Numerical Techniques for Non-Linear Ordinary Differential Equations

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MS THESIS WORK

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Dedication

This effort is dedicated to my parents, sister, and late grandparents, for their infinite support and encouragement.

May ALLAH Rub ul Izzat bless them with the best of health, life and akhira.

Ameen

Acknowledgments

I lower my head to **ALLAH Almighty**, Who is most merciful and beneficial, Who utterly has all the power and knowledge, and Who blessed me with such an opportunity to enhance my knowledge.

I am grateful to my supervisor **Prof. Azad A. Siddiqui** for his availability, and for teaching me the key elements of research work. I wish to convey my gratitude to the respected institute **National University of Science and Technology** for giving me this opportunity of learning, also my classmates, faculty members, and the **Department of Mathematics**.

I am indebted to my parents and my sister, their support provided me with a comfortable environment to spend time on education, work, and extracurricular activities equally. They always stayed by my side in every struggling situation, without their moral support and forbearance, it would have been much harder to keep up the motivation to complete this thesis.

Abstract

This thesis provides the development of families of Runge Kutta methods up to 4th order for solving non-linear ordinary differential equations. Our motive is to deeply study and compare several third and fourth order Runge Kutta methods for the sake of error analysis. First, the basics of differential equations and numerical methods are elaborated along with development of a few elementary methods. Subsequently, second and third order Runge Kutta methods are developed from a general framework. The comparison of several third order Runge Kutta methods applied to a few non-linear problems is provided. Endmost, development and comparisons of several fourth order Runge Kutta methods applied to a bunch of non-linear problems are provided.

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Chapter 1

Preliminaries

1.1 Introduction

Most physical problems contain a rate of change of any quantity with respect to any other quantity. For example, population growth or decay problems involve rate of change of population or mass over time. The mathematical modeling of such problems results in differential equations, either linear or non-linear. The motivation behind solving a differential equation is to find an explicit relation between the dependent and independent variables, that is free of derivatives. Other than that, finding a solution is like calculating values for dependent variable at all points of the domain of problem. When a mathematical problem is solved analytically, its solution is perhaps exact; however such technique is not always applicable, for instance it fails for transcendental functions.

Linear differential equations mostly end up with analytical solutions, whereas one can approximate solution for a non-linear differential equation via numerical techniques. That is why the numerical approach is applied to find solutions of such problems. A numerical method is an approach to solve mathematical equations via computer coding. Moreover, the independent variable is discretized which is ideal for coding. The main concern of research is the analysis of numerical methods for non-linear differential equations.

Elementary technique to obtain an approximate solution to differential equations or initial value problems was first developed in 1768 by Leonhard Euler [1]. In the beginning, Leonhard Euler, Kendall Atkinson, Weimin Han, and David Stewart worked to develop elementary numerical techniques for non-linear differential equations. Primary idea is to truncate the Taylor series and approximate it as a solution to an initial value problem.

1.2 Differential Equations and their Classification

Definition 1.2.1. *An equation expressed in terms of a function of one or more independent variables along with finite derivatives of the function is called a Differential Equation(DE) [2].*

There are vast applications of differential equations, from simple mixing problems to logistic equations of chaotic mathematics. The differential equations are classified mainly as ordinary and partial differential equations, defined as;

Definition 1.2.2. *An equation that involves one or more unknown functions in terms of a single independent variable and its finite derivatives, is known as an Ordinary Differential Equation (ODE) [2].*

Definition 1.2.3. *An equation involving one or more unknown functions in terms of more than a single independent variable, and its partial derivatives is called a Partial Differential Equation (PDE) [2].*

The ordinary and partial differential equations have there own specifications and types, and different methods for finding solutions. In general PDE is harder to solve as compared to an ODE. Often a higher order PDE is converted to a set of ordinary differential equations, and is solved by methods of ODE. It declares the significance of developments and improvements in methods for solving ordinary differential equations.

Further Types of Differential Equations

The differential equations have further types defined as;

Definition 1.2.4. *A DE is linear in y if it is represented as*

$$f(x) = \alpha_n(x)\frac{d^n y}{dx^n} + \alpha_{n-1}(x)\frac{d^{n-1}y}{dx^{n-1}} + \cdots + \alpha_1\frac{dy}{dx} + \alpha_0(x)y. \tag{1.1}$$

Also, it satisfies the following conditions:

1) Dependent variable y and it's derivatives have power 1.

2) Coefficients $\alpha_n, \alpha_{n-1}, \ldots, \alpha_0$, are functions of independent variable x only.

3) Dependent variable y does not appear as a multiple of its own derivative or in the form of any transcendental function [2].

The linear ODE has analytical solution and is solved via different methods, such as variable separable or integrating factor and other methods. Often to solve non-linear ODE one requires numerical methods,some elementary numerical methods are discussed in section 1.8 and 1.9.

Definition 1.2.5. *A DE is said to be non-linear if any of the conditions provided in definition 1.2.4, is violated.*

Simply, for a non-linear DE the coefficients $\alpha_n, \alpha_{n-1}, \ldots, \alpha_0$ in eq. (1.1), can appear as functions defined in dependent variable or as transcendental functions. Moreover, dependent variable and its derivatives can have power more than 1.

Definition 1.2.6. *If $f(x) = 0$ in eq. (1.1), then such DE is said to be homogeneous; on the other hand if $f(x) \neq 0$ then such DE is said to be a non-homogeneous differential equation [2].*

1.3 Numerical Method

An iterative technique is a mathematical process that utilizes an initial guess to generate a sequence of approximated solutions for a problem. Here the solution is obtained by repeating the same step to make the computations automatic. This systematic approach is called the numerical method.

Explicit and Implicit Numerical Methods

There are two main categories of numerical methods, i.e., explicit and implicit numerical methods. Such categorization is based on calculation steps involved in the process of estimating the desired value. This helps one to choose an efficient method based on ease in calculations and sometimes to avoid complex algebraic calculations. A brief discussion on explicit and implicit methods is given in subsequent sections.

Explicit Numerical Methods

The explicit numerical method calculates a value at a future state or time using only the current value. It is simple and does not require any tough calculations to compile the final formula. Let $y(x)$ be the current state and $y(x+h)$ is the future state; and h is the small step-size, then general form of an explicit numerical method is given as

$$y(x+h) = \phi(h, y(x)),$$

i.e., ϕ is any function defined only in terms of $y(x)$. Euler method is a famous example of explicit numerical methods, for reference check section 1.8.1.

Implicit Numerical Methods

An implicit numerical method calculates the desired future value by using both a current state or time and the future one. In such a case, there is a high chance that calculations are tedious. There arises a situation where one must estimate the future value that is being used in the formula. Let $y(x)$ be the current state and $y(x+h)$ is the future state; and for a small step size h general form of an implicit numerical technique is given as

$$y(x+h) = \varphi\Big(h, y(x), y(x+h)\Big),$$

where φ is a function defined in both $y(x)$ and $y(x+h)$. That is why it is necessary either to estimate $y(x+h)$ via some elementary technique or figure it out by algebraic calculations. Such obstacles are dealt according to the nature of numerical method. For example, improved Euler method is an implicit method and its process utilizes the estimation from Euler method. The brief discussion on this case is provided in section 1.9.1.

Some limitations associated with the numerical methods for ordinary differential equations are listed below:

- Always requires an initial guess to initiate the iterative process.
- Generates result in a discretized domain of the problem.
- Generally numerical solution has some error when compared to exact solution.

Though error occurs while using a numerical technique but these techniques are developed in such a way that results meet the error tolerance of a problem. Some problems have small while some have high error permissiveness, One may define error tolerance prior and then use an appropriate technique, i.e., higher order method for smaller error tolerance.

1.4 Order of a Numerical Method

Step-size (h) is a crucial element for investigating the error of numerical solution, while solving an initial value problem by any numerical technique. For instance, if step-size is decreased then the error ultimately reduces. How much change occurs in the error of numerical solution when the step-size is decreased can be measured. Such measurement is associated with a numerical method as the order of method. Generally, let $e(h)$ be the error occurred while solving an initial value problem by a specific numerical method. if $|e(h)| \approx ph^n$ as $h \to 0$ then n is order of the numerical method, where p is a constant.

1.5 Errors in Numerical Methods

The main observation of a numerical technique is that some difference between exact and numerical solutions occurs, which is known as error. Over the years mathematicians are trying to develop methods which yield less error. In this research, we discuss the most significant types of error, i.e., truncation error for numerical methods. Moreover, for the sake of comparison, the results are generated and depicted as absolute error graphs. In current section the brief knowledge of different types of errors in numerical methods is provided.

Absolute Error

Definition 1.5.1. *Difference between the true solution and approximated solution in the approximation process is the absolute error (Abs. error).*

Let $X^\star$ be the approximation to X then

$$Abs.\ error = |X - X^\star|.$$

Relative Error

Definition 1.5.2. *Difference between true value and approximated value represented in percentage of true value is the relative error.*

$$\textit{Relative error} = \frac{|X - X^{\star}|}{|X|}, \quad X \neq 0,$$

where X is the true value and $X^{\star}$ is the approximated value.

Local Truncation Error

As mentioned earlier that numerical solutions are approximate solutions. For solution of non-linear differential equations, the truncation of Taylor series up to desired terms is required. Simply, the higher order terms are ignored, such ignored terms do have impact on the solution. Thus such truncation process results in truncation error. The difference between the exact solution at a future point and the numerical solution at the same point, is called the Local Truncation Error (LTE).

Global Error

Numerical techniques are not applicable on the continuous domain, thus one must define a domain of problem and discretize it to start iterations. In this way the numerical solution is generated on such a descritized domain. The cumulative error over the range of solution is known as Global Error (GE), and is calculated as

$$GE = \frac{LTE}{h}.$$

The order of GE is actually the order of the numerical method. Details of such error, are mentioned along with each method described in section 1.8 and 1.9.

1.6 Initial Value Problem (IVP)

Definition 1.6.1. *An initial value problem is the one which has all conditions defined at a single value of independent variable.*

Generally an IVP defined in a specific interval $[a, b]$ of independent variable is given by

$$\frac{dy}{dx} = f(x, y), \quad y(x_o) = y_o, \tag{1.2}$$

where x_o is a point from the interval $[a, b]$. Often it is assumed to be the initial point of interval as well, i.e., $x_o = a$. One intends to solve an IVP to fetch a solution free of derivatives, just an explicit relation between the dependent and independent variables.

Definition 1.6.2. *A solution to an IVP as given in eq. (1.2), is a differentiable function $y = y(x)$ in the interval $[x_o, b]$, i.e., $y(x_o) = y_o$ and $y'(x) = f(x, y(x))$ for all $x \in [x_o, b]$.*

An initial condition associated to the ODE generates a solution $y = y(x)$, i.e., the point (x_o, y_o) lies on solution curve. Implies that for various initial conditions the general solution to the problem generates a set of solution curves. Each of these solutions satisfy the relevant initial condition [3].

