1 = \frac{\cos^2\theta - 1}{\theta^2[4\cos\theta - 1]}, \quad \beta_1 = \frac{1 - \cos\theta}{\theta^2[4\cos\theta - 1]}.$$

The coefficients α_0, α_1 and β_1 are undefined when $\cos\theta = 1/4$ or $\theta = 0$.

Following Definition 3.4, the stability boundaries are the curves

$$\nu_+(\theta) = \left\{2\theta^2\left(\frac{2 + \cos\theta}{1 - \cos\theta}\right)\right\}^{1/2} \quad \text{and} \quad \nu_-(\theta) = \left\{2\theta^2\left(\frac{1 - \cos\theta}{2 + \cos\theta}\right)\right\}^{1/2}$$

and the lines corresponding to any values of θ for which

$$\alpha_0 - 1 = \frac{2(\cos\theta - 1)^2}{4\cos\theta - 1} = 0, \quad \alpha_1 - \beta_1 = \frac{2\cos\theta(\cos\theta + 2)}{4\cos\theta - 1} = 0$$

and

$$\alpha_0 + 1 = \frac{2\cos\theta(\cos\theta + 2)}{4\cos\theta - 1} = 0, \quad \alpha_1 + \beta_1 = \frac{\cos\theta(\cos\theta - 1)}{4\cos\theta - 1}.$$

We have

$$\begin{aligned} \alpha_0 - 1 = 0 &\quad \text{when} \quad \theta = 2n\pi \\ \alpha_1 - \beta_1 = \alpha_1 + 1 = 0 &\quad \text{when} \quad \theta = (2n+1)\tfrac{\pi}{2} \\ \alpha_1 + \beta_1 = 0 &\quad \text{when} \quad \theta = (2n+1)\tfrac{\pi}{2} \text{ and } \theta = 2n\pi \end{aligned}$$

where n is a non-negative integer. Also method (6.6) is undefined when $\cos\theta = 1/4$.

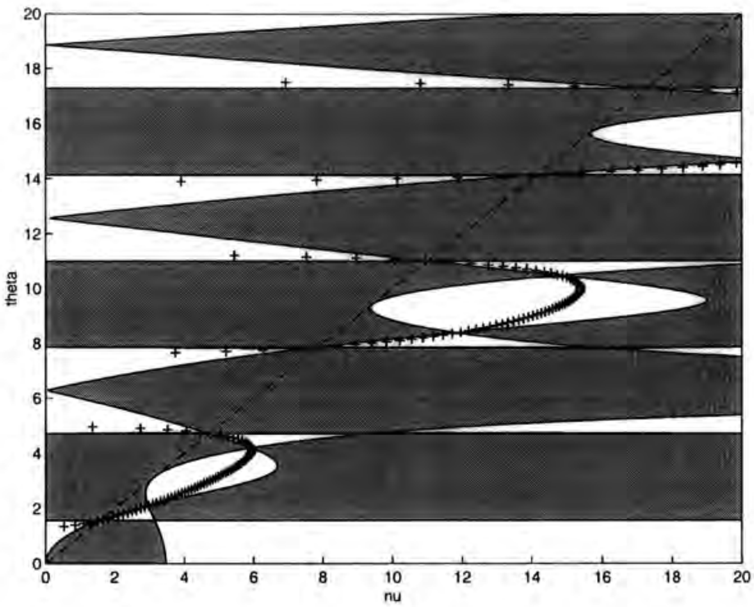

Figure 6.10: $\nu - \theta$ plot for extended mixed collocation method II : $c_1 = 0$ and $c_2 = 1$

When $\theta = \nu$ the stability function is

$$R_{11}(\nu^2;\nu) = \frac{\nu^2[1+2\cos^2\nu] + \nu^2[\cos^2\nu - 1]}{\nu^2[4\cos\nu - 1] + \nu^2[1-\cos\nu]} = \cos\nu.$$

Also for $\theta = 2n\pi$,

$$R_{11}(\nu^2;2n\pi) = \frac{4n^2\pi^2(3) + \nu^2(0)}{4n^2\pi^2(3) + \nu^2(0)} = 1.$$

The stability regions are shown in figure 6.10. When $\theta = 2n\pi$, the modulus of the stability function is 1 but the lines do not affect the stability regions. For $r < 1$, there is an interval of periodicity $(0, h_0)$ where h_0 decreases from $\sqrt{12}/w$ to $\pi/2w$ as r increases from 0 to 1, for fixed w. For $r > 1$, the primary interval of periodicity decreases from $\pi/2k$ to 0 as r increases.

A number of apparent inconsistencies occur in figure 6.10. When the stability curves $\nu_+(\theta)$ and $\nu_-(\theta)$ are substituted into the stability function, we obtain

$$R_{11}(\nu_+^2;\theta) = 1 \text{ and } R_{11}(\nu_-^2;\theta) = -1$$

so wherever the curves cross, $R_{11}(\nu^2;\theta)$ is of different values. Also, on the lines $\theta = (2n+1)\pi/2$, where n is a non-negative integer, $R_{11}(\nu^2;\theta) = -1$ but as $R_{11}(\nu_+^2;\theta) = 1$, then this must be checked also.

As in earlier work, we find where the stability function is undefined. Thus, the denominator of the stability function set to zero gives

$$\theta^2[4\cos\theta - 1] + \nu^2[1 - \cos\theta] = 0$$

$$\Rightarrow \quad \bar{\nu} = \left\{\frac{\theta^2[1 - 4\cos\theta]}{1 - \cos\theta}\right\}^{1/2}$$

and the curves $\bar{\nu}(\theta)$ are plotted '+' in figure 6.10. The curves pass through all the places where the inconsistencies occur.

6.3 Steplength dependent collocation points

The motivation behind steplength dependent collocation nodes is to see whether we can improve the order or the stability of the mixed collocation methods of chapter 4.

6.3.1 Order conditions for one collocation point

First, let

$$c = c^{(0)} + c^{(1)}h + c^{(2)}h^2 + c^{(3)}h^3 + \dots$$

where $c^{(i)}$ for $i = 0, 1, 2, \dots$ are constants.

Then, from section 4.2.1, after some simplification, the linear difference operators become

$$L_1[y] = \frac{h^3}{6}(1 - 3c^{(0)})\left\{y^{(3)}(x_n) + k^2y'(x_n)\right\} +$$

$$\frac{h^4}{24}\left\{[1 - 6(c^{(0)})^2][y^{(4)}(x_n) + k^2y''(x_n)] - 12c^{(1)}[y^{(3)}(x_n) + k^2y'(x_n)]\right\} + O(h^5)$$

and

$$L_2[y] = \frac{h^2}{2}(1 - 2c^{(0)})\left\{y^{(3)}(x_n) + k^2y'(x_n)\right\} +$$

$$\frac{h^3}{6}\left\{[1 - 3(c^{(0)})^2][y^{(4)}(x_n) + k^2y''(x_n)] - 6c^{(1)}[y^{(3)}(x_n) + k^2y'(x_n)]\right\} + O(h^4).$$

Thus

$$
\begin{aligned}
\text{if } c^{(0)} \neq \frac{1}{2}, \quad L_1[y] &= O(h^3) \text{ or higher}, \\
L_2[y] &= O(h^2) \quad \Rightarrow \textbf{Order 1}. \\
\text{If } c^{(0)} = \frac{1}{2}, \quad L_1[y] &= O(h^3), \\
L_2[y] &= O(h^3) \quad \Rightarrow \textbf{Order 2}.
\end{aligned}
$$

Thus, the highest attainable order is 2 when $c^{(0)} = \frac{1}{2}$, and so it is not possible to improve the order for the one-point mixed collocation method with the nodes dependent on the steplength.

6.3.2 Stability for one collocation point

The characteristic equation for the one-point mixed collocation method is given by (5.6). For the method to have an interval of periodicity we require $P(\nu^2;\theta) = 1$ from which $\nu = \theta$ or $\cos(\theta c) - \cos\theta(1-c) = 0$. From section 5.1.1 the latter equation is satisfied when $c = 1/2$ and so it is easily verified that when $c = c^{(0)} + c^{(1)}h + c^{(2)}h^2 + c^{(3)}h^3 + \ldots$, then $P(\nu^2;\theta) = 1$ if

$$c^{(0)} = \frac{1}{2} \quad \text{and} \quad c^{(n)} = 0 \quad \text{where} \quad n = 1, 2, \ldots$$

Once again, no improvement has been made for the one-point mixed collocation method and so we shall turn our attention to the two-point method.

6.3.3 Order conditions for two or more collocation points

First of all, let

$$c_i = c_i^{(0)} + c_i^{(1)}h + c_i^{(2)}h^2 + c_i^{(3)}h^3 + \ldots, \quad \text{for } i = 1, \ldots, s. \tag{6.7}$$

As with the one-point mixed collocation method, the order conditions may be found by substituting the above expansion for the collocation nodes into the linear difference operators (c.f. section 3.4.2) and then collect in terms of h.

The Order Conditions for the Mixed Collocation methods for $s \geq 2$

(With steplength dependent coefficients and collocation nodes)

For **order 1**,

$$1.)\ \sum_{i=1}^{s} d_i^{(0)} = 1.$$

For **order 2**,

$$2.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^{(0)} = \frac{1}{2},\quad 3.)\ \sum_{i=1}^{s} b_i^{(0)} = \frac{1}{2}.$$

For **order 3**,

$$4.)\ \sum_{i=1}^{s} d_i^{(0)} (c_i^{(0)})^2 = \frac{1}{3},\quad 5.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^{(1)} = 0,\quad 6.)\ \sum_{i=1}^{s} d_i^{(2)} = 0;$$

$$7.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} = \frac{1}{6},\quad 8.)\ \sum_{i=1}^{s} b_i^{(0)} c_i^{(0)} = \frac{1}{6}.$$

For **order 4**,

$$9.)\ \sum_{i=1}^{s} d_i^{(0)} (c_i^{(0)})^3 = \frac{1}{4},\quad 10.)\ \sum_{i=1}^{s} \left\{ d_i^{(0)} c_i^{(2)} + d_i^{(2)} c_i^{(0)} \right\} = 0,$$

$$11.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j^{(0)} = \frac{1}{24},\quad 12.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} c_i^{(0)} a_{ij}^{(0)} = \frac{1}{8},$$

$$13.)\ \sum_{i=1}^{s} d_i^{(0)} c_i^{(0)} c_i^{(1)} = 0,\quad 14.)\ \sum_{i=1}^{s} b_i^{(0)} (c_i^{(0)})^2 = \frac{1}{12},$$

$$15.)\ \sum_{i=1}^{s} b_i^{(0)} c_i^{(1)} = 0,\quad 16.)\ \sum_{i=1}^{s} b_i^{(2)} = 0,\quad 17.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} = \frac{1}{24}.$$

For **order 5**,

$$18.)\ \sum_{i=1}^{s} d_i^{(0)} (c_i^{(0)})^4 = \frac{1}{5},\quad 19.)\ \sum_{i=1}^{s} \left\{ d_i^{(2)} (c_i^{(0)})^2 + d_i^{(0)} (c_i^{(1)})^2 + 2 d_i^{(0)} c_i^{(2)} c_i^{(0)} \right\} = 0,$$

$$20.)\ \sum_{i=1}^{s} d_i^{(4)} = 0, \quad 21.)\ \sum_{i=1}^{s} d_i^{(0)}(c_i^{(0)})^2 c_i^{(1)} = 0, \quad 22.)\ \sum_{i=1}^{s} \left\{ d_i^{(0)} c_i^{(3)} + d_i^{(2)} c_i^{(1)} \right\} = 0,$$

$$23.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} \left\{ d_i^{(2)} a_{ij}^{(0)} + d_i^{(0)} a_{ij}^{(2)} \right\} = 0, \quad 24.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} (c_j^{(0)})^2 = \frac{1}{60},$$

$$25.)\ \sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} d_i^{(0)} a_{ij}^{(0)} a_{jk}^{(0)} = \frac{1}{120}, \quad 26.)\ \sum_{i=1}^{s} d_i^{(0)} \left(\sum_{j=1}^{s} a_{ij}^{(0)} \right)^2 = \frac{1}{20},$$

$$27.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_i^{(0)} c_j^{(0)} = \frac{1}{30}, \quad 28.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} (c_i^{(0)})^2 = \frac{1}{10},$$

$$29.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} a_{ij}^{(0)} c_j^{(1)} = 0, \quad 30.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} d_i^{(0)} c_i^{(1)} a_{ij}^{(0)} = 0,$$

$$31.)\ \sum_{i=1}^{s} b_i^{(0)} (c_i^{(0)})^3 = \frac{1}{20}, \quad 32.)\ \sum_{i=1}^{s} \left\{ b_i^{(0)} c_i^{(2)} + b_i^{(2)} c_i^{(0)} \right\} = 0, \quad 33.)\ \sum_{i=1}^{s} b_i^{(0)} c_i^{(0)} c_i^{(1)} = 0,$$

$$34.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(0)} c_j^{(0)} = \frac{1}{120}, \quad 35.)\ \sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} c_i^{(0)} a_{ij}^{(0)} = \frac{1}{40}.$$

Example: $s = 2$
When the collocation nodes are given by

$$c_1 = c_1^{(0)} + c_1^{(1)}h + c_1^{(2)}h^2 + c_1^{(3)}h^3 + \dots$$

$$c_2 = c_2^{(0)} + c_2^{(1)}h + c_2^{(2)}h^2 + c_2^{(3)}h^3 + \dots$$

then the method has default order 2.

For order 3, we require

$$c_1^{(0)} = \frac{1}{3}\left\{\frac{3c_2^{(0)} - 2}{2c_2^{(0)} - 1}\right\} \text{ and } c_1^{(1)} = -\frac{1}{3}\left\{\frac{c_2^{(1)}}{4(c_2^{(0)})^2 - 4c_2^{(0)} + 1}\right\}$$

with $c_2^{(0)} \neq 1/2$, and the maximum order of 4 is obtained when, in addition to the above, we have

$$c_2^{(0)} = \frac{3+\sqrt{3}}{6} \text{ and } c_2^{(1)} = 0,$$

that is

$$c_1 = \frac{3-\sqrt{3}}{6} + c_1^{(2)}h^2 + c_1^{(3)}h^3 + \dots \text{ and } c_2 = \frac{3+\sqrt{3}}{6} + c_2^{(2)}h^2 + c_2^{(3)}h^3 + \dots$$

Once again, we cannot improve on the order conditions for two collocation points.

For an s-stage mixed collocation method

It we set to zero any coefficients of c_i which have a superscript greater than 0, then the above conditions reduce to those for the mixed collocation methods of section 4.2.2 where the collocation nodes do not depend on the steplength h. As these original conditions still have to be satisfied plus the extra ones obtained in this section, it is not possible to improve on the algebraic order for an s-stage mixed collocation method by making c_i depend on the steplength.

6.3.4 Stability for two collocation points

When the expressions for the expansions of the collocation nodes are substituted into $P(\nu^2; \theta)$, equation (5.10), for the two-point mixed collocation method, and we perform a series expansion about $h = 0$, then the requirements for $P(\nu^2; \theta) = 1$ are

$$c_1^{(0)} + c_2^{(0)} = 1 \text{ and } c_1^{(i)} = -c_2^{(i)} \text{ for } i = 1, 2, \ldots$$

Thus, the nodes $c_1 = \mathcal{A}_0 + \mathcal{A}_1\theta + \mathcal{A}_2\theta^2 + \ldots$ and $c_2 = 1 - c_1$ satisfy the requirements for the two-point mixed collocation method to have an interval of periodicity where the $\mathcal{A}_i$ are constants.

The two-point mixed collocation method with $c_1 = a\theta^2$ and $c_2 = 1 - c_1$ is undefined when $\sin\theta(c_2 - c_1) = 0 \Rightarrow \theta(1 - 2a\theta^2) = n\pi$ where n is a non-negative integer. Our aim is to find values of a for which the method is always defined.

Let $f(\theta) = \theta - 2a\theta^3 - n\pi$. Then as $f(-\infty) = \infty$, $f(\infty) = -\infty$ and $f(0) = -n\pi$, there is at least one negative real root. The function has a maximum when $\theta = 1/\sqrt{6a}$ and a minimum when $\theta = -1/\sqrt{6a}$. As $\theta = kh$ is real and positive, then the mixed collocation method will always be defined if the roots of $f(\theta)$ are real and negative or they are complex for a particular value of a. So, for the other two roots of $f(\theta)$ to be complex, we require the value $f(\theta)$ at the maximum point to be less than zero, i.e. $f(1/\sqrt{6a}) < 0$

$$\Rightarrow a > \frac{2}{27n^2\pi^2}.$$

With the choice $a = 7.6 \times 10^{-3}$, the stability regions are given in figure 6.11. As a is increased, the stability regions become more complicated as can be seen in figures 6.12 and 6.13 for $a = 2 \times 10^{-2}$ and $a = 4 \times 10^{-2}$ respectively.

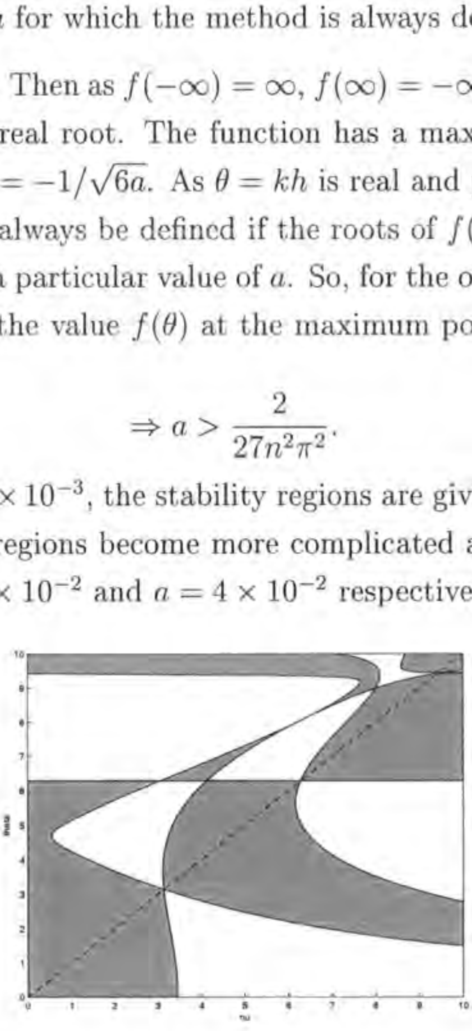

Figure 6.11: Stability regions for $c_1 = a\theta^2$ and $c_2 = 1 - c_1$ with $a = 7.6 \times 10^{-3}$

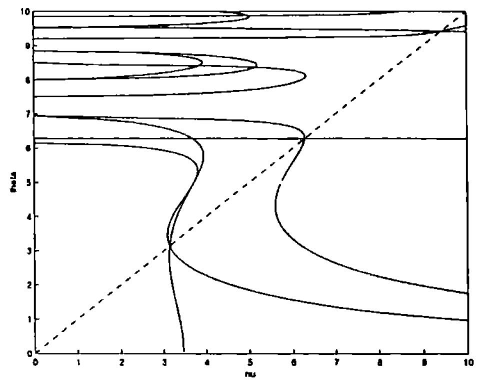

Figure 6.12: Stability curves for $a = 2 \times 10^{-2}$

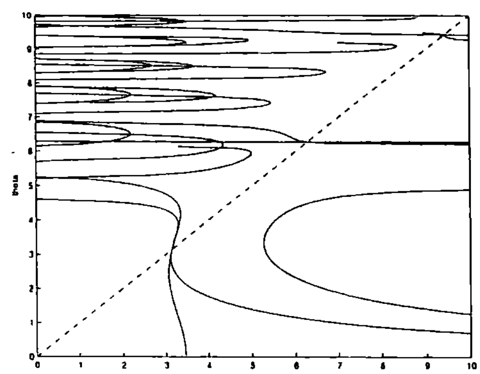

Figure 6.13: Stability curves for $a = 4 \times 10^{-2}$

Chapter 7

Numerical Results

In this chapter, numerical results are given for the mixed collocation methods. All the results in this chapter were generated using Matlab Version 4.2b.

The Mixed Collocation Methods

Method	Stage number	Collocation points ($c_i, i = 1..s$)	Algebraic order
Ia	1	0	1
Ib	1	1/2	2
Ic	1	1	1
IIa	2	0, 1	2
IIb	2	$(3-\sqrt{3})/6$, $(3+\sqrt{3})/6$	4
$IIIa$	3	0, 1/2, 1	4
$IIIb$	3	$(5-\sqrt{15})/10$, 1/2, $(5+\sqrt{15})/10$	6
IVa^*	2	0, 1	2
IVb^*	2	$(3-\sqrt{3})/6$, $(3+\sqrt{3})/6$	4
V^*	2	0, 1	2

Methods I refers to methods Ia, Ib and Ic; methods II are methods IIa and IIb, methods III are methods $IIIa$ and $IIIb$, and similarly, methods IV^* refers to methods IVa^* and IVb^*.

In methods I, II and III, we approximate the solution $y(x)$ of problem (1.1) on the interval $[x_n, x_{n+1}]$ by a function $u(x)$ of the form

$$u(x) = a\cos[k(x-x_n)] + b\sin[k(x-x_n)] + \sum_{i=1}^{s-1} r_i(x-x_n)^i.$$

In methods IV^* we approximate $y(x)$ by

$$u(x) = [a_0 + a_1 t]\cos(kt) + [b_0 + b_1 t]\sin(kt) + \sum_{i=1}^{s-3} r_i t^i$$

and in method V^*, $y(x)$ is approximated by

$$u(x) = a_0 \cos(k_1 t) + a_1 \cos(k_2 t) + b_0 \sin(k_1 t) + b_1 \sin(k_2 t) + \sum_{i=1}^{s-3} r_i t^i$$

where $t = x - x_n$.

In some of the following numerical examples, we also include results from Numerov's 4th order method and three 4th order exponentially-fitted multistep methods used by Coleman and Ixaru [18].

The multistep methods are of the form

$$y_{n+1} - 2\,\alpha_0\, y_n + y_{n-1} = h^2[\beta_1(f_{n+1} + f_{n-1}) - 2\,\alpha_1\, f_n].$$

Method S_0 is Numerov's method with coefficients given by

$$\alpha_0 = 1,\quad \alpha_1 = -\frac{5}{12} \text{ and } \beta_1 = \frac{1}{12}.$$

Method S_1 is the Stiefel-Bettis method which is exact for $[1, x, x^2, x^3, \exp(\pm ikx)]$ with steplength dependent coefficients given by

$$\alpha_0 = 1,\quad \alpha_1 = \beta_1 - \frac{1}{2} \text{ and } \beta_1 = \frac{\theta^2 - 2(1-\cos\theta)}{2\theta^2(1-\cos\theta)}.$$

As $k \to 0$, we obtain Numerov's method S_0.

