# SOLVING NONLINEAR CHEMICAL KINETICS SYSTEM BY USING BERNSTEIN POLYNOMIALS

**Tufa Gonfa Bekele**

**A Thesis Submitted to Department of Applied Mathematics**

**School of Applied Natural Science**

**Presented in Partial Fulfillment of the Requirement for the Degree of Master's in Applied Mathematics (Differential Equations)**

**Office of Graduate Studies**

**Adama Science and Technology University**

**August 20, 2021**

**Adama, Ethiopia**

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**Tufa Gonfa Bekele**

**Advisor:**

**Feyissa Kebede (Ph.D.)**

**Co-Advisor:**

**Sileshi Mebrate**

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# Declaration

I hereby declare that this Master Thesis entitled ”Solving nonlinear chemical kinetics system by using Bernstein polynomials ” is my oririgal work. That is, it has not been submitted for the award of any academic degree,diploma or certificate in any other univeristy. All sources of materials that are used for this thesis have been duly acknowledged through citation.

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# Recommendation

We, the advisors of this thesis, hereby certify that we have read the revised version of the thesis entitled ”Solving nonlinear chemical kinetics system by using Bernstein polynomials ” prepared under our guidance by Tufa Gonfa Bekele submitted in partial fulfillment of the requirements for the degree of Master's of Science in Applied Mathematics. Therefore, we recommend the submission of revised version of the thesis to the department following the applicable procedures.

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# Approval Page

We, the advisors of the thesis entitled ” Solving nonlinear chemical kinetics system by using Bernstein polynomials ” and developed by Tufa Gonfa Bekele, hereby certify that the recommedantion and suggestions made by the board of examiners are appropriately incorporated into the final version of the thesis.

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We, the undersigned, members of the Board of Examiners of the thesis by Tufa Gonfa Bekele have read and evaluated the thesis entitled ”Solving nonlinear chemical kinetics system by using Bernstein polynomials ” and examined the candidate during open defense. This is, therefore, to certify that the thesis has been accepted in partial fulfillment of the requirement of the degree of Master’s of Science in Applied Mathematics.

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# TABLE OF CONTENTS

# LIST OF FIGURES

# List of Symbols and Acronyms

| | |
|---|---|
| $\Gamma$ | Gamma function |
| $\gamma$ | Order of fractional derivative |
| $\mathbf{I}^{\gamma}$ | Bernstein polynomials operational matrix of fractional integration |
| $\widehat{C}$ | Bernstein operational Matrix of product |
| $A$ | Matrix formulation of Bernstein polynomials |
| $C$ | Coefficient of Bernstein polynomials |
| $D_t^{\gamma}$ | Caputo Fractional derivative of order $\gamma$ |
| $H_m$ | Hilbert matrix |
| $I_a^{\gamma}$ | Fractional integral of Riemann-Liouville |
| $m$ | Degree of Bernstein polynomials |
| $Q$ | Symmetric matrix of Bernstein polynomials |
| $t$ | time(seconds) |
| BPs | Bernstein polynomials |
| HAM | Homotopy analysis method |
| HPM | Homotopy perturbation method |
| VIM | Variational iteration method |

# Abstract

*In this study, we solve a nonlinear fractional model of chemical kinetics system. The numerical solution of this nonlinear fractional model has been obtained by using Bernstein polynomials. The basic idea is to apply operational matrices of fractional integration and multiplication of Bernstein polynomials. The significance point to note here is the given problem turns into a set of nonlinear algebraic equations by expanding the solution as Bernstein polynomials with unknown coefficients. Then, by solving nonlinear algebraic equations, the approximate solution of a fractional model of chemical kinetics system are obtained. In addition, to solve this nonlinear algebraic equations we have used the Newton iterations method. Also, this result explained by the fact that the suggested technique is computationally powerful for solving a fractional model of chemical kinetics system. To manifest about the performance and applicability of the method, one test example is deliberated. In this work we use of Mathematica for computations and programming.*

**Keywords:-** Gamma function; Fractional model of chemical kinetics system; Riemann-Liouville integral; Caputo fractional derivative; Approximation of function; Operational matrix; Bernstein polynomials.

Chapter 1

# INTRODUCTION

## 1.1 Background of the Study

Differential equations are extremely important in the history of mathematics and science, because the laws of nature are generally expressed in terms of differential equations. One of the most significant current subjects in pure and applied mathematics is fractional calculus (Hairer, Nørsett, & Wanner, 1993). Fractional calculus is a branch of mathematical analysis in which derivatives and integrals of fractional order are defined and studied, is nearly as old as the classical calculus of integer orders. It is a generalization of ordinary differentiation and integration to arbitrary noninteger order (Weyl, 1959).

Fractional integrals and derivatives arise in many engineering and scientific disciplines as the mathematical modeling of systems and processes in the fields of physics, chemistry, aerodynamics, electrodynamics of a complex medium (Kareem, 2018). Many problems in physics, chemistry and biology can be represented by either linear or nonlinear ordinary or partial differential equations (AL-Jawary & Raham, 2016). In every phenomena in real life, there are many parameters and variables. When the relations between the parameters and variables are presented in mathematical language we usually derive a mathematical model of the problem (Khader, 2013).

Mathematical modelling is the best way to formulating problems from an application area and it is well known that several mathematical characterization of numerous growth in chemical and physical sciences is described by differential equations (Kumar, Kumar, Singh, & Al-Zhour, 2020). A model is a simplified representation of a real world process. These models are an equation, a differential equation, an integral equation, a system of integral

equations,etc(Weyl, 1959).

In Chemistry the laws governing chemical kinetics can be written as systems of ordinary differential equations based on the law of mass action. A chemical kinetics system is represented by a nonlinear system of ordinary differential equations. Chemical kinetics deals with chemistry experiments and interprets them in terms of a mathematical model. The experiments are perfomed on chemical reactions as they proceed with time. The models are differential equations for the rates at which reactants are consumed and products are produced (Hairer et al., 1993).

The law of mass action says that the rate of the chemical reaction is directly proportional to the product of the activities or concentrations of the reactants. It explains and predicts behaviors of solutions in dynamic equilibrium. Specifically, it implies that for a chemical reaction mixture that is in equilibrium, the ratio between the concentration of reactants and products is constant (Hairer et al., 1993).

Suppose that two chemicals $X$ and $Y$ react to form a product chemical $Z$, written as (Chasnov et al., 2009)

$$X + Y \xrightarrow{\theta} Z$$

where $\theta$ is the constant chemical reaction rate. For simplicity, we will use the same symbol $Z$, say to refer to both the chemical $Z$ and its concentration. The law of mass action says that $\frac{dZ}{dt}$ is proportional to the product of the concentrations $X$ and $Y$, with proportionality constant $\theta$.