Discretization

The primary step in numerically solving an IVP as given in eq (1.2), is to discretize domain of the problem. Discretization is a process which transforms a continuous domain into a finite set of discrete points, also known as mesh or nodal points. Since the initial point x_o is provided thus to initiate the process x_o acts as an input. Suppose domain of interest is $[a, b]$, i.e., $x_o = a$, and to discretize such domain, identify the points between a and b at which the solution is obtained through iterations. Let there are total $N+1$ points, defined as

$$x_{n+1} = x_n + (n+1)h, \quad n = 0, 1, 2, \ldots, N,$$

where N is total number of sub-intervals the domain $[a, b]$ is divided into. The step length or step-size of these sub-intervals is a constant h, defined as

$$h = \frac{b-a}{N}.$$

Definition 1.6.3. *A function $f(x, y)$ continuous on a region $R = [(x, y) : a \leq x \leq b, c \leq y \leq d]$, is said to satisfy the Lipschitz condition if there exist $L > 0$ and*

$$|f(x, y_1) - f(x, y_2)| \leq L|y_1 - y_2|,$$

where L is the Lipschitz constant for f and $(x, y_1), (x, y_2) \in R$ [3].

Theorem 1.6.1. *If $f(x, y)$ is defined in the region R and there exists $L > 0$ such that,*

$$|f_y(x, y)| \leq L \quad \forall (x, y) \in R,$$

then f satisfies the Lipschitz Condition in variable y.

Theorem 1.6.2. *If $f(x, y)$ is continuous in a region R, f satisfies the Lipschitz condition on R in variable y and $(x_o, y_o) \in R$, then the IVP (1.2) has a unique solution $y = y(x)$ on some sub-interval $x_o \leq x \leq x_o + \delta$ [3].*

1.7 Taylor Series

Theorem 1.7.1 (Taylor Theorem)**.** *Suppose $f : (a, b) \to \mathbb{R}$ is a function defined on (a, b), where $a, b \in \mathbb{R}$ and $a < b$. Assume that for a positive integer n, f is n-times differentiable in the interval (a, b), i.e., f^n exists on (a, b), and $f, f', f'', \ldots, f^{n-1}$ be continuous on $[a, b]$, then there exists $\alpha \in (a, b)$ such that,*

$$f(x) = f(\alpha) + f'(\alpha)(x-\alpha) + \frac{f''(\alpha)}{2!}(x-\alpha)^2 + \cdots + \frac{f^{n-1}(\alpha)}{(n-1)!}(x-\alpha)^{n-1} + \frac{f^n(\alpha)}{n!}(x-\alpha)^n$$

1.7.2 Taylor Series Method

Consider an IVP as

$$\frac{dy}{dx} = f(x, y), \quad y(x_o) = y_o,$$

where (x_o, y_o) is a known point on the solution curve.
If all higher order derivatives of y exist at $x = x_o$ then by Taylor series method the value of y at point $x_o + h$ is given by

$$y(x_0 + h) = y(x_o) + hy'(x_o) + \frac{h^2}{2!}y''(x_o) + \frac{h^3}{3!}y'''(x_o) + \dots$$

The sum of above infinite series yields the value of y at a neighboring point $x_o + h$, but calculating infinite derivatives is not practically possible. Thus the summation process needs to be terminated after some finite terms, for instance truncate the series after k^{th} term as

$$y(x_0 + h) = y(x_o) + hy'(x_o) + \frac{h^2}{2!}y''(x_o) + \cdots + \frac{h^k}{k!}y^k(x_o) + O(h^{k+1}).$$

The above formula is the k^{th} order Taylor series approximation of y, and order of error is $k + 1$.

1.7.3 Error in Taylor Series Approximation

Taylor series method of order k has the LTE of $O(h^{k+1})$, so h can be chosen small as per requirement and ultimately error becomes smaller. Since,

$$E_k = \frac{1}{(k+1)!}h^{k+1}y^{k+1}(x + h).$$

The above expression can be further simplified by substituting derivative of y^{k+1} as

$$E_k = \frac{1}{(k+1)!}h^k\Big(y^k(x + h) - y^k(x)\Big).$$

However, one can fix k and vary the step size h to compare the error.

1.8 Euler Method

A Swiss mathematician Leonhard Euler developed the Euler method in 1768. It is the first and basic approach for solving initial value problems numerically. It is a single-step and first order method requiring just one value to initiate the process. Other than that, the process determines a future value of slope with the help of the current slope thus it is an explicit method.

1.8.1 Derivation of Euler Method

Consider an IVP as

$$\frac{dy}{dx} = f(x,y), \quad y(x_o) = y_o, \quad [a,b], \tag{1.3}$$

where $y(x_o) = y_o$ is initial condition associated with the problem and $[a,b]$ is domain of the problem. The Taylor series of $y(x+h)$ is given as

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \dots \tag{1.4}$$

Truncate the Taylor series up-to first two terms as

$$y(x+h) \approx y(x) + hf(x,y).$$

To solve the IVP (1.3) numerically, first discretize its domain as $x_0 < x_1 < x_2 < x_3 < \cdots < x_N$, thus we have

$$y(x_n + h) \approx y(x_n) + hf(x_n, y_n), \quad n = 0, 1, 2, 3, ..., N-1,$$

where n is the index for iterations and N is the number of intervals to which the domain is descritized. N is calculated by the formula as

$$N = \frac{b-a}{h}. \tag{1.5}$$

The final form of Euler method is

$$y_{n+1} = y_n + hf(x_n, y_n), \quad n = 0, 1, 2, 3, ..., N-1. \tag{1.6}$$

1.8.2 Order of Euler Method

Global truncation error of Euler method is calculated by the help of truncation process that is given in section 1.8.1. The significant term after truncating the series is $\frac{1}{2}y''(x)h^2$, that shows the LTE is of second order, i.e., $O(h^2)$. To calculate the global error multiply this term with total number of sub-intervals N, it results the impact of this second order term on the whole interval as

$$\frac{1}{2}y''(x)h^2N.$$

Use eq. (1.5) and simplify as

$$\frac{1}{2}(b-a)y''(x)h.$$

If the constant terms are ignored then we are left with h, that implies the global error is of first order; and hence Euler method is of first order, denoted as $O(h)$.

Graphical interpretation of Euler method

Consider a general IVP as

$$\frac{dy}{dx} = f(x,y), \quad y(x_0) = y_{0.}$$

Initial value at x_0 is already given, one can estimate the successive value, i.e., y_1, by the help of slope at initial point. The tangent at initial point (x_0, y_0), approximates the curve in interval $[x_0, x_1]$, where $x_1 = x_0 + h$.

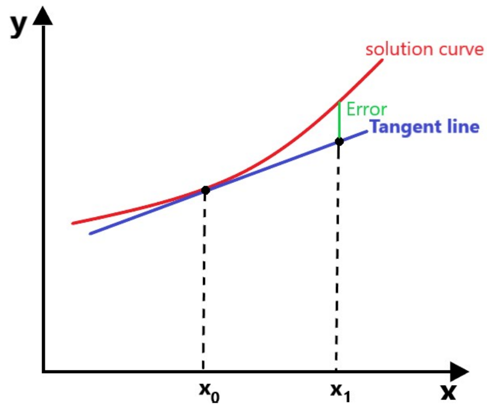

Figure 1.1: Graphical interpretation of Euler method.

In Figure 1.1, solution curve to the IVP is shown in red solid colored curve, and slope at (x_0, y_0) is shown in blue dotted line. The gap between exact value and estimated value at x_1 is the error. Similarly, one can figure out values at all points of discretized domain, i.e, $x_0, x_1, x_2, \ldots, x_n, \quad n = 1, 2, \ldots$ and $x_n = x_{n-1} + nh$. The equation of tangent line for the interval $[x_{n-1}, x_n]$ is given as

$$y - y_{n-1} = \left.\frac{dy}{dx}\right|_{(x_{n-1}, y_{n-1})} (x - x_{n-1}).$$

Thus, corresponding value of y at $x = x_n$ is

$$y_n = y_{n-1} + (x_n - x_{n-1}) f(x_{n-1}, y_{n-1}),$$

or

$$y_n = y_{n-1} + h f(x_{n-1}, y_{n-1}), \quad n = 1, 2, \ldots$$

That is how Euler method generates a sequence of tangent lines at each point of discretized domain, but these tangent lines when joined, are not too close to actual curve. Also, it has lower order of accuracy and requires a very small step size to achieve high accuracy.

1.9 Improved Euler Method

Typical Euler method was frequently used as an elementary method, but there was a need for improvement to minimize the error. There are two main reasons for improving Euler method. First, Euler method is a first-order technique with low order of convergence. Second, decreasing step size after a certain point increases round-off errors. In such cases, results are not acceptable as per error tolerance associated with the problem.

1.9.1 Derivation of Improved Euler Method

The initial steps of derivation are same as Euler one, first consider the IVP (1.2) and the Taylor series as given in eq. (1.4). In this case to reduce the error in solution, the Taylor series is truncated up to second order of h as

$$y(x+h) \approx y(x) + hy'(x) + \frac{h^2}{2!}y''(x). \tag{1.7}$$

The forward differnce formula for second order derivative of $y(x)$ is given by

$$y''(x) = \frac{y'(x+h) - y'(x)}{h}.$$

Thus eq. (1.7) can be written as

$$y(x+h) \approx y(x) + \frac{h}{2}\Big(y'(x) + y'(x+h)\Big). \tag{1.8}$$

After discretizing the domain as $x_0 < x_1 < x_2 < x_3 < \cdots < x_N$, the eq. (1.8) can be written as

$$y(x_n+h) \approx y(x_n) + \frac{h}{2}\Big(y'(x_n) + y'(x_n+h)\Big).$$

By IVP (1.2), $y'(x) = f(x, y)$ hence,

$$y_{n+1} = y_n + \frac{h}{2}\Big(f(x_n, y_n) + f(x_{n+1}, y^{\star}_{n+1})\Big), \quad n = 0, 1, 2, 3, ..., N-1, \tag{1.9}$$

where $y^{\star}_{n+1}$ is unknown yet, but here it is estimated using the Euler formula given in eq. (1.6), i.e., $y^{\star}_{n+1} = y_n + hf(x_n, y_n)$. Thus, improved Euler method is an implicit method.

1.9.2 Order of Improved Euler Method

Error of improved Euler method is estimated by the help of truncation process that is given in previous section. The significant term after truncating the Taylor series is $\frac{1}{3}y'''(x)h^3$, which shows that local truncation error is of third order, denoted as $O(h^3)$. To calculate the global error multiply this term with total number of sub-intervals N, it results the impact of this third order term in the whole range as

$$\frac{1}{3!}y'''(x)h^3N.$$

Use eq. (1.5) and simplify to get

$$\frac{1}{3!}(b-a)y'''(x)h^2.$$

If the constant terms are ignored then we are left with h^2, that implies the GTE is of second order; And hence improved Euler method is of second order, denoted as $O(h^2)$.

Graphical Interpretation of Improved Euler Method

Considere the IVP (1.2), and recall eq. (1.9) where for $n = 0$ the equation gets the following form

$$y_1 = y_0 + \frac{1}{2}(f(x_0, y_0), f(x_1, y^{\star}_1)), \tag{1.10}$$

where $y^{\star}_1 = y_0 + hf(x_0, y_0)$. Let the slope at initial point be m_0 and the estimated slope at $(x_1, y^{\star}_1)$ be m_1. From eq. (1.10), it is clear that the average of these two slopes is used to estimate the value y_1, let such average slope be m_{avg}.