Method S_2 is exact for $[1, x, \exp(\pm ikx), x\exp(\pm ikx)]$ with coefficients

$$\alpha_0 = 1,\quad \alpha_1 = \frac{2\tan(\theta/2)\cos\theta - \theta}{\theta^3} \text{ and } \beta_1 = \frac{2\tan(\theta/2) - \theta}{\theta^3}$$

and finally method S_3 is exact for $[\exp(\pm ikx), x\exp(\pm ikx), x^2\exp(\pm ikx)]$ with

$$\alpha_0 = \frac{2\theta + \cos\theta\,(3\sin\theta - \theta\cos\theta)}{3\sin\theta + \theta\cos\theta},\quad \alpha_1 = \frac{\cos\theta\,(\sin\theta + \theta\cos\theta) - 2\theta}{(3\sin\theta + \theta\cos\theta)\theta^2}$$

$$\text{and} \quad \beta_1 = \frac{\sin\theta - \theta\cos\theta}{(3\sin\theta + \theta\cos\theta)\theta^2}.$$

Again, as $k \to 0$, both methods S_2 and S_3 reduce to Numerov's method S_0.

For each example unless otherwise stated, a tolerance of 10^{-14} is set and for each step, we require this to be satisfied within a maximum of 10 iterations. Many authors tend to look only at the absolute errors at the end point of the interval $[a, b]$. For some problems though, the maximum absolute error over the interval is much larger than the absolute error at the end-point of the interval. In the following results, the absolute errors at certain step points are presented but the main result that we are interested in is the maximum absolute error over the interval $[a, b]$.

7.1 One-dimensional problems

Example 1.1

For our first linear test problem, consider the scalar equation

$$y'' = -y, \;\; y(0) = 1, \;\; y'(0) = 0$$

where the exact solution is $y(x) = \cos x$. The methods which are exact for this problem are the mixed collocation methods $I - IV$, and the exponentially-fitted multistep methods $S_1 - S_3$, all with fitted frequency $k = 1$.

In table 7.1, the maximum absolute errors are given over the interval $[0, 40\pi]$ for four different values of the steplength h. The top values are found using the mixed collocation methods with fitted angular frequency $k = 1$, and for comparison, the bottom values are found using the classical polynomial collocation method, that is $k = 0$. In table 7.2, results are given for the extended method IV^* with $k = 1$ and the two frequency method V^* with various values of the frequencies k_1 and k_2. For method V_1^*, we let $k_1 = 1$ and $k_2 = 0.1$, for method V_2^*, $k_1 = 1$ and $k_2 = 0.01$, and for method V_3^*, $k_1 = 1$ and $k_2 = 0.001$. Finally, in table 7.3, the maximum absolute errors are given for S_0 (Numerov's method) and the exponentially-fitted 4th order multistep methods S_1, S_2 and S_3 of Coleman and Ixaru [23] with angular frequency $k = 1$.

h		Ia	Ib	Ic	IIa
$\pi/4$	$k=1$	1.24×10^{-14}	9.76×10^{-15}	9.25×10^{-15}	1.75×10^{-14}
	$k=0$	$1.49\times10^{+9}$	1.3465	1.0025	1.9926
$\pi/8$	$k=1$	1.08×10^{-14}	1.04×10^{-14}	9.88×10^{-15}	2.11×10^{-14}
	$k=0$	$1.30\times10^{+5}$	3.82×10^{-1}	1.0000	7.66×10^{-1}
$\pi/16$	$k=1$	9.55×10^{-15}	1.24×10^{-14}	1.06×10^{-14}	7.02×10^{-14}
	$k=0$	$3.95\times10^{+2}$	9.90×10^{-2}	9.98×10^{-1}	1.98×10^{-1}
$\pi/32$	$k=1$	5.10×10^{-14}	2.70×10^{-14}	1.02×10^{-14}	5.54×10^{-13}
	$k=0$	$2.06\times10^{+1}$	2.49×10^{-2}	9.54×10^{-1}	4.98×10^{-2}

h		IIb	$IIIa$	$IIIb$
$\pi/4$	$k=1$	2.45×10^{-14}	4.37×10^{-14}	1.74×10^{-14}
	$k=0$	1.04×10^{-2}	2.38×10^{-2}	3.50×10^{-5}
$\pi/8$	$k=1$	1.28×10^{-13}	3.97×10^{-13}	5.42×10^{-13}
	$k=0$	6.75×10^{-4}	1.52×10^{-3}	5.60×10^{-7}
$\pi/16$	$k=1$	5.77×10^{-13}	1.59×10^{-12}	4.15×10^{-12}
	$k=0$	4.26×10^{-5}	9.59×10^{-5}	8.80×10^{-9}
$\pi/32$	$k=1$	6.89×10^{-13}	7.62×10^{-12}	1.92×10^{-12}
	$k=0$	2.67×10^{-6}	6.00×10^{-6}	1.38×10^{-10}

Table 7.1: Ex 1.1 - Mixed Collocation and Polynomial Collocation Methods $I - III$

h	IVa^*	IVb^*	V_1^*	V_2^*	V_3^*
$\pi/4$	2.54×10^{-14}	9.51×10^{-13}	2.79×10^{-14}	3.39×10^{-14}	4.13×10^{-14}
$\pi/8$	1.17×10^{-14}	2.29×10^{-13}	6.39×10^{-14}	1.92×10^{-14}	2.98×10^{-14}
$\pi/16$	4.10×10^{-14}	1.12×10^{-12}	9.10×10^{-15}	4.70×10^{-14}	1.24×10^{-13}
$\pi/32$	2.66×10^{-13}	1.10×10^{-11}	2.50×10^{-13}	2.11×10^{-13}	7.27×10^{-13}

Table 7.2: Ex 1.1 - Mixed Collocation Methods IV^* and V^*

h	S_0	S_1	S_2	S_3
$\pi/4$	1.00×10^{-1}	9.79×10^{-15}	9.79×10^{-15}	2.17×10^{-14}
$\pi/8$	6.17×10^{-3}	1.24×10^{-14}	6.79×10^{-14}	9.77×10^{-15}
$\pi/16$	3.84×10^{-4}	4.01×10^{-14}	1.43×10^{-13}	1.46×10^{-13}
$\pi/32$	2.40×10^{-5}	5.43×10^{-13}	4.79×10^{-13}	2.28×10^{-12}

Table 7.3: Ex 1.1 - Multistep methods S_0, S_1, S_2 and S_3

Conclusions

From the stability theory for the mixed collocation methods $I - V^*$ in chapter 5 and sections 6.1.2 and 6.2.2, all the results in tables 7.1 and 7.2 are stable for the frequency $k = 1$ and for the particular values of ν and θ. As the mixed collocation methods $I - III$, IV^* and the multistep methods $S_1 - S_3$ are exact when solving the test problem with $k = 1$, then if the calculations are performed exactly, we would expect the numerical results to be zero. Because of the errors in evaluating the coefficients of the methods using double precision, then we must take into account the accumulation of rounding error over the interval and so the results are very close to zero.

The polynomial collocation methods struggle for low order methods but start to show signs of improvement when the 4th and 6th order methods IIb, $IIIa$ and $IIIb$ are used with small steplengths. The 4th order methods IIb and $IIIa$ are more accurate than the 4th order method S_0.

Example 1.2

Next, consider the harmonic oscillator as in Example 1.1 but with a higher frequency so the solution contains a more rapidly oscillating function. The differential equation is

$$y'' = -25y, \quad y(0) = 1, \quad y'(0) = 0$$

with the exact solution $y(x) = \cos(5x)$.

In tables 7.4 - 7.7, the maximum absolute error over the interval $[0, 40\pi]$ is given. In table 7.4 we have Numerov's method S_0, and for the multistep methods $S_1 - S_3$ in table 7.5, the angular frequency is $k = 5$ and $k = 4$. In table 7.6, $k = 5$ for methods IVa^* and IVb^*, for method V_1^* we take $k_1 = 5$ and $k_2 = 0.1$, for method V_2^*, $k_1 = 5$ and $k_2 = 0.01$, and for method V_3^*, $k_1 = 5$ and $k_2 = 0.001$. Three different values for k are considered in table 7.7, $k = 5$ and $k = 4$ for the mixed collocation methods, and $k = 0$ which is the polynomial collocation method. Also included in tables 7.5 and 7.7 is whether the methods are stable (S) or unstable (U) and this was found from the work of Coleman and Ixaru [23] for methods $S_1 - S_3$ and the stability analysis of chapter 5 for the mixed collocation methods.

Where 'Undefined' occurs in table 7.7, this means that the steplength dependent coefficients of the mixed collocation method are undefined for those particular values of $\theta = kh$.

	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$	$h = \pi/32$
S_0	$4.09 \times 10^{+5}$ U	1.9995 S	1.1627 S	7.58×10^{-2} S

Table 7.4: Ex 1.2 - Multistep Method S_0

h	k	S_1		S_2		S_3	
$\pi/4$	5	7.43×10^{-14}	S	8.63×10^{-14}	S	7.19×10^{-14}	S
	4	$*^1$	U	$*^2$	U	$*^3$	U
$\pi/8$	5	1.67×10^{-13}	S	9.47×10^{-14}	S	6.77×10^{-14}	S
	4	2.0004	S	1.9990	S	1.4153	S
$\pi/16$	5	9.86×10^{-14}	S	9.61×10^{-14}	S	1.66×10^{-13}	S
	4	4.60×10^{-1}	S	1.70×10^{-1}	S	6.29×10^{-2}	S
$\pi/32$	5	1.07×10^{-13}	S	1.30×10^{-13}	S	3.03×10^{-13}	S
	4	2.75×10^{-2}	S	9.99×10^{-3}	S	3.62×10^{-3}	S

Table 7.5: Ex 1.2 - Multistep Methods $S_1 - S_3$

h	IVa^*	IVb^*	V_1^*	V_2^*	V_3^*
$\pi/4$	6.44×10^{-14}	8.62×10^{-12}	1.79×10^{-13}	1.09×10^{-13}	8.27×10^{-14}
$\pi/8$	2.59×10^{-13}	8.11×10^{-13}	6.73×10^{-14}	9.92×10^{-14}	9.16×10^{-14}
$\pi/16$	1.33×10^{-13}	1.91×10^{-12}	1.52×10^{-13}	1.12×10^{-13}	1.27×10^{-13}
$\pi/32$	1.95×10^{-13}	1.78×10^{-12}	9.74×10^{-14}	1.17×10^{-13}	1.42×10^{-13}

Table 7.6: Ex 1.2 - Mixed Collocation Methods IV^* and V^*

For $*^1$, at the 9th step the tolerance was not satisfied within 10 iterations and the method was interrupted. The maximum absolute error at this point is $2.02 \times 10^{+2}$. At $*^2$, after 154 steps, the maximum absolute error is $4.45 \times 10^{+1}$ and at $*^3$, after 58 steps, the maximum absolute error is $1.64 \times 10^{+1}$. This agrees with the stability analysis and figures from the paper by Coleman and Ixaru [23] that their methods are unstable for the particular values of θ and ν.

h	k	Ia		Ib		Ic		IIa	
$\frac{\pi}{4}$	5	7.59×10^{-14}	S	1.43×10^{-13}	S	9.36×10^{-14}	S	6.79×10^{-14}	S
	4	$2.38 \times 10^{+52}$	U	Undefined	-	1.0490	S	Undefined	-
	0	$2.36 \times 10^{+75}$	U	$*^4$	U	1.0009	S	$*^5$	U
$\frac{\pi}{8}$	5	9.51×10^{-14}	S	1.33×10^{-13}	S	1.35×10^{-13}	S	7.12×10^{-14}	S
	4	$8.74 \times 10^{+30}$	U	1.9992	S	Undefined	-	1.9998	S
	0	$5.05 \times 10^{+74}$	U	1.9471	S	1.0488	S	2.0000	S
$\frac{\pi}{16}$	5	1.17×10^{-13}	S	8.30×10^{-14}	S	9.39×10^{-14}	S	1.24×10^{-13}	S
	4	$1.45 \times 10^{+21}$	U	1.9997	S	1.0025	S	1.9974	S
	0	$4.63 \times 10^{+54}$	U	2.0000	S	1.0019	S	1.9808	S
$\frac{\pi}{32}$	5	9.70×10^{-14}	S	1.12×10^{-13}	S	8.49×10^{-14}	S	1.43×10^{-13}	S
	4	$4.20 \times 10^{+11}$	U	1.0607	S	1.0000	S	1.7971	S
	0	$3.96 \times 10^{+31}$	U	1.9963	S	1.0001	S	1.9975	S

h	k	IIb		$IIIa$		$IIIb$	
$\frac{\pi}{4}$	5	1.08×10^{-13}	S	1.10×10^{-13}	S	9.92×10^{-14}	S
	4	1.9999	S	1.9974	S	9.92×10^{-1}	S
	0	1.9999	S	1.9986	S	1.2163	S
$\frac{\pi}{8}$	5	8.25×10^{-14}	S	1.33×10^{-13}	S	1.26×10^{-13}	S
	4	8.14×10^{-1}	S	1.3606	S	2.32×10^{-2}	S
	0	1.3064	S	1.9996	S	3.58×10^{-2}	S
$\frac{\pi}{16}$	5	1.17×10^{-13}	S	2.37×10^{-13}	S	4.38×10^{-13}	S
	4	6.09×10^{-2}	S	1.04×10^{-1}	S	3.96×10^{-4}	S
	0	1.23×10^{-1}	S	2.82×10^{-1}	S	6.57×10^{-4}	S
$\frac{\pi}{32}$	5	3.83×10^{-13}	S	1.29×10^{-12}	S	6.88×10^{-13}	S
	4	3.95×10^{-3}	S	6.73×10^{-3}	S	6.35×10^{-6}	S
	0	8.23×10^{-3}	S	1.86×10^{-2}	S	1.07×10^{-5}	S

Table 7.7: Ex 1.2 - Mixed Collocation and Polynomial Collocation Methods $I - III$

At $*^4$, the method exceeded the maximum number of iterations but 6 steps were reached and the maximum absolute error at this point was $3.14 \times 10^{+2}$, therefore agreeing with the stability analysis that the method is unstable for these values of θ and ν.

At $*^5$, 38 steps were reached and the maximum absolute error at this point was $8.06 \times 10^{+8}$, again unstable.

Conclusions

For $k = 5$, the mixed collocation methods are exact, except for rounding error and this agrees with the stability theory and the fact that we have used the same frequency as the test equation $w = k = 5$. For $k = 4$, the results appear to be very similar to the classical polynomial collocation methods.

The multistep methods S_1, S_2 and S_3 give very similar results to the mixed collocation methods and all the methods show how varied the results can be when choosing different values for the fitted angular frequency. Comparing the 4th order methods IIb and $IIIa$ with the multistep methods $S_1 - S_3$ when $k = 4$, the mixed collocation methods are more accurate for large steplengths but we can see that the S_3 method shows signs of improvement when $h = \pi/32$. The 6th order mixed collocation method $IIIb$ is the most accurate for $k = 4$.

Again, the 4th order polynomial collocation methods IIb and $IIIa$ are superior to Numerov's method S_0, especially for small steplengths. The 6th order polynomial collocation $IIIb$ is the most accurate for $k = 0$.

Example 1.3

For the next example we solve the differential equation

$$y'' = -100y + 2, \;\; y(0) = 3, \;\; y'(0) = 0$$

where the exact solution is $y(x) = 2.98\cos 10x + 0.02$.

In tables 7.8 - 7.11, the absolute errors at $x = \pi, 7\pi/4, 2\pi$ and $11\pi/4$ are given, and in the final column, MAX, we give the maximum absolute error on the interval $[0, 11\pi/4]$. Two steplengths are taken for comparison, $h = \pi/24$ and $h = \pi/48$ and the fitted angular frequency is $k = 10$ for methods $I - IV^*$ and $S_1 - S_3$. For the two frequency mixed collocation method V_1^*, $k_1 = 10$ and $k_2 = 1$ and for method V_2^*, $k_1 = 10$ and $k_2 = 0.001$.

In table 7.12 the maximum absolute error on the interval $[0, 11\pi/4]$ is given for the polynomial collocation methods IIb, $IIIa$ and $IIIb$ and Numerov's method S_0.

In table 7.13, numerical results obtained from a 2-step 4th order P-stable hybrid method with phase-lag of order 6 by Chawla et al [15] are presented. The absolute errors only are given at $x = \pi, 7\pi/4, 2\pi$ and $11\pi/4$ for this method.

	$x = \pi$	$x = 7\pi/4$	$x = 2\pi$	$x = 11\pi/4$	MAX
Ia	9.33×10^{-15}	1.23×10^{-14}	1.51×10^{-14}	2.12×10^{-15}	3.60×10^{-14}
Ib	1.33×10^{-15}	1.69×10^{-14}	1.78×10^{-15}	9.67×10^{-15}	4.33×10^{-14}
Ic	5.33×10^{-15}	5.61×10^{-14}	3.55×10^{-15}	7.15×10^{-14}	9.88×10^{-14}
IIa	2.22×10^{-15}	1.27×10^{-14}	4.00×10^{-15}	1.89×10^{-15}	3.62×10^{-14}
IIb	1.15×10^{-14}	2.96×10^{-15}	2.13×10^{-14}	1.50×10^{-14}	3.60×10^{-14}
$IIIa$	4.00×10^{-15}	1.01×10^{-14}	8.88×10^{-15}	2.55×10^{-15}	3.53×10^{-14}
$IIIb$	3.06×10^{-14}	1.52×10^{-14}	5.82×10^{-14}	7.00×10^{-15}	8.84×10^{-14}
IVa^*	6.23×10^{-15}	3.55×10^{-3}	8.00×10^{-15}	3.55×10^{-3}	7.10×10^{-3}
IVb^*	1.91×10^{-12}	1.03×10^{-4}	3.83×10^{-12}	1.03×10^{-4}	2.06×10^{-4}
V_1^*	2.66×10^{-15}	2.95×10^{-5}	8.88×10^{-16}	2.95×10^{-5}	5.89×10^{-5}
V_2^*	4.44×10^{-15}	2.94×10^{-11}	7.99×10^{-15}	2.94×10^{-11}	5.88×10^{-11}

Table 7.8: Ex 1.3 - Mixed Collocation Methods $I - V^*$: $h = \pi/24$

	$x = \pi$	$x = 7\pi/4$	$x = 2\pi$	$x = 11\pi/4$	MAX
Ia	7.99×10^{-15}	1.41×10^{-14}	1.55×10^{-14}	4.06×10^{-15}	4.37×10^{-14}
Ib	5.77×10^{-15}	6.20×10^{-15}	9.77×10^{-15}	9.40×10^{-15}	2.95×10^{-14}
Ic	1.78×10^{-15}	1.65×10^{-14}	4.00×10^{-15}	6.11×10^{-15}	4.20×10^{-14}
IIa	4.00×10^{-15}	3.02×10^{-14}	9.33×10^{-15}	2.90×10^{-14}	6.35×10^{-14}
IIb	7.99×10^{-15}	2.19×10^{-14}	1.60×10^{-14}	1.68×10^{-14}	5.46×10^{-14}
$IIIa$	5.42×10^{-14}	7.48×10^{-14}	1.12×10^{-13}	1.04×10^{-13}	1.88×10^{-13}
$IIIb$	4.09×10^{-14}	3.20×10^{-13}	8.39×10^{-14}	4.85×10^{-13}	4.85×10^{-13}
IVa^*	1.02×10^{-14}	7.51×10^{-4}	2.00×10^{-14}	7.51×10^{-4}	1.50×10^{-3}
IVb^*	1.22×10^{-13}	6.06×10^{-6}	2.40×10^{-13}	6.06×10^{-6}	1.21×10^{-5}
V_1^*	8.88×10^{-16}	7.19×10^{-6}	1.78×10^{-15}	7.19×10^{-6}	1.44×10^{-5}
V_2^*	8.88×10^{-16}	7.17×10^{-12}	2.22×10^{-15}	7.17×10^{-12}	1.44×10^{-11}

Table 7.9: Ex 1.3 - Mixed Collocation Methods $I - V^*$: $h = \pi/48$

	$x = \pi$	$x = 7\pi/4$	$x = 2\pi$	$x = 11\pi/4$	MAX
S_1	4.44×10^{-16}	2.96×10^{-15}	1.78×10^{-15}	1.40×10^{-14}	2.70×10^{-14}
S_2	1.33×10^{-15}	6.38×10^{-15}	8.88×10^{-16}	9.43×10^{-15}	2.69×10^{-14}
S_3	1.33×10^{-15}	5.40×10^{-4}	1.33×10^{-15}	5.40×10^{-4}	6.87×10^{-4}

Table 7.10: Ex 1.3 - Multistep Methods $S_1 - S_3$: $h = \pi/24$

	$x = \pi$	$x = 7\pi/4$	$x = 2\pi$	$x = 11\pi/4$	MAX
S_1	1.78×10^{-15}	3.20×10^{-14}	8.88×10^{-16}	3.25×10^{-14}	6.31×10^{-14}
S_2	0	2.95×10^{-14}	8.88×10^{-16}	2.69×10^{-14}	5.87×10^{-14}
S_3	1.78×10^{-15}	2.16×10^{-5}	1.33×10^{-15}	2.16×10^{-5}	3.31×10^{-5}

Table 7.11: Ex 1.3 - Multistep Methods $S_1 - S_3$: $h = \pi/48$

	$h = \pi/24$	$h = \pi/48$
IIb	1.50×10^{-1}	1.06×10^{-2}
$IIIa$	3.56×10^{-1}	2.40×10^{-2}
$IIIb$	1.47×10^{-3}	2.46×10^{-5}
S_0	1.6128	9.95×10^{-2}

Table 7.12: Ex 1.3 - Methods IIb, $IIIa$, $IIIb$ and S_0 : $k = 0$

	$x = \pi$	$x = 7\pi/4$	$x = 2\pi$	$x = 11\pi/4$
$h = \pi/24$	5.68×10^{-5}	3.29×10^{-2}	2.38×10^{-4}	5.21×10^{-2}
$h = \pi/48$	1.71×10^{-8}	5.63×10^{-4}	6.98×10^{-8}	8.89×10^{-4}

Table 7.13: Ex 1.3 - Hybrid Method of Chawla, Rao and Neta

Conclusions

When $k = 10$, the mixed collocation methods $I - III$ are exact, except for the accumulation of rounding errors and are far superior to the numerical results by Chawla et al [15]. For methods IVa^* and IVb^*, the reason why the results are poor at $x = 7\pi/4$ and $11\pi/4$ is because the method is only exact for the trigonometric functions $[\sin kx, \cos kx, x \sin kx, x \cos kx]$. Method IVb^* is more accurate than the 4th order method S_3. Also for method V_2^*, when k_2 is closer to zero, the results improve compared to V_1^* because the basis of functions are $[\sin k_1x, \cos k_1x, \sin k_2x, \cos k_2x]$ and thus $\cos k_2x$ becomes a close approximation for the constant term in the theoretical solution. This is also the case for the multistep method S_3 which has only trigonometric functions, or products of trigonometric functions and powers in the basis, whilst methods S_1 and S_2 are exact for this problem and are comparable to the mixed collocation methods $I - III$.

Again, the 4th order polynomial collocation methods are superior to S_0 but the 6th order method $IIIb$ is more accurate than the 4th order hybrid methods of Chawla et al [15] as the maximum absolute errors over the interval $[0, 11\pi/4]$ for both steplengths are smaller than the last errors for the hybrid method.