That is,

$$\frac{dZ}{dt} = \theta XY.$$

Similarly, the law of mass action enables us to write equations for the time derivatives of the reactant concentrations $X$ and $Y$:

$$\frac{dX}{dt} = -\theta XY, \frac{dY}{dt} = -\theta XY.$$

Notice that when using the law of mass action to find the rate-of-change of a concentration, the chemical that the arrow points towards is increasing in concentration (positive sign) and the chemical that the arrow points away from is decreasing in concentration (negative sign). The product of concentrations on the right-hand-side is always that of the reactants from which the arrow points away, multiplied by the rate constant that is on top of the arrow and studied by Vallance in (Vallance, 2017).

A wide variety of chemical reactions can be modeled with coupled (often nonlinear) differential equations. These equations describe the time evolution of the concentrations of the various chemical species: reactants, intermediaties, catalysts, and products. The problem of dealing with chemical reactions of systems involving two variable intermediates, together with a number of initial and final products whose concentrations are assumed to be controlled throughout the reaction process is an important one under quite realistic conditions (Bank, Graham, Stoer, Varga, & Yserentant, n.d.).

Consider the model of a chemical kinetics system has form of

$$\begin{cases} P + X \xrightarrow{\theta_1} X + X, \\ X + Y \xrightarrow{\theta_2} Y + Y, \\ Y \xrightarrow{\theta_3} Z \end{cases} \tag{1.1}$$

where $\theta_1$, $\theta_2$ and $\theta_3$ are the constant chemical reaction rates.

The rate equations for chemical kinetics system are fundamentally nonlinear differential equation. The solution of differential equation is specific function that satisfies equation. Unfortunately most of nonlinear differential equation cannot be solved analytically. To investigate the predictions of model of such phenomena it is necessary to approximate their solution numerically (Hairer et al., 1993).

In the study by Hossein Aminikhah, the homotopy perturbation method was applied for solving the nonlinear system of chemical kinetics. In this case numerical methods such as Runge-Kutta and Euler methods commonly used for solving these equations, either need a lot of computations and have less convergence speed and accuracy or solve only certain types of problems (Aminikhah, 2011).

In this thesis, we apply the method of Bernstein polynomials (Bps) for solving the model of nonlinear chemical kinetics system (1.1). Here, we also use the operational matrices of fractional integration and multiplication of Bernstein polynomials.

## 1.2 Statement of the Problem

In this work we consider four species in the model of chemical process which are denoted by $P$, $X$, $Y$ and $Z$ where $P$ is reactant, $Z$ is product and $X$ and $Y$ are the intermediates. We can define the three reactions as:

$$P + X \xrightarrow{\theta_1} X + X, \tag{1.2}$$

$$X + Y \xrightarrow{\theta_2} Y + Y, \tag{1.3}$$

$$Y \xrightarrow{\theta_3} Z. \tag{1.4}$$

where $\theta_1$, $\theta_2$ and $\theta_3$ are the constant chemical reaction rates.

Assume that the concentrations of $P$, $X$, $Y$ and $Z$ are indicated by $\zeta$, $\eta$, $\kappa$ and $\mu$, respectively. We suppose that these concentrations are scaled so that the sum of four concentrations is one and that all of four constituent reactions are added with the concentration of some of the species accurately at the rate of the corresponding values of the reactants. The law of mass action in the chemical reactions leads to the following system of differential equations for the variation with time $t$:

$$\begin{aligned}
\frac{d\zeta}{dt} &= -\theta_1\zeta(t)\eta(t),\\
\frac{d\eta}{dt} &= \theta_1\zeta(t)\eta(t) - \theta_2\eta(t)\kappa(t),\\
\frac{d\kappa}{dt} &= \theta_2\eta(t)\kappa(t) - \theta_3\kappa(t),\\
\frac{d\mu}{dt} &= \theta_3\kappa(t).
\end{aligned} \tag{1.5}$$

with initial condition $\zeta(0) = 0.5$, $\eta(0) = 0.3$, $\kappa(0) = 0.2$ and $\mu(0) = 0$.

Fractional differential equations are generalized from classical integer order ones, which are obtained by replacing integer-order derivatives by fractional ones. The main issue why we replace the fractional order differential equations with integer order differential equations are the capability of simulating natural physical process and dynamic system more accurately. So we replace the time-derivative in equation (1.5) by the Caputo fractional derivative and

yields:

$$\begin{aligned} D_t^{\gamma}\zeta(t) &= -\theta_1\zeta(t)\eta(t), \\ D_t^{\gamma}\eta(t) &= \theta_1\zeta(t)\eta(t) - \theta_2\eta(t)\kappa(t), \\ D_t^{\gamma}\kappa(t) &= \theta_2\eta(t)\kappa(t) - \theta_3\kappa(t), \\ D_t^{\gamma}\mu(t) &= \theta_3\kappa(t) \end{aligned} \tag{1.6}$$

with initial condition $\zeta(0) = 0.5$, $\eta(0) = 0.3$, $\kappa(0) = 0.2$ and $\mu(0) = 0$.

In equation (1.6), $D^{\gamma}\zeta(t)$ is indicated to be the Caputo fractional derivative of order $\gamma$.

The focus of this work is to study how to solve fractional model of system (1.6) by the method of Bernstein polynomials.

Therefore, this study was intended to answer the following basic questions;

1. How to apply Bernstein polynomials method for solving fractional model of chemical kinetics system?
2. How to reduce the fractional model of chemical kinetics system into nonlinear algebraic equation by the method of Bernstein polynomials?
3. What is numerical result?

## 1.3 Objectives of the Study

### 1.3.1 General Objective of the Study

The general objective of this study is to solve a fractional model of nonlinear chemical kinetics system using Bernstein polynomials method.

### 1.3.2 Specific Objectives

The specific objectives of this study are to:

- introduce Caputo fractional derivative on the model of chemical kinetics system.
- reduce the fractional model of chemical kinetics system into nonlinear algebraic equation by using Bernstein polynomials.
- compare the approximate solution with exact solution.

## 1.4 Significance of the Study

The result of this study will helpful to:

1. understand how to apply Bernstein polynomials for solving fractional chemical kinetics system.
2. great contribution to the existing knowledge on the application of fractional model of chemical kinetics system.
3. the researchers as a starting point for further studies on fractional model of chemical kinetics system and related studies.
4. apply the proposed method to other non-linear differential equations to get an approximate solution.

Chapter 2

# LITERATURE REVIEW

In the recent years, an increasing interest of scientists and engineers has been devoted to the analytical asymptotic techniques for solving nonlinear problems. Many new numerical techniques have been widely applied to the nonlinear problems of chemical kinetics system.