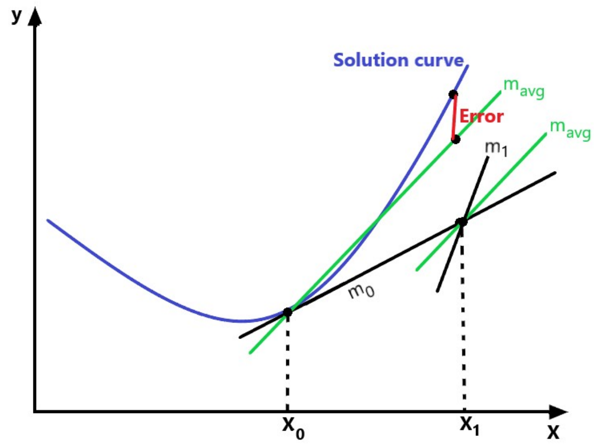

Figure 1.2: Graphical interpretation of improved Euler method.

In Figure 1.2, the exact solution of the problem is given in blue solid curve, the average slope m_{avg} is shown in green solid line while the estimated slopes at x_o and x_1 are given in black solid lines. Here the approximate solution curve is estimated by joining the lines obtained by taking an average of slopes at x_o and x_1, which is closer to true solution.

Example 1.9.1 Consider the initial value problem

$$\frac{dy}{dx} = 1 + y^2, \quad y(0) = 1, \quad [0, 0.5]. \tag{1.11}$$

Solve the problem with Euler and improved Euler methods, and compare the results. Problem (1.11) has exact solution $y = tan(x + \frac{\pi}{4})$, for $h = 0.025$ the results obtained by both methods are listed below

Points (x)	Exact solution	Improved Euler method	Euler method
0.000	1.0000	1.0000	1.0000
0.025	1.1054	1.1053	1.1026
0.050	1.1625	1.1624	1.158
0.075	1.2230	1.223	1.2165
0.100	1.2874	1.2873	1.2785
0.125	2.1497	2.1413	1.9906
0.150	1.3561	1.356	1.3443
0.175	1.4296	1.4294	1.4145
0.200	1.5085	1.5083	1.4895
0.225	1.5936	1.5933	1.5700
0.250	1.6858	1.6854	1.6566
0.275	1.7861	1.7856	1.7502
0.300	1.8958	1.8951	1.8518
0.325	2.0164	2.0155	1.9625
0.350	2.1497	2.1486	2.0838
0.375	2.2983	2.2968	2.2174
0.400	2.4650	2.4630	2.3653
0.425	2.6535	2.6509	2.5302
0.450	2.8689	2.8654	2.7152
0.475	3.1175	3.1128	2.9245
0.500	3.4082	3.4017	3.1634

Table 1.1: Comparison of Euler and improved Euler methods.

The data in Table 1.1, clearly shows that result obtained by improved Euler method is more closer to the exact solution as compared to Euler method.

Points (x)	Abs. error for Euler method	Abs. error for improved Euler method
0.000	0.0000000	0.0000000
0.025	0.0012930	0.0000176
0.050	0.0027931	0.0000267
0.075	0.0045381	0.0000455
0.100	0.0065739	0.0000693
0.125	0.0089566	0.0000991
0.150	0.0117550	0.0001366
0.175	0.0150550	0.0001837
0.200	0.0189630	0.0002432
0.225	0.0236120	0.0003184
0.250	0.0291720	0.0004139
0.275	0.0358570	0.0005359
0.300	0.0439470	0.0006929
0.325	0.0538050	0.0008961
0.350	0.0659090	0.0011618
0.375	0.0808990	0.0015127
0.400	0.0996430	0.0019816
0.425	0.1233300	0.0026172
0.450	0.1536500	0.0034927
0.475	0.1929800	0.0047212
0.500	0.2448500	0.0064837

Table 1.2: Absolute errors obtained by Euler and improved Euler methods.

In Table 1.2, the maximum absolute error obtained by Euler method is 0.2448500, whereas by Improved Euler method maximum absolute error is 0.0064837 which is comparatively small. The absolute error curves are given in Figure 1.3.

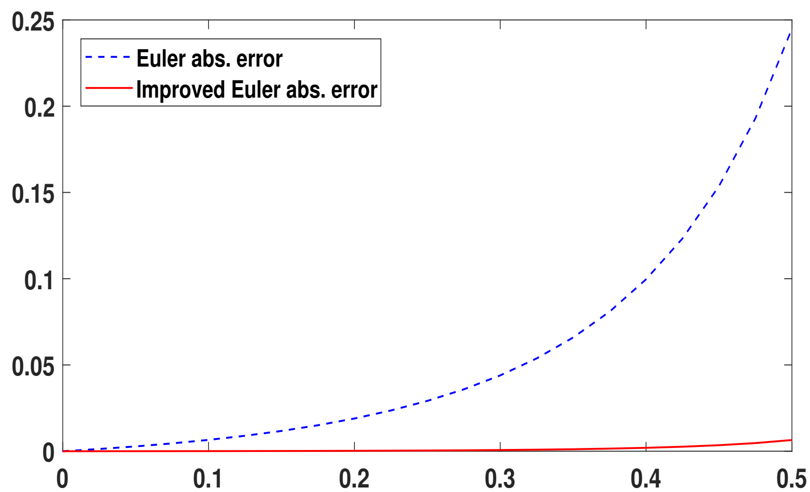

Figure 1.3: Absolute error curves obtained by Euler and improved Euler method.

in Figure 1.3 the absolute error curve obtained by Euler method is given by black dotted line and the absolute error curve obtained by improved Euler's method is given by red solid line. The Figure 1.3 shows that absolute error obtained by improved Euler method is much less than Euler method. The maximum absolute error for improved Euler method is 0.0064837, which is arguable if error tolerance of the problem is extremely small. In such case, one can skip a second order method and move to higher order methods , or one can try decreasing the step size. As discussed earlier, the step size is related to the error per step, so a small step size could help in decreasing error.

Step Size (h) versus Error

Example 1.9.2 The Initial value problem,

$$\frac{dy}{dx} = \frac{x}{y}, \quad y(0) = 1, \quad 0 \leq x \leq 5,$$

has exact solution $y = \sqrt{1 + x^2}$, solve by improved Euler method. Use multiple step sizes starting from $h = 1$ then decreasing by half, and compare results.

Step size (h)	Numerical solution at $x = 5$	Max. Abs. error for improved Euler method
1.0000	5.1252	0.0858
0.5000	5.1013	0.0075
0.2500	5.0993	0.0008
0.0625	5.0990	0.00001

Table 1.3: Maximum absolute errors in improved Euler method for different step sizes.

Observations in Table 1.3 show that decreasing the step size reduces the error. However, a small step size indicates more mesh points and calculations on each of these points would consume more time. Moreover round-off error might also increase hence, one can opt for a higher order method, to get lesser error.

Chapter 2

Runge-Kutta Methods (RK Methods)

The German mathematician Carl Runge worked on the scheme of Euler method and developed the Rung-Kutta method in 1895 [4]. His idea was to extend the approximation in Euler method and hence improve accuracy. Karl Heun and Martin Kutta contributed to develop higher order schemes; Karl Heun enhanced their work up-to 4th order RK methods.

The background of Runge-Kutta methods is linked to Taylor's series and improved Euler method. The idea is same but with small amendment in truncation process of Taylor's series. That is to keep more terms that involve higher order of h in series and truncate it, this results in a higher-order accuracy.

If series is truncated after second-order h terms, then it is a second order RK method and improved Euler method is a special case of such process. If series is truncated after third order h terms, then it results a third order RK method. One can generate a higher order method as per requirement of the modeled problem. It is convenient to first define a general form of RK methods; afterwards one can derive the RK method of desired order out of such mathematical formulae.

2.1 General Form of RK Methods

Consider the IVP (1.2) and the formula of improved Euler method given in eq. (1.9). If $a_1 = \frac{1}{2}, \quad k_1 = f(x_n, y_n), \quad a_2 = \frac{1}{2} \quad and \quad k_2 = f(x_{n+1}, y^*_{n+1})$, then eq. (1.9) can be written as

$$y_{n+1} = y_n + h(a_1 k_1 + a_2 k_2).$$

Likewise, one can write the general form up to mth order as

$$y_{n+1} = y_n + h[a_1 k_1 + a_2 k_2 + \cdots + a_m k_m], \tag{2.1}$$

where

$$\begin{aligned}
k_1 &= f(x_n, y_n),\\
k_2 &= f(x_n + c_1 h, y_n + b_{11} h k_1),\\
k_3 &= f(x_n + c_2 h, y_n + h(b_{21} k_1 + b_{22} k_2)),\\
&.\\
&.\\
&.\\
k_m &= f\left(x_n + c_{n-1} h, y_n + h \sum_{i=1}^{m-1} b_{mi} k_i\right).
\end{aligned} \tag{2.2}$$

The set of equations (2.1) and (2.2) is the general frame work for RK Methods upto mth order with a condition, $\sum_{j=1}^{m} a_j = 1$. Moreover, one can drive a set of RK methods out of it for a specific order. These methods are widely used as they have eliminated the efforts of calculating higher order derivatives a compared to Taylor's series method. Euler method is a first order RK method. In this chapter discussions on second and third order RK methods are provided. For the sake of ease notations of $b_1, b_2, b_3, \ldots, b_6$ instead of $b_{11}, b_{21}, b_{22}, \ldots, b_{33}$ are used respectively .

2.2 General Framework for 2nd Order RK-Methods

The second order RK methods have a general formula as given below

$$y_{n+1} = y_n + h(a_1k_1 + a_2k_2), \tag{2.3}$$

where

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f(x_n + c_1h, y_n + hb_1k_1). \end{aligned} \tag{2.4}$$

The expantion of k_2 by Taylor's series up to first order h term is given as

$$k_2 = f + c_1f_xh + b_1ff_yh. \tag{2.5}$$

For the sake of ease use f as a notation for $f(x_n, y_n)$, and use equations (2.4) and (2.5) in eq. (2.3) to get

$$y_{n+1} = y_n + h\Bigg(a_1f + a_2(f + c_1f_xh + b_1ff_yh)\Bigg),$$

or

$$y_{n+1} = y_n + hf(a_1 + a_2) + h^2a_2c_1f_x + h^2a_2b_1ff_y. \tag{2.6}$$

Now use the Tayor series from eq. (1.4), up to second order h terms as

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2!}y''_n, \tag{2.7}$$

where $y'_n = f$ by IVP (1.2), so eq. (2.7) can be written as

$$y_{n+1} = y_n + hf + \frac{h^2}{2!}(f_x + ff_y). \tag{2.8}$$

The comparison of equations (2.6) and (2.8) results the following set of equations

$$\begin{aligned} a_1 + a_2 &= 1, \\ a_2c_1 &= \frac{1}{2}, \\ a_2b_1 &= \frac{1}{2}. \end{aligned} \tag{2.9}$$

The set of equations (2.9) has three equations and four arbitrary parameters, and $a_2,\ b_1\ and\ c_2$ can not be equal to 0. One can choose any one parameter arbitrarily and obtain a specific type of second order RK method. For MATLAB code, any one of these unknown parameters is kept as input parameter and rest are found using the set of equations (2.9). Let us choose a_1 as input parameter and generate some specific second order RK methods.