Example 1.4

We now consider a highly oscillatory problem where the solution to the differential equation involves two frequencies. The differential equation is

$$y'' = -100y + 99\sin x, \quad y(0) = 1, \quad y'(0) = 11$$

with exact solution $y(x) = \cos(10x) + \sin(10x) + \sin x$.

The results for the mixed collocation methods in table 7.14 are given for $k = 10$, $k = 1$ and $k = 0$, the polynomial collocation methods. In table 7.15, the maximum absolute error over the interval $[0, 20\pi]$ is given for the two frequency method V^* with various values for the fitted angular frequencies k_1 and k_2. For comparison, results are presented for the exponentially-fitted multistep methods $S_1 - S_3$ in table 7.16. The top values in tables 7.14 and 7.16 are the maximum absolute errors over the interval $[0, 20\pi]$ and the bottom values are the absolute errors at $x = 20\pi$. The steplength is $h = \pi/40$.

The method used by Paternoster [53] is a 2-stage Runge-Kutta-Nyström method of trigonometric order 1 and algebraic order 2. It has been shown in chapter 4 that this method is also the 2-point mixed collocation method with nodes $c_1 = 1/4$ and $c_2 = 3/4$. Over the interval $[0, 20\pi]$, the method gave a maximum absolute error of 6.42×10^{-5}.

Also in table 7.17 are sd-values for the interval $[0, 100]$ with $k = 10$ where

$$sd_{max} = -\log_{10}(\max |y(x_n) - y_n|)$$

is the number of correct digits for the maximum absolute error over the interval $[0, 100]$. The results in table 7.18 are the sd-values obtained by Simos et al [65] from the methods shown below:

Method	Description	Algebraic order	Dispersive order
1	Runge-Kutta-Nyström-Fehlberg	4	8
2	Runge-Kutta-Nyström	2	8
3	Runge-Kutta-Nyström	4	10

	$k = 10$	$k = 1$	Polynomial
Ia	7.85×10^{-2}	$2.40 \times 10^{+46}$	$5.89 \times 10^{+46}$
	1.37×10^{-14}	$2.40 \times 10^{+46}$	$5.89 \times 10^{+46}$
Ib	5.41×10^{-3}	2.8009	2.8008
	2.20×10^{-14}	1.3893	1.4798
Ic	7.85×10^{-2}	1.4170	1.4174
	3.00×10^{-14}	1.0000	1.0004
IIa	5.63×10^{-4}	2.8466	2.8473
	1.33×10^{-13}	2.4315	2.4070
IIb	5.43×10^{-6}	7.43×10^{-2}	7.46×10^{-2}
	1.27×10^{-13}	5.37×10^{-2}	5.40×10^{-2}
$IIIa$	5.72×10^{-7}	1.68×10^{-1}	1.69×10^{-1}
	9.50×10^{-14}	1.26×10^{-1}	1.27×10^{-1}
$IIIb$	2.41×10^{-9}	2.49×10^{-4}	2.49×10^{-4}
	1.03×10^{-13}	1.77×10^{-4}	1.77×10^{-4}
IVa^*	5.94×10^{-2}	2.8471	2.8473
	8.92×10^{-14}	2.4263	2.4070
IVb^*	6.42×10^{-4}	7.39×10^{-2}	7.46×10^{-2}
	5.83×10^{-12}	5.35×10^{-2}	5.40×10^{-2}

Table 7.14: Ex 1.4 - Methods $I - IV^*$, $h = \pi/40$

This problem highlights the fact that when one looks at the absolute error at the end-point of the interval, the value can differ greatly from the absolute maximum error over the whole interval and so this information may be misleading. This is seen especially for $k = 10$ in table 7.14 where the error at the end-point is very close to zero but the maximum absolute error is much larger. Note that as $k \to 0$, methods IVa^* and IVb^* reduce to the polynomial collocation methods IIa and IIb respectively and this can be seen in the results for $k = 1$.

	$k_1 = 10$, $k_2 = 1$	$k_1 = 10.1$, $k_2 = 1$	$k_1 = 9.9$, $k_2 = 1$	$k_1 = 10$, $k_2 = 10^{-5}$
V^*	1.88×10^{-13}	4.38×10^{-1}	4.34×10^{-1}	5.63×10^{-4}

Table 7.15: Ex 1.4 - Mixed Collocation Method V^*

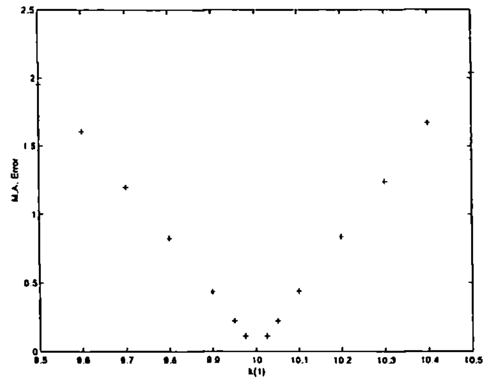

Figure 7.1: Ex 1.4 - Varying the frequency k_1 with $k_2 = 1$

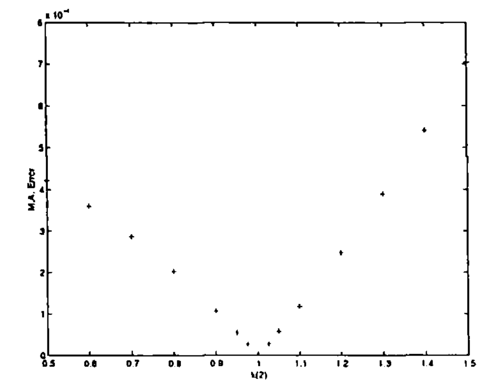

Figure 7.2: Ex 1.4 - Varying the frequency k_2 with $k_1 = 10$

In figures 7.1 and 7.2, the maximum absolute errors are given for the two-frequency method V^* with one frequency fixed and varying the other to show how the errors behave. When $k_1 = 10$ and $k_2 = 1$, the maximum error is 1.79×10^{-13}. From the figures, when the lower frequency k_2 is varied but the high frequency is kept fixed, then the results are comparable to the lower order mixed collocation methods. If we vary the high frequency then the results are very poor.

	$k = 10$	$k = 1$
S_1	1.79×10^{-7}	6.86×10^{-1}
	9.46×10^{-14}	3.60×10^{-1}
S_2	1.81×10^{-5}	6.80×10^{-1}
	6.25×10^{-14}	3.58×10^{-1}
S_3	1.84×10^{-3}	6.74×10^{-1}
	1.57×10^{-13}	3.56×10^{-1}

Table 7.16: Ex 1.4 - Multistep Methods $S_1 - S_3$

	$h = 0.05$	$h = 0.025$
Ia	1.3	1.6
Ib	2.7	3.3
Ic	1.3	1.6
IIa	3.6	4.2
IIb	6.1	7.3
$IIIa$	7.0	8.2
$IIIb$	9.8	11.5

Table 7.17: Ex 1.4 - Mixed Collocation Methods $I - III$: $k = 10$

	$h = 0.05$	$h = 0.025$
1	2.8	4.3
2	1.1	0.0
3	1.7	2.3

Table 7.18: Ex 1.4 - Methods of Simos et al

Conclusions

With $k = 10$, the numerical results for the mixed collocation methods are poor for the lower stage methods but the higher stage methods show some improvement. Comparing the mixed collocation methods with the multistep methods $S_1 - S_3$, we see that the method S_1 is more accurate compared to the 4th order mixed collocation methods IIb and $IIIa$ for $k = 10$ but not for $k = 1$.

The 2nd order two frequency method V^* is exact except for rounding error when $k_1 = 10$ and $k_2 = 1$ but if one of the frequencies is changed by a small amount, then we can obtain poor results. The results do show the advantage of having a method with two frequencies. Comparing method IIb with the result given by Paternoster's TRKN1 method, both methods have 2 stages but the higher order method IIb is more accurate. With $k = 1$, the results are not so good and they are very similar to the polynomial collocation results. Comparing the results of table 7.18 with table 7.17, the mixed collocation methods of algebraic order greater or equal to four are more accurate than methods 1-3 and the 2nd order method IIa is comparable to method 1 which is a 4th order method.

By the stability work in chapter 5 and section 6.1.2, methods Ib, Ic, II, III and IV^* are stable for $k = 10$, $k = 1$ and $k = 0$ in table 7.14 and method Ia is unstable for $k = 0$ and $k = 1$, and stable for $k = 10$. This agrees with the results found.

Example 1.5

Again, we look at a highly oscillatory problem which involves two frequencies as suggested by Krishnaiah [1]

$$y'' = -100y + 100\sin x, \quad y(0) = 0, \quad y'(0) = \frac{595}{99}$$

where the exact solution is $y(x) = \frac{100}{99}\sin x + \frac{1}{2}\sin(10x)$.

The numerical values in tables 7.19 - 7.21 are the maximum absolute errors on the interval $[0, 100]$ for $k = 1$, 0 and 10 respectively. For the method V^* in table 7.21, the frequencies are $k_1 = 10$ and $k_2 = 1$. Also given in tables 7.19 and 7.20 are whether the methods are stable (S) or unstable (U). When (-) appears in the table then the iterative process breaks down and the method only managed to reach a certain number of steps. The methods in table 7.21 are all stable for the particular values of ν and θ.

In table 7.22, the numerical solutions given are the absolute errors at $x = 100$. The 2-step methods used by Krishnaiah [1] are

Method	Description of method	Trigonometric order	Algebraic order
1	Explicit involving $f''(x, y)$	1	4
2	Implicit involving $f''(x, y)$	1	6
3	Implicit involving $f''(x, y)$ (Hairer)	0	4

In table 7.23, the maximum absolute errors over the interval $[0, 100]$ and the end-point errors at $x = 100$ are calculated using methods 1-3. Krishnaiah states that method 3 is P-stable but using our definition for stability, the method has an interval of stability given by $(0, 12)$.

	$h = 1/2$		$h = 1/4$		$h = 1/8$		$h = 1/16$	
Ia	$1.87 \times 10^{+189}$	U	$7.54 \times 10^{+121}$	U	$1.23 \times 10^{+99}$	U	$1.15 \times 10^{+61}$	U
Ib	–	U	7.33×10^{-1}	S	9.39×10^{-1}	S	9.88×10^{-1}	S
Ic	6.62×10^{-1}	S	5.20×10^{-1}	S	5.00×10^{-1}	S	5.00×10^{-1}	S
IIa	–	U	1.2144	S	1.0352	S	1.0057	S
IIb	7.17×10^{-1}	S	1.0673	S	2.41×10^{-1}	S	1.64×10^{-2}	S
$IIIa$	1.3694	S	9.47×10^{-1}	S	5.31×10^{-1}	S	3.69×10^{-2}	S
$IIIb$	8.05×10^{-1}	S	9.90×10^{-2}	S	2.11×10^{-3}	S	3.49×10^{-5}	S
IVa^*	–	U	1.2175	S	1.0333	S	1.0053	S
IVb^*	7.18×10^{-1}	S	1.0654	S	2.40×10^{-1}	S	1.63×10^{-2}	S
S_1	–	U	–	U	9.86×10^{-1}	S	1.58×10^{-1}	S
S_2	–	U	–	U	9.83×10^{-1}	S	1.57×10^{-1}	S
S_3	–	U	–	U	9.79×10^{-1}	S	1.55×10^{-1}	S

Table 7.19: Ex 1.5 - Methods $I - IV^*$ and $S_1 - S_3$: $k = 1$

	$h = 1/2$		$h = 1/4$		$h = 1/8$		$h = 1/16$	
Ia	$2.37 \times 10^{+190}$	U	$5.85 \times 10^{+122}$	U	$7.42 \times 10^{+99}$	U	$4.75 \times 10^{+61}$	U
Ib	–	U	7.32×10^{-1}	S	9.35×10^{-1}	S	9.87×10^{-1}	S
Ic	6.62×10^{-1}	S	5.21×10^{-1}	S	5.01×10^{-1}	S	5.00×10^{-1}	S
IIa	–	U	1.2178	S	1.0358	S	1.0060	S
IIb	7.15×10^{-1}	S	1.0686	S	2.42×10^{-1}	S	1.65×10^{-2}	S
$IIIa$	1.3750	S	9.46×10^{-1}	S	5.35×10^{-1}	S	3.72×10^{-2}	S
$IIIb$	7.62×10^{-1}	S	9.87×10^{-2}	S	2.10×10^{-3}	S	3.49×10^{-5}	S
S_0	–	U	–	U	9.89×10^{-1}	S	1.60×10^{-1}	S

Table 7.20: Ex 1.5 - Methods $I - III$ and S_0 : $k = 0$

	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
Ia	8.72×10^{-1}	2.65×10^{-1}	1.28×10^{-1}	6.33×10^{-2}
Ib	6.57×10^{-1}	5.93×10^{-2}	1.40×10^{-2}	3.45×10^{-3}
Ic	8.79×10^{-1}	2.65×10^{-1}	1.28×10^{-1}	6.33×10^{-2}
IIa	6.37×10^{-2}	6.15×10^{-3}	1.46×10^{-3}	3.59×10^{-4}
IIb	3.62×10^{-2}	6.49×10^{-4}	3.59×10^{-5}	2.20×10^{-6}
$IIIa$	3.52×10^{-3}	6.57×10^{-5}	3.77×10^{-6}	2.31×10^{-7}
$IIIb$	7.45×10^{-4}	3.03×10^{-6}	4.03×10^{-8}	6.14×10^{-10}
IVa^*	5.6780	1.6435	1.71×10^{-1}	3.70×10^{-2}
IVb^*	*	8.72×10^{-2}	4.34×10^{-3}	2.58×10^{-4}
V^*	2.29×10^{-14}	1.04×10^{-13}	1.53×10^{-13}	1.39×10^{-14}
S_1	2.55×10^{-3}	3.04×10^{-5}	1.23×10^{-6}	7.15×10^{-8}
S_2	1.0414	3.93×10^{-3}	1.29×10^{-4}	7.19×10^{-6}
S_3	6.5864	6.99×10^{-1}	1.38×10^{-2}	7.23×10^{-4}

Table 7.21: Ex 1.5 - Methods $I - V^*$ and $S_1 - S_3$: $k = 10$

Method	$h = 1/2$	$h = 1/4$
1	2.21×10^{-4}	1.47×10^{-5}
2	1.89×10^{-6}	1.52×10^{-6}
3	2.83×10^{-1}	1.73×10^{-1}

Table 7.22: Ex 1.5 - Results of Krishnaiah

Method	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
1	3.55×10^{-3}	2.40×10^{-5}	8.52×10^{-7}	4.81×10^{-8}
	2.22×10^{-4}	1.45×10^{-5}	4.68×10^{-7}	2.61×10^{-8}
2	2.52×10^{-5}	1.14×10^{-7}	8.79×10^{-10}	1.15×10^{-11}
	1.57×10^{-6}	6.90×10^{-8}	4.82×10^{-10}	6.24×10^{-12}
3	1.1487	9.46×10^{-1}	9.97×10^{-1}	1.00×10^{-1}
	2.83×10^{-1}	1.33×10^{-1}	8.44×10^{-1}	6.66×10^{-2}

Table 7.23: Ex 1.5 - Our results using methods 1-3

Conclusions

As expected, the numerical results for the 2nd order two frequency method V^* are exact except for rounding error. The higher order mixed collocation methods show an improvement when the steplength is decreased and with $k = 10$, method $IIIb$ is comparable to methods 1 and 2. For $k = 10$, the 4th order multistep method S_1 gives slightly better results than the 4th order mixed collocation methods IIb and $IIIa$ whilst methods S_2 and S_3 are less accurate.

* Note that for method IVb^* with steplength $h = 1/2$, the iterative process breaks down when the tolerance is 10^{-14}. If we use a less stringent tolerance of 10^{-13}, then the error is given by 18.967 and as the steplength is halved, the ratio between the errors become closer to 16.

For $k = 1$, the results were very poor and it appears from this problem and the previous example that we obtain more accurate results when the higher frequency is chosen. The polynomial collocation methods gave very similar results to the mixed collocation methods with $k = 1$ and all of the multistep methods $S_1 - S_3$ were unstable for $h = 1/2$ and $h = 1/4$.

If we compare the end-point errors of method 2 in table 7.22 to those in 7.23, they are relatively close for $h = 1/2$ but very different for $h = 1/4$. The ratios between the errors in table 7.23 are satisfied but not by Krishnaiah's results. Possible explanations are that Krishnaiah used only single precision in his calculations or it could be a typing error.

Example 1.6

Consider the popular almost periodic problem introduced by Stiefel and Bettis [67]

$$z'' = -z + 0.001e^{ix}, \quad z(0) = 1, \quad z'(0) = 0.9995i, \quad z \in C \tag{7.1}$$

where the exact solution is $z(x) = e^{ix}(1 - 0.0005ix)$. If we set $z = y_1 + iy_2$, then the differential problem can be written in the equivalent form

$$y_1'' = -y_1 + 0.001\cos x, \quad y_1(0) = 1, \quad y_1'(0) = 0$$

$$y_2'' = -y_2 + 0.001\sin x, \quad y_2(0) = 0, \quad y_2'(0) = 0.9995$$

with the exact solution

$$y_1(x) = \cos x + 0.0005x\sin x \text{ and } y_2(x) = \sin x - 0.0005x\cos x.$$

In table 7.24, results are presented for the real part of the differential problem (7.1)

$$y_1'' = -y_1 + 0.001\cos x, \quad y_1(0) = 1, \quad y_1'(0) = 0$$

and in table 7.25, the imaginary part of the differential problem (7.1)

$$y_2'' = -y_2 + 0.001\sin x, \quad y_2(0) = 0, \quad y_2'(0) = 0.9995.$$

For methods $I - IV^*$ and $S_1 - S_3$ in tables 7.24 and 7.25, the top values are the maximum absolute error on $[0, 40\pi]$, and the bottom values are the absolute errors at $x = 40\pi$. For the angular frequency, $k = 1$.

	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
Ia	2.34×10^{-2}	1.22×10^{-2}	6.15×10^{-3}
	2.34×10^{-2}	1.22×10^{-2}	6.15×10^{-3}
Ib	1.58×10^{-3}	3.98×10^{-4}	9.96×10^{-5}
	1.89×10^{-15}	4.44×10^{-16}	6.33×10^{-15}
Ic	2.34×10^{-2}	1.22×10^{-2}	6.15×10^{-3}
	2.34×10^{-2}	1.22×10^{-2}	6.15×10^{-3}
IIa	3.12×10^{-3}	7.93×10^{-4}	1.99×10^{-4}
	9.55×10^{-15}	1.00×10^{-15}	5.55×10^{-16}
IIb	1.62×10^{-5}	1.02×10^{-6}	6.40×10^{-8}
	1.00×10^{-15}	6.81×10^{-14}	2.63×10^{-14}
$IIIa$	2.42×10^{-5}	1.53×10^{-6}	9.60×10^{-8}
	2.45×10^{-14}	1.23×10^{-13}	7.61×10^{-14}
$IIIb$	7.14×10^{-8}	1.13×10^{-9}	2.18×10^{-11}
	1.72×10^{-14}	1.34×10^{-13}	4.49×10^{-13}
IVa^*	2.66×10^{-14}	1.80×10^{-14}	4.13×10^{-14}
	1.22×10^{-15}	9.21×10^{-15}	3.87×10^{-14}
IVb^*	9.59×10^{-13}	2.26×10^{-13}	1.12×10^{-12}
	9.59×10^{-13}	4.21×10^{-14}	1.12×10^{-12}
S_1	1.03×10^{-4}	6.20×10^{-6}	3.85×10^{-7}
	1.67×10^{-15}	2.22×10^{-16}	3.66×10^{-15}
S_2	1.01×10^{-14}	7.42×10^{-14}	1.34×10^{-13}
	7.77×10^{-16}	3.33×10^{-16}	1.22×10^{-13}
S_3	2.28×10^{-14}	9.21×10^{-15}	1.43×10^{-13}
	2.44×10^{-15}	3.66×10^{-15}	5.44×10^{-15}

Table 7.24: Ex 1.6 - Methods $I - IV^*$ and $S_1 - S_3$: (Real)

	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
Ia	2.31×10^{-2}	1.20×10^{-2}	6.07×10^{-3}
	6.26×10^{-3}	1.60×10^{-3}	4.03×10^{-4}
Ib	1.60×10^{-3}	4.03×10^{-4}	1.01×10^{-4}
	1.60×10^{-3}	4.03×10^{-4}	1.01×10^{-4}
Ic	2.31×10^{-2}	1.20×10^{-2}	6.07×10^{-3}
	6.26×10^{-3}	1.60×10^{-3}	4.03×10^{-4}
IIa	3.16×10^{-3}	8.03×10^{-4}	2.02×10^{-4}
	3.16×10^{-3}	8.03×10^{-4}	2.02×10^{-4}
IIb	1.64×10^{-5}	1.03×10^{-6}	6.48×10^{-8}
	1.64×10^{-5}	1.03×10^{-6}	6.48×10^{-8}
$IIIa$	2.45×10^{-5}	1.55×10^{-6}	9.72×10^{-8}
	2.45×10^{-5}	1.55×10^{-6}	9.72×10^{-8}
$IIIb$	7.23×10^{-8}	1.14×10^{-9}	2.21×10^{-11}
	7.23×10^{-8}	1.14×10^{-9}	2.21×10^{-11}
IVa^*	2.63×10^{-14}	1.67×10^{-14}	4.03×10^{-14}
	2.21×10^{-14}	7.49×10^{-15}	1.09×10^{-14}
IVb^*	9.51×10^{-13}	2.32×10^{-13}	1.11×10^{-12}
	1.70×10^{-13}	2.32×10^{-13}	3.80×10^{-14}
S_1	1.05×10^{-4}	6.30×10^{-6}	3.90×10^{-7}
	1.05×10^{-4}	6.30×10^{-6}	3.90×10^{-7}
S_2	1.27×10^{-14}	7.89×10^{-14}	1.43×10^{-13}
	6.34×10^{-15}	7.51×10^{-14}	1.43×10^{-13}
S_3	2.14×10^{-14}	8.26×10^{-15}	1.46×10^{-13}
	1.76×10^{-14}	4.30×10^{-16}	1.44×10^{-13}

Table 7.25: Ex 1.6 - Methods $I - IV^*$ and $S_1 - S_3$: (Imag.)

Conclusions (i)

This problem again highlights the fact that the absolute error at the end-point of the interval can differ greatly from the maximum absolute error as we can see in table 7.24, but in table 7.25, the errors at the end-point are very close or equivalent to the maximum absolute errors for the imaginary part of problem (7.1). The methods IV^*, S_2 and S_3 are exact except for rounding error. The 4th order methods IIb and $IIIa$ are more accurate than S_1, and the mixed collocation methods with the Gauss points show better results than others of the same order.