Aminikhah (2011) obtained the analytical approximation of chemical kinetics system using a homotopy perturbation method. Perturbation method is one of the well-known methods for solving nonlinear equations. However, perturbation method has some limitations, and the small parameter assumption is over restricted, so its application is strongly limited.

Khader (2013) studied the chemical kinetics problem using the Picard-Pade technique. In this case, he introduced modification of the Picard iteration method (PIM) using Pade-approximation and the so called Picard-Pade technique. The chemical kinetics problem is formed by a system of nonlinear ordinary differential equations. Also he studied the convergence analysis of the chemical kinetics system. Convergence analysis is reliable enough to estimate the maximum absolute error of the solution given by Picard iteration method (PIM). Besides to this he compared the numerical results against with the conventional numerical method, fourth-order Runge-Kutta method (RK4). Numerical results were obtained for these two methods and he found that Picard-Pade technique and RK4 are in excellent conformance. The results obtained ensure that the presented procedure needs less work in comparison with the traditional methods and decreases considerable volume of calculation and is a powerful tool for solving large amount of other problems in physics and engineering.

Singh, Kumar, and Baleanu (2017) proposed the analysis of chemical kinetics system with a fractional derivative with the Mittag-Leffler type kernel and numerous papers have been published on the analytical and numerical methods for solving nonlinear fractional differential equations such as: decomposition method, second order finite difference method, collocation method, Runge kutta, dual reciprocity boundary element method, differential quadrature algorithms and more recently, variation multiscale element free Galerkin and local discontinuous Galerkin methods, modified trigonometric cubic B-spline function based differential quadrature algorithm etc.

AL-Jawary and Raham (2016) proposed the system of ordinary differential equations which represent one of a mathematical models of a chemical kinetics problems using iterative methods. In this iterative method the solution is obtained in the series form with easily computed components. The results of the maximal error remainder values show that the iterative method is very effective and reliable.

Ganji, Nourollahi, and Mohseni (2007) proposed the He's Homotopy perturbation method (HPM) and Variation iteration method (VIM) for solving analytically two systems of ordinary differential equations that often appear in chemical applications. In both methods, the initial approximations can be freely chosen with possible unknown constants which can be determined by imposing the boundary and initial conditions. The solution procedure is of utter simplicity, and the obtained solution is of high accuracy.

Matinfar, Saeidy, Gharahsuflu, and Eslami (2014) proposed the homotopy analysis method (HAM) to solve analytic solutions of nonlinear systems that often appear in chemical problems. In this case the variational iteration method (VIM) and the homotopy perturbation method (HPM) has a solution of the chemical kinetics problem, but the paper contained some evident mistakes that we could easily identify. The results show that the HAM is very effective and convenient and the solutions obtained using this method have high accuracy with respect to VIM and HPM.

Patade and Bhalekar (2015) proposed that a new iterative method for solving linear and nonlinear functional equations namely (DJM). The DJM has been successfully implemented

by many authors for solving linear and nonlinear ordinary and partial differential equations of integer and fractional order. This method converges to the exact solution if it exists through successive approximations. However, for concrete problems, a few number of approximations can be used for numerical purposes with high degree of accuracy. The DJM does not require any restrictive assumptions for nonlinear terms as required by some existing techniques.

In all above reviewed literature excpet (Sheybak & Tajadodi, 2019) a fractional model of nonlinear chemical kinetics system has studied in different technique. But in this thesis we intended to extend a fractional model of nonlinear chemical kinetics system in (Sheybak & Tajadodi, 2019) by introducing one more concentration of chemical. Then we will use Bernstein polynomial method to solve a fractional model of nonlinear chemical kinetics system.

Chapter 3

# RESEARCH METHODOLOGY

The way of approximation of the numerical solution of the fractional chemical kinetics model is using the operational matrices of fractional integration and multiplication based on Bernstein polynomials. To describe the system of chemical kinetics, we utilize system of non linear differential equations. The study involves numerical implementation with Mathematica. Again, to attain the objective of this study we validate the method using numerical examples and show results using graphs. Plotting the graphs of solutions of each method and exact solution is performed working with Mathematica code. Finally, the exact and numerical solutions of the methods can be compared using graphs.

Chapter 4

# MATHEMATICAL PRELIMINARIES

In this chapter, we state some theorems and give the definitions of terminologies which are most crucial for the thesis as an input.

## 4.1 Existence and Uniqueness Theorem

The fundamental existence-uniqueness theorem for a non-linear autonomous system of ordinary differential equations

$$\dot{u} = f(u(t)), \quad u(t_0) = u_0 \tag{4.1}$$

under the hypothesis that $f \in C^1(E)$ where $E$ is an open subset of $\mathbb{R}^n$.

**Definition 1** *(The Fundamental Existence-Uniqueness Theorem) (Perko, 2013) Suppose that $f \in C(E)$ where $E$ is an open subset of $\mathbb{R}^n$. Then $u(t)$ is a solution of the differential equation (4.1) on an interval $I$ if $u(t)$ is differentiable on $I$ and if for all $t \in I$, $u(t) \in E$ and*

$$\dot{u} = f(u(t)).$$

*And given $u_0 \in E$, $u(t)$ is a solution of the initial value problem*

$$\dot{u} = f(u(t)), \quad u(t_0) = u_0$$

*on an interval $I$ if $t_0 \in I$, $u(t_0) = u_0$ and $u(t)$ is a solution of the differential equation (4.1) on the interval $I$.*

**Definition 2** *(Perko, 2013) A solution $u(t)$ of (4.1) is stable if every solution that starts sufficiently close to $u(t)$ at $t = t_0$ remains close to $u(t)$ for all $t > t_0$. The solution $u(t)$ is unstable if there exists at least one solution starting close to $u(t)$ at $t = t_0$, which does not remain close to $u(t)$ for all $t > t_0$.*

## 4.2 Gamma and Beta function

**Definition 3** *The Gamma function is a generalization of the factorial function $m!$ and defined as (Kareem, 2018)*

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}dt, \quad \mathbb{R}ez > 0. \tag{4.2}$$

The following are the most important properties of the Gamma function:

1. $\Gamma(z+1) = z\Gamma(z)$.

   **Proof:** By definition,

$$\begin{aligned}
\Gamma(z+1) &= \int_0^\infty t^z e^{-t}dt \\
&= \lim_{b\to\infty}\left[\left[-t^z e^{-t}\right]_0^b + z\int_0^b t^{z-1}e^{-t}dt\right] \\
&= \lim_{b\to\infty}\left[-\frac{t^z}{e^t}\right]_0^b + z\int_0^\infty t^{z-1}e^{-t}dt \\
&= z\int_0^\infty t^{z-1}e^{-t}dt \\
&= z\Gamma(z).
\end{aligned}$$

2. $\Gamma(m) = (m-1)!$, for all $m \in \mathbb{N}$.