Derivation of Mid-point Method using the General Framework for 2nd Order RK Methods

Choose $a_1 = 0$, then the set of equations (2.9) results

$$a_2 = 1, \quad c_1 = \tfrac{1}{2} \quad \text{and} \quad b_1 = \tfrac{1}{2},$$

and the formula of Mid-point method is obtained as

$$y_{n+1} = y_n + k_2,$$

$$k_1 = f(x_n, y_n),$$
$$k_2 = f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1\right).$$

Derivation of Improved Euler Method using the General Framework for 2nd Order RK Methods

Choose $a_1 = \frac{1}{2}$, then the set of equations (2.9) results

$$a_2 = \tfrac{1}{2}, \quad c_1 = 1 \quad \text{and} \quad b_1 = 1,$$

hence the formula of Improved Euler method is obtained as

$$y_{n+1} = y_n + \frac{1}{2}h(k_1 + k_2),$$

$$k_1 = f(x, y),$$

$$k_2 = f(x + h, y + k_1h).$$

Derivation of Ralston Method using the General Framework for 2nd Order RK Methods

Choose $a_1 = \frac{1}{3}$, then the set of equations (2.9) results

$$a_2 = \tfrac{2}{3}, \quad c_1 = \tfrac{3}{4} \quad \text{and} \quad b_1 = \tfrac{3}{4},$$

and the formula of Ralston method is obtained as

$$y_{n+1} = y_n + h\left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right),$$

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f\left(x_n + \frac{3}{4}h, y_n + \frac{3}{4}hk_1\right). \end{aligned}$$

One can fetch a desired method by fixing the value for a_1 in the set of equations (2.9) and simplifying as shown in the previous cases.

2.3 General Framework of 3rd Order RK Methods

Like the second order RK methods, one can generate a set of 3rd order RK methods via a general framework. The general form of 3rd order RK methods is given as

$$y_{n+1} = y_n + h(a_1k_1 + a_2k_2 + a_3k_3), \tag{2.10}$$

where

$$\begin{aligned} k_1 &= f(x_n, y_n) = f, \\ k_2 &= f(x_n + c_1h, y_n + hb_1k_1), \\ k_3 &= f(x_n + c_2h, y_n + h(b_2k_1 + b_3k_2)). \end{aligned} \tag{2.11}$$

Use eq. (2.4), i.e., $k_1 = f$, in k_2 and k_3, then expand the Taylor series of both k_2 and k_3. The exapanded forms are given below

$$k_2 = f + c_1f_xh + b_1ff_yh + \frac{1}{2!}\left(c_1^2f_{xx}h^2 + 2c_1b_1ff_{xy}h^2 + b_1^2f^2f_{yy}h^2\right), \tag{2.12}$$

and

$$k_3 = f+c_2f_xh+h(b_2k_1+b_3k_2)f_y+\frac{1}{2!}\left(c_2^2h^2f_{xx}+2c_2(b_2k_1+b_3k_2)h^2f_{xy}+h^2(b_2k_1+b_3k_2)^2\right).$$

Use eq. (2.11) in k_3 and simplify as

$$\begin{aligned} k_3 &= f + c_2f_xh + (b_2+b_3)ff_yh + b_3c_1f_xf_yh^2 + b_1b_3ff_y^2h^2 \\ &+ \frac{1}{2}(b_3c_1^2f_yf_{xx})h^3 + c_1b_1b_3ff_yf_{xy}h^3 + \frac{1}{2}(b_3f^2f_yf_{yy})h^3 + \frac{1}{2}(c_2^2f_{xx})h^2 \\ &+ c_2b_2ff_{xy}h^2 + c_2b_3ff_{xy}h^2 + c_1c_2b_3f_xf_{xy}h^3 + c_2b_1b_3ff_yf_{xy}h^3 + b_2^2f^2h^2 \\ &+ b_2b_3f^2h^2 + b_2b_3c_1ff_xh^3 + b_1b_2b_3f^2f_yh^3 + \frac{1}{2}(c_1^2b_2b_3ff_{xx})h^3. \end{aligned} \tag{2.13}$$

Now use equations (2.4), (2.12) and (2.13) in eq. (2.10) and simplify to get

$$\begin{aligned} y_{n+1} &= y_n + (a_1+a_2)fh + a_2c_1f_xh^2 + a_2b_1ff_yh^2 + \frac{1}{2}(a_2c_1^2f_{xx})h^3 \\ &+ a_2c_1b_1ff_{xy}h^3 + \frac{1}{2}(a_2b_1^2f^2f_{yy})h^3 + a_3fh + a_3c_2f_xh^2 + a_3b_2ff_yh^2 \\ &+ a_3b_3ff_yh^2 + a_3b_3c_1f_xf_yh^3 + a_3b_1b_3ff_y^2h^3 + \frac{1}{2}(a_3c_2^2f_{xx})h^3 \\ &+ a_3c_2b_2ff_{xy}h^3 + a_3c_2b_3ff_{xy}h^3 + a_3b_2^2f^2h^3 + a_3b_2b_3f^2h^3. \end{aligned} \tag{2.14}$$

The Taylor series expansion of y_{n+1} given by eq. (1.4) up to 3rd order h terms in simplified form is given as

$$y_{n+1} = y_n + fh + \frac{1}{2}(f_x+ff_y)h^2 + \frac{1}{3!}(f_{xx}+2ff_{xy}+f_xf_y+f^2f_{yy}+ff_y^2)h^3. \tag{2.15}$$

The comparison of equations (2.14) and (2.15) yields the following set of equations

$$a_1+a_2+a_3 = 1, \tag{2.16}$$

$$a_2c_1+a_3c_2 = \frac{1}{2}, \tag{2.17}$$

$$a_2b_1+a_3b_2+a_3b_3 = \frac{1}{2}, \tag{2.18}$$

$$a_1c_1^2 + a_3c_2^2 = \frac{1}{3}, \tag{2.19}$$

$$a_2b_1c_1 + a_3b_2c_2 + a_3b_3c_2 = \frac{1}{3}, \tag{2.20}$$

$$a_3b_3c_1 = \frac{1}{6}, \tag{2.21}$$

$$a_3b_1b_3 = \frac{1}{6}. \tag{2.22}$$

Set of equations (2.16)-(2.22) has seven equations and eight unknown parameters, which indicates that one of these parameters is arbitrary. However, some more algebraic calculations on this set results in two equations to be identical. Following are the brief calculations of such process.

Simultaneously solve equations (2.21) and (2.22) and simplify as

$$b_1 = c_1. \tag{2.23}$$

Thus, one may rewrite eq. (2.22) as eq. (2.23). Now, use eq. (2.23) in eq.(2.17) as

$$a_2b_1 + a_3c_2 = \frac{1}{2}. \tag{2.24}$$

Subtract eq. (2.24) from eq. (2.18) and simplify as,

$$c_2 = b_2 + b_3. \tag{2.25}$$

Now use equations (2.23) and (2.25) in eq. (2.20) to get

$$a_1c_1^2 + a_3c_2^2 = \frac{1}{3}. \tag{2.26}$$

Observe that eq. (2.26) is same as eq. (2.19), further simplifications lead to the following set of equations

$$
\begin{aligned}
&a_1 + a_2 + a_3 = 1,\\
&a_2 = \frac{3c_2 - 2}{6c_1(c_2 - c_1)}, \quad c_1 \neq c_2,\\
&a_3 = \frac{2 - 3c_1}{6c_2(c_2 - c_1)}, \quad c_1 \neq c_2,\\
&b_2 = \frac{1}{a_3}\left(\frac{1}{2} - (a_2 b_1 + a_3 b_3)\right),\\
&b_3 = \frac{1}{6a_3 c_1},\\
&b_1 = c_1.
\end{aligned}
\tag{2.27}
$$

The set of equations (2.27) has six equations and eight unknown parameters, thus one is free to choose any two parameters and generate different 3rd order RK methods. Some conditions rise here, i.e., $c_1 \neq 0$, $c_2 \neq 0$ and $c_1 \neq c_2$, while making choices such conditions must be fulfilled. Moreover, one can use same set of equations to write a MATLAB code while inserting c_1 and c_2 as inputs.

2.3.1 Derivation of Standard 3rd Order RK Method using General Framework for 3rd order RK Methods

Recall the set of equations (2.27) and choose $c_1 = \frac{1}{2}$ and $c_2 = 1$ to get the values of remaining parameters as

$$
\begin{aligned}
&a_1 = \frac{1}{6}, \quad a_2 = \frac{2}{3}, \quad a_3 = \frac{1}{6},\\
&b_1 = \frac{1}{2}, \quad b_2 = -1, \quad b_3 = 2.
\end{aligned}
\tag{2.28}
$$

Plug the values listed in set of equations (2.27) into the set of equations (2.10) and (2.11) to get the standard 3rd order RK method as

$$\begin{aligned}
y_{n+1} &= y_n + h\left(\frac{1}{6}k_1 + \frac{2}{3}k_2 + \frac{1}{6}k_3\right), \\
k_1 &= f(x_n, y_n), \\
k_2 &= f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1), \\
k_3 &= f(x_n + h, y_n - hk_1 + 2hk_2).
\end{aligned} \tag{2.29}$$

Chapter 3

Comparison of Various 3rd Order RK Methods

The comparison of various 3rd order RK methods applied to different non-linear initial value problems are provided in this chapter.

Problem 1

In general relativity solutions of the Einstein field equations lead to models of space-time geometry. The spherically symmetric static solutions of the field equations led to a non-linear ordinary differential equation given as

$$\frac{dy}{dx} = \frac{y}{\sqrt{y^2 + \alpha_1 y + \alpha_2 y^4}}, \quad y(0) = 0, \tag{3.1}$$

where α_1 and α_2 are arbitrary constants. Take $\alpha_1 = 0$ and $\alpha_2 = 1$ in eq. (3.1) we obtain a specific case given as

$$\frac{dy}{dx} = \frac{1}{\sqrt{1 + y^2}}, \quad y(0) = 0. \tag{3.2}$$

The domain of the problem is $[0, 1]$ and exact solution is $x = \frac{1}{2}\Big(y\sqrt{1+y^2} + ln|\sqrt{1+y^2}|\Big)$. For a fixed step size $h = 0.05$ numerical solution obtained by standard 3rd order RK method and the exact solution are displayed in Figure 3.1.

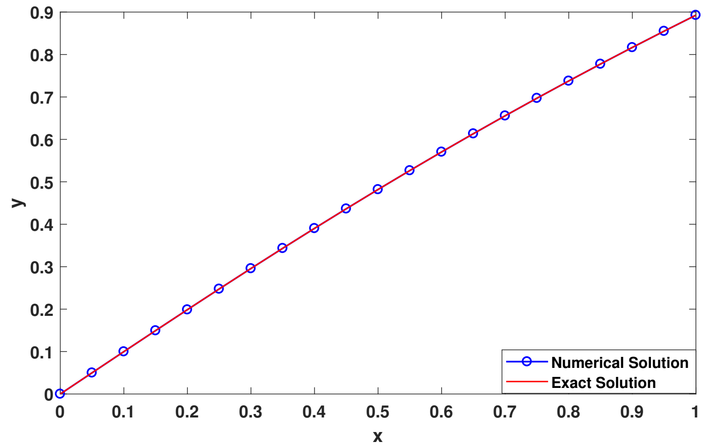

Figure 3.1: Solution obtained numerically via standard 3rd order RK method vs exact solution.