We now follow the approach taken by Raptis and Simos [58]. First define

$$\Sigma(x) = \gamma(x) - \sqrt{(y_1^2 + y_2^2)},$$

where y_1 and y_2 are the approximations for $y_1(x)$ and $y_2(x)$ respectively at the step x, and

$$\gamma(x) = [y_1^2(x) + y_2^2(x)]^{1/2} = [1 + (0.0005x)^2]^{1/2}$$

is the distance of the point $z(x)$ from the centre of the orbit at time x. In tables 7.26 and 7.27, the top entry in each box is the value of max $\{|\Sigma(x)|\}$ over the interval $[0, 40\pi]$ and the bottom values are the absolute errors at the end-point given by $|\Sigma(40\pi)|$. When only one value appears, the maximum absolute error and the end-point error are the same.

In tables 7.28 and 7.29, the top entry is the value max $\{\Omega(x)\}$ over the interval $[0, 40\pi]$ where we define

$$\Omega(x) = |z(x) - z| = \sqrt{[y_1(x) - y_1]^2 + [y_2(x) - y_2]^2},$$

and the bottom entry is $\Omega(40\pi)$. Again, if there is only one entry, then the end-point error is the same as the maximum absolute error for Ω.

For comparison, results are given for the polynomial collocation methods *IIb*, *IIIa* and *IIIb* and Numerov's method S_0 in tables 7.27 and 7.29. In table 7.30, the errors are $|\Sigma(40\pi)|$ for the 4-step methods 1-4 used by Raptis and Simos [58], and our results for methods 5-7 are the values max $\{|\Sigma(x)|\}$ over the interval $[0, 40\pi]$ for the 2-step methods used by Krishnaiah [1]. The methods are listed below:

Method	Description	Algebraic order	Trigonometric order
1	Classical - [35]	6	0
2	P-stable hybrid - [43]	6	0
3	3-stage Predictor-Corrector - [76]	6	0
4	Hybrid - [58]	6	0
5	Explicit involving $f''(x, y)$	4	1
6	Implicit involving $f''(x, y)$	6	1
7	Implicit involving $f''(x, y)$ (Hairer)	4	0

Method	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
Ia	2.38×10^{-2}	1.23×10^{-2}	6.16×10^{-3}
Ib	9.92×10^{-5}	2.52×10^{-5}	6.32×10^{-6}
Ic	2.30×10^{-2}	1.21×10^{-2}	6.11×10^{-3}
IIa	2.16×10^{-4}	5.53×10^{-5}	1.39×10^{-5}
	1.93×10^{-4}	5.01×10^{-5}	1.26×10^{-5}
IIb	1.53×10^{-6}	9.41×10^{-8}	5.86×10^{-9}
	1.03×10^{-6}	6.49×10^{-8}	4.06×10^{-9}
$IIIa$	1.54×10^{-6}	9.72×10^{-8}	6.09×10^{-9}
$IIIb$	4.53×10^{-9}	7.16×10^{-11}	9.35×10^{-13}
IVa^*	4.66×10^{-15}	1.00×10^{-14}	3.95×10^{-14}
	2.44×10^{-15}	8.66×10^{-15}	3.82×10^{-14}
IVb^*	9.46×10^{-13}	2.73×10^{-14}	1.12×10^{-12}
S_1	7.15×10^{-6}	4.35×10^{-7}	2.70×10^{-8}
	6.58×10^{-6}	3.95×10^{-7}	2.45×10^{-8}
S_2	8.88×10^{-16}	4.44×10^{-15}	5.77×10^{-15}
	4.44×10^{-16}	4.44×10^{-15}	2.89×10^{-15}
S_3	1.11×10^{-15}	3.11×10^{-15}	6.44×10^{-15}
	1.55×10^{-15}	4.00×10^{-15}	8.44×10^{-15}

Table 7.26: Ex 1.6 - Methods $I - IV^*$ and $S_1 - S_3$, $k = 1$: Error in Σ

Method	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
IIb	7.92×10^{-4}	4.88×10^{-5}	3.04×10^{-6}
	3.30×10^{-4}	2.14×10^{-5}	1.35×10^{-6}
$IIIa$	7.48×10^{-4}	4.81×10^{-5}	3.03×10^{-6}
$IIIb$	2.21×10^{-6}	3.24×10^{-8}	4.99×10^{-10}
	1.10×10^{-6}	1.77×10^{-8}	2.77×10^{-10}
S_0	3.79×10^{-3}	2.39×10^{-4}	1.49×10^{-5}
	3.15×10^{-3}	1.95×10^{-4}	1.22×10^{-5}

Table 7.27: Ex 1.6 - Methods IIb, $IIIa$, $IIIb$ and S_0, $k = 0$: Error in Σ

Method	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
Ia	2.43×10^{-2}	1.23×10^{-2}	6.16×10^{-3}
Ib	1.60×10^{-3}	4.03×10^{-4}	1.01×10^{-4}
Ic	2.43×10^{-2}	1.23×10^{-2}	6.16×10^{-3}
IIa	3.16×10^{-3}	8.03×10^{-4}	2.02×10^{-4}
IIb	1.65×10^{-5}	1.04×10^{-6}	6.54×10^{-8}
	1.64×10^{-5}	1.03×10^{-6}	6.48×10^{-8}
$IIIa$	2.45×10^{-5}	1.55×10^{-6}	9.72×10^{-8}
$IIIb$	7.23×10^{-8}	1.14×10^{-9}	2.21×10^{-11}
IVa^*	2.75×10^{-14}	1.82×10^{-14}	4.13×10^{-14}
	2.21×10^{-14}	1.19×10^{-14}	3.89×10^{-14}
IVb^*	9.74×10^{-13}	2.36×10^{-13}	1.12×10^{-12}
S_1	1.05×10^{-4}	6.30×10^{-6}	3.90×10^{-7}
S_2	1.27×10^{-14}	8.18×10^{-14}	1.46×10^{-13}
	6.39×10^{-15}	7.51×10^{-14}	1.42×10^{-13}
S_3	2.32×10^{-14}	9.35×10^{-15}	1.48×10^{-13}
	1.78×10^{-14}	3.54×10^{-15}	1.41×10^{-13}

Table 7.28: Ex 1.6 - Methods $I - IV^*$ and $S_1 - S_3$, $k = 1$: Error in Ω

Method	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
IIb	1.07×10^{-2}	6.93×10^{-4}	4.37×10^{-5}
	1.05×10^{-2}	6.84×10^{-4}	4.31×10^{-5}
$IIIa$	2.40×10^{-2}	1.54×10^{-3}	9.69×10^{-5}
$IIIb$	3.58×10^{-5}	5.72×10^{-7}	8.98×10^{-9}
	3.54×10^{-5}	5.65×10^{-7}	8.88×10^{-9}
S_0	1.02×10^{-1}	6.25×10^{-3}	3.89×10^{-4}

Table 7.29: Ex 1.6 - Methods IIb, $IIIa$, $IIIb$ and S_0, $k = 0$: Error in Ω

Method	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$
1	1.01×10^{-3}	1.23×10^{-5}	1.80×10^{-7}
2	3.14×10^{-5}	5.07×10^{-7}	8.23×10^{-9}
3	2.19×10^{-6}	2.45×10^{-8}	1.70×10^{-10}
4	1.00×10^{-6}	1.34×10^{-8}	2.00×10^{-10}
5	4.92×10^{-6}	2.93×10^{-7}	1.80×10^{-8}
6	1.85×10^{-7}	2.70×10^{-9}	4.15×10^{-11}
7	2.38×10^{-3}	1.57×10^{-4}	9.92×10^{-6}

Table 7.30: Ex 1.6 - Methods 1-4, $|\Sigma(40\pi)|$: Methods 5-7, $\max|\Sigma|$

Conclusions (ii)

As expected, methods IV^*, S_2 and S_3 are exact except for rounding error because the methods are exact for problems which have the trigonometric functions $\cos kx$, $\sin kx$, $x\cos kx$ and $x\sin kx$ in the solution. The errors in Σ by the 6th order mixed collocation method $IIIb$ are smaller than those of method 4 by approximately a factor of 200 and those of method 6 by approximately a factor of 40 which shows the superiority of the method. Even when $k = 0$, the polynomial collocation method $IIIb$ is comparable to methods 3 and 4 of Raptis and Simos, more accurate than method 5, and the errors in Σ are larger by a factor of approximately 6 than the errors of method 6. The errors in both Σ and Ω by the two 4th order mixed collocation methods IIb and $IIIa$ are smaller than those of the exponentially-fitted multistep method S_1 by a factor of 6 and 4 respectively. Methods 3 and 4 of Raptis and Simos are comparable to the higher order mixed collocation methods and as we can see from the results, for tables 7.26 - 7.29, the absolute error at the end-point is pretty close to the maximum absolute error over the interval $[0, 40\pi]$.

Example 1.7

We now consider the nonlinear problem [51]

$$y'' = -(1 + 0.01y^2)y + 0.01\cos^3 x, \quad y(0) = 1, \quad y'(0) = 0$$

where the exact solution is $y(x) = \cos x$.

Presented in table 7.31 are the results obtained by Ozawa with two 4th order implicit Runge-Kutta-Nyström methods of trigonometric order 1 with orders of dispersion 4 and 6 respectively. Ozawa's results are the absolute end-point errors at $x = 8.25\pi$. In Ozawa's paper [51], he does not give the value of the frequency for the results in table 7.31 for this particular problem but with $k = 0.1$ our results are very close to those in table 7.31. The values in tables 7.32 - 7.36 are the maximum absolute errors over the interval $[0, 8.25\pi]$. Polynomial collocation is used in table 7.32, and the angular frequency for methods $I - IV^*$ and $S_1 - S_3$ is $k = 1$ in tables 7.33 and 7.34, and $k = 0.1$ in tables 7.35 and 7.36. For the two frequency method V_1^*, we take $k_1 = 1$ and $k_2 = 0.1$, and for method V_2^*, $k_1 = 1$ and $k_2 = 0.01$.

In tables 7.34 and 7.36, the maximum absolute errors are presented for the mixed collocation methods IIb, $IIIa$ and $IIIb$ where the coefficients have been written as series expansions in terms of θ. This is because, for small θ, the exact form of the coefficients of the mixed collocation method are inaccurate because of the accumulation of rounding error resulting from the loss of significant digits, whilst the power series expansions are more accurate.

Dispersive order	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$	$h = \pi/32$	$h = \pi/64$
4	1.87×10^{-2}	1.54×10^{-3}	1.07×10^{-4}	7.01×10^{-6}	4.47×10^{-7}
6	1.07×10^{-2}	3.15×10^{-4}	7.86×10^{-6}	1.46×10^{-7}	1.05×10^{-9}

Table 7.31: Ex 1.7 - Methods by Ozawa

	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$	$h = \pi/32$	$h = \pi/64$
IIb	2.08×10^{-3}	1.35×10^{-4}	8.48×10^{-6}	5.31×10^{-7}	3.32×10^{-8}
$IIIa$	4.48×10^{-3}	2.87×10^{-4}	1.81×10^{-5}	1.31×10^{-6}	7.08×10^{-8}
$IIIb$	6.57×10^{-6}	1.06×10^{-7}	1.66×10^{-9}	2.60×10^{-11}	4.06×10^{-13}

Table 7.32: Ex 1.7 - Methods $IIb, IIIa$ and $IIIb$: $k = 0$

	$h=\pi/4$	$h=\pi/8$	$h=\pi/16$	$h=\pi/32$	$h=\pi/64$
Ia	3.23×10^{-15}	3.66×10^{-15}	3.55×10^{-15}	1.10×10^{-14}	8.99×10^{-15}
Ib	2.65×10^{-15}	2.77×10^{-15}	2.80×10^{-15}	6.99×10^{-15}	3.18×10^{-15}
Ic	2.00×10^{-15}	2.18×10^{-15}	2.83×10^{-15}	2.66×10^{-15}	1.44×10^{-14}
IIa	3.92×10^{-15}	5.58×10^{-15}	1.48×10^{-14}	1.04×10^{-13}	1.20×10^{-13}
IIb	5.78×10^{-15}	2.46×10^{-14}	1.10×10^{-13}	1.34×10^{-13}	1.42×10^{-12}
$IIIa$	9.44×10^{-15}	7.69×10^{-14}	3.04×10^{-13}	1.44×10^{-12}	4.71×10^{-12}
$IIIb$	3.55×10^{-15}	9.94×10^{-14}	7.88×10^{-13}	3.64×10^{-13}	6.00×10^{-12}
IVa^*	4.95×10^{-15}	3.95×10^{-15}	9.10×10^{-15}	5.31×10^{-14}	4.35×10^{-14}
IVb^*	1.87×10^{-13}	4.90×10^{-14}	2.21×10^{-13}	2.12×10^{-12}	3.98×10^{-12}
V_1^*	4.28×10^{-15}	1.27×10^{-14}	2.55×10^{-15}	4.91×10^{-14}	8.45×10^{-13}
V_2^*	6.70×10^{-15}	4.33×10^{-15}	9.21×10^{-15}	4.06×10^{-14}	5.36×10^{-13}
S_1	3.26×10^{-15}	3.34×10^{-15}	1.23×10^{-14}	1.06×10^{-13}	1.27×10^{-13}
S_2	2.14×10^{-15}	1.61×10^{-14}	2.57×10^{-14}	8.70×10^{-14}	2.25×10^{-13}
S_3	5.25×10^{-15}	2.06×10^{-15}	3.05×10^{-14}	4.22×10^{-13}	1.52×10^{-13}

Table 7.33: Ex 1.7 - Methods $I - V^*$ and $S_1 - S_3$ (Exact form): $k=1$

	$h=\pi/4$	$h=\pi/8$	$h=\pi/16$	$h=\pi/32$	$h=\pi/64$
IIb	1.91×10^{-10}	4.35×10^{-14}	4.19×10^{-15}	2.75×10^{-15}	2.66×10^{-15}
$IIIa$	5.12×10^{-12}	3.55×10^{-15}	2.54×10^{-15}	3.07×10^{-15}	3.22×10^{-15}
$IIIb$	8.86×10^{-9}	1.72×10^{-11}	3.38×10^{-14}	2.24×10^{-15}	3.32×10^{-15}

Table 7.34: Ex 1.7 - Methods $IIb, IIIa$ and $IIIb$ (Series expansions): $k=1$

	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$	$h = \pi/32$	$h = \pi/64$
Ib	2.73×10^{-1}	7.30×10^{-2}	1.85×10^{-2}	4.65×10^{-3}	1.16×10^{-3}
IIa	5.37×10^{-1}	1.46×10^{-1}	3.71×10^{-2}	9.30×10^{-3}	2.33×10^{-3}
IIb	2.07×10^{-3}	1.34×10^{-4}	8.44×10^{-6}	5.28×10^{-7}	3.30×10^{-8}
$IIIa$	4.43×10^{-3}	2.85×10^{-4}	1.79×10^{-5}	1.12×10^{-6}	7.04×10^{-8}
$IIIb$	6.58×10^{-6}	1.06×10^{-7}	1.60×10^{-9}	1.47×10^{-10}	7.37×10^{-11}
IVa^*	5.33×10^{-1}	1.45×10^{-1}	3.67×10^{-2}	9.21×10^{-3}	2.30×10^{-3}
IVb^*	2.06×10^{-3}	1.33×10^{-4}	8.39×10^{-6}	5.26×10^{-7}	3.32×10^{-8}
S_1	1.83×10^{-2}	1.14×10^{-3}	7.13×10^{-5}	4.47×10^{-6}	2.78×10^{-7}
S_2	1.81×10^{-2}	1.13×10^{-3}	7.06×10^{-5}	4.42×10^{-6}	2.77×10^{-7}
S_3	1.79×10^{-2}	1.11×10^{-3}	6.99×10^{-5}	4.38×10^{-6}	2.74×10^{-7}

Table 7.35: Ex 1.7 - Methods $I - IV^*$ and $S_1 - S_3$ (Exact form): $k = 0.1$

	$h = \pi/4$	$h = \pi/8$	$h = \pi/16$	$h = \pi/32$	$h = \pi/64$
$IIIb$	6.58×10^{-6}	1.06×10^{-7}	1.66×10^{-9}	2.60×10^{-11}	4.05×10^{-13}

Table 7.36: Ex 1.7 - Method $IIIb$ (Series expansions): $k = 0.1$

Conclusions

The mixed collocation methods and the multistep methods $S_1 - S_3$ are exact except for the accumulation of rounding error when $k = 1$. For our own results for Ozawa's method and the 3-stage TRKN1 method in Appendix A, we found that they are also exact when $k = 1$ except for rounding error. Comparing methods IIb, $IIIa$ and $IIIb$ in tables 7.33 and 7.34, we see the difference in using the series expansion for the coefficients especially for small steplengths. For large steplengths, the results in table 7.34 are quite poor but as the steplength decreases, they are superior to those in table 7.33. For $h = \pi/64$, the errors in table 7.33 for the methods IIb, $IIIa$ and $IIIb$ are larger than those in table 7.34 by a factor of approximately 533, 1462 and 1807 respectively.

For $k = 0.1$, comparing the 4th order methods with Ozawa's methods, we see that the most accurate method appears to be Ozawa's TRKN41 method with order of dispersion 6 when the steplength is decreased. Although he presented only the absolute end-point error, the maximum absolute error is slightly smaller than that of method IIb. The polynomial collocation method $IIIb$ is considerably more accurate than Ozawa's methods and all the mixed collocation methods of order 4 or less when $k = 0.1$.

Example 1.8

Consider the initial value problem

$$z'' = -[1 + \gamma + \gamma\,\delta\,\mathrm{e}^{-2ix}]\,z + \gamma\,\mathrm{e}^{-ix}\,z^2,$$

$$z(0) = 1 + \delta, \;\; z'(0) = i(1 - \delta), \;\; \gamma \geq 0, \; 0 \leq \delta \leq 1$$

where γ is a nonlinearity parameter, δ is a distortion parameter and the exact solution is an ellipse given by

$$z(x) = \mathrm{e}^{ix} + \delta\mathrm{e}^{-ix}.$$

We take the approach of Jain et al [43] and set $z = y_1 + iy_2$, then,

$$\begin{aligned} y_1'' &= -[1 + \gamma + \gamma\,\delta\,\cos(2x)]\,y_1 + 2y_1\,y_2\,\gamma\,\sin x - y_2\,\delta\,\gamma\,\sin(2x) + \gamma\,(y_1^2 - y_2^2)\,\cos x \\ y_2'' &= -[1 + \gamma + \gamma\,\delta\,\cos(2x)]\,y_2 + 2y_1\,y_2\,\gamma\,\cos x + y_1\,\delta\,\gamma\,\sin(2x) - \gamma\,(y_1^2 - y_2^2)\,\sin x \end{aligned}$$

where

$$\begin{aligned} y_1(0) &= 1 + \delta, \quad & y_1'(0) &= 0, \\ y_2(0) &= 0, & y_2'(0) &= 1 - \delta \end{aligned}$$

and the exact solution is

$$y_1(x) = (1 + \delta)\cos x \;\text{ and }\; y_2(x) = (1 - \delta)\sin x.$$

We define

$$\Omega(x) = |z(x) - z| = \left\{[y_1(x) - y_1]^2 + [y_2(x) - y_2]^2\right\}^{1/2}$$

and the entries in tables 7.37 and 7.38 are the values $\max\{\Omega(x)\}$ over the interval $[0, 10\pi]$. In table 7.39 the value $\Omega(10\pi)$ is given for the methods used by Jain et al [43].

The steplength is $h = \pi/12$, the nonlinearity parameter is $\gamma = 1/10$ and the fitted angular frequency is $k = 1$ for the exponentially-fitted methods. For the distortion parameter, we take five different values for δ. The methods used by Jain et al [43] are as follows:

Method	Description	P-stable	Algebraic order
1	5-step classical : Störmer-Cowell	No	6
2	4-step implicit : Lambert & Watson	No	6
3	2-step hybrid : Cash	Yes	6
4	4-step hybrid : Jain et al	Yes	6

	$\delta = 0$	$\delta = 0.1$	$\delta = 0.2$	$\delta = 0.3$	$\delta = 0.4$
Ia	3.26×10^{-15}	3.69×10^{-15}	2.90×10^{-15}	3.75×10^{-15}	2.70×10^{-15}
Ib	5.20×10^{-15}	3.87×10^{-15}	3.66×10^{-15}	4.88×10^{-15}	3.54×10^{-15}
Ic	9.48×10^{-15}	8.72×10^{-15}	7.83×10^{-15}	8.12×10^{-15}	9.72×10^{-15}
IIa	9.56×10^{-15}	1.03×10^{-14}	1.12×10^{-14}	1.20×10^{-14}	1.33×10^{-14}
IIb	5.87×10^{-14}	5.99×10^{-14}	6.22×10^{-14}	6.46×10^{-14}	6.72×10^{-14}
$IIIa$	3.71×10^{-13}	3.73×10^{-13}	3.89×10^{-13}	4.06×10^{-13}	4.23×10^{-13}
$IIIb$	3.34×10^{-13}	3.34×10^{-13}	3.46×10^{-13}	3.59×10^{-13}	3.73×10^{-13}
IVa^*	1.32×10^{-14}	1.37×10^{-14}	1.93×10^{-14}	1.40×10^{-14}	2.36×10^{-14}
IVb^*	8.89×10^{-14}	1.00×10^{-13}	1.10×10^{-13}	1.31×10^{-13}	1.40×10^{-13}
S_1	9.42×10^{-15}	9.70×10^{-15}	8.77×10^{-15}	8.91×10^{-15}	1.01×10^{-14}
S_2	4.75×10^{-14}	4.53×10^{-14}	5.30×10^{-14}	5.17×10^{-14}	5.64×10^{-14}
S_3	5.35×10^{-14}	7.27×10^{-14}	5.12×10^{-14}	6.17×10^{-14}	6.68×10^{-14}

Table 7.37: Ex 1.8 - Methods $I - IV$ and $S_1 - S_3$: $k = 1$

	$\delta = 0$	$\delta = 0.1$	$\delta = 0.2$	$\delta = 0.3$	$\delta = 0.4$
IIb	2.75×10^{-5}	2.57×10^{-5}	2.49×10^{-5}	2.61×10^{-5}	2.73×10^{-5}
$IIIa$	6.91×10^{-5}	7.35×10^{-5}	7.80×10^{-5}	8.25×10^{-5}	8.70×10^{-5}
$IIIb$	1.16×10^{-8}	1.22×10^{-8}	1.29×10^{-8}	1.35×10^{-8}	1.42×10^{-8}
S_0	2.89×10^{-4}	2.92×10^{-4}	3.11×10^{-4}	3.30×10^{-4}	3.49×10^{-4}

Table 7.38: Ex 1.8 - Methods IIb, $IIIa$, $IIIb$ and S_0 : $k = 0$

Method	$\delta = 0$	$\delta = 0.1$	$\delta = 0.2$	$\delta = 0.3$	$\delta = 0.4$
1	1.54×10^{-5}	1.65×10^{-5}	1.66×10^{-5}	1.67×10^{-5}	1.68×10^{-5}
2	5.51×10^{-6}	5.24×10^{-6}	4.97×10^{-6}	4.73×10^{-6}	4.51×10^{-6}
3	1.30×10^{-7}	1.24×10^{-7}	1.18×10^{-7}	1.12×10^{-7}	1.06×10^{-7}
4	7.15×10^{-7}	7.25×10^{-7}	7.38×10^{-7}	7.55×10^{-7}	7.75×10^{-7}

Table 7.39: Ex 1.8 - Methods of Jain, Kambo and Goel

Conclusions

The mixed collocation methods $I - IV^*$ and exponentially-fitted methods $S_1 - S_3$ are exact for this problem except for the accumulation of rounding error and are far superior to the 6th order methods used by Jain et al. The 4th order polynomial collocation methods IIb and $IIIa$ are superior to Numerov's method S_0 and method $IIIb$ is the most accurate of the polynomial based methods and superior to the 6th order methods 1-4.