   **Proof:** We have

$$\begin{aligned}
\Gamma(m) &= \int_0^\infty t^{m-1}e^{-t}dt \\
&= \left[-t^{m-1}e^{-t}\right]_0^\infty + (m-1)\int_0^\infty t^{m-2}e^{-t}dt \\
&= (m-1)\int_0^\infty t^{m-2}e^{-t}dt \\
&= (m-1)\int_0^\infty t^{(m-1)-1}e^{-t}dt \\
&= (m-1)\Gamma(m-1).
\end{aligned}$$

Now, to start working through the proof of the property we expand out $\Gamma(m)$ as follows.

$$\begin{aligned}\Gamma(m) &= (m-1)\Gamma(m-1)\\ &= (m-1)(m-2)\Gamma(m-2)\\ &= (m-1)(m-2)(m-3)\cdots(3)(2)(1)\Gamma(1).\end{aligned}$$

We now have $\Gamma(1)$ multiplied by a large coefficient. This coefficient, as it turns out, is the definition for $(m-1)!$. That means,

$$(m-1)(m-2)(m-3)\cdots(3)(2)(1) = (m-1)!.$$

Thus

$$\Gamma(m) = (m-1)(m-2)(m-3)\cdots(3)(2)(1)\Gamma(1) = (m-1)!.$$

3. $\Gamma(m+1) = m!, \quad \forall m \in \mathbb{N}.$

   **Proof:**

   Since

$$\begin{aligned}\Gamma(m+1) &= \int_0^\infty t^m e^{-t}dt\\ &= \lim_{b\to\infty}\left[\left[-t^m e^{-t}\right]_0^b + m\int_0^b t^{m-1}e^{-t}dt\right]\\ &= \lim_{b\to\infty}\left[-\frac{t^m}{e^t}\right]_0^b + m\int_0^\infty t^{m-1}e^{-t}dt\\ &= m\int_0^\infty t^{m-1}e^{-t}dt\\ &= m\Gamma(m)\\ &= m(m-1)! = m!.\end{aligned}$$

**Remark:**

1. $\Gamma(1) = \Gamma(2) = 1.$
2. $\Gamma(\frac{1}{2}) = \sqrt{\pi}.$

**Definition 4** *The Beta function is defined by the integral(Kareem, 2018)*

$$B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}dt$$

*where x and y are positive real numbers.*

**Remark**: The Gamma and Beta functions are related as follows:

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}, \quad for \quad x,y \in (0,\infty).$$

## 4.3 Riemann-Liouville Fractional Integral

**Definition 5** *The Riemann-Liouville fractional integral of order $\gamma$ which is denoted by $I_a^\gamma$, of a function $f$ in $L_1[a,b]$ is defined as(Haghbin & Jafari, 2017)*

$$I_a^\gamma f(x) = \frac{1}{\Gamma(\gamma)} \int_a^x (x-t)^{\gamma-1} f(t)dt \quad \gamma > 0, \quad a \leq x \leq b. \tag{4.3}$$

It is a manner of generalization of the repeated antiderivative of $f$ in the sense that for values of order $\gamma$ and $I^\gamma f$ is an iterated antiderivative of $f$ of order $\gamma$. The integral is well-defined provided that $f(t)$ is a locally integrable function.

The main properties of the Riemann-Liouville fractional integral of order $\gamma$ are (Haghbin & Jafari, 2017):

1. $I_a^\gamma I_a^\beta f(x) = I_a^{\gamma+\beta} f(x)$.

   **Proof:** We have

$$\begin{aligned}
I_a^\gamma I_a^\beta f(x) &= I_a^\gamma \left[ \frac{1}{\Gamma(\beta)} \int_s^x (t-s)^{\beta-1} f(s)ds \right] \\
&= \frac{1}{\Gamma(\gamma)} \int_a^x (x-t)^{\gamma-1} \left[ \frac{1}{\Gamma(\beta)} \int_s^x (t-s)^{\beta-1} f(s)ds \right] dt \\
&= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x (x-t)^{\gamma-1} \int_s^x (t-s)^{\beta-1} f(s)dtds \\
&= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x \int_s^x (x-t)^{\gamma-1} (t-s)^{\beta-1} f(s)dtds \\
&= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x f(s) \int_s^x (x-t)^{\gamma-1} (t-s)^{\beta-1} dtds.
\end{aligned}$$

   The substitution $t = s + r(x-s)$ yields

$$\begin{aligned}
I_a^\gamma I_a^\beta f(x) &= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x f(s) \int_0^1 [(x-s)(1-r)]^{\gamma-1} [r(x-s)]^{\beta-1} (x-s)drds \\
&= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x f(s)(x-s)^{\gamma+\beta-1} \int_0^1 (1-r)^{\gamma-1} r^{\beta-1} drds.
\end{aligned}$$

   Since the integral of

$$\int_0^1 (1-r)^{\gamma-1} r^{\beta-1} dr,$$

   is the beta function formula and which is equal to $\frac{\Gamma(\gamma)\Gamma(\beta)}{\Gamma(\gamma+\beta)}$.

Thus,

$$\begin{aligned} I_a^{\gamma} I_a^{\beta} f(x) &= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x f(s)(x-s)^{\gamma+\beta-1} \int_0^1 (1-r)^{\gamma-1} r^{\beta-1} dr ds \\ &= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \int_a^x f(s)(x-s)^{\gamma+\beta-1} \left( \frac{\Gamma(\gamma)\Gamma(\beta)}{\Gamma(\gamma+\beta)} \right) ds \\ &= \frac{1}{\Gamma(\gamma)\Gamma(\beta)} \frac{\Gamma(\gamma)\Gamma(\beta)}{\Gamma(\gamma+\beta)} \int_a^x f(s)(x-s)^{\gamma+\beta-1} ds \\ &= I_a^{\gamma+\beta} f(x). \end{aligned}$$

2. $I_a^{\gamma} I_a^{\beta} f(x) = I_a^{\beta} I_a^{\gamma} f(x)$.

3. $I_0^{\gamma} x^{\beta} = \frac{\Gamma(\beta+1)}{\Gamma(\gamma+\beta+1)} t^{\gamma+\beta}$.