In Figure 3.1, solution curve obtained numerically embeds closely on the exact solution curve. Here results are obtained by a MATLAB code that utilizes formula given in eq. (2.29). Small increment generates better results, on the other hand, a large increment yields more difference between the exact and numerical solutions. In order to have meaningful comparisons let us keep the same step size and vary the parameters c_1 and c_2 within $(0, 1]$ to generate different 3rd order RK methods. By such process the solution curves obtained numerically embed closely on the exact solution curve thus generating similar figures as of Figure 3.1. No difference is visible by such plotting, the difference can only be observed by zooming into the graphs.
A better way to seek and analyze the difference between numerical and exact solutions is to plot absolute error curves. The strategy followed here is to plot the absolute error curves for standard 3rd order RK method and the methods generated by varying parameters.
The standard 3rd order RK method has the form given in set of equations (2.29), where $c_1 = \frac{1}{2}$ and $c_2 = 1$. Vary both parameters and compare the absolute error curves for various 3rd order RK methods applied to eq. (3.2). The results are dis-

played in Figure 3.2, while step size and domain both are same as defined with the problem.

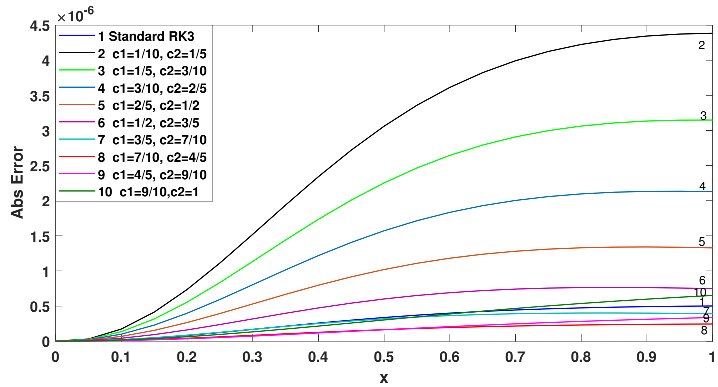

Figure 3.2: Absolute error curves of various 3rd order RK methods vs standard 3rd order RK method.

The choices of parameters follow a pattern, firstly choices closer to 0, secondly choices closer to $\frac{1}{2}$ and lastly choices closer to 1 are taken under consideration. The tabular data of Figure 3.2 is given in Table 3.1, along with maximum absolute errors in each each case.

	Parameters		
Method	c_1	c_2	Max. Abs. Error
*Standard RK*3	$\frac{1}{2}$	1	$5.01440416078580 \times 10^{-07}$
	$\frac{1}{10}$	$\frac{1}{5}$	$4.38410888214946 \times 10^{-06}$
	$\frac{1}{5}$	$\frac{3}{10}$	$3.14822215230492 \times 10^{-06}$
	$\frac{3}{10}$	$\frac{2}{5}$	$2.13477371580062 \times 10^{-06}$
	$\frac{2}{5}$	$\frac{1}{2}$	$1.34151276476313 \times 10^{-06}$
	$\frac{1}{2}$	$\frac{3}{5}$	$7.65325713358855 \times 10^{-07}$
	$\frac{3}{5}$	$\frac{7}{10}$	$4.01521781268066 \times 10^{-07}$
	$\frac{7}{10}$	$\frac{4}{5}$	$\mathbf{2.44962246265246 \times 10^{-07}}$
	$\frac{4}{5}$	$\frac{9}{10}$	$3.3742029670325 \times 10^{-07}$
	$\frac{9}{10}$	1	$6.51449542976579 \times 10^{-07}$

Table 3.1: Comparison of different 3rd order RK methods with standard 3rd order RK method.

Discussion

The trend observed in Figure 3.2 is that error reduces when choices are taken closer to 1. From Table 3.1 it is clear that the choice $c_1 = \frac{7}{10}$ and $c_2 = \frac{4}{5}$ results in comparatively less error. Observe that standard third order RK method produces error closer to this particular choice and the minute difference is $2.564781698133340 \times 10^{-07}$.

Problem 2

A logistic map differential equation is given as

$$\frac{dy}{dx} = \frac{1}{4}\left(y - \frac{y^2}{20}\right), \quad y(0) = 1. \tag{3.3}$$

The exact solution of problem is $y = \frac{20}{1+19e^{-x/4}}$. and domain of problem is [0,1]. For a fixed step size of 0.05, numerical solution obtained by 3rd order RK method and exact solution both embed closely to each other and are presented in the Figure 3.3.

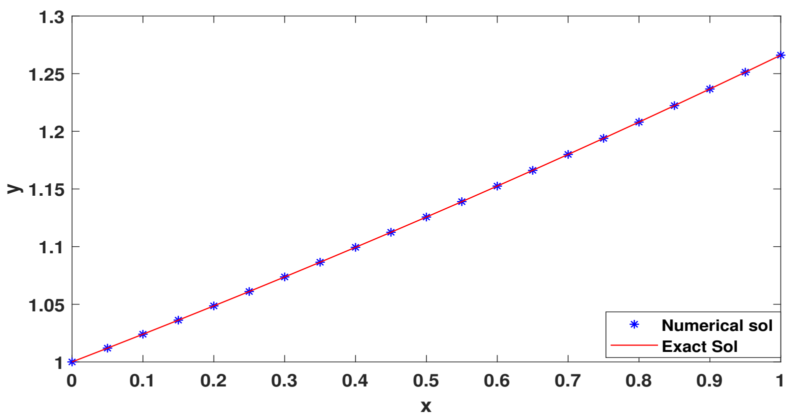

Figure 3.3: Solution obtained numerically via standard 3rd order RK method vs exact solution.

Following the process and strategy of varying the parameters c_1 and c_2 as followed for Problem 1. Multiple choices of parameters are considered which follow the same pattern as in Problem 1 and the absolute error curves are shown in Figure 3.4.

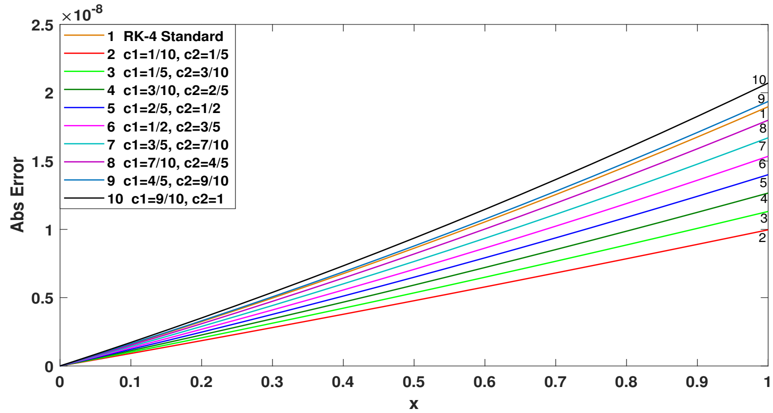

Figure 3.4: Absolute error curves of various 3rd order RK methods vs standard 3rd order RK method.

	Parameters		
Method	c_1	c_2	Max. Abs. Error
*Standard RK*3	$\frac{1}{2}$	1	$1.89756526047802 \times 10^{-08}$
	$\frac{1}{10}$	$\frac{1}{5}$	$\mathbf{9.96657978369342 \times 10^{-09}}$
	$\frac{1}{5}$	$\frac{3}{10}$	$1.13112714750230 \times 10^{-08}$
	$\frac{3}{10}$	$\frac{2}{5}$	$1.26560919522234 \times 10^{-08}$
	$\frac{2}{5}$	$\frac{1}{2}$	$1.40013334259947 \times 10^{-08}$
	$\frac{1}{2}$	$\frac{3}{5}$	$1.53479990938621 \times 10^{-08}$
	$\frac{7}{10}$	$\frac{4}{5}$	$1.79895247587325 \times 10^{-08}$
	$\frac{4}{5}$	$\frac{9}{10}$	$1.93614886345728 \times 10^{-08}$
	$\frac{9}{10}$	1	$2.07088410864031 \times 10^{-08}$

Table 3.2: Comparison of different 3rd order RK methods with standard 3rd order RK method.

Discussion

The trend observed in Figure 3.4 is that error reduces when choices are taken closer to 0. From Table 3.2 it is clear that the choice $c_1 = \frac{1}{10}$ and $c_2 = \frac{1}{5}$ results in comparatively less error. Observe that standard third order RK methods produces error closer to this particular choice and the minute difference is $9.009072821086779 \times 10^{-09}$.

Chapter 4

Fourth Order RK Methods

Derivation of a general framework to develop various 4th order RK methods is provided in this chapter.

4.1 General Framework of 4th Order RK Methods

The general form of a 4th order RK method is given as

$$y_{n+1} = y_n + h(a_1k_1 + a_2k_2 + a_3k_3 + a_4k_4), \tag{4.1}$$

$$\begin{aligned} k_1 &= f(x_n, y_n) = f, \\ k_2 &= f(x_n + c_1h, y_n + hb_1k_1), \\ k_3 &= f(x_n + c_2h, y_n + h(b_2k_1 + b_3k_2)), \\ k_4 &= f(x_n + c_3h, y_n + h(b_4k_1 + b_5k_2 + b_6k_3)). \end{aligned} \tag{4.2}$$

Taylor's series expansions of k_2, k_3 and k_4 in simplified forms are given below

$$\begin{aligned} k_2 = f + c_1f_xh + b_1ff_yh + \frac{h^2}{2!}\left(c_1^2f_{xx}h^2 + 2c_1b_1ff_{xy}h^2 + b_1^2f^2f_{yy}h^2\right) \\ + \frac{h^3}{6}\left(c_1^3f_{xxx} + 3c_1^2b_1ff_{xxy} + 3c_1b_1^2ff_{xyy} + b_1^3f^3f_{yyy}\right), \end{aligned} \tag{4.3}$$

$$
\begin{aligned}
k_3 = f + h\Bigg(& c_2 f_x + b_2 f f_y + b_3 f f_y + b_3(c_1 f_x + b_1 f f_y) f_y h + \frac{b_3}{2}\Bigg(c_1^2 f_{xx} \\
&+ 2c_1 b_1 f f_{xy} + b_1^2 f^2 f_{yy}\Bigg) f_y h^2\Bigg) + \frac{h^2}{2}\Bigg(c_2^2 f_{xxx} + 2c_2 b_2 f f_{xy} + 2c_2 b_3 (f + c_1 f_x h \\
&+ b_1 f f_y h) f_{xy} + b_2^2 f^2 f_{yy} + 2b_2 b_3 f(f + c_1 f_x h + b_1 f f_y h) f_{yy} + b_3^2 f^2 f_{yy}\Bigg) \\
&+ \frac{h^3}{6}\Bigg(c_2^3 f_{xxx} + 3c_2^2 b_2 f f_{xxy} + 3c_2^2 b_3 f f_{xxy} + 3c_2 b_2^2 f^2 f_{xyy} + 6c_2 b_2 b_3 f^2 f_{xyy} \\
&+ 3c_2 b_3^2 f f_{xyy} + (b_2 + b_3)^3 f^3 f_{yyy}\Bigg),
\end{aligned}
\tag{4.4}
$$