Example 1.9
For our next example, consider the nonlinear Duffing's equation

$$y'' = -y - y^3 + \mathcal{A}\cos(\sigma x)$$

where $\mathcal{A} = 0.002$, $\sigma = 1.01$, the initial conditions are

$$y(0) = \sum_{i=0}^{4} A_{2i+1} = 2.00426728067 \times 10^{-1}, \;\; y'(0) = 0$$

where the coefficients

$$A_1 = 0.200179477536, \;\; A_3 = 0.246946143 \times 10^{-3},$$

$$A_5 = 0.304014 \times 10^{-6}, \;\; A_7 = 0.374 \times 10^{-9}, \;\; A_9 = 0.0$$

are computed by Galerkin's approximation method with a precision of 10^{-12}, see Van Dooren [75] and the solution is given by

$$y(x) = A_1 \cos \sigma x + A_3 \cos 3\sigma x + A_5 \cos 5\sigma x + A_7 \cos 7\sigma x + A_9 \cos 9\sigma x.$$

The interval for x is $[0, 40\pi]$. In tables 7.40 and 7.41, the absolute maximum errors are given on the interval $[0, 40\pi]$. The angular frequency is $k = 1.01$ for table 7.40 and $k = 0$ for table 7.41.

For comparison we look at three 4th order polynomial based methods used by Chawla and Neta [11] and the results in table 7.42 for methods 1-3 are the absolute errors at $x = 40\pi$.

In table 7.43, we present our results for the 2-step Störmer extrapolation and interpolation methods 4-7 by Gautschi [28]. The results are the maximum absolute errors over the interval $[0, 40\pi]$. These methods are of Störmer type but the coefficients are chosen so that the linear functional of the method annihilates all trigonometric polynomials of order p (c.f. Definition 3.1). The fitted angular frequency is $k = 1.01$.

Method	Description of method
1	2-step P-stable hybrid method by Chawla [7]
2	2-step P-stable hybrid method by Cash [4]
3	2-step P-stable hybrid method by Costabile & Costabile [24]

Method	Description of method	Algebraic order	Trigonometric order
4	2-step extrapolation	2	1
5	2-step extrapolation	3	2
6	2-step interpolation	1	1
7	2-step interpolation	4	2

	$h = \pi/5$	$h = \pi/10$	$h = \pi/20$	$h = \pi/40$
Ia	1.06×10^{-3}	5.19×10^{-4}	2.49×10^{-4}	1.21×10^{-4}
Ib	1.46×10^{-4}	2.69×10^{-5}	6.18×10^{-6}	1.51×10^{-6}
Ic	8.90×10^{-4}	4.53×10^{-4}	2.32×10^{-4}	1.17×10^{-4}
IIa	1.50×10^{-4}	4.58×10^{-5}	1.19×10^{-5}	3.00×10^{-6}
IIb	8.73×10^{-6}	4.81×10^{-7}	2.93×10^{-8}	1.82×10^{-9}
$IIIa$	1.11×10^{-5}	5.82×10^{-7}	3.47×10^{-8}	2.14×10^{-9}
$IIIb$	1.17×10^{-7}	1.43×10^{-9}	1.46×10^{-11}	8.39×10^{-12}
S_1	5.42×10^{-5}	2.60×10^{-6}	1.44×10^{-7}	8.67×10^{-9}
S_2	4.90×10^{-5}	2.32×10^{-6}	1.28×10^{-7}	7.71×10^{-9}
S_3	4.43×10^{-5}	2.07×10^{-6}	1.14×10^{-7}	6.86×10^{-9}

Table 7.40: Ex 1.9 - Methods $I - IV^*$ and $S_1 - S_3 : k = 1.01$

	$h = \pi/5$	$h = \pi/10$	$h = \pi/20$	$h = \pi/40$
Ib	1.30×10^{-1}	3.46×10^{-2}	8.70×10^{-3}	2.18×10^{-3}
Ic	2.00×10^{-1}	2.02×10^{-1}	2.06×10^{-1}	2.10×10^{-1}
IIa	2.75×10^{-1}	6.96×10^{-2}	1.75×10^{-2}	4.36×10^{-3}
IIb	7.17×10^{-4}	4.57×10^{-5}	2.87×10^{-6}	1.80×10^{-7}
$IIIa$	1.36×10^{-3}	8.69×10^{-5}	3.46×10^{-6}	3.43×10^{-7}
$IIIb$	1.26×10^{-6}	2.05×10^{-8}	3.32×10^{-10}	1.28×10^{-11}
S_0	5.67×10^{-3}	3.51×10^{-4}	2.19×10^{-5}	1.37×10^{-6}

Table 7.41: Ex 1.9 - Methods I, II, III and $S_0 : k = 0$

Method	$h = \pi/5$	$h = \pi/10$	$h = \pi/20$	$h = \pi/40$
1	4.50×10^{-3}	2.85×10^{-4}	1.79×10^{-5}	1.12×10^{-6}
2	4.54×10^{-3}	2.88×10^{-4}	1.81×10^{-5}	1.13×10^{-6}
3	3.10×10^{-2}	2.05×10^{-3}	1.30×10^{-4}	8.15×10^{-6}

Table 7.42: Ex 1.9 - Methods 1-3

Method	$h = \pi/5$	$h = \pi/10$	$h = \pi/20$	$h = \pi/40$
4	3.10×10^{-4}	5.76×10^{-5}	1.27×10^{-5}	3.05×10^{-6}
5	2.18×10^{-4}	3.39×10^{-5}	5.13×10^{-6}	6.41×10^{-7}
6	8.37×10^{-4}	7.56×10^{-4}	4.35×10^{-4}	2.30×10^{-4}
7	3.23×10^{-5}	1.48×10^{-6}	8.06×10^{-8}	4.84×10^{-9}

Table 7.43: Ex 1.9 - Our results using Methods 4-7 of Gautschi

Conclusions

For $k = 1.01$, the mixed collocation methods with Gauss points are more accurate than other mixed collocation methods of the same algebraic order. The 4th order methods IIb and $IIIa$ and method 7 by Gautschi give slightly better results than the multistep methods $S_1 - S_3$. Also, the mixed collocation methods are more accurate than the methods 4-7 by Gautschi when we look at those of the same algebraic order.

Note that for $h = \pi/40$ for the mixed collocation and polynomial collocation methods $IIIb$, the ratios of the error to the previous error for $h = \pi/20$ are 1.7 and 26 respectively, instead of $2^6 = 64$. We take into consideration that the solution of the problem is not exact because the coefficients A_{2i+1}, for $i = 0, \ldots, 4$ are calculated with a precision of 10^{-12} and so this effects the error each time it is calculated. When the coefficients are written as series expansions in terms of θ for the mixed collocation method $IIIb$, we obtain the errors 1.51×10^{-11} for $h = \pi/20$ and 7.74×10^{-12} for $h = \pi/40$. The ratio is 1.95 but as we require the ratio to be 64, this again shows the effects of the accumulation of rounding error.

Example 1.10

For the next problem, we follow Coleman [18]. The differential equation is

$$y'' = -\left\{16\pi^2 e^{2x} - \frac{1}{4}\right\} y, \quad y(0) = 1, \quad y'(0) = -\frac{1}{2}$$

with exact solution

$$y(x) = e^{-x/2}\cos(4\pi\, e^x).$$

The interval is $[x_0, x_{max}]$ where $x_0 = 0$ and $x_{max} = x_0 + Nh = \log(209/8)$ is the hundredth positive zero of $y(x)$. The sd-values are computed for the maximum absolute error over the interval where we define

$$sd_{max} = -\log_{10}[\max(|y(x_n) - y_n|)]$$

as the number of significant digits for the maximum absolute error over the interval $[x_0, x_{max}]$ in the approximate solution. Also

$$sd_{last} = -\log_{10}(|y(x_{max}) - y_N|)$$

is the absolute error at the end-point x_{max} in the approximate solution. The sd_{max} value is the top value in each box of table 7.44 and the bottom value is the sd_{last} value. In table 7.44, the angular frequency is $k = 1$. The polynomial collocation methods IIb, $IIIa$ and $IIIb$ are used in table 7.45, and in table 7.46 the frequency parameter is $k = \sqrt{16\pi^2 e^{2x} - 1/4}$ where the sd_{max} values have been given for both tables 7.45 and 7.46. The steplength is $h = \dfrac{x_{max}}{400 \times 2^m}$, where $m = 1, 2, 3$ and 4.

In table 7.47, results are shown for various methods used by Coleman [18] which are listed below. The sd_{last} values only are given.

Method	Step/Stage number	Description of method	Algebraic order	Order of dispersion
1	2-step	Explicit	4	4
2	2-step	Singly-implicit	4	6
3	2-step	Diagonally implicit	4	6
4	2-step	Implicit	4	8
5	2-stage	DIRKN	2	6
6	3-stage	DIRKN	2	8

Method	$m=1$	$m=2$	$m=3$	$m=4$
Ia	-19.1	-10.5	-5.16	-2.24
	-19.1	-10.5	-5.16	-1.84
Ib	0.41	0.74	1.31	1.91
	1.14	0.79	1.31	1.91
Ic	0.41	0.49	0.56	0.64
	14.7	12.1	6.60	4.19
IIa	0.35	0.50	1.02	1.61
	0.82	0.76	1.03	1.61
IIb	2.07	3.23	4.43	5.62
	2.07	3.23	4.43	5.62
$IIIa$	1.70	2.88	4.08	5.41
	1.70	2.89	4.08	5.65
$IIIb$	4.22	6.00	7.80	9.60
	4.22	6.00	7.80	9.60
IVa^*	0.36	0.50	1.02	1.61
	0.82	0.76	1.03	1.61
IVb^*	2.07	3.23	4.43	5.65
	2.07	3.23	4.43	5.65
S_1	1.04	2.26	3.35	4.15
	1.04	2.26	3.35	4.15
S_2	1.04	2.26	3.47	4.68
	1.04	2.26	3.47	4.68
S_3	1.04	2.26	3.47	4.68
	1.04	2.26	3.47	4.68

Table 7.44: Ex 1.10 - Methods $I - IV^*$ and $S_1 - S_3$: $k = 1$

Method	$m = 1$	$m = 2$	$m = 3$	$m = 4$
IIb	2.07	3.23	4.43	5.63
$IIIa$	1.70	2.88	4.08	5.28
$IIIb$	4.22	6.00	7.80	9.60
S_0	1.04	2.26	3.47	4.68

Table 7.45: Ex 1.10 - Methods $IIb, IIIa$ and $IIIb$ and S_0: $k = 0$

Method	$m = 1$	$m = 2$	$m = 3$	$m = 4$
Ia	0.92	1.21	1.50	1.80
Ib	3.97	4.62	5.23	5.84
Ic	0.91	1.20	1.50	1.80
IIa	1.58	2.15	2.75	3.34
IIb	3.85	5.06	6.26	7.46
$IIIa$	3.38	4.58	5.78	6.98
$IIIb$	5.67	7.47	9.28	11.10
IVa^*	1.56	2.15	2.74	3.35
IVb^*	3.55	4.76	5.95	7.16
S_1	2.54	3.78	5.00	6.20
S_2	2.84	4.09	5.30	6.50
S_3	4.23	5.55	6.78	7.98

Table 7.46: Ex 1.10 - Methods $I - IV^*$ and $S_1 - S_3$: $k = \sqrt{16\pi^2 e^{2x} - 1/4}$

Method	$m=1$	$m=2$	$m=3$	$m=4$
1	1.1	2.4	3.6	4.9
2	2.7	4.4	6.0	7.5
3	2.8	4.4	6.0	7.5
4	3.1	4.6	6.1	7.5
5	3.2	5.1	7.1	7.5
6	5.1	5.6	6.6	7.5

Table 7.47: Ex 1.10 - Methods of Coleman, sd_{last} values

Conclusions

For the mixed collocation methods with $k = 1$, the results are poor for the lower order methods but they improve for the higher order methods and the 6th order mixed collocation method $IIIb$ is superior to all the other methods in this example. The multistep methods $S_1 - S_3$ are not as good as the 4th order mixed collocation methods IIb, $IIIa$ and IVb^*. Note that methods IVa^* and IVb^* give similar results to the methods IIa and IIb respectively.

When the polynomial collocation method is used for IIb, $IIIa$ and $IIIb$, the results are similar to the mixed collocation methods. Also, the results of the polynomial based method S_0 are the same as those of the exponentially-fitted methods S_2 and S_3. This is perhaps because none of the methods are exact for this problem and so the polynomial based methods approximate the solution as well as the exponentially-fitted methods. Also, the choice of $k = 1$ for the angular frequency may not be a good approximation for the problem, and as we have seen in earlier problems, the results for the polynomial collocation methods can be similar to the mixed collocation methods for certain values of the frequency parameter k.

When $k = \sqrt{16\pi^2 e^{2x} - 1/4}$, the results are greatly improved for the exponentially-fitted methods. The superiority of the mixed collocation methods with Gauss nodes can be seen compared to other methods of the same algebraic order. Once again, the mixed collocation method $IIIb$ is the most accurate method.

Example 1.11

Our final one-dimensional problem is,

$$y'' = -\left\{100 + \frac{1}{4x^2}\right\} y, \quad y(1) = J_0(10), \quad y'(1) = \frac{J_0(10)}{2} - 10J_1(10)$$

with exact solution $y(x) = \sqrt{x}\,J_0(10x)$ where J_0 is the Bessel function of the first kind of order 0. The interval of x is $[1, 10]$.

In tables 7.48 - 7.50, the maximum absolute error over the interval $[1, 10]$ is given. In table 7.48 the angular frequency is $k = 10$. In table 7.49 we use the polynomial collocation method, i.e. $k = 0$, and in table 7.50, $k = \sqrt{100 + 1/(4x^2)}$.

Method	$h = 0.09$	$h = 0.045$	$h = 0.0225$	$h = 0.01125$
Ia	1.23×10^{-3}	6.30×10^{-4}	3.15×10^{-4}	1.58×10^{-4}
Ib	9.35×10^{-5}	2.36×10^{-5}	5.91×10^{-6}	1.48×10^{-6}
Ic	1.29×10^{-3}	6.34×10^{-4}	3.16×10^{-4}	1.58×10^{-4}
IIa	1.88×10^{-4}	4.75×10^{-5}	1.19×10^{-5}	2.99×10^{-6}
IIb	1.26×10^{-6}	7.99×10^{-8}	5.10×10^{-9}	3.19×10^{-10}
$IIIa$	1.59×10^{-6}	1.23×10^{-7}	7.86×10^{-9}	4.92×10^{-10}
$IIIb$	8.31×10^{-9}	1.29×10^{-10}	2.08×10^{-12}	1.24×10^{-12}
IVa^*	4.25×10^{-5}	1.02×10^{-5}	2.57×10^{-6}	6.42×10^{-7}
IVb^*	3.68×10^{-7}	2.26×10^{-8}	1.41×10^{-9}	8.75×10^{-11}
S_1	7.00×10^{-6}	4.30×10^{-7}	2.78×10^{-8}	1.74×10^{-9}
S_2	1.95×10^{-6}	1.15×10^{-7}	7.14×10^{-9}	4.48×10^{-10}
S_3	6.13×10^{-7}	3.97×10^{-8}	2.59×10^{-9}	1.66×10^{-10}

Table 7.48: Ex 1.11 - Methods $I - IV^*$ and $S_1 - S_3$: $k = 10$

Method	$h = 0.09$	$h = 0.045$	$h = 0.0225$	$h = 0.01125$
Ia	$4.25 \times 10^{+6}$	$3.83 \times 10^{+3}$	$3.42 \times 10^{+1}$	2.7337
Ib	3.07×10^{-1}	9.19×10^{-2}	2.36×10^{-2}	5.92×10^{-3}
Ic	2.52×10^{-1}	2.52×10^{-1}	2.51×10^{-1}	2.31×10^{-1}
IIa	4.82×10^{-1}	1.82×10^{-1}	4.75×10^{-2}	1.20×10^{-2}
IIb	3.17×10^{-3}	2.10×10^{-4}	1.35×10^{-5}	8.49×10^{-7}
$IIIa$	7.18×10^{-3}	4.66×10^{-4}	3.00×10^{-5}	1.88×10^{-6}
$IIIb$	1.37×10^{-5}	2.22×10^{-7}	3.58×10^{-9}	5.60×10^{-11}

Table 7.49: Ex 1.11 - Polynomial Collocation Methods $I - III$: $k = 0$

Method	$h = 0.09$	$h = 0.045$	$h = 0.0225$	$h = 0.01125$
Ia	1.48×10^{-4}	7.37×10^{-5}	3.72×10^{-5}	1.86×10^{-5}
Ib	7.45×10^{-6}	1.85×10^{-6}	4.62×10^{-7}	1.16×10^{-7}
Ic	1.45×10^{-4}	7.29×10^{-5}	3.70×10^{-5}	1.85×10^{-5}
IIa	3.78×10^{-5}	9.85×10^{-6}	2.52×10^{-6}	6.37×10^{-7}
IIb	2.08×10^{-7}	1.26×10^{-8}	7.96×10^{-10}	5.02×10^{-11}
$IIIa$	5.97×10^{-7}	3.76×10^{-8}	2.35×10^{-9}	1.47×10^{-10}
$IIIb$	2.59×10^{-9}	3.89×10^{-11}	6.08×10^{-13}	5.35×10^{-14}
IVa^*	4.25×10^{-5}	1.02×10^{-5}	2.58×10^{-6}	6.43×10^{-7}
IVb^*	3.70×10^{-7}	2.27×10^{-8}	1.41×10^{-9}	8.75×10^{-11}
S_1	3.30×10^{-6}	2.05×10^{-7}	1.31×10^{-8}	8.28×10^{-10}
S_2	1.95×10^{-6}	1.15×10^{-7}	7.15×10^{-9}	4.48×10^{-10}
S_3	6.13×10^{-7}	3.96×10^{-8}	2.59×10^{-9}	1.66×10^{-10}

Table 7.50: Ex 1.11 - Mixed Collocation Methods $I - IV$: $k = \sqrt{100 + 1/(4x^2)}$

Conclusions (i)

The most accurate method is the 6th order mixed collocation method $IIIb$ for $k = 10, 0$ and $\sqrt{100 + 1/(4x^2)}$. Method IVb^* which is exact for the functions $\cos(kx)$, $\sin(kx)$, $x\cos(kx)$ and $x\sin(kx)$ is the best 4th order method for $k = 10$ whilst method IIb improves when $k = \sqrt{100 + 1/(4x^2)}$. The mixed collocation methods with Gauss nodes for the collocation points are more accurate than the other mixed collocation methods of the same order. The polynomial collocation methods are not so good for this problem although method $IIIb$ improves and is comparable to the 4th order methods IIb, $IIIa$, IVb^* and $S_1 - S_3$ with $k = 1$ and $k = \sqrt{100 + 1/(4x^2)}$ for small steplengths.

Note that the ratios of the maximum absolute errors for $h = 0.0225$ and $h = 0.01125$ for method $IIIb$ in tables 7.48 and 7.50 do not agree with the required value of

$2^6 = 64$. For $h = 0.01125$, when the coefficients are evaluated as series expansions in terms of θ we obtain the error 3.45×10^{-14} for $k = 10$, and 1.16×10^{-14} for $k = \sqrt{100 + 1/(4x^2)}$ for method *IIIb*. The ratios between these and the previous errors at $h = 0.0225$ are 60 and 52 respectively which are closer to 64. We must also take into account any rounding error incurred by Matlab from the evaluation of the Bessel function for the starting values and each time the exact solution is evaluated.

Results are also given for the 2-step methods used by Jain et al [42] and the 2-step Störmer extrapolation and interpolation methods by Gautschi [28] which are listed below. The methods by Gautschi are described in Example 1.9. In table 7.51 we present our results for the maximum absolute errors over the interval $[1, 10]$ for methods 1-8. Methods 2 and 3 are of the form

$$y_{n+1} - 2y_n + y_{n-1} = h^2[\lambda f_{n+1} + (1 - 2\lambda)f_n + \lambda f_{n-1}], \qquad (7.2)$$

where

$$\lambda = \frac{1}{4}\left(\frac{1}{\sin^2(\theta/2)} - \frac{4}{\theta^2}\right).$$

Method	Description of method	Algebraic order	Stability Interval
1	Lambert-Watson method	2	P-stable
2	Method (7.2) with $\theta = \pi/2$	2	$(0, \pi^2/4)$
3	Method (7.2) with $\theta = \pi$	2	$(0, \pi^2)$
4	Numerov (S_0)	4	$(0, 6)$

Method	Description of method	Algebraic order	Trigonometric order
5	2-step extrapolation	2	1
6	2-step extrapolation	3	2
7	2-step interpolation	1	1
8	2-step interpolation	4	2

Jain et al [42] describe a method which is of the form (7.2) with frequency $k = 10$. This method is equivalent to the Stiefel-Bettis method S_1 with $k = 10$ but the coefficients still depend on the steplength h. The definition used by Jain et al for an interval of periodicity differs from Definition 3.5 in that they consider the stability of exponentially-fitted methods when the angular frequency of the problem is the same as the frequency of the test equation. They applied Lambert and Watson's definition of P-stability which is concerned with constant coefficients and not steplength-dependent coefficients. Because θ is fixed in methods 2 and 3, then the coefficients are independent of the steplength and Definitions 2.6 and 2.7 of chapter 2 can be applied.

Method	$h = 0.09$	$h = 0.045$	$h = 0.0225$	$h = 0.01125$
1	4.97×10^{-1}	5.04×10^{-1}	2.22×10^{-1}	5.95×10^{-2}
2	7.12×10^{-2}	2.36×10^{-2}	6.40×10^{-3}	1.63×10^{-3}
3	4.25×10^{-1}	1.44×10^{-1}	3.72×10^{-2}	9.37×10^{-3}
4	3.04×10^{-2}	1.91×10^{-3}	1.21×10^{-4}	7.57×10^{-6}
5	1.88×10^{-4}	4.65×10^{-5}	1.17×10^{-5}	2.96×10^{-6}
6	4.41×10^{-4}	6.16×10^{-5}	7.98×10^{-6}	1.00×10^{-6}
7	2.47×10^{-3}	1.26×10^{-3}	6.32×10^{-4}	3.17×10^{-4}
8	2.63×10^{-5}	1.49×10^{-6}	9.23×10^{-8}	5.82×10^{-9}

Table 7.51: Ex 1.11 - Methods 1-8

Conclusions (ii)

Comparing the 2nd order methods 1, 2 and 3 with methods Ib and IIa, the latter methods are far superior and even the 1st order methods Ia and Ic are more accurate. The 4th order polynomial methods IIb and $IIIa$ are better than Numerov's method and finally comparing methods 5-8 with the mixed collocation methods of the same algebraic order in tables 7.48 and 7.50, the mixed collocation methods are the most accurate.