   **Proof:** We have

$$\begin{aligned} I_0^{\gamma} x^{\beta} &= \frac{1}{\Gamma(\gamma)} \int_0^x (x-t)^{\gamma-1} t^{\beta} dt \\ &= \frac{1}{\Gamma(\gamma)} \int_0^1 (x-sx)^{\gamma-1} (sx)^{\beta} x ds \quad putting \quad t = sx \\ &= \frac{1}{\Gamma(\gamma)} x^{\gamma+\beta} \int_0^1 s^{\beta} (1-s)^{\gamma-1} ds \\ &= \frac{1}{\Gamma(\gamma)} x^{\gamma+\beta} \left[ \frac{\Gamma(\gamma)\Gamma(\beta+1)}{\Gamma(\gamma+\beta+1)} \right] \\ &= \frac{\Gamma(\beta+1)}{\Gamma(\gamma+\beta+1)} x^{\gamma+\beta}. \end{aligned}$$

## 4.4 Caputo Fractional Derivative

**Definition 6** *The fractional derivative of $f(t)$ in the Caputo sense is defined as (Rehman, Darus, & Salah, 2018)*

$$D_t^{\gamma} f(x) = \frac{1}{\Gamma(m-\gamma)} \int_0^x (x-t)^{m-\gamma-1} f^{(m)}(t) dt, \tag{4.4}$$

which is called the Caputo Fractional derivative or Caputo fractional differential operator of order $\gamma$. In this definition first differentiate $f(t)$ m-times then integrate $m-\gamma$ times.

Main advantages of Caputo fractional derivative are:

**(i)**. The Caputo fractional derivative of a constant function is zero.

**(ii)**. The initial conditions for the fractional-order differential equations with the Caputo derivatives are in the same form as for the integer-order differential equations.

**Theorem 1** *The Caputo fractional derivative of the power function is (Kareem, 2018):*

$$D_t^{\gamma} x^p = \begin{cases} \frac{\Gamma(p+1)}{\Gamma(1+p-\gamma)} t^{p-\gamma}, p \in \mathbb{N}, p > \gamma \\ 0, otherwise \end{cases} \tag{4.5}$$

**Proof:**

The first case since $p \in \mathbb{N}$, $p > \gamma$ then

$$\begin{aligned} D_t^{\gamma} x^p &= \frac{1}{\Gamma(m-\gamma)} \int_0^x (x-t)^{m-\gamma-1} (t^p)^m dt \\ &= \frac{1}{\Gamma(m-\gamma)} \int_0^x \frac{\Gamma(p+1)}{\Gamma(p-m+1)} t^{p-m} (x-t)^{m-\gamma-1} dt. \end{aligned}$$

And using substitution $t = \lambda x$, $0 \leq \lambda \leq 1$

$$\begin{aligned} D_t^{\gamma} x^p &= \frac{\Gamma(p+1)}{\Gamma(m-\gamma)\Gamma(p-m+1)} \int_0^x (x-\lambda x)^{m-\gamma-1} (\lambda x)^{p-m} t d\lambda \\ &= \frac{\Gamma(p+1)}{\Gamma(m-\gamma)\Gamma(p-m+1)} t^{p-\gamma} \int_0^x (1-\lambda)^{m-\gamma-1} \lambda^{p-m} t d\lambda \\ &= \frac{\Gamma(p+1)}{\Gamma(m-\gamma)\Gamma(p-m+1)} t^{p-\gamma} \beta(p-m+1, m-\gamma) \\ &= \frac{\Gamma(p+1)}{\Gamma(m-\gamma)\Gamma(p-m+1)} t^{p-\gamma} \frac{\Gamma(p-m+1)\Gamma(m-\gamma)}{\Gamma(p-\gamma+1)} \\ &= \frac{\Gamma(p+1)}{\Gamma(p-\gamma+1)} t^{p-\gamma}. \end{aligned}$$

The second case $D_t^{\gamma} x^p = 0$, follows from the differentiation of the constant function. So, the proof of the theorem is complete.

**Example:**

Let $\gamma = \frac{1}{2}$, $m = 1, f(t) = t$. Then substituting in equation (4.4) we get,

$$\begin{aligned} D^{\frac{1}{2}} x &= \frac{1}{\Gamma(1-\frac{1}{2})} \int_0^x (x-t)^{1-\frac{1}{2}-1} dt \\ &= \frac{1}{\Gamma(\frac{1}{2})} \int_0^x (x-t)^{-\frac{1}{2}} dt \\ &= \frac{1}{\sqrt{\pi}} \int_0^x (x-t)^{-\frac{1}{2}} dt \\ &= \frac{1}{\sqrt{\pi}} \int_0^x \frac{1}{(x-t)^{\frac{1}{2}}} dt. \end{aligned}$$

Taking into account the properties of the Gamma function and using the subsitution $u = (x-t)^{\frac{1}{2}}$, we obtain:

$$\begin{aligned} D^{\frac{1}{2}}x &= \frac{1}{\sqrt{\pi}}\int_0^x \frac{1}{(x-t)^{\frac{1}{2}}}dt \\ &= \frac{1}{\sqrt{\pi}}\int_{\sqrt{t}}^0 -\frac{2u}{u}du \\ &= \frac{1}{\sqrt{\pi}}\int_0^{\sqrt{t}} \frac{2u}{u}du \\ &= \frac{2}{\sqrt{\pi}}(\sqrt{t}-0). \end{aligned}$$

Thus, it holds

$$D^{\frac{1}{2}}t = \frac{2\sqrt{t}}{\sqrt{\pi}}.$$

## 4.5 Bernstein Polynomials

The Bernstein polynomials(BPs) of the m-th degree on the interval [0, 1] is given by (Jafari & Tajadodi, 2016):

$$B_{i,m}(t) = \binom{m}{i} t^i(1-t)^{m-i}, \quad 0 \le i \le m, \tag{4.6}$$

where

$$\binom{m}{i} = \frac{m!}{i!(m-i)!}.$$

The Bernstein polynomials satisfy the recursive definition given by

$$B_{i,m}(t) = (1-t)B_{i,m-1}(t) + tB_{i-1,m-1}(t), \quad i = 0, 1, \cdots, m. \tag{4.7}$$

A recursive definition of a function defines values of the function for some inputs in terms of the values of the same function for other (usually smaller) inputs. By using the binomial expansion of $(1-t)^{m-i}$, Bernstein polynomials can be shown in terms of linear combination of the basis functions (Jafari & Tajadodi, 2016):

$$\begin{aligned} B_{i,m}(t) &= \binom{m}{i} t^i(1-t)^{m-i} \\ &= \binom{m}{i} t^i \left(\sum_{j=0}^{m-i}(-1)^j \binom{m-1}{j} t^j\right) \\ &= \sum_{j=i}^{m-i}(-1)^j \binom{m}{i}\binom{m-i}{j} t^{i+j}, \quad i = 0, 1, \cdots, m \end{aligned} \tag{4.8}$$