$$
\begin{aligned}
k_4 = f &+ (c_3 f_x + (b_4 + b_5 + b_6) f f_y) h + \Bigg((c_1 b_5 + c_2 b_6) f_x f_y + (b_1 b_5 \\
&+ b_2 b_6) f f_y^2 + \frac{1}{2} c_3^2 f_{xx} + (b_4 + b_5 + b_6) c_3 f f_{xy} + ((c_1 b_5 + c_2 b_6) f_x \\
&+ (b_1 b_5 + b_2 b_6 + b_3 b_6) f f_y) c_3 f_{xy} h + \Bigg(\frac{1}{2}(b_4^2 + b_5^2 + b_6^2) + (b_4 b_5 + b_5 b_6 \\
&+ b_4 b_6) h\Bigg) f^2 f_{yy} + ((c_1 b_5 + c_2 b_6) b_4 f_x + (b_1 b_5 + b_2 b_6 + b_3 b_6) f_y) f f_{yy} h\Bigg) h^2 \\
&+ \Bigg(\Bigg(\frac{1}{2} c_1^2 b_5 + (c_1 b_1 b_5 + c_2 b_2 b_6) f\Bigg) f_{xx} f_y + \frac{1}{2}\Bigg((b_1^2 b_5 + b_2^2 b_6 + 2b_2 b_3 b_6) f^2 f_{yy} \\
&+ (c_2^2 f_{xxx} + 2c_2 b_3 f f_y + b_3^2 f^2 f_{yy}^2) b_6\Bigg) f_y + \frac{1}{6} c_3^3 f_{xxx} + \frac{1}{2}(b_4 + b_5 + b_6) c_3^2 f f_{xxy} \\
&+ \frac{1}{2}(b_4 + b_5 + b_6)^2 f^2 f_{xyy} + \frac{1}{6}(b_4 + b_5 + b_6)^3 f^3 f_{yyy}\Bigg) h^3.
\end{aligned}
\tag{4.5}
$$

Use equations (4.3), (4.4) and (4.5) in eq. (4.1) and simplify as

$$
\begin{aligned}
y_{n+1} &= y_n + (a_1 + a_2 + a_3 + a_4) f h + (a_2 c_1 + a_3 c_2 + a_4 c_3) f_x h^2 + (a_2 b_1 \\
&+ a_3 b_2 + a_3 b_3 + a_4 b_4 + a_4 b_5 + a_4 b_6) f f_y h^2 + \frac{1}{2}(a_2 c_1^2 + a_3 c_2^2 + a_4 c_3^2) f_{xx} h^3 \\
&+ (a_2 b_1 c_1 + a_3 b_2 c_2 + a_3 b_3 c_2 + a_4 b_4 c_3 + a_4 b_5 c_3 + a_4 b_6 c_3) f f_{xy} h^3 \\
&+ \frac{1}{6}(a_2 c_1^3 + a_3 c_2^3 + a_4 c_3^3) f_{xxx} h^4 + \frac{1}{2}(a_2 b_1 c_1^2 + a_3 b_2 c_2^2 + a_3 b_3 c_2^2 \\
&+ a_4 b_4 c_3^2 + a_4 b_5 c_3^2 + a_4 b_6 c_3^2) f f_{xxy} h^4 + (a_3 b_3 c_1 + a_4 b_5 c_1 + a_4 b_6 c_2) f_x f_y h^3 \\
&+ (a_3 b_1 b_3 + a_4 b_1 b_5 + a_4 b_2 b_6 + a_4 b_3 b_6) f f_y^2 h^3 + (a_3 b_3 c_1 c_2 + a_4 b_5 c_1 c_3 \\
&+ a_4 b_6 c_2 c_3) f_x f_{xy} h^4 + (a_3 b_1 b_3 c_2 + a_3 b_1 b_3 c_1 + a_4 b_1 b_5 + a_4 b_2 b_6 c_2 + a_4 b_3 b_6 c_2 \\
&+ a_4 b_1 b_5 c_3 + a_4 b_2 b_6 c_3 + a_4 b_3 b_6 c_3) f f_y f_{xy} h^4 + \frac{1}{2}(a_3 b_3 c_1^2 + a_4 b_5 c_1^2 \\
&+ a_4 b_6 c_2^2) f_y f_{xx} h^4 + a_4 b_3 b_6 c_1 f f_x f_y^2 h^4 + a_4 b_1 b_3 b_6 f f_y^3 h^4.
\end{aligned} \tag{4.6}
$$

The Taylor series expansion of y_{n+1} by eq. (1.4) is given as

$$
\begin{aligned}
y_{n+1} &= y_n + f h + \frac{1}{2}(f_x + f f_y) h^2 + \frac{1}{3!}(f_{xx} + 2 f f_{xy} + f_x f_y + f^2 f_{yy} + f f_y^2) h^3 \\
&+ \frac{1}{4!}(f_{xxx} + 3 f f_{xxy} + 3 f^2 f_{xyy} + f_3 f_{yyy} + f_y f_{xx} + 5 f f_y f_{xy} + 4 f^2 f_y f_{yy} \\
&+ 3 f_x f_{xy} + 3 f f_x f_{yy} + f_x f_y^2 + f f_y^3) h^4.
\end{aligned} \tag{4.7}
$$

After comparing eq. (4.6) with eq. (4.7), we get following set of equations

$$a_1 + a_2 + a_3 + a_4 = 1, \tag{4.8}$$

$$a_2 c_1 + a_3 c_2 + a_4 c_3 = \frac{1}{2}, \tag{4.9}$$

$$a_2 b_1 + a_3 b_2 + a_3 b_3 + a_4 b_4 + a_4 b_5 + a_4 b_6 = \frac{1}{2}, \tag{4.10}$$

$$a_2 c_1^2 + a_3 c_2^2 + a_4 c_3^2 = \frac{1}{3}, \tag{4.11}$$

$$2 a_2 b_1 c_1 + a_3 b_2 c_2 + a_3 b_3 c_2 + a_4 b_4 c_3 + a_4 b_5 c_3 + a_4 b_6 c_3 = \frac{1}{3}, \tag{4.12}$$

$$a_2 c_1^3 + a_3 c_2^3 + a_4 c_3^3 = \frac{1}{4}, \tag{4.13}$$

$$a_2b_1c_1^2 + a_3b_2c_2^2 + a_3b_3c_2^2 + a_4b_4c_3^2 + a_4b_5c_3^2 + a_4b_6c_3^2 = \frac{1}{4}, \tag{4.14}$$

$$a_3b_3c_1 + a_4b_5c_1 + a_4b_6c_2 = \frac{1}{6}, \tag{4.15}$$

$$a_3b_1b_3 + a_4b_1b_5 + a_4b_2b_6 + a_4b_3b_6 = \frac{1}{6}, \tag{4.16}$$

$$a_3b_3c_1c_2 + a_4b_5c_1c_3 + a_4b_6c_2c_3 = \frac{1}{8}, \tag{4.17}$$

$$\begin{aligned} &a_3b_1b_3c_2 + a_3b_1b_3c_3 + a_4b_1b_5c_1 + a_4b_2b_6c_2 + a_4b_3b_6c_2 + a_4b_1b_5c_3 + a_4b_2b_6c_3 \\ &+ a_4b_3b_6c_3 = \frac{1}{8}, \end{aligned} \tag{4.18}$$

$$a_3b_3c_1^2 + a_4b_5c_1^2 + a_4b_6c_2^2 = \frac{1}{12}, \tag{4.19}$$

$$a_4b_3b_6c_1 = \frac{1}{24}, \tag{4.20}$$

$$a_4b_1b_3b_6 = \frac{1}{24}. \tag{4.21}$$

The set of equations (4.8)-(4.21) has fourteen equations and thirteen unknown parameters; whereas simultaneously solving the set shows a few equations to be identical. Following are the brief calculations of the process.
Simultaneously solve equations (4.20) and (4.21) as

$$c_1 = b_1. \tag{4.22}$$

Use eq. (4.22) in equations (4.15) and (4.16), and simplify as

$$c_2 = b_2 + b_3. \tag{4.23}$$

Use equations (4.22) and (4.23) in eq. (4.9), and subtract the resultant equation from eq. (4.10) to get

$$c_3 = b_4 + b_5 + b_6. \tag{4.24}$$

Use equations (4.22), (4.23) and (4.24) in eq. (4.9) to get

$$a_2b_1 + a_3b_2 + a_3b_3 + a_4b_4 + a_4b_5 + a_4b_6 = \frac{1}{2}. \tag{4.25}$$

Equation (4.25) identical to eq. (4.10). Now use equations (4.22), (4.23) and (4.24) in eq. (4.11), shows that eq. (4.11) is identical to eq. (4.12). Similarly, continue the process, use equations (4.22), (4.23) and (4.24) in equations (4.13), (4.15), (4.17) and (4.20), the resultant equations are identical to equations (4.14), (4.16), (4.18) and (4.21), respectively. Thus, we get the following simplified set of equations

$$\begin{aligned}
&a_1 + a_2 + a_3 + a_4 = 1,\\
&a_2c_1 + a_3c_2 + a_4c_3 = \frac{1}{2},\\
&a_2c_1^2 + a_3c_2^2 + a_4c_3^2 = \frac{1}{3},\\
&a_2c_1^3 + a_3c_2^3 + a_4c_3^3 = \frac{1}{4},\\
&a_3b_3c_1 + a_4b_5c_1 + a_4b_6c_2 = \frac{1}{6},\\
&a_3b_3c_1c_2 + a_4b_5c_1c_3 + a_4b_6c_2c_3 = \frac{1}{8},\\
&a_3b_3c_1^2 + a_4b_5c_1^2 + a_4b_6c_2^2 = \frac{1}{12},\\
&a_4b_3b_6c_1 = \frac{1}{24},\\
&c_1 = b_1,\\
&c_2 = b_2 + b_3,\\
&c_3 = b_4 + b_5 + b_6.
\end{aligned} \tag{4.26}$$

In the set of equations (4.26) there are eleven equations and thirteen unknown parameters, hence two parameters are arbitrary. Some fixed values of these parameters can generate a specific 4th order RK method [10].