7.1.1 Comparisons of two-point mixed collocation methods

In this section, we study the effects of varying the collocation point c_1 for the symmetric two-point mixed collocation method (4.19). Because the collocation nodes are symmetric, i.e. $c_2 = 1 - c_1$, then we shall only consider values of c_1 in the region $0 \leq c_1 < 1/2$.

In figures 7.3 - 7.12, a dot (.) represents the maximum absolute error for a number of problems selected from section 7.1 using the 2nd-order two-point mixed collocation method (4.19). When $c_1 = 0$ and $c_2 = 1$, the method is the second-order mixed collocation method IIa. The point marked by a circle (o) is the maximum absolute error obtained when the collocation points c_1 and c_2 are the Gauss nodes, that is the 4th-order method IIb.

The following examples are labelled according to the particular problems of section 7.1.

Example 1.4
Figure 7.3 is the plot of the maximum absolute error for Problem 1.4 for various values of c_1 with fitted parameter $k = 10$ and steplength $h = \pi/40$.

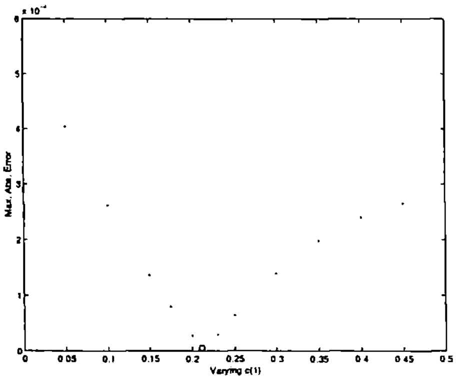

Figure 7.3: Problem 1.4 with $k = 10$ and $h = \pi/40$

Conclusions
As the value of c_1 approaches the Gauss node $(3 - \sqrt{3})/6$, then the maximum absolute error decreases and as c_1 approaches $1/2$ from the Gauss node, then the error increases. Thus, the 4th order method IIb gives the more accurate results.

Example 1.5

Figures 7.4, 7.5 and 7.6 are the plots of the maximum absolute error for Problem 1.5. The fitted frequency is 10 and the steplength is given by $h = 1/2$, $1/4$ and $1/8$ respectively.

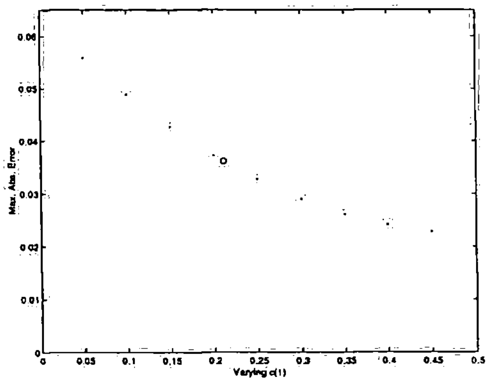

Figure 7.4: Problem 1.5 with $k = 10$ and $h = 1/2$

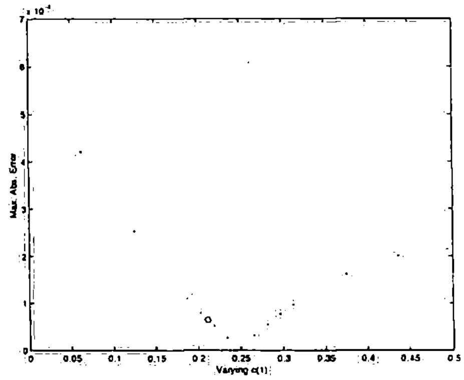

Figure 7.5: Problem 1.5 with $k = 10$ and $h = 1/4$

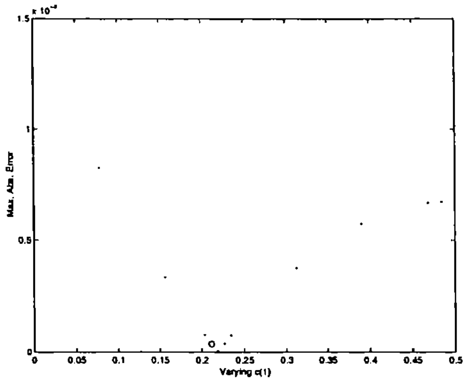

Figure 7.6: Problem 1.5 with $k = 10$ and $h = 1/8$

Conclusions

For $h = 1/2$, as $c_1 \to 1/2$, the maximum absolute error decreases but we can'improve on the Gauss nodes and the 4th order method does not give the best results. As the steplength decreases, then method IIb improves (with the Gauss nodes) but there are still values of c_1 for which the results are more accurate.

Example 1.6

The figures 7.7 and 7.8 are the plots of the maximum absolute error for Problem 1.6, the Stiefel-Bettis problem.

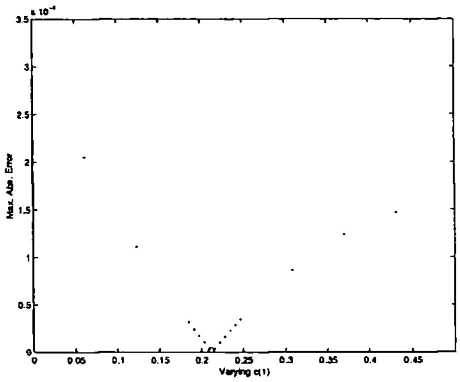

Figure 7.7: Problem 1.6 with $k = 1$ and $h = \pi/4$

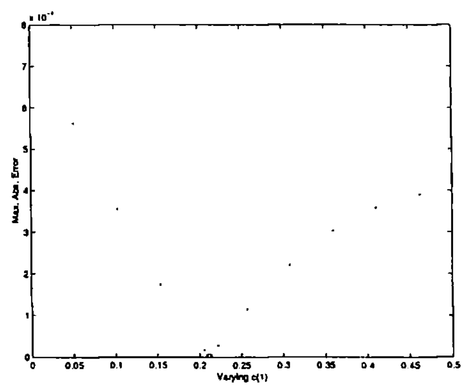

Figure 7.8: Problem 1.6 with $k = 1$ and $h = \pi/8$

Conclusions

It is easily seen that the most accurate method is the 4th order mixed collocation method IIb with the Gauss nodes.

Example 1.9

The figures 7.9 and 7.10 are the plots of the maximum absolute error for Problem 1.9. The fitted frequency is $k = 1.01$ and the steplengths are $\pi/5$ and $\pi/10$.

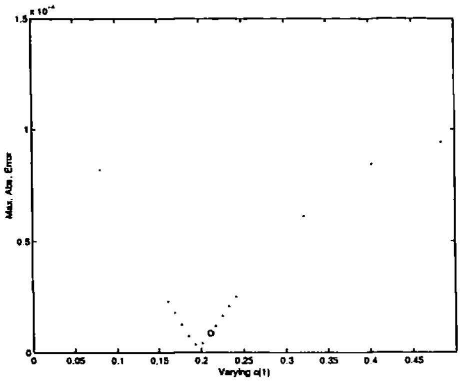

Figure 7.9: Problem 1.9 with $k = 1.01$ and $h = \pi/5$

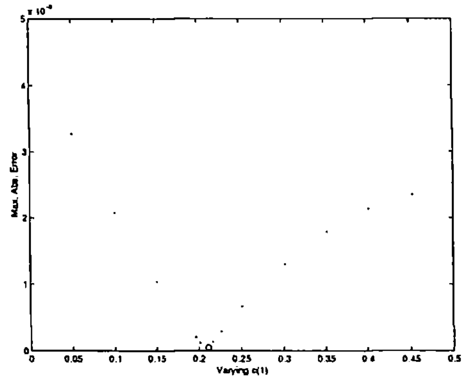

Figure 7.10: Problem 1.9 with $k = 1.01$ and $h = \pi/10$

Conclusions

For $h = \pi/5$, we can improve on the results of the 4th order method IIb but as h decreases, then the results for method IIb improve.

Example 1.11

The figures 7.11 and 7.12 are the plots of the maximum absolute error for Problem 1.11.

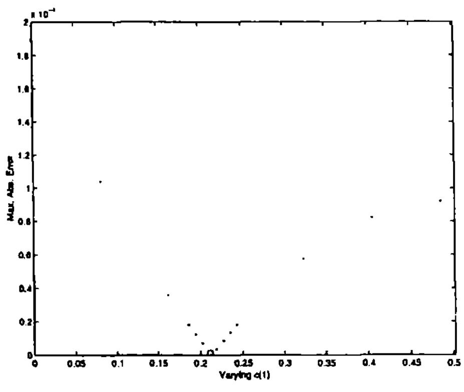

Figure 7.11: Problem 1.11 with $k = 10$ and $h = 0.09$

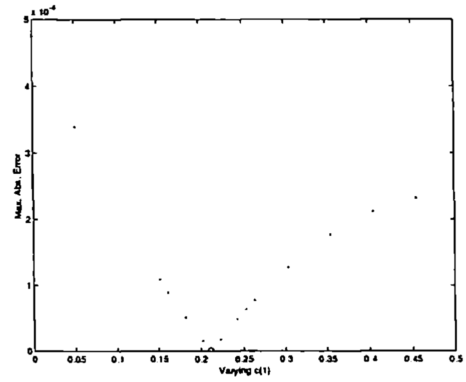

Figure 7.12: Problem 1.11 with $k = 10$ and $h = 0.045$

Conclusions

Again, as with example 1.6, the 4th order method IIb with the Gauss nodes for collocation points give the best results.

General Conclusions

Generally for small steplengths, the 4th-order mixed collocation method IIb gave the most accurate results. For large steplengths, it is sometimes possible to improve on the results with a lower order method.

7.2 Two-dimensional problems

Example 2.1
For our first two-dimensional example consider Kramarz' test problem [45]

$$y_1'' = 2498y_1 + 4998y_2, \quad y_1(0) = 2, \quad y_1'(0) = 0$$

$$y_2'' = -2499y_1 - 4999y_2, \quad y_2(0) = -1, \quad y_2'(0) = 0$$

where the exact solution is $y_1(x) = 2\cos x$ and $y_2(x) = -\cos x$.

The error is given by the maximum of the 1-norm, i.e.

$$\text{Error } = \max\{|y_1(x_n) - y_1| + |y_2(x_n) - y_2|\}$$

where y_1 and y_2 are the numerical approximations to $y_1(x_n)$ and $y_2(x_n)$ respectively. The steplength is $h = 0.01$. Because a small steplength is used throughout this problem, the difference is shown in the numerical solution when the coefficients of the methods are written as power series expansions in terms of θ compared to the exact form.

The maximum absolute errors over the interval $[0, 80]$ are given in tables 7.52 - 7.54. For the exponentially-fitted methods in tables 7.52, 7.53 and 7.55, the top entries are the numerical solutions when the coefficients b_i, d_i and a_{ij} of the mixed collocation methods are in exact form. The bottom entries are the coefficients written as power series expansions. The fitted angular frequency is $k = 1$ and for the two frequency method V_1^*, we take $k_1 = 1$ and $k_2 = 0.1$ and for V_2^*, $k_1 = 1$ and $k_2 = 50$. In table 7.56, results are presented for the polynomial collocation methods IIb, $IIIa$ and $IIIb$, and Numerov's method S_0.

The methods used by Coleman and Booth [21] in table 7.54 are a 6th order Panovsky-Richardson method which we will denote by (PR4), and the equivalent 6th order Runge-Kutta-Nyström method given by (RKN6).

	Ia	Ib	Ic	IIa
$x = 1$	1.40×10^{-13}	1.07×10^{-13}	1.65×10^{-14}	3.75×10^{-13}
	1.56×10^{-13}	6.86×10^{-14}	1.47×10^{-13}	1.91×10^{-14}
$x = 2$	4.23×10^{-11}	2.26×10^{-13}	5.37×10^{-14}	7.73×10^{-13}
	4.88×10^{-11}	1.27×10^{-13}	1.63×10^{-13}	3.76×10^{-14}
$x = 5$	2.44×10^{-3}	2.98×10^{-13}	9.20×10^{-14}	2.12×10^{-12}
	1.88×10^{-3}	3.74×10^{-13}	2.77×10^{-13}	4.50×10^{-14}
$x = 10$	$1.24 \times 10^{+10}$	3.23×10^{-13}	1.25×10^{-13}	3.40×10^{-12}
	$1.44 \times 10^{+10}$	3.74×10^{-13}	2.77×10^{-13}	3.08×10^{-13}
$x = 20$	$4.70 \times 10^{+35}$	4.35×10^{-13}	4.92×10^{-13}	8.07×10^{-12}
	$5.31 \times 10^{+35}$	5.60×10^{-13}	4.26×10^{-13}	5.02×10^{-13}
$x = 40$	$6.77 \times 10^{+86}$	4.35×10^{-13}	8.15×10^{-13}	1.73×10^{-11}
	$5.92 \times 10^{+86}$	7.94×10^{-13}	1.05×10^{-12}	6.69×10^{-13}
$x = 80$	$1.40 \times 10^{+189}$	7.82×10^{-13}	1.97×10^{-12}	3.41×10^{-11}
	$1.12 \times 10^{+189}$	1.33×10^{-12}	2.04×10^{-12}	7.53×10^{-13}

	IIb	$IIIa$	$IIIb$
$x = 1$	1.13×10^{-12}	5.00×10^{-12}	2.75×10^{-11}
	2.18×10^{-14}	1.13×10^{-13}	9.90×10^{-14}
$x = 2$	2.42×10^{-12}	1.10×10^{-11}	6.00×10^{-11}
	2.18×10^{-14}	1.33×10^{-13}	1.71×10^{-13}
$x = 5$	6.17×10^{-12}	2.96×10^{-11}	1.59×10^{-10}
	9.67×10^{-14}	3.45×10^{-13}	2.23×10^{-13}
$x = 10$	1.01×10^{-11}	4.88×10^{-11}	2.61×10^{-10}
	2.31×10^{-13}	3.45×10^{-13}	2.24×10^{-13}
$x = 20$	2.33×10^{-11}	1.13×10^{-10}	5.99×10^{-10}
	2.67×10^{-13}	6.64×10^{-13}	3.50×10^{-13}
$x = 40$	4.96×10^{-11}	2.43×10^{-10}	1.29×10^{-9}
	9.55×10^{-13}	6.78×10^{-13}	4.20×10^{-13}
$x = 80$	1.01×10^{-10}	4.91×10^{-10}	2.61×10^{-9}
	9.55×10^{-13}	6.78×10^{-13}	6.26×10^{-13}

Table 7.52: Ex 2.1 - Mixed Collocation Methods $I - III$: $k = 1$

	IVa^*	IVb^*	V_1^*	V_2^*
$x = 1$	2.82×10^{-14}	1.86×10^{-12}	5.57×10^{-13}	4.57×10^{-14}
	1.25×10^{-13}	3.86×10^{-14}	6.16×10^{-14}	6.86×10^{-12}
$x = 2$	1.70×10^{-13}	6.01×10^{-12}	1.30×10^{-12}	7.68×10^{-14}
	2.61×10^{-13}	4.21×10^{-14}	1.03×10^{-13}	1.50×10^{-11}
$x = 5$	2.11×10^{-13}	1.58×10^{-11}	3.20×10^{-12}	8.29×10^{-14}
	3.38×10^{-13}	1.17×10^{-13}	1.06×10^{-13}	3.97×10^{-11}
$x = 10$	4.46×10^{-13}	2.63×10^{-11}	5.35×10^{-12}	2.40×10^{-13}
	5.96×10^{-13}	1.17×10^{-13}	1.06×10^{-13}	6.54×10^{-11}
$x = 20$	1.02×10^{-12}	5.72×10^{-11}	1.24×10^{-11}	4.20×10^{-13}
	8.14×10^{-13}	3.75×10^{-13}	2.55×10^{-13}	1.50×10^{-10}
$x = 40$	1.96×10^{-12}	1.30×10^{-10}	2.73×10^{-11}	6.89×10^{-13}
	1.82×10^{-12}	4.06×10^{-13}	4.74×10^{-13}	3.25×10^{-10}
$x = 80$	4.62×10^{-12}	2.54×10^{-10}	5.47×10^{-11}	1.28×10^{-12}
	3.55×10^{-12}	4.21×10^{-13}	6.90×10^{-13}	6.56×10^{-10}

Table 7.53: Ex 2.1 - Mixed Collocation Methods IVa^*, IVb^* and V_J^*.

	PR4	RKN6
$x = 1$	6.8×10^{-14}	1.1×10^{-15}
$x = 2$	1.0×10^{-13}	1.9×10^{-15}
$x = 5$	2.2×10^{-13}	2.2×10^{-15}
$x = 10$	2.2×10^{-13}	5.8×10^{-15}
$x = 20$	4.6×10^{-13}	1.4×10^{-14}
$x = 40$	6.4×10^{-13}	2.3×10^{-14}
$x = 80$	9.0×10^{-13}	4.3×10^{-14}

Table 7.54: Ex 2.1 - Booth's Methods

	S_1	S_2	S_3
$x = 1$	1.27×10^{-12}	9.50×10^{-13}	3.84×10^{-12}
	6.16×10^{-13}	7.85×10^{-13}	7.47×10^{-13}
$x = 2$	3.23×10^{-12}	2.09×10^{-12}	8.55×10^{-12}
	1.17×10^{-12}	1.49×10^{-12}	2.00×10^{-12}
$x = 5$	8.63×10^{-12}	5.07×10^{-12}	2.32×10^{-11}
	1.98×10^{-12}	4.55×10^{-12}	5.66×10^{-12}
$x = 10$	1.47×10^{-11}	7.72×10^{-12}	3.86×10^{-11}
	4.66×10^{-12}	8.15×10^{-12}	9.55×10^{-12}
$x = 20$	3.32×10^{-11}	1.44×10^{-11}	8.55×10^{-11}
	1.12×10^{-11}	1.84×10^{-11}	2.06×10^{-11}
$x = 40$	7.13×10^{-11}	3.56×10^{-11}	1.87×10^{-10}
	2.20×10^{-11}	3.91×10^{-11}	4.38×10^{-11}
$x = 80$	1.41×10^{-10}	7.10×10^{-11}	3.77×10^{-10}
	4.80×10^{-11}	7.67×10^{-11}	8.80×10^{-11}

Table 7.55: Ex 2.1 - Multistep Methods $S_1 - S_3$: $k = 1$

	S_0	IIb	$IIIa$	$IIIb$
$x = 1$	3.58×10^{-11}	6.02×10^{-12}	1.32×10^{-11}	9.30×10^{-14}
$x = 2$	7.81×10^{-11}	1.29×10^{-11}	2.84×10^{-11}	1.30×10^{-13}
$x = 5$	2.06×10^{-10}	3.37×10^{-11}	7.52×10^{-11}	1.30×10^{-13}
$x = 10$	3.40×10^{-10}	5.52×10^{-11}	1.24×10^{-10}	2.07×10^{-13}
$x = 20$	7.84×10^{-10}	1.27×10^{-10}	2.86×10^{-10}	2.07×10^{-13}
$x = 40$	1.69×10^{-9}	2.73×10^{-10}	6.14×10^{-10}	2.07×10^{-13}
$x = 80$	3.41×10^{-9}	5.52×10^{-10}	1.24×10^{-9}	4.75×10^{-13}

Table 7.56: Ex 2.1 - Methods S_0, IIb, $IIIa$ and $IIIb$: $k = 0$

Conclusions

In tables 7.52 and 7.53, the results are generally more accurate when the coefficients of the steplength dependent methods are power series expansions. For method *IIIb*, when the exact form for the coefficients is used, the maximum absolute errors over the interval are poor compared to the one and two-point mixed collocation methods and this is because of the accumulation of rounding errors in calculating the coefficients which are more complicated. The results greatly improve using the series expansions. The exponentially-fitted multistep methods $S_1 - S_3$ give similar results to the mixed collocation methods and show an improvement when the coefficients are written as series expansions with the exception of method S_2 towards the end of the interval. The mixed collocation methods are superior when the series expansions are used.

When $k = 0$, the 6th order method *IIIb* is one of the most accurate methods whilst the method RKN6 is the best method. The polynomial collocation method *IIIb* gives slightly better results than the corresponding mixed collocation method when the coefficients are in the exact form because of the accumulation of rounding error in the latter method.

Example 2.2

For our next example, consider the problem,

$$y_1'' = -7y_1 + 3y_2, \quad y_1(0) = y_1'(0) = 0,$$

$$y_2'' = 2y_1 - 6y_2, \quad y_2(0) = y_2'(0) = 1.$$

where the theoretical solution is

$$y_1(x) = \frac{3}{5}\cos(2x) - \frac{3}{5}\cos(3x) + \frac{3}{10}\sin(2x) - \frac{1}{5}\sin(3x),$$

$$y_2(x) = \frac{3}{5}\cos(2x) + \frac{2}{5}\cos(3x) + \frac{3}{10}\sin(2x) + \frac{2}{15}\sin(3x).$$

The errors in tables 7.57 - 7.60 are given by the 2-norm which we define by $\Omega(x) = \sqrt{[y_1(x) - y_1]^2 + [y_2(x) - y_2]^2}$ where y_1 and y_2 are the numerical approximations to $y_1(x)$ and $y_2(x)$ respectively at the step x. In tables 7.57 - 7.60, the top value is the maximum absolute error over the interval $[0, 10]$ and the bottom value is the end-point error given by $\Omega(10)$. If only one entry appears then the end-point error is the same as the maximum absolute error. In tables 7.57, 7.59 and 7.60, three different values for the frequency parameter k are given, $k = 2$, $k = 3$ and $k = 0$ respectively. In table 7.58, the two frequencies are given by $k_1 = 2$ and $k_2 = 3$.