For mathematical convenience, we usually set $B_{i,m} = 0$, if $i < 0$ or $i > m$. The coefficients $\binom{m}{i}$ can be obtained from Pascal's triangle; the exponents on the $t$ term increase by one as $i$ increases; and the exponents on the $(1-t)$ term decrease by one as $i$ increases. In the simple cases, we obtain

- The Bernstein polynomials of degree 1 are

$$B_{0,1}(t) = 1 - t$$

$$B_{1,1}(t) = t$$

and can plotted for $0 \leq t \leq 1$ as

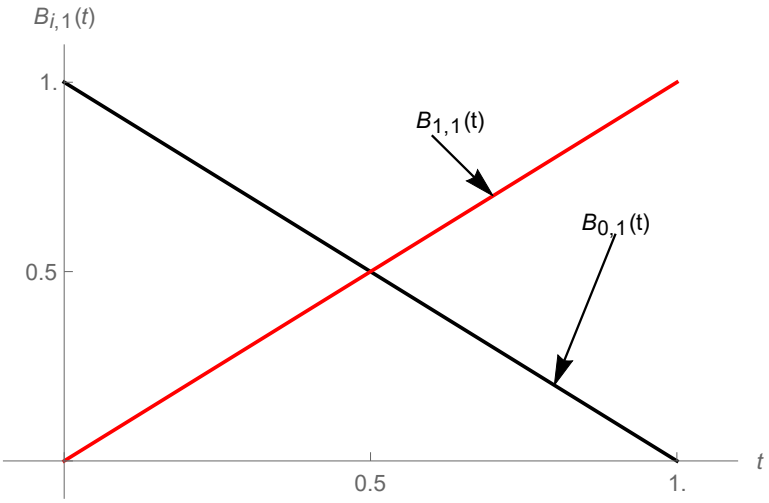


Figure 4.1: Bernstein Basis polynomial of degree 1

- The Bernstein polynomials of degree 2 are

$$B_{0,2}(t) = (1-t)^2$$

$$B_{1,2}(t) = 2t(1-t)$$

$$B_{2,2}(t) = t^2$$

and can plotted for $0 \leq t \leq 1$ as

It can easily be shown that each of the Bernstein polynomials is positive and also the sum of all the Bernstein polynomials is unity for all real $t \in [0, 1]$. That means (Jafari & Tajadodi, 2016)

$$\sum_{i=0}^{m} B_{i,m}(t) = 1.$$

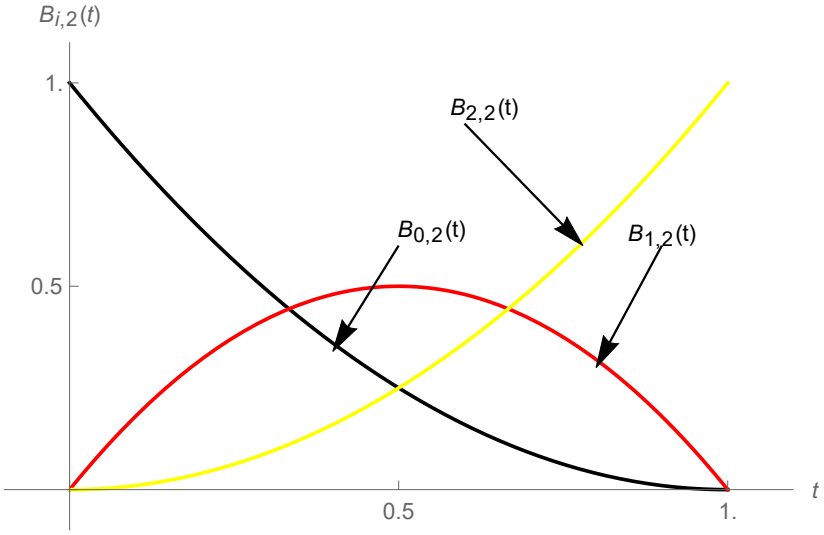


Figure 4.2: Bernstein Basis polynomial of degree 2

In many applications, a matrix formulation for the Bernstein polynomials is useful. These are straightforward to develop if one only looks at a linear combination in terms of dot products. Given a polynomial written as a linear combination of the Bernstein basis functions,

$$B(t) = c_0 B_{0,m}(t) + c_1 B_{1,m}(t) + \cdots + c_m B_{m,m}(t). \tag{4.9}$$

It is easy to write this as a dot product of two vectors

$$B(t) = \begin{bmatrix} B_{0,m}(t) & B_{1,m}(t) & \cdots & B_{m,m}(t) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_m \end{bmatrix}.$$

We can convert this in to

$$B(t) = \begin{bmatrix} 1 & t & t^2 & \cdots & t^m \end{bmatrix} \begin{bmatrix} b_{0,0} & 0 & 0 & \cdots & 0 \\ b_{1,0} & b_{1,1} & 0 & \cdots & 0 \\ b_{2,0} & b_{2,1} & b_{2,2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{m,0} & b_{m,1} & b_{m,2} & \cdots & b_{m,m} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix},$$

where the $b_{i,j}, i, j = 0, 1, 2, \cdots, m$ are the coefficients of the power basis that are used to determine the respective Bernstein polynomials. We note that the matrix in this case is lower triangular.

We can write the Bernstein polynomials in the form

$$B(t) = \phi_m(t) C$$

where $\phi_m(t) = [B_{0,m}(t) \;\; B_{1,m}(t) \;\; \cdots \;\; B_{m,m}(t)]$ and $C = [c_0 \;\; c_1 \;\; \cdots \;\; c_m]^T$. Again we can write $\phi_m(t) = T_m(t)A$, where

$$A = \begin{bmatrix} b_{0,0} & 0 & 0 & \cdots & 0 \\ b_{1,0} & b_{1,1} & 0 & \cdots & 0 \\ b_{2,0} & b_{2,1} & b_{2,2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{m,0} & b_{m,1} & b_{m,2} & \cdots & b_{m,m} \end{bmatrix},$$

and

$$T_m(t) = \begin{bmatrix} 1 \\ t \\ t^2 \\ \vdots \\ t^m \end{bmatrix}^T.$$

In the quadratic case ($m = 2$), the matrix representation is

$$B(t) = [1 \;\; t \;\; t^2] \begin{bmatrix} 1 & 0 & 0 \\ -2 & 2 & 0 \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix},$$

and in the cubic case ($m = 3$), the matrix representation is

$$B(t) = [1 \;\; t \;\; t^2 \;\; t^3] \begin{bmatrix} 1 & 0 & 0 & 0 \\ -3 & 3 & 0 & 0 \\ 3 & -6 & 3 & 0 \\ -1 & 3 & -3 & 1 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix}.$$