Creating an algorithm for MATLAB code by using the set of equations (4.26) is a tedious task. In this thesis, c_1 and c_2 are considered to be input parameters and for remaining parameters use crammers rule to get the following set as

$$a_1 = 1 - a_2 - a_3 - a_4, \tag{4.27}$$

$$a_2 = \frac{6c_2c_3 - 4(c_2 + c_3) + 3}{12c_1(c_1 - c_2)(c_1 - c_3)}, \quad c_1 \neq c_2 \neq c_3, \tag{4.28}$$

$$a_3 = \frac{6c_1c_3 - 4(c_1 + c_3) + 3}{12c_2(c_3 - c_2)(c_1 - c_2)}, \quad c_1 \neq c_2 \neq c_3, \tag{4.29}$$

$$a_4 = \frac{4(c_1 + c_2) - 6c_1c_2 - 3}{12c_3(c_3 - c_2)(c_1 - c_3)}, \quad c_1 \neq c_2 \neq c_3, \tag{4.30}$$

$$b_1 = c_1, \tag{4.31}$$

$$b_2 = c_2 - b_3, \tag{4.32}$$

$$b_3 = \frac{c_2(4c_3 - 3)(c_1 - c_2)}{12c_1^2c_3 - 8c_1(c_3 + c_1) + 6c_1}, \tag{4.33}$$

$$b_4 = c_3 - b_5 - b_6, \tag{4.34}$$

$$b_5 = \frac{c_2(5 - 4c_2) - c_1(3 - 4c_3) - 2c_3}{24a_4c_1(c_3 - c_2)(c_2 - c_1)}, \quad c_1 \neq c_2 \neq c_3, \tag{4.35}$$

$$b_6 = \frac{1 - 2c_1}{12a_4c_2(c_2 - c_1)}, \quad c_1 \neq c_2, \tag{4.36}$$

$$a_4 = \frac{1}{24b_3b_6c_1}. \tag{4.37}$$

In set of equations(4.27)-(4.37), each unknown parameter is defined in terms of c_1 and c_2, except for c_3. Which means, an expression of c_3 in terms of c_1 and c_2 is required, further simplifications for c_3 leads to an interesting result. Calculations of this result are given subsequently.
Use eq. (4.37) in eq. (4.36) and simplify for b_3 as

$$b_3 = \frac{c_2(c_2 - c_1)}{2(1 - 2c_1)}. \tag{4.38}$$

Simultaneously solve equations (4.33) and (4.38) to get

$$c_3 = 1.$$

Upon utilizing $c_3 = 1$ in the set of equations (4.27)-(4.37) a simplified set of equations is formed as

$$
\begin{aligned}
a_1 &= 1 - a_2 - a_3 - a_4, \\
a_2 &= \frac{2c_2 - 1}{12c_1(c_1 - c_2)(c_1 - 1)}, \\
a_3 &= \frac{2c_1 - 1}{12c_2(1 - c_2)(c_1 - c_2)}, \\
a_4 &= \frac{4(c_1 + c_2) - 6c_1c_2 - 3}{12(1 - c_2)(c_1 - 1)}, \\
b_1 &= c_1, \\
b_2 &= c_2 - b_3, \\
b_3 &= \frac{c_2(c_1 - c_2)}{2c_1(2c_1 - 1)}, \\
b_4 &= 1 - b_5 - b_6, \\
b_5 &= \frac{c_2(5 - 4c_2) + c_1 - 2}{24a_4c_1(1 - c_2)(c_2 - c_1)}, \\
b_6 &= \frac{1 - 2c_1}{12a_4c_2(c_2 - c_1)}.
\end{aligned}
\tag{4.39}
$$

The set of equations (4.39) is used to generate an algorithm for the MATLAB code, where c_1 and c_2 are input parameters. Choices for c_1 and c_2 must be made under some conditions deduced by the set of equations (4.39), i.e., c_1 and c_2 both can not be equal to 0 or 1, also $c_1 \neq c_2$. Exceptionally, most widely used standard 4th order RK method can not be driven using set of equations (4.39), it can be driven from set of equations (4.26), the derivation is provided in subsequent section.

4.1.1 Derivation of Standard 4th Order RK Method using General Framework for 4th order RK Methods

Recall the set of equations (4.26), and choose $c_1 = \frac{1}{2}$ and $b_2 = 0$, we get the follwoing set of equations

$$
\begin{aligned}
& a_1 + a_2 + a_3 + a_4 = 1, \\
& \frac{1}{2}a_2 + a_3 c_2 + a_4 c_3 = \frac{1}{2}, \\
& \frac{1}{4}a_2 + a_3 c_2^2 + a_4 c_3^2 = \frac{1}{3}, \\
& \frac{1}{8}a_2 + a_3 c_2^3 + a_4 c_3^3 = \frac{1}{4}, \\
& \frac{1}{2}a_3 b_3 + \frac{1}{2}a_4 b_5 + a_4 b_6 c_2 = \frac{1}{6}, \\
& \frac{1}{2}a_3 b_3 c_2 + \frac{1}{2}a_4 b_5 c_3 + a_4 b_6 c_2 c_3 = \frac{1}{8}, \\
& \frac{1}{4}a_3 b_3 + \frac{1}{4}a_4 b_5 + a_4 b_6 c_2^2 = \frac{1}{12}, \\
& a_4 b_3 b_6 = \frac{1}{12}, \\
& b_1 = \frac{1}{2}, \\
& c_2 = b_3, \\
& c_3 = b_4 + b_5 + b_6.
\end{aligned}
\tag{4.40}
$$

Solve the set of equations (4.40) and determine the remaining parameters as

$$
\begin{aligned}
& a_1 = \frac{1}{6}, \quad a_2 = \frac{1}{3}, \quad a_3 = \frac{1}{3}, \quad a_4 = \frac{1}{6}, \\
& c_2 = \frac{1}{2}, \quad c_3 = 1, \quad b_1 = \frac{1}{2}, \quad b_3 = \frac{1}{2}, \\
& b_4 = 0, \quad b_5 = 0, \quad and \quad b_6 = 1.
\end{aligned}
\tag{4.41}
$$

Now plug the values listed in the set of equations (4.41) into the set of equations (4.1) and (4.2) to get the standard 4th order RK method as

$$\begin{aligned}
&y_{n+1} = y_n + h\left(\frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4\right),\\
&k_1 = f(x_n, y_n) = f,\\
&k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1),\\
&k_3 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2)\\
&k_4 = f(x_n + h, y_n + hk_3).
\end{aligned} \tag{4.42}$$

Graphical Interpretation of Standard 4th order RK Method

Recall initial value problem as given in eq. (1.2), and formula of standard 4th order RK method given by eq. (4.42). For $n = 0$ we have

$$\begin{aligned}
&y_1 = y_0 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),\\
&k_1 = f(x_0, y_0),\\
&k_2 = f(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}hk_1),\\
&k_3 = f(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}hk_2)\\
&k_4 = f(x_0 + h, y_0 + hk_3).
\end{aligned} \tag{4.43}$$

Likewise Euler method the standard 4th order RK method utilizes $y(x_0)$ to figure out y_1 but approximation involves average of four slopes $k_1,\ k_2,\ k_3$ and k_4. That is y_1 is approximated as

$$y_1 = y_0 + h(\textit{average slope}),$$

where,

$$\textit{Average slope} = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

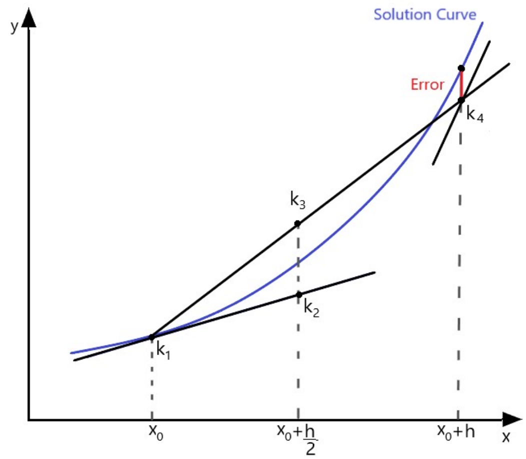

Figure 4.1: Graphical interpretation of standard 4th order RK method.

In Figure 2.1, the solution curve of problem is given in blue solid curve and all the approximated slopes are given in black solid lines while error is shown by a red solid line. Here the initial slope k_0 estimates the slope at midpoint of $[x_0, x_0 + h]$, i.e., k_2. From set of equations (4.42), witness that there is an upgrade in k_2 which estimates a slope k_3 at $x_0 + \frac{h}{2}$. Hence this upgraded slope at k_3 leads to a better estimation at $x_1 = x_0 + h$, i.e., k_4.

Chapter 5

Comparison of Various 4th Order RK Methods

The comparison of various 4th order RK methods applied to non-linear initial value problems are provided in this chapter.

Problem 1

A special case of Riccati equations has IVP as

$$\frac{dy}{dx} = \frac{-y^3}{2}, \quad y(0) = 1. \tag{5.1}$$

The domain of the problem is $[0, 2]$ and exact solution is $y = \frac{1}{\sqrt{1+x}}$. For a fixed step size $h = 0.05$, numerical solution obtained by standard 4th order RK method and the exact solution are plotted in Figure 5.1.

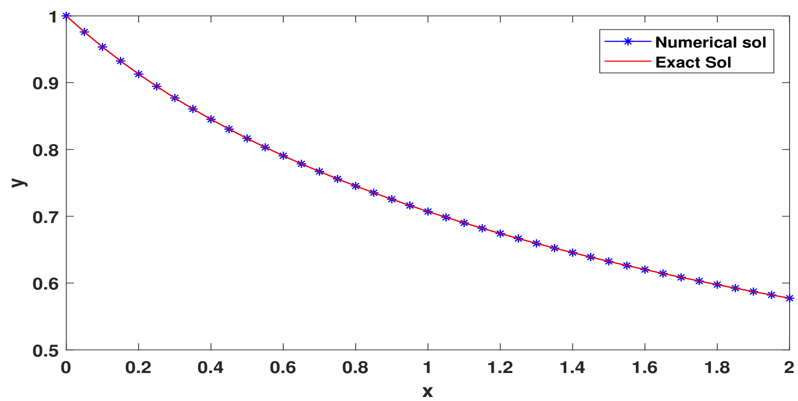

Figure 5.1: Solution obtained numerically via Standard RK-4 method vs exact solution.

In Figure 5.1, solution curve obtained numerically embeds closely on the exact solution curve. Here results are obtained by a MATLAB code that utilizes formula given in eq. (4.42). Small increment generates better results, on the other hand, a large increment yields more difference between the exact and numerical solutions. In order to have a meaningful comparison let us keep the same step size and vary the parameters c_1 and c_2 within (0,1) to generate different 4th order RK methods. By such process the solution curves obtained numerically embed closely on the exact solution curve thus the process yields similar figures as of Figure 3.1. No difference is visible by such plotting, the difference can only be observed by zooming into the graphs.

A better way to seek and analyze the difference between numerical and exact solutions is to plot absolute error curves. The strategy followed here is to plot the absolute error curves for standard 4th order RK method and the methods generated by varying parameters. The standard 4th order RK method has the form given in eq. (4.42), where $c_1 = c_2 = \frac{1}{2}$. The choices closer to 0, $\frac{1}{2}$ and 1 are taken under consideration and an important point here is that $c_1 = c_2$ only for standard 4th order RK method. The rest of variations are made with conditions that both parameters can not be 0 or 1, and $c_1 \neq c_2$. Compare the absolute error curves for different 4th order RK methods applied on eq. (5.1). Results are displayed in Figure 5.2, while step size and domain both are same as defined with the problem.

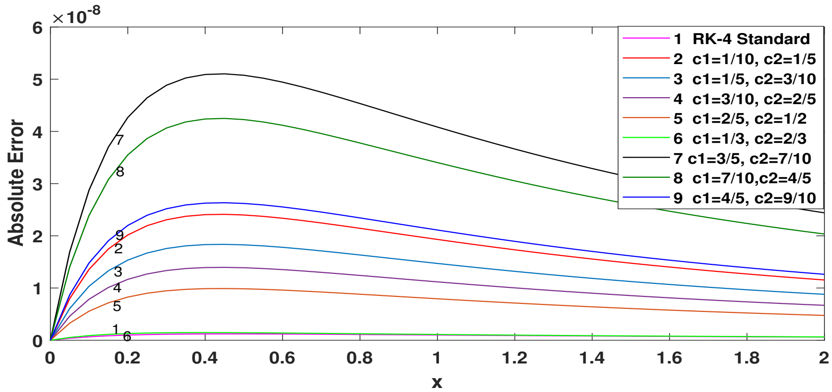

Figure 5.2: Absolute error curves of various 4th order VS standard 4th order RK method.