Method	$h = 0.1$	$h = 0.05$	$h = 0.025$
Ia	1.6915	6.09×10^{-1}	2.60×10^{-1}
	5.78×10^{-1}	1.34×10^{-1}	4.58×10^{-2}
Ib	2.24×10^{-2}	5.66×10^{-3}	1.42×10^{-3}
Ic	5.26×10^{-1}	3.38×10^{-1}	1.94×10^{-1}
	4.85×10^{-2}	3.54×10^{-2}	2.32×10^{-2}
IIa	4.68×10^{-2}	1.18×10^{-2}	2.96×10^{-3}
IIb	2.98×10^{-5}	1.87×10^{-6}	1.17×10^{-7}
$IIIa$	5.16×10^{-5}	3.23×10^{-6}	2.02×10^{-7}
$IIIb$	1.53×10^{-8}	2.42×10^{-10}	8.53×10^{-12}
IVa^*	2.61×10^{-2}	6.57×10^{-3}	1.64×10^{-3}
IVb^*	1.95×10^{-5}	1.22×10^{-6}	7.63×10^{-8}
S_1	2.12×10^{-4}	1.33×10^{-5}	8.30×10^{-7}
S_2	1.18×10^{-4}	7.37×10^{-6}	4.61×10^{-7}
S_3	6.57×10^{-5}	4.10×10^{-6}	2.56×10^{-7}

Table 7.57: Ex 2.2 - Methods $I - IV^*$ and $S_1 - S_3$: $k = 2$

Method	$h = 0.1$	$h = 0.05$	$h = 0.025$
V^*	5.31×10^{-14}	2.35×10^{-13}	5.09×10^{-13}
	4.63×10^{-14}	2.04×10^{-13}	5.09×10^{-13}

Table 7.58: Ex 2.2 - Mixed Collocation Method V^* : $k_1 = 2$ and $k_2 = 3$

Method	$h = 0.1$	$h = 0.05$	$h = 0.025$
Ia	6.58×10^{-1}	4.23×10^{-1}	2.43×10^{-1}
	5.18×10^{-1}	3.32×10^{-1}	1.89×10^{-1}
Ib	1.65×10^{-2}	4.11×10^{-3}	1.03×10^{-3}
	1.15×10^{-2}	2.84×10^{-3}	7.08×10^{-4}
Ic	2.1510	7.65×10^{-1}	3.26×10^{-1}
	1.5737	5.80×10^{-1}	2.50×10^{-1}
IIa	3.59×10^{-2}	8.97×10^{-3}	2.24×10^{-3}
	2.66×10^{-2}	6.51×10^{-3}	1.62×10^{-3}
IIb	1.77×10^{-5}	1.10×10^{-6}	6.89×10^{-8}
	1.30×10^{-5}	8.09×10^{-7}	5.05×10^{-8}
$IIIa$	1.69×10^{-5}	1.06×10^{-6}	6.61×10^{-8}
	1.19×10^{-5}	7.41×10^{-7}	4.63×10^{-8}
$IIIb$	5.06×10^{-9}	7.95×10^{-11}	4.06×10^{-12}
	3.49×10^{-9}	5.48×10^{-11}	4.05×10^{-12}
IVa^*	4.56×10^{-2}	1.13×10^{-2}	2.81×10^{-3}
	3.17×10^{-2}	8.05×10^{-3}	2.02×10^{-3}
IVb^*	3.34×10^{-5}	2.08×10^{-6}	1.30×10^{-7}
	2.43×10^{-5}	1.52×10^{-6}	9.48×10^{-8}
S_1	7.15×10^{-5}	4.47×10^{-6}	2.80×10^{-7}
	5.13×10^{-5}	3.22×10^{-6}	2.02×10^{-7}
S_2	8.97×10^{-5}	5.60×10^{-6}	3.50×10^{-7}
	6.44×10^{-5}	4.03×10^{-6}	2.52×10^{-7}
S_3	1.13×10^{-4}	7.00×10^{-6}	4.47×10^{-7}
	8.08×10^{-5}	5.04×10^{-6}	3.15×10^{-7}

Table 7.59: Ex 2.2 - Methods $I - IV^*$ and $S_1 - S_3$: $k = 3$

Method	$h = 0.1$	$h = 0.05$	$h = 0.025$
Ia	5.8687 3.0168	1.6342 6.37×10^{-1}	6.28×10^{-1} 2.39×10^{-1}
Ib	4.28×10^{-2}	1.08×10^{-2}	2.72×10^{-3}
Ic	1 step $2.23 \times 10^{+9}$	1 step $1.06 \times 10^{+14}$	1 step $4.02 \times 10^{+18}$
IIa	8.96×10^{-2}	2.28×10^{-2}	5.72×10^{-3}
IIb	4.54×10^{-5}	2.85×10^{-6}	1.78×10^{-7}
$IIIa$	9.50×10^{-5}	5.96×10^{-6}	3.73×10^{-7}
$IIIb$	1.89×10^{-8}	2.96×10^{-10}	4.63×10^{-12}
S_0	2.63×10^{-4}	1.64×10^{-5}	1.02×10^{-6}

Table 7.60: Ex 2.2 - Methods $I - III$ and S_0 : $k = 0$

Conclusions

On comparing the results, for all the methods except IVa^*, IVb^* and S_3, they are more accurate for the higher frequency $k = 3$. Once again, the 4th order methods IIb and $IIIa$ are superior to the multistep methods $S_1 - S_3$ for all values of the fitted frequency k. For $k = 2$, the 4th order method IVb^* is superior to all the other 4th order methods but for $k = 3$, methods IIb and $IIIa$ are more accurate. The two frequency method V^* is exact except for rounding error and the 6th order method $IIIb$ is the second best method. If we look at the ratios of the methods as the steplength is halved, then we should obtain 2^p where p is the order of the method. For the mixed collocation method $IIIb$, when $h = 0.025$, the ratio is approximately 28 and 20 for $k = 2$ and $k = 3$ respectively. This is because of the effects of rounding error from evaluating the coefficients. When we use the series expansion in terms of θ for the coefficients, the errors are 3.77×10^{-12} and 1.24×10^{-12} for $k = 2$ and $k = 3$ respectively when $h = 0.025$.

The polynomial collocation method $IIIb$ gives very similar results to the corresponding mixed collocation method. Therefore the polynomial collocation method $IIIb$ is very useful because the coefficients are independent of the steplength and so there is less rounding error.

Example 2.3

Consider the problem

$$y_1'' = -\lambda^2 y_1 + 0.0025e^{(-0.05x)} + \lambda^2 e^{(-0.05x)}$$

$$y_2'' = -\lambda^2 y_2 + 0.0025e^{(-0.05x)} + \lambda^2 e^{(-0.05x)}$$

with initial conditions

$$y_1(0) = a + 1, \quad y_1'(0) = -0.05$$

$$y_2(0) = 1, \quad y_2'(0) = \lambda a - 0.05$$

and whose theoretical solution is

$$y_1(x) = a\cos(\lambda x) + e^{(-0.05x)}, \quad y_2(x) = a\sin(\lambda x) + e^{(-0.05x)}.$$

It was pointed out by Lambert and Watson [47] that this problem is intended to illustrate numerically the property of P-stability. With the choice of parameter $a = 0$, the 2-dimensional problem corresponds to the high frequency oscillations not being present. The results for the mixed collocation methods and exponentially-fitted methods $S_1 - S_3$ with fitted angular frequency $k = \lambda$ are presented in table 7.61, and the polynomial collocation methods and Numerov's method S_0 in table 7.62 with $k = 0$. The errors in tables 7.61 and 7.62 are given by the maximum of $|\Sigma(x)|$ over the interval $[0, 20\pi]$ where

$$\Sigma(x) = \gamma(x) - \sqrt{y_1^2 + y_2^2} \quad \text{and}$$

$$\gamma(x) = \sqrt{y_1^2(x) + y_2^2(x)} = \sqrt{a^2 + 2ae^{(-0.05x)}[\cos(\lambda x) + \sin(\lambda x)] + 2e^{(-0.1x)}}.$$

The absolute error in the radius $\sqrt{y_1^2 + y_2^2}$ at $x = 20\pi$ for $a = 0$ is given in table 7.63 for methods 1-6 used by Cash [3] and Jain et al [43] which are listed below. In tables 7.64 and 7.66, results are presented for the mixed collocation methods $I - III$ and multistep methods $S_1 - S_3$ with $a = 0.1$ and 0.2 respectively, and in tables 7.65 and 7.67, the polynomial based methods $I - III$ and S_0 are used with $a = 0.1$ and 0.2 respectively. The steplength is $h = \pi/32$ throughout this example.

Method	Description of method	Algebraic order
1	2-step P-stable [3]	2
2	2-step P-stable hybrid [3]	4
3	2-step P-stable hybrid [3]	6
4	5-step Störmer-Cowell [43]	6
5	4-step symmetric [43]	6
6	4-step P-stable hybrid [43]	6

	$\lambda = 5$	$\lambda = 10$	$\lambda = 15$	$\lambda = 20$
Ia	6.76×10^{-3}	6.74×10^{-3}	6.78×10^{-3}	7.07×10^{-3}
Ib	2.86×10^{-4}	5.78×10^{-4}	8.85×10^{-4}	1.22×10^{-3}
Ic	6.83×10^{-3}	6.93×10^{-3}	7.01×10^{-3}	6.95×10^{-3}
IIa	5.57×10^{-6}	5.68×10^{-6}	5.81×10^{-6}	5.96×10^{-6}
IIb	2.24×10^{-8}	9.18×10^{-8}	2.13×10^{-7}	3.94×10^{-7}
$IIIa$	1.15×10^{-10}	2.34×10^{-10}	3.61×10^{-10}	5.03×10^{-10}
$IIIb$	8.04×10^{-13}	1.61×10^{-12}	5.64×10^{-12}	1.41×10^{-11}
IVa^*	5.71×10^{-2}	2.51×10^{-1}	6.69×10^{-1}	1.5607
IVb^*	2.63×10^{-4}	4.38×10^{-3}	2.35×10^{-2}	8.07×10^{-2}
S_1	6.88×10^{-12}	7.39×10^{-12}	8.59×10^{-12}	1.11×10^{-11}
S_2	6.95×10^{-8}	3.07×10^{-7}	8.44×10^{-7}	2.08×10^{-6}
S_3	7.02×10^{-4}	1.28×10^{-2}	8.49×10^{-2}	4.25×10^{-1}

Table 7.61: Ex 2.3 - Methods $I - IV^*$ and $S_1 - S_3$: $a = 0$ and $k = \lambda$

	$\lambda = 5$	$\lambda = 10$	$\lambda = 15$	$\lambda = 20$
Ia	$1.89 \times 10^{+9}$	$3.71 \times 10^{+47}$	$3.01 \times 10^{+94}$	$3.05 \times 10^{+141}$
Ib	2.81×10^{-8}	1.33×10^{-8}	8.09×10^{-9}	5.11×10^{-9}
Ic	2.28×10^{-5}	3.86×10^{-5}	1.70×10^{-5}	2.02×10^{-5}
IIa	5.53×10^{-10}	1.39×10^{-10}	6.17×10^{-11}	3.47×10^{-11}
IIb	1.86×10^{-12}	1.87×10^{-12}	1.87×10^{-12}	1.86×10^{-12}
$IIIa$	1.18×10^{-14}	7.11×10^{-15}	4.40×10^{-15}	8.64×10^{-15}
$IIIb$	1.33×10^{-15}	2.41×10^{-15}	2.45×10^{-15}	2.28×10^{-15}
S_0	1.65×10^{-15}	1.41×10^{-15}	2.20×10^{-15}	2.20×10^{-15}

Table 7.62: Ex 2.3 - Methods $I - III$ and S_0 : $a = 0$ and $k = 0$

	$\lambda = 5$	$\lambda = 10$	$\lambda = 15$	$\lambda = 20$
1	6.35×10^{-10}	6.00×10^{-11}	7.21×10^{-12}	3.61×10^{-11}
2	4.39×10^{-15}	9.42×10^{-16}	2.83×10^{-15}	7.22×10^{-15}
3	4.40×10^{-16}	3.21×10^{-14}	4.93×10^{-13}	1.40×10^{-12}
4	3.74×10^{-16}	2.24×10^{-16}	6.94×10^{-18}	2.08×10^{-16}
5	5.42×10^{-15}	2.03×10^{-15}	1.35×10^{-15}	2.56×10^{-15}
6	4.18×10^{-14}	1.51×10^{-13}	2.15×10^{-12}	1.79×10^{-12}

Table 7.63: Ex 2.3 - Methods 1-6 : $a = 0$

Conclusions (i)

For the exponentially-fitted methods $I - IV^*$ and $S_1 - S_3$, the methods that give the best results are those of algebraic order 4 or 6 and which have a high polynomial order. By this we mean the methods which have the highest degree of polynomial in the basis of functions. Comparing the 4th order methods, S_1 fits polynomials up to degree 3, method $IIIa$ up to degree 2, methods IIb and S_2 up to degree 1, and S_3 is not exact for polynomials. From table 7.61, S_1 gives the best results for the 4th order methods followed by $IIIa$. The 6th order method $IIIb$ is again the most accurate when $k = \lambda$. For $k = 0$, the methods with the higher algebraic and polynomial order do well and methods $IIIb$ and S_0 are superior to the exponentially-fitted methods. They are also comparable to methods 2, 4 and 5 although only the absolute error at the end-point is given in table 7.63.

	$\lambda = 5$	$\lambda = 10$
Ia	6.76×10^{-3}	6.73×10^{-3}
Ib	2.86×10^{-4}	5.77×10^{-4}
Ic	6.81×10^{-3}	6.92×10^{-3}
IIa	5.56×10^{-6}	5.67×10^{-6}
IIb	2.24×10^{-8}	9.16×10^{-8}
$IIIa$	1.15×10^{-10}	2.34×10^{-10}
$IIIb$	1.96×10^{-13}	1.61×10^{-12}
S_1	6.88×10^{-12}	7.39×10^{-12}
S_2	6.95×10^{-8}	3.07×10^{-7}
S_3	7.02×10^{-4}	1.28×10^{-2}

Table 7.64: Ex 2.3 - Methods $I - III$ and $S_1 - S_3$: $a = 0.1$ and $k = \lambda$

	$\lambda = 5$	$\lambda = 10$
Ia	$6.36 \times 10^{+14}$	$5.12 \times 10^{+53}$
Ib	1.16×10^{-1}	1.97×10^{-1}
Ic	1 step $6.36 \times 10^{+14}$	1 step $2.40 \times 10^{+1}$
IIa	1.90×10^{-1}	2.01×10^{-1}
IIb	3.41×10^{-4}	1.04×10^{-2}
$IIIa$	7.78×10^{-4}	2.40×10^{-2}
$IIIb$	4.53×10^{-7}	5.60×10^{-5}
S_0	2.17×10^{-3}	7.56×10^{-2}

Table 7.65: Ex 2.3 - Methods $I - III$ and S_0 : $a = 0.1$ and $k = 0$

The polynomial collocation method Ic was unable to satisfy the tolerance within a suitable number of iterations in tables 7.65 and 7.67.

	$\lambda = 5$	$\lambda = 10$
Ia	6.74×10^{-3}	6.72×10^{-3}
Ib	2.83×10^{-4}	5.74×10^{-4}
Ic	6.77×10^{-3}	6.87×10^{-3}
IIa	5.52×10^{-6}	5.63×10^{-6}
IIb	2.22×10^{-8}	9.11×10^{-8}
$IIIa$	1.14×10^{-10}	2.32×10^{-10}
$IIIb$	1.95×10^{-13}	1.60×10^{-12}
S_1	6.86×10^{-12}	7.38×10^{-12}
S_2	6.93×10^{-8}	3.07×10^{-7}
S_3	7.00×10^{-4}	1.28×10^{-2}

Table 7.66: Ex 2.3 - Methods $I - III$ and $S_1 - S_3$: $a = 0.2$ and $k = \lambda$

	$\lambda = 5$	$\lambda = 10$
Ia	$1.27 \times 10^{+15}$	$1.02 \times 10^{+54}$
Ib	1.82×10^{-1}	3.94×10^{-1}
Ic	1 step $1.74 \times 10^{+6}$	1 step $4.81 \times 10^{+1}$
IIa	3.24×10^{-1}	4.03×10^{-1}
IIb	5.00×10^{-4}	1.53×10^{-2}
$IIIa$	1.15×10^{-3}	3.52×10^{-2}
$IIIb$	6.64×10^{-7}	8.33×10^{-5}
S_0	3.19×10^{-3}	1.13×10^{-1}

Table 7.67: Ex 2.3 - Methods $I - III$ and S_0 : $a = 0.2$ and $k = 0$

Conclusions (ii)

For $k = \lambda$, again the methods with the higher polynomial order are more accurate than others of the same algebraic order. When $k = 0$, the polynomial collocation methods with the Gauss points are superior to other polynomial collocation methods of the same order and the results are not as good as when $a = 0$ because trigonometric terms appear in the exact solution. The results for the mixed collocation methods $I - III$ are similar when the parameter $a = 0.1$ and $a = 0.2$. The exponentially-fitted methods show a slight improvement in the results as a is increased whilst the results for the polynomial based methods are slightly worse.

Example 2.4

For our final example, we study the two-body problem

$$y_1'' = \frac{-y_1}{r^3}, \quad y_1(0) = 1 - \epsilon, \quad y_1'(0) = 0$$

$$y_2'' = \frac{-y_2}{r^3}, \quad y_2(0) = 0, \quad y_2'(0) = \sqrt{\frac{1+\epsilon}{1-\epsilon}}$$

where $r = \sqrt{y_1^2 + y_2^2}$. The exact solution is $y_1(x) = \cos(u) - \epsilon$ and $y_2(x) = \sqrt{1-\epsilon^2}\sin(u)$ where $u = x + \epsilon\sin(u)$. Because we are interested in problems with oscillatory solutions we take $\epsilon < 1$.

The method derived by Ozawa [51] is a four-stage 4th order implicit Runge-Kutta-Nyström method of trigonometric order 1 with order of dispersion 4, and we shall denote the method by TRKN1(4). The top entries in tables 7.68 - 7.79 are the maximum absolute errors on the interval $[0, 20]$ with the coefficients b_i, d_i and a_{ij} in their exact form, whilst the bottom entries are the maximum absolute errors with the coefficients as power series expansions. If only one value appears, then the same result is obtained. The angular frequency is $k = 1$.

The error is given by

$$\text{Error} = \max\{|y_1(x_n) - y_1| + |y_2(x_n) - y_2|\}$$

where y_1 and y_2 are the numerical approximations to $y_1(x_n)$ and $y_2(x_n)$ respectively.

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	1.35×10^{-14}	2.61×10^{-13}	5.62×10^{-13}
	1.35×10^{-14}	1.38×10^{-13}	2.94×10^{-13}
0.01	2.16×10^{-1}	6.71×10^{-2}	2.47×10^{-2}
0.1	4.4084	1.5880	6.62×10^{-1}
0.5	5.0812	12.447	4.8388

Table 7.68: Ex 2.4 - Mixed Collocation Method *Ia*

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	2.55×10^{-14}	5.36×10^{-13}	5.87×10^{-13}
	1.81×10^{-13}	4.94×10^{-14}	1.17×10^{-14}
0.01	2.07×10^{-3}	5.08×10^{-4}	1.26×10^{-4}
0.1	3.02×10^{-2}	7.48×10^{-3}	1.86×10^{-3}
0.5	1.9016	6.19×10^{-1}	1.60×10^{-1}

Table 7.69: Ex 2.4 - Mixed Collocation Method *Ib*

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	8.56×10^{-11}	1.28×10^{-11}	2.44×10^{-12}
0.01	$*^1$	6.01×10^{-1}	3.60×10^{-2}
0.1	$*^2$	$*^3$	1.5709
0.5	$*^4$	$*^5$	$*^6$

Table 7.70: Ex 2.4 - Mixed Collocation Method *Ic*

In table 7.70, the maximum number of iterations were exceeded for $*$.

	Steps taken	|Max Error|
$*^1$	58	1.5013
$*^2$	32	1.2276
$*^3$	128	1.9312
$*^4$	12	1.7654
$*^5$	34	1.7965
$*^6$	116	2.2376

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	9.88×10^{-14}	5.67×10^{-13}	1.57×10^{-12}
	1.80×10^{-13}	4.23×10^{-14}	3.65×10^{-14}
0.01	2.14×10^{-2}	5.16×10^{-3}	1.28×10^{-3}
0.1	2.84×10^{-1}	6.86×10^{-2}	1.70×10^{-2}
0.5	3.0993	2.3480	7.66×10^{-1}

Table 7.71: Ex 2.4 - Mixed Collocation Method *IIa*

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	2.27×10^{-13}	4.28×10^{-12}	3.72×10^{-12}
	1.12×10^{-14}	1.64×10^{-14}	4.40×10^{-14}
0.01	7.65×10^{-6}	4.81×10^{-7}	3.01×10^{-8}
0.1	8.61×10^{-5}	5.39×10^{-6}	3.37×10^{-7}
0.5	2.17×10^{-2}	1.09×10^{-3}	6.52×10^{-5}

Table 7.72: Ex 2.4 - Mixed Collocation Method *IIb*

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	3.75×10^{-12}	3.12×10^{-12}	1.92×10^{-12}
	1.65×10^{-14}	1.31×10^{-14}	3.74×10^{-14}
0.01	1.89×10^{-5}	1.18×10^{-6}	7.40×10^{-8}
0.1	2.28×10^{-4}	1.43×10^{-5}	8.94×10^{-7}
0.5	5.66×10^{-3}	7.10×10^{-4}	4.90×10^{-5}

Table 7.73: Ex 2.4 - Mixed Collocation Method *IIIa*

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	2.59×10^{-12}	2.20×10^{-12}	1.42×10^{-11}
	3.23×10^{-14}	5.96×10^{-14}	8.83×10^{-14}
0.01	5.60×10^{-9}	8.59×10^{-11}	1.57×10^{-11}
0.1	5.02×10^{-8}	7.90×10^{-10}	2.80×10^{-11}
0.5	3.68×10^{-4}	4.21×10^{-6}	6.24×10^{-8}

Table 7.74: Ex 2.4 - Mixed Collocation Method *IIIb*

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	4.09×10^{-14}	8.80×10^{-13}	1.22×10^{-12}
	1.69×10^{-13}	4.94×10^{-13}	2.20×10^{-12}
0.01	1.66×10^{-4}	1.04×10^{-5}	6.53×10^{-7}
0.1	2.90×10^{-3}	1.84×10^{-4}	1.15×10^{-5}
0.5	7.65×10^{-1}	6.74×10^{-2}	4.55×10^{-3}

Table 7.75: Ex 2.4 - Multistep Method S_1

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	5.09×10^{-13}	1.26×10^{-12}	2.31×10^{-12}
	1.26×10^{-13}	2.94×10^{-13}	3.35×10^{-13}
0.01	1.26×10^{-4}	7.89×10^{-6}	4.94×10^{-7}
0.1	2.37×10^{-3}	1.50×10^{-4}	9.42×10^{-6}
0.5	7.46×10^{-1}	6.59×10^{-2}	4.46×10^{-3}

Table 7.76: Ex 2.4 - Multistep Method S_2

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	7.20×10^{-13}	2.00×10^{-12}	5.57×10^{-13}
	3.69×10^{-13}	6.85×10^{-13}	6.49×10^{-12}
0.01	8.14×10^{-5}	5.10×10^{-6}	3.19×10^{-7}
0.1	1.79×10^{-3}	1.14×10^{-4}	7.15×10^{-6}
0.5	7.28×10^{-1}	6.45×10^{-2}	4.36×10^{-3}

Table 7.77: Ex 2.4 - Multistep Method S_3

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	1.21×10^{-14}	4.64×10^{-14}	2.17×10^{-13}
0.01	9.67×10^{-5}	6.21×10^{-6}	3.92×10^{-7}
0.1	7.65×10^{-4}	6.03×10^{-5}	4.15×10^{-6}
0.5	3.00×10^{-1}	6.45×10^{-3}	1.49×10^{-4}

Table 7.78: Ex 2.4 - Ozawa's Method TRKN1(4)

ϵ	$h = 0.2$	$h = 0.1$	$h = 0.05$
0	5.84×10^{-4}	3.66×10^{-5}	2.29×10^{-6}
0.01	5.94×10^{-4}	3.62×10^{-5}	2.27×10^{-6}
0.1	8.35×10^{-4}	5.24×10^{-5}	3.28×10^{-6}
0.5	2.12×10^{-2}	1.49×10^{-3}	9.55×10^{-5}

Table 7.79: Ex 2.4 - 2-stage Gauss Runge-Kutta Method

Conclusions

For $\epsilon = 0$, the exponentially-fitted methods give very good results and when the coefficients are power series expansions, then the results do show improvement. The 4th order methods IIb and $IIIa$ are more accurate for $\epsilon \neq 0$ compared to the methods $S_1 - S_3$, Ozawa's TRKN1(4) method and the 2-stage Gauss Runge-Kutta method. The mixed collocation methods with the Gauss nodes are superior to other mixed collocation methods of the same algebraic order with the exception of methods IIb and $IIIa$ in tables 7.72 and 7.73 when $\epsilon = 0.5$. For method $IIIb$ in table 7.74, with $\epsilon = 0.01$ and $\epsilon = 0.1$, the ratios of the errors are not satisfied for $h = 0.05$. Again, this is due to rounding error accumulated from the error in calculating the coefficients. When we use the series expansions for the coefficients, the errors are 1.35×10^{-12} and 1.24×10^{-11} for $\epsilon = 0.01$ and $\epsilon = 0.1$ respectively, and the ratios are close to 64 as required.