## 4.6 Approximation of Function

**Definition 7** *A Hilbert space $H$ is a real or complex inner product space that is also a complete metric space with respect to the distance function induced by the inner product and satisfies the following properties:*

1. The inner product is conjugate symmetric; that is, the inner product of a pair of elements is equal to the complex conjugate of the inner product of the swapped elements:

$$\langle y, x \rangle = \overline{\langle x, y \rangle}.$$

2. The inner product is linear in its first argument.

$$\langle ax_1 + bx_2, y\rangle = a\langle x_1, y\rangle + b\langle x_2, y\rangle.$$

3. The inner product of an element with itself is positive definite:

$$\begin{cases} \langle x, x\rangle > 0 & x \neq 0, \\ \langle x, x\rangle = 0 & x = 0. \end{cases}$$

Suppose that $H = L^2[0,1]$ is the Hilbert space and $\{B_{0,m}(t), B_{1,m}(t), \cdots, B_{m,m}(t)\} \subset H$ be the set of Bernstein polynomials of $m$th-degree and (Yousefi, Barikbin, & Behroozifar, 2010)

$$Y = span\{B_{0,m}(t), B_{1,m}(t), \cdots, B_{m,m}(t)\} \tag{4.10}$$

and $f(t)$ be an arbitrary element in $H$. Since $Y$ is a finite dimensional vector space, $f(t)$ has the unique best approximation out of $Y$ such as $y_0 \in Y$, that is $\exists! y_0 \in Y; \forall y \in Y$

$$\|f(t) - y_0\| \leq \|f(t) - y\|. \tag{4.11}$$

Since $y_0 \in Y$, there exist the unique coefficients $c_0, c_1, \cdots, c_m$ such that

$$f(t) \simeq y_0 = \sum_{j=0}^{m} c_j B_{j,m}(t) = C^T \phi_m(t), \tag{4.12}$$

where $C = [c_0, c_1, \cdots, c_m]^T$ is called the coefficient vector and

$$\phi_m(t) = [B_{0,m}(t), B_{1,m}(t), \cdots, B_{m,m}(t)]^T$$

is the Bernstein function vector and $T$ is the transpose. From eqution (4.12) we can find $C^T$ multiplying both sides by $\phi_m(t)$ and we have:

$$C^T \langle \phi_m(t), \phi_m(t)\rangle = \langle f(t), \phi_m(t)\rangle. \tag{4.13}$$

We know that,

$$\begin{aligned} \langle f(t), \phi_m(t)\rangle &= \int_0^1 f(t)\phi_m(t)^T dt \\ &= \left[\langle f, B_{0,m}\rangle, \langle f, B_{1,m}\rangle, \cdots, \langle f, B_{m,m}\rangle\right], \end{aligned}$$

and $\langle \phi_m(t), \phi_m(t)\rangle$ is called dual matrix(symmetric matrix) of $\phi_m(t)$ which is showed by $Q$, where

$$Q = \langle \phi_m(t), \phi_m(t)\rangle = \int_0^1 \phi_m(t)\phi_m(t)^T dt. \tag{4.14}$$

This implies that,

$$\begin{aligned} Q &= \int_0^1 \phi_m(t)\phi_m(t)^T dt \\ &= \int_0^1 (AT_m(t))(AT_m(t))^T dt, \quad since \quad \phi_m(t) = AT_m(t) \\ &= \int_0^1 A(T_m(t))(T_m(t))^T A^T dt \\ &= A\left[\int_0^1 T_m(t)T_m(t)^T dt\right] A^T \\ &= AH_mA^T \end{aligned}$$

where $H_m$ is a well-known Hilbert matrix,

$$H_m = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{m+1} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{m+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{m+1} & \frac{1}{m+2} & \frac{1}{m+3} & \cdots & \frac{1}{2m+1} \end{bmatrix}.$$

Thus equation (4.13) becomes,

$$C^T = Q^{-1}\langle f(t), \phi_m(t)\rangle = \left(\int_0^1 f(t)\phi_m(t)^T dt\right) Q^{-1}, \tag{4.15}$$

In particular for $m = 2$, we have

$$Q = AH_2A^T = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 2 & 0 \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \end{bmatrix} \begin{bmatrix} 1 & -2 & 1 \\ 0 & 2 & -2 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0.3333 \\ -1 & 1.3333 & -0.5 \\ 0.3333 & -0.5 & 0.2 \end{bmatrix},$$

and

$$Q^{-1} = \begin{bmatrix} 9 & 18 & 30 \\ 18 & 48 & 90 \\ 30 & 90 & 180 \end{bmatrix}.$$

**Lemma 1** *: Suppose that the function $f : [0,1] \to \mathbb{R}$ is $m+1$ times differentiable, $f(t) \in C^{m+1}[0,1]$ and $Y = span\{B_{0,m}(t), B_{1,m}(t), \cdots, B_{m,m}(t)\}$. If $y_0(t) = C^T\phi_m(t)$ is the best approximation of $f(t)$ out of $Y$, then the mean error bounded is presented as follows (Yousefi et al., 2010):*

$$\|f(t) - C^T\phi_m(t)\|_{L^2[0,1]} \leq \frac{K}{(m+1)!\sqrt{2m+3}}$$

*where $K = max_{t\in[0,1]}|f^{(m+1)}(t)|$.*

**Proof:**

We consider the Taylor polynomial

$$y_0(t) = f(0) + tf'(0) + \frac{t^2}{2!}f''(0) + \cdots + \frac{t^m}{m!}f^{(m)}(0).$$

From Taylor expansion we have

$$|f(t) - y_0(t)| \leq |f^{(m+1)}(\eta(t))\frac{t^{m+1}}{(m+1)!}| \tag{4.16}$$

where $\eta(t) \in (0,1)$. Since $C^T\phi_m(t)$ is the best approximation $f(t)$ out of $Y$, $y_0(t) \in Y$ and using equation (4.16), we have

$$\begin{aligned}
\|f(t) - C^T\phi_m(t)\|^2 &= \|f(t) - y_0(t)\|^2 \\
&= \int_0^1 |f(t) - y_0(t)|^2 dt \\
&\leq \int_0^1 \left[f^{(m+1)}(\eta)\frac{t^{m+1}}{(m+1)!}\right]^2 dt \\
&\leq \frac{K^2}{[(m+1)!]^2}\int_0^1 t^{2m+2}dt \\
&= \frac{K^2}{[(m+1)!]^2\,(2m+3)},
\end{aligned}$$

and by taking square roots we have the above bound.