The choices of parameters follow a pattern, first $c_1, c_2 < \frac{1}{2}$, second $c_1 \leq \frac{1}{2}$ and $c_2 \geq \frac{1}{2}$ and third $c_1, c_2 > \frac{1}{2}$. The tabular data of Figure 5.2 is given in subsequent Table 5.1, along with maximum absolute errors in each of the distinct methods.

	Parameters		
Method	c_1	c_2	Max. Abs. Error
Standard RK4	$\frac{1}{2}$	$\frac{1}{2}$	$\mathbf{1.21718835011109 \times 10^{-09}}$
	$\frac{1}{10}$	$\frac{1}{5}$	$2.41163832237490 \times 10^{-08}$
	$\frac{1}{5}$	$\frac{3}{10}$	$1.83668016351390 \times 10^{-08}$
	$\frac{3}{10}$	$\frac{2}{5}$	$1.39585784042495 \times 10^{-08}$
	$\frac{2}{5}$	$\frac{1}{2}$	$9.90654291932458 \times 10^{-09}$
	$\frac{1}{3}$	$\frac{2}{3}$	$1.46270173750906 \times 10^{-09}$
	$\frac{3}{5}$	$\frac{7}{10}$	$5.10261441988291 \times 10^{-08}$
	$\frac{7}{10}$	$\frac{4}{5}$	$4.24873145554727 \times 10^{-08}$
	$\frac{4}{5}$	$\frac{9}{10}$	$2.63350745655089 \times 10^{-08}$

Table 5.1: Comparison of different 4th order RK methods with standard 4th order RK method.

Discussion

Observations in Table 5.1 show that 4th order RK method is the best choice, as it generates comparatively less error. Otherwise, maximum absolute error increases for choosing the parameters either closer to 0 or 1.

Problem 2

The Gompertz tumor growth model is given as

$$\frac{dN}{dt} = a\ N\ ln\left(\frac{b}{N}\right). \tag{5.2}$$

In this modal $N(t)$ is the number of cells in a tumor that grows over time. The positive contants a and b depend on the type of tumor, whether the tumor is being treated, and on the kind of treatment.

Consider a simple case by choosing $a = b = 1$ and initial number of tumor cells to be 2 units we get the IVP as

$$\frac{dN}{dt} = N\ ln\left(\frac{1}{N}\right), \quad N(0) = 2. \tag{5.3}$$

The exact solution of problem is $N = 2^{e^{-t}}$ and domain of problem is [0,1]. For a fixed step size of 0.05, numerical solution obtained by 4th order RK method and exact solution, both embed closely on each other and are presented in Figure 5.5.

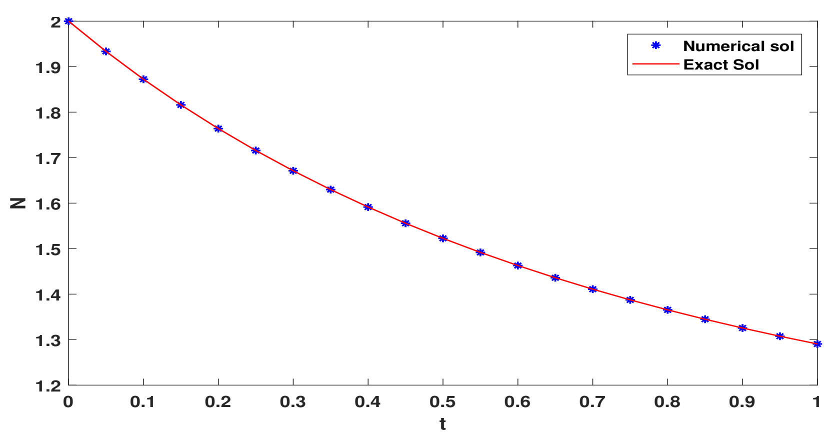

Figure 5.3: Exact solution vs numerical solution obtained by standard 4th order RK method.

Follow the process as followed for Problem 1 and plot absolute error curves obtained for multiple choices of both parameters.

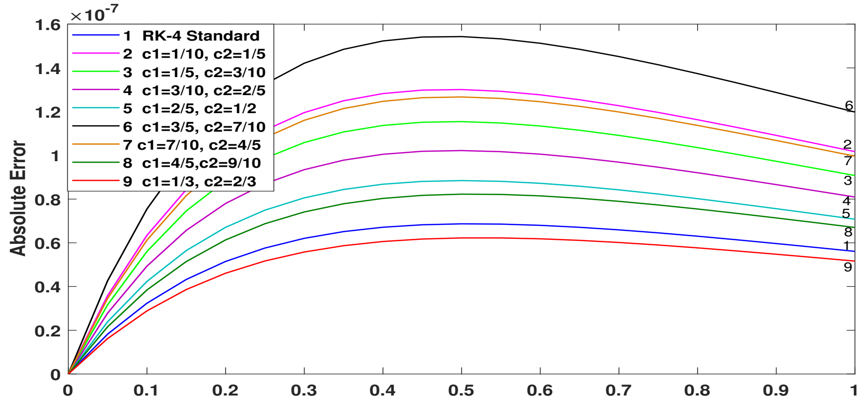

Figure 5.4: Absolute error curves of various 4th order RK methods vs standard 4th order RK method.

	Parameters		
Method	c_1	c_2	Max. Abs. Error
Standard RK4	$\frac{1}{2}$	$\frac{1}{2}$	$6.86767844815250 \times 10^{-08}$
	$\frac{1}{10}$	$\frac{1}{5}$	$1.30088052774369 \times 10^{-07}$
	$\frac{1}{5}$	$\frac{3}{10}$	$1.15432211122979 \times 10^{-07}$
	$\frac{3}{10}$	$\frac{2}{5}$	$1.02181226369069 \times 10^{-07}$
	$\frac{2}{5}$	$\frac{1}{2}$	$8.84544968382528 \times 10^{-08}$
	$\boldsymbol{\frac{1}{3}}$	$\boldsymbol{\frac{2}{3}}$	$\mathbf{6.22314431097948 \times 10^{-08}}$
	$\frac{3}{5}$	$\frac{7}{10}$	$1.54315801914606 \times 10^{-07}$
	$\frac{7}{10}$	$\frac{4}{5}$	$1.26705950398431 \times 10^{-07}$
	$\frac{4}{5}$	$\frac{9}{10}$	$8.22473413819580 \times 10^{-08}$

Table 5.2: Comparison of different 4th order RK methods with standard 4th order RK method.

Discussion

There is no trend observed in Figure 5.6 and from Table 5.4 the choice $c_1 = \frac{1}{3}$ and $c_2 = \frac{2}{3}$ that is a choice closer to $\frac{1}{2}$, results in minimum error. Otherwise, maximum absolute error increases for choosing the parameters either closer to 0 or 1. Some more choices of the form $c_1 < \frac{1}{2}$ and $c_2 > \frac{1}{2}$ to compare the absolute error curves are displayed in Figure 5.7.

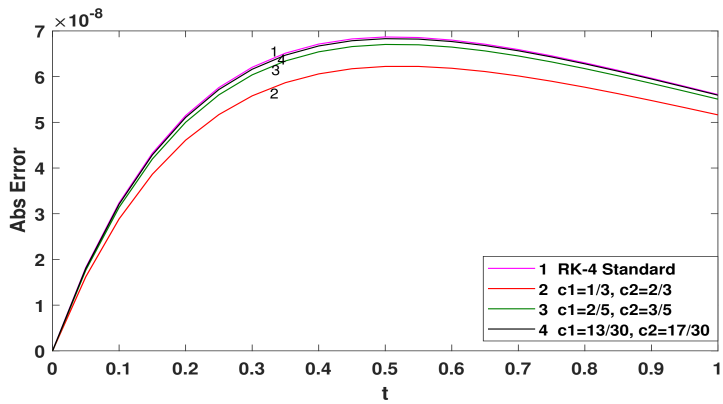

Figure 5.5: Absolute error curves of different 4th order RK methods, where $c_1 < \frac{1}{2}$ and $c_2 > \frac{1}{2}$.

	Parameters		
Method	c_1	c_2	Max. Abs. Error
*Standard RK*4	$\frac{1}{2}$	$\frac{1}{2}$	$6.86767844815250 \times 10^{-08}$
	$\frac{2}{5}$	$\frac{3}{5}$	$\mathbf{6.22314431097948 \times 10^{-08}}$
	$\frac{3}{10}$	$\frac{7}{10}$	$6.70403315083945 \times 10^{-08}$
	$\frac{9}{20}$	$\frac{13}{20}$	$6.83056864403397 \times 10^{-08}$

Table 5.3: Comparison of different 4th order RK methods, where $c_1 < c_2$, with standard 4th order RK method.

In Table 5.5 the difference between maximum absolute errors of standard RK-4 and second choice is $6.445341371730211 \times 10^{-09}$. Second choice has slightly less error as compared to the standard RK-4, hence it is comparatively a better choice for the Problem 2.

Observations from last problem show that standard 4th order RK method is not necessarily a best method. Also, if both parameters are chosen closer to $\frac{1}{2}$ results in minimum error. Furthermore, no change occurs by enhancing the domain of problem in each case.

Chapter 6

Conclusion

This thesis discusses numerical methods for solving non-linear ordinary differential equations. The study and development of RK methods up to the 4th order are provided. The families of second, third and fourth order RK methods are developed by truncating the Taylor series, and a set of non-linear equations with some unknown parameters in each case are obtained. Each set has some input parameters, i.e., one can generate a specific method by varying these parameters. Each method's mathematical set of equations is further simplified to generate MATLAB codes. While deriving such a set for third and fourth order RK methods, some important constraints are discussed to choose the input parameters. The comparisons of various third and fourth order RK methods applied to non-linear problems, such as the special case of the Riccati equation, logistic map IVP and Gompertz tumor growth model, are provided in chapter 3 and 5.

In case of family of third and fourth order RK methods, there are two free parameters c_1 and c_2. These parameters are chosen under some conditions, such as, $c_1 \neq c_2$, also c_1 and c_2 both are non-zero real numbers. The comparison of various third order RK methods applied to considered problems leads to a main observation that for considered problems standard 3rd order RK method is not a better choice. For first problem the choice $c_1 = \frac{7}{10}$ and $c_2 = \frac{4}{5}$ generates solution with comparatively less error. For second problem the choice $c_1 = \frac{1}{10}$ and $c_2 = \frac{1}{5}$ is better. Prominent

observation from comparison of different fourth order RK methods is that both of these parameters generate accurate results if these are chosen closer to $\frac{1}{2}$, that is closer to the choices in standard fourth order RK method. In problem 1 the standard 4th order RK method generates solution with less error and in problem 2 the choice $c_1 = \frac{1}{3}$ and $c_2 = \frac{2}{3}$ results in minimum error.
Thus, on the basis of considered problems one can not conclude that only standard third and fourth order RK methods are better. Moreover, observations from each problem shows that the standard third and fourth order RK methods are suitable if the error tolerance associated with the problem is not sensitive. For the error tolerance up to fifth decimal place of value, any method from both families is suitable. Else, if a sensitive tolerance appears then one can vary the parameters and choose a best suitable method from the family. The sensitive error tolerance can be tackled by upgrading the mesh points or taking a small step size.

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