CONCLUSIONS

By far the most accurate method out of all those used in the examples is the 6th order 3-stage mixed collocation method $IIIb$ with Gauss points for the collocation parameters. The only disadvantage of this method is the complexity of the coefficients and the time it took the program to run for small steplengths, especially for problems where the angular frequency k is dependent on the steplength. To avoid significant losses in evaluating the coefficients, writing the coefficients as power series expansions generally gave more accurate results.

For problems which involve two frequencies or combinations of products of trigonometric and polynomial functions, the extended methods IV^* and V^* are very useful and give good results whilst higher order methods struggle to come close. The mixed collocation methods of order 4 are comparable to the exponentially-fitted multistep methods of Coleman and Ixaru [23] and more often than not are more accurate. The high order mixed collocation methods are comparable or superior to other methods tested such as the polynomial based hybrid methods or exponentially-fitted multistep methods.

When the theoretical solution of the problem is included in the basis of function for the methods, then the results are exact, taking into the account the accumulation of rounding error. Generally, the mixed collocation methods with the Gauss points are slightly more accurate than those of the same algebraic order with the exception of examples 1.4, 1.5 and 2.2. The theoretical solutions in examples 1.4 and 1.5 contains two frequencies and the methods with the higher polynomial order are more accurate for particular values of the frequency parameter k.

In conclusion, the mixed collocation methods are a useful family of methods for solving problems which have oscillatory solutions. The high algebraic order methods can be quite accurate when the fitted frequency k is suitably chosen. For $k = 0$, the 6th order polynomial collocation method gave good results for certain problems.

Chapter 8

Conclusions

It was shown that the mixed collocation methods developed in chapter 4 for the initial value problem (1.1) may be regarded as Runge-Kutta-Nyström methods with steplength dependent coefficients and the order conditions up to and including order 6 are given. When the collocation points are the Gauss nodes, the maximum order is obtained and the criteria for the methods to have an interval of periodicity are satisfied. We have shown that every 2-stage Runge-Kutta-Nyström method of trigonometric order 1 is a 2-stage mixed collocation method. A general theory for the stability of exponentially-fitted methods was described and we analysed the stability of the one, two and three-point mixed collocation methods. As the fitted angular frequency approaches zero, the mixed collocation methods reduce to the corresponding polynomial collocation methods. Although it is true for up to 3 stages, we have still to prove that the order of an s-stage mixed collocation method is the same as that of the corresponding polynomial collocation method, and that an s-stage mixed collocation method has an interval of periodicity when the collocation nodes are symmetric.

Two other types of mixed collocation methods were also developed. The first involves combinations of products of polynomial and trigonometric functions, and the second method is exact for two frequencies. Although we only considered methods with low algebraic orders, the methods generally produced good results. It is clear how to obtain methods with more than two frequencies but the coefficients become complicated. For the two-frequency method, the stability analysis could only be done by setting one frequency as a multiple of the other and so a possible further area of research is the stability analysis of methods with more than one frequency.

Although the derivation of the mixed collocation methods becomes complicated because of the length of the formulae for 3 or more stages, the numerical results show that the 2-stage and 3-stage methods of order 4 or higher are very powerful methods. More often than not, they are more accurate for problems with oscillatory solutions than other exponentially-fitted methods or higher order polynomial based methods.

In section 6.3, the two-point symmetric mixed collocation method was adapted so that the collocation nodes depended on the steplength h. Although this does not improve the order of the method, for $c_1 = a\theta^2$ and $c_2 = 1 - c_1$ it was shown that the method is always defined when $a > 2/(27n^2\pi^2)$, where n is a non-negative integer.

One area not considered in this thesis is error estimation for the mixed collocation methods. Because the methods are exponentially-fitted, the techniques used for polynomial based methods cannot be applied here. As there is little literature on this subject then this is a possible area of research for future work.

Appendix A

Coefficients for the 3-stage TRKN1 method

(From section 3.2). For a 3-stage Runge-Kutta-Nyström method to have trigonometric order 1 and algebraic order 4, we require the collocation nodes to be symmetric, that is $c_3 = 1 - c_1$ and $c_2 = 1/2$, and the coefficients of the method are given by

$$b_1 = \frac{1}{2}\frac{\theta^2\,\mathcal{F}_{32} + 2\,(\mathcal{B}_3 - \mathcal{B}_2)\,\theta + 2\,\mathcal{H}_3 - 2\,\mathcal{A}_3 + 2\,\mathcal{A}_2 - 2\,\mathcal{H}_2}{\theta^2\,E},$$

$$b_2 = \frac{1}{2}\frac{\theta^2\,\mathcal{F}_{13} + 2\,(\mathcal{B}_1 - \mathcal{B}_3)\,\theta + 2\,\mathcal{H}_1 - 2\,\mathcal{H}_3 - 2\,\mathcal{A}_1 + 2\,\mathcal{A}_3}{\theta^2\,E},$$

$$b_3 = \frac{1}{2}\frac{\theta^2\,\mathcal{F}_{21} + 2\,(\mathcal{B}_2 - \mathcal{B}_1)\,\theta + 2\,\mathcal{H}_2 - 2\,\mathcal{H}_1 + 2\,\mathcal{A}_1 - 2\,\mathcal{A}_2}{\theta^2\,E},$$

$$d_1 = \frac{\theta\,\mathcal{F}_{32} - \mathcal{K}_3 + \mathcal{B}_3 + \mathcal{K}_2 - \mathcal{B}_2}{\theta\,E}, \quad d_2 = \frac{\theta\,\mathcal{F}_{13} - \mathcal{K}_1 + \mathcal{K}_3 - \mathcal{B}_3 + \mathcal{B}_1}{\theta\,E},$$

$$d_3 = \frac{\theta\,\mathcal{F}_{21} + \mathcal{K}_1 - \mathcal{B}_1 - \mathcal{K}_2 + \mathcal{B}_2}{\theta\,E},$$

$$a_{11} = \frac{\theta^2\,\alpha_1\,\mathcal{F}_{32} - \theta\,c_1\,\mathcal{B}_2 - \mathcal{F}_{21} + \mathcal{A}_2}{\mathcal{F}_{21}\,\theta^2}, \quad a_{12} = \frac{\theta^2\,\alpha_1\,\mathcal{F}_{13} + \mathcal{B}_1\,\theta\,c_1 - \mathcal{A}_1}{\mathcal{F}_{21}\,\theta^2},$$

$$a_{21} = \frac{\theta^2\,\alpha_2\,\mathcal{F}_{32} - \theta\,c_2\,\mathcal{B}_2 + \mathcal{A}_2}{\mathcal{F}_{21}\,\theta^2}, \quad a_{22} = \frac{\theta^2\,\alpha_2\,\mathcal{F}_{13} + \mathcal{B}_1\,\theta\,c_2 - \mathcal{F}_{21} - \mathcal{A}_1}{\mathcal{F}_{21}\,\theta^2},$$

$$a_{31} = \frac{\theta^2\,\alpha_3\,\mathcal{F}_{32} - \theta\,c_3\,\mathcal{B}_2 + \mathcal{F}_{32} + \mathcal{A}_2}{\mathcal{F}_{21}\,\theta^2}, \quad a_{32} = \frac{\theta^2\,\alpha_3\,\mathcal{F}_{13} + \mathcal{B}_1\,\theta\,c_3 + \mathcal{F}_{13} - \mathcal{A}_1}{\mathcal{F}_{21}\,\theta^2},$$

and $a_{13} = \alpha_1$, $a_{23} = \alpha_2$ and $a_{33} = \alpha_3$ where for j from 1 to 3,

$$\mathcal{A}_j = \sin(\theta\, c_j),\quad \mathcal{B}_j = \cos(\theta\, c_j),\quad \mathcal{H}_j = \sin(\theta\,(c_j - 1)),\quad \mathcal{K}_j = \cos(\theta\,(c_j - 1))$$

with

$$\mathcal{F}_{21} = \sin(\theta\,(c_2 - c_1)),\quad \mathcal{F}_{32} = \sin(\theta\,(c_3 - c_2)),\quad \mathcal{F}_{13} = \sin(\theta\,(c_1 - c_3))$$

and

$$E = \sin(\theta\,(c_1 - c_3)) + \sin(\theta\,(c_3 - c_2)) + \sin(\theta\,(c_2 - c_1)).$$

The method has default order 4. When the off-step points are the Gauss nodes

$$c_1 = \frac{5-\sqrt{15}}{10},\quad c_2 = \frac{1}{2},\quad c_3 = \frac{5+\sqrt{15}}{10},$$

and

$$\alpha_1 = \frac{1}{5} - \frac{\sqrt{15}}{20} - \frac{8}{5}\alpha_2 - \alpha_3,$$

then the method has order at least 5, and the maximum possible order of 6 is obtained when

$$\alpha_2 = \frac{1}{16} - \frac{\sqrt{15}}{72} - \frac{5}{4}\alpha_3.$$

As $k \to 0$, the coefficients of the TRKN1 method with algebraic order 6 reduce to those for the polynomial based 3-stage Runge-Kutta-Nyström method of order 6, i.e.

$\frac{5-\sqrt{15}}{10}$	α_3	$\frac{9-2\sqrt{15}-180\alpha_3}{90}$	$\frac{18-5\sqrt{15}+180\alpha_3}{180}$
$1/2$	$\frac{9+2\sqrt{15}-180\alpha_3}{144}$	$\frac{5}{2}\alpha_3$	$\frac{9-2\sqrt{15}-180\alpha_3}{144}$
$\frac{5+\sqrt{15}}{10}$	$\frac{18+5\sqrt{15}+180\alpha_3}{180}$	$\frac{9+2\sqrt{15}-180\alpha_3}{90}$	α_3
	$(5+\sqrt{15})/36$	$2/9$	$(5-\sqrt{15})/36$
	$5/18$	$4/9$	$5/18$

Appendix B

The Mixed Collocation Methods

In this section, the Maple programs for the derivation of the mixed collocation methods of Chapter 4 and the extended mixed collocation methods I and II of Chapter 6 are given. Maple V Release 5 was used. For the extended mixed collocation methods I and II, values of the collocation points have to be substituted for $s \geq 3$ to avoid Maple running out of memory.

B.1 The Mixed Collocation Methods : $s \geq 1$

Example

The two-point mixed collocation method (4.19) with nodes $c_1 = 0$ and $c_2 = 1$.

```
> restart;
Enter number of collocation points:
> s:=2;
If known, substitute the values of the collocation points:
> c[1]:=0; c[2]:=1;

Consider a function of the form:
> U:=a[0]*cos(k*(x-X[n]))+b[0]*sin(k*(x-X[n]))+sum(r[i]*(x-X[n])^i,
  i=0..s-1);
> UU:=diff(U,x);
> UUU:=diff(UU,x);

Apply the initial and collocation conditions and solve:
> x:=X[n];
```

```
> y[n]=U; a[0]:=solve(",a[0]);
> z[n]=UU; b[0]:=solve(",b[0]);
> for j from 1 to s do x:=X[n]+c[j]*h;
  f[n+c[j]]=combine(simplify(UUU),trig);
  r[j-1]:=simplify(solve(",r[j-1])); od;
```

```
Substitute the coefficients back into u(x) and u'(x) to obtain the
Mixed Collocation formulae:
> k:=theta/h;
> x:=X[n]+h;
> y[n+1]:=collect(combine(simplify(U),trig),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor);
> z[n+1]:=collect(combine(simplify(UU),trig),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor);
> for j from 1 to s do x:=X[n]+c[j]*h;
  Y[j]:=collect(combine(simplify(U),trig),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor); od;
```

B.2 Mixed Collocation Method I : $s \geq 2$

Example

The extended two-point mixed collocation method I (6.3) with nodes $c_1 = 0$ and $c_2 = 1$.

```
> restart;
Enter number of collocation points:
> s:=2;
If known, substitute the values of the collocation points:
> c[1]:=0; c[2]:=1;
```

```
Consider a function of the form:
> U:=(a[0]+a[1]*(x-X[n]))*cos(k*(x-X[n]))
  +(b[0]+b[1]*(x-X[n]))*sin(k*(x-X[n]))
  +sum(r[i]*(x-X[n])^i,i=0..s-3);
> UU:=diff(U,x);
> UUU:=diff(UU,x);
```

Apply the initial and collocation conditions and solve:

```
> x:=X[n];
> y[n]=U; a[0]:=solve(",a[0]);
> z[n]=UU; a[1]:=solve(",a[1]);
> for j from 2 by -1 to 1 do x:=X[n]+c[j]*h;
  f[n+c[j]]=combine(simplify(UUU),trig); b[j-1]:=solve(",b[j-1]); od;
> for j from 3 to s do x:=X[n]+c[j]*h;
  f[n+c[j]]=combine(simplify(UUU),trig); r[j-3]:=solve(",r[j-3]); od;
```

Substitute coefficients back into function u(x) and u'(x) to obtain the mixed collocation formulae:

```
> k:=theta/h;
> x:=X[n]+h;
> y[n+1]:=collect(combine(simplify(U),trig),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor);
> z[n+1]:=collect(combine(simplify(UU),trig),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor);
> for j from 1 to s do x:=X[n]+c[j]*h;
  y[n+c[j]]:=collect(combine(simplify(U),trig),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor); od;
```

We list the coefficients for the two-point method (6.3) with arbitrary collocation points c_1 and c_2. First, define

$$S_1 = \sin(\theta\, c_1),\;\; C_1 = \cos(\theta\, c_1),\;\; S_2 = \sin(\theta\, c_2),\;\; C_2 = \cos(\theta\, c_2),$$

$$S_3 = \sin(\theta\,(c_1 - c_2)),\;\; C_3 = \cos(\theta\,(c_1 - c_2)),\;\; S_4 = \sin(\theta\,(c_1 + c_2)),$$

$$C_4 = \cos(\theta\,(c_1 + c_2)),\;\; S_5 = \sin(\theta\,(1 + c_1)),\;\; C_5 = \cos(\theta\,(1 + c_1)),$$

$$S_6 = \sin(\theta\,(-1 + c_1)),\;\; C_6 = \cos(\theta\,(-1 + c_1)),\;\; S_7 = \sin(\theta\,(1 + c_2)),$$

$$C_7 = \cos(\theta\,(1 + c_2)),\;\; S_8 = \sin(\theta\,(-1 + c_2)),\;\; C_8 = \cos(\theta\,(-1 + c_2)),$$

$$S_9 = \sin(\theta\,(-c_2 + 2\,c_1)),\;\; C_9 = \cos(\theta\,(-c_2 + 2\,c_1)),\;\; S_{10} = \sin(\theta\,(2\,c_2 - c_1)),$$

$$C_{10} = \cos(\theta\,(2\,c_2 - c_1)),\;\; S_{11} = \sin(\theta\,(c_2 - 1 + c_1)),\;\; C_{11} = \cos(\theta\,(c_2 - 1 + c_1)),$$

$$S_{12} = \sin(\theta\,(-c_2 - 1 + c_1)),\quad C_{12} = \cos(\theta\,(-c_2 - 1 + c_1)),$$

$$S_{13} = \sin(\theta\,(-c_2 + 1 + c_1)),\quad C_{13} = \cos(\theta\,(-c_2 + 1 + c_1)),$$

then the coefficients are given by

$$A_1 = -\Big\{[(c_1 - c_2)\,S_{11} + c_1\,S_{12}\,(1 - c_2) + c_2\,S_{13}\,(1 - c_1)]\,\theta^2$$

$$+[(c_2 - c_1)\,C_{11} + C_{12}\,(c_2 - 2\,c_1 - 1) + C_{13}\,(2\,c_2 - c_1 + 1)]\,\theta - 2\,S_{13} - 2\,S_{12}\}\,/\mathcal{E},$$

$$A_2 = \Big\{[(c_1 - c_2)\,C_{11} + c_1\,C_{12}\,(c_2 - 1) + c_2\,C_{13}\,(1 - c_1)]\,\theta^2$$

$$+2\,[S_{12}\,(c_2 - c_1 - 1) + S_{13}\,(c_1 - c_2 - 1)]\,\theta + 4\,C_{12} - 4\,C_{13}\}\,/(\theta\,\mathcal{E}),$$

$$A_3 = \frac{2\,c_2\,S_8\,\theta^2 + [C_7\,(c_2 - 1) - C_8\,(c_2 + 3)]\,\theta + 2\,S_7 - 2\,S_8}{\mathcal{E}\,\theta^2},$$

$$A_4 = -\frac{2\,c_1\,S_6\,\theta^2 + [C_5\,(c_1 - 1) - C_6\,(c_1 + 3)]\,\theta + 2\,S_5 - 2\,S_6}{\mathcal{E}\,\theta^2},$$

$$B_1 = -\theta\,\Big\{[(c_2 - c_1)\,C_{11} + c_1\,C_{12}\,(c_2 - 1) + c_2\,C_{13}\,(1 - c_1)]\,\theta^2$$

$$+[S_{12}\,(c_2 - c_1 - 1) + S_{13}\,(c_1 - c_2 - 1)]\,\theta + C_{12} - C_{13}\}\,/\mathcal{E},$$

$$B_2 = \Big\{[(c_1 - c_2)\,S_{11} + c_1\,S_{12}\,(c_2 - 1) + c_2\,S_{13}\,(c_1 - 1)]\,\theta^2$$

$$+[(c_1 - c_2)\,C_{11} + C_{12}\,(c_1 - 2\,c_2 + 2) + C_{13}\,(2\,c_1 - c_2 - 2)]\,\theta + 2\,S_{12} + 2\,S_{13}\}\,/\mathcal{E},$$

$$B_3 = -\frac{2\,c_2\,C_8\,\theta^2 + [(c_2 - 1)\,S_7 + S_8\,(3 - c_2)]\,\theta + C_8 - C_7}{\theta\,\mathcal{E}},$$

$$B_4 = \frac{2\,c_1\,C_6\,\theta^2 + [(c_1 - 1)\,S_5 + S_6(3 - c_1)]\,\theta + C_6 - C_5}{\theta\,\mathcal{E}},$$

$$P_1 = -2\,\frac{(c_2\,C_2 - 2\,c_1\,C_2 + c_2\,C_9)\,\theta + S_2 - S_9}{\mathcal{E}},$$

$$P_2 = 2\,\frac{(2\,S_2\,c_1 - S_2\,c_2 - S_9\,c_2)\,\theta + 2\,C_2 - 2\,C_9}{\theta\,\mathcal{E}},$$

$$P_3 = -\frac{2\,\theta^2\,c_2\,c_1\,S_3 + [(c_2 + 3\,c_1)\,C_3 + (c_1 - c_2)\,C_4]\,\theta - 2\,S_3 - 2\,S_4}{\mathcal{E}\,\theta^2},$$

$$P_4 = 4\,\frac{\theta\,c_1 - S_1\,C_1}{\mathcal{E}\,\theta^2},$$

and

$$Q_1 = -2\,\frac{(2\,c_2\,C_1 - c_1\,C_1 - c_1\,C_{10})\,\theta - S_1 + S_{10}}{\mathcal{E}},$$

$$Q_2 = 2\,\frac{(S_1\,c_1 - 2\,S_1\,c_2 + S_{10}\,c_1)\,\theta - 2\,C_1 + 2\,C_{10}}{\theta\,\mathcal{E}},$$

$$Q_3 = 4\,\frac{S_2\,C_2 - \theta\,c_2}{\mathcal{E}\,\theta^2},$$

$$Q_4 = -\frac{2\,\theta^2\,c_2\,c_1\,S_3 + [(c_1 - c_2)\,C_4 - (c_1 + 3\,c_2)\,C_3]\,\theta - 2\,S_3 + 2\,S_4}{\mathcal{E}\,\theta^2}$$

where

$$\mathcal{E} = 2\theta^2 c_2 c_1 S_3 - (3C_3 + C_4)(c_2 - c_1)\theta + 4S_3.$$

B.3 Mixed Collocation Method II : $s \geq 2$

Example

The two-point mixed collocation method with two frequencies (6.6) with nodes $c_1 = 0$ and $c_2 = 1$.

```
> restart;
Enter number of collocation points:
> s:=2;
If known, substitute the values of the collocation points:
> c[1]:=0; c[2]:=1;

Consider a function of the form:
> U:=a[0]*cos(k[1]*(x-X[n]))+b[0]*cos(k[2]*(x-X[n]))+
  a[1]*sin(k[1]*(x-X[n]))+b[1]*sin(k[2]*(x-X[n]))
  +sum(r[i]*(x-X[n])^i,i=0..s-3);
> UU:=diff(U,x);
> UUU:=diff(UU,x);

Apply the initial and collocation conditions and solve:
> x:=X[n];
> y[n]=U; a[0]:=solve(",a[0]);
> z[n]=UU; a[1]:=solve(",a[1]);
> for j from 2 by -1 to 1 do x:=X[n]+c[j]*h;
  f[n+c[j]]=combine(simplify(UUU),trig); b[j-1]:=solve(",b[j-1]); od;
```

```
> for j from 3 to s do x:=X[n]+c[j]*h;
  f[n+c[j]]=combine(simplify(UUU),trig); r[j-3]:=solve(",r[j-3]); od;
```

Substitute coefficients back into function u(x) and u'(x) to obtain two-frequency mixed collocation formulae:

```
> k[1]:=theta[1]/h; k[2]:=theta[2]/h;
> x:=X[n]+h;
> y[n+1]:=collect(simplify(U),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor);
> x:=X[n]+h;
> z[n+1]:=collect(simplify(UU),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor);
> for j from 1 to s do x:=X[n]+c[j]*h;
  y[n+c[j]]:=collect(simplify(U),
  {y[n],z[n],f[n+c[1]],f[n+c[2]],f[n+c[3]]},factor); od;
```

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