## 4.7 Operational Matrix for Fractional Integration Based on Bernstein Polynomials

In this section, we want to investigate an operational matrix for the Riemann-Liouville fractional integral on the basis of Bernstein polynomials from order $m$ as (Jafari & Tajadodi, 2016)

$$I_t^{\gamma}\phi_m(t) \approx \mathbf{I}^{\gamma}\phi_m(t), \tag{4.17}$$

where $\mathbf{I}^{\gamma}$ is the $(m+1) \times (m+1)$ Bernstein polynomials operational matrix of fractional integration.

Instead of using $\phi_m(t)$ we can substitute $AT_m(t)$, in consequence we get to:

$$\begin{aligned} I_t^{\gamma}\phi_m(t) &= I_t^{\gamma}AT_m(t) \\ &= AI_t^{\gamma}T_m(t) \\ &= AI_t^{\gamma}\left[1, t, \cdots, t^m\right]^T \\ &= A\left[I^{\gamma}1, I^{\gamma}t, \cdots, I^{\gamma}t^m\right]^T \\ &= A\left[\frac{0!}{\Gamma(\gamma+1)}t^{\gamma}, \frac{1!}{\Gamma(\gamma+2)}t^{\gamma+1}, \cdots, \frac{m!}{\Gamma(\gamma+m+1)}t^{\gamma+m}\right]^T \\ &= AD\overline{T}_m, \end{aligned}$$

where $D$ is $(m+1)\times(m+1)$ matrix and $\overline{T}_m$ are given by

$$D = \begin{bmatrix} \frac{0!}{\Gamma(\gamma+1)} & 0 & \cdots & 0 \\ 0 & \frac{1!}{\Gamma(\gamma+2)} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \frac{m!}{\Gamma(\gamma+m+1)} \end{bmatrix} \quad or \quad D_{i,j} = \begin{cases} \frac{i!}{\Gamma(\gamma+i+1)} & i=j, \\ 0 & i\neq j \end{cases}$$

and

$$\overline{T}_m = \begin{bmatrix} t^{\gamma} \\ t^{\gamma+1} \\ \vdots \\ t^{\gamma+m} \end{bmatrix}.$$

For example, if we take $m=2$ and $\gamma=0.97$, then:

$$D = \begin{bmatrix} 1.0125 & 0 & 0 \\ 0 & 0.5139 & 0 \\ 0 & 0 & 0.3461 \end{bmatrix}.$$

In the same way as in section 3.5, we approximate $t^{\gamma+i}$ by $m+1$ as follows:

$$t^{\gamma+i} \simeq E_i^T\phi_m(t), \quad i=0,1,\cdots,m. \tag{4.18}$$

We have

$$\begin{aligned} E_i &= Q^{-1}\left(\int_0^1 t^{\gamma+i}\phi_m(t)dt\right) \\ &= Q^{-1}\left[\int_0^1 t^{\gamma+i}B_{0,m}(t)dt, \int_0^1 t^{\gamma+i}B_{1,m}(t)dt, \cdots, \int_0^1 t^{\gamma+i}B_{m,m}(t)dt\right]^T \\ &= Q^{-1}\overline{E}_i, \end{aligned}$$

where,

$$\overline{E}_i = \left[\overline{E}_{i,0}, \overline{E}_{i,1}, \cdots, \overline{E}_{i,m}\right]$$

and

$$\overline{E}_{i,j} = \int_0^1 t^{\gamma+i} B_{j,m}(t)dt = \frac{m!\Gamma(i+j+\gamma+1)}{j!\Gamma(i+m+\gamma+2)},\ i,j = 0,1,2,\cdots,m. \tag{4.19}$$

That means,

$$\begin{aligned}
\overline{E}_{i,j} &= \int_0^1 t^{\gamma+i} B_{j,m}(t)dt \\
&= \int_0^1 t^{\gamma+i} \binom{m}{j} t^j (1-t)^{m-j} dt \\
&= \int_0^1 \binom{m}{j} t^{\gamma+i+j} (1-t)^{m-j} dt \\
&= \binom{m}{j} \int_0^1 t^{\gamma+i+j} (1-t)^{m-j} dt \\
&= \frac{m!\Gamma(i+j+\gamma+1)\Gamma(m-j+1)}{j!(m-j)!\Gamma(i+m+\gamma+2)} \\
&= \frac{m!\Gamma(i+j+\gamma+1)}{j!\Gamma(i+m+\gamma+2)},\ i,j = 0,1,2,\cdots,m.
\end{aligned} \tag{4.20}$$

Then, $E_i$ is an $(m+1)\times(m+1)$ matrix that has vector $Q^{-1}\overline{E}_i$ for $i^{th}$ columns.

For $m = 2$, we have

$$E_2 = \begin{bmatrix} 1.8957 & 5.3736 & 10.9128 \\ 4.7076 & 13.9860 & 29.2650 \\ 8.6940 & 26.3460 & 55.8120 \end{bmatrix}.$$

Therefore, we can write

$$I^{\gamma}\phi_m(x) = AD\left[E_0^T\phi_m(t), E_1^T\phi_m(t), \cdots, E_m^T\phi_m(t)\right]^T = ADE_i^T\phi_m(t). \tag{4.21}$$

Thus from equation (4.21) we obtain

$$I_t^{\gamma}\phi_m(t) \simeq \mathbf{I}^{\gamma}\phi_m(t), \tag{4.22}$$

where

$$\mathbf{I}^{\gamma} = ADE_i^T \tag{4.23}$$

which is called the Bernstein polynomials operational matrix of fractional integration.

For example, let $\gamma = 0.97$ and $m = 2$, the Bernstein polynomials operational matrix of

fractional integration $\mathbf{I}^{\gamma}$ is equal to:

$$\begin{aligned}
\mathbf{I}^{0.97} &= ADE_2^T \\
&= \begin{bmatrix} 1 & 0 & 0 \\ -2 & 2 & 0 \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1.0125 & 0 & 0 \\ 0 & 0.5139 & 0 \\ 0 & 0 & 0.3461 \end{bmatrix} \begin{bmatrix} 1.8957 & 5.3736 & 10.9128 \\ 4.7076 & 13.9860 & 29.2650 \\ 8.6940 & 26.3460 & 55.8120 \end{bmatrix}^T \\
&= \begin{bmatrix} 1.9194 & 4.7664 & 8.8027 \\ 1.6842 & 4.8419 & 9.4731 \\ 0.1733 & 0.5203 & 1.0408 \end{bmatrix}.
\end{aligned}$$

## 4.8 Operational Matrix of Multiplication

It is always necessary to assess the product of $\phi_m(t)$ and $\phi_m(t)^T$, which is called the product matrix for the Bernstein polynomial basis. The operational matrices for the product $\widehat{C}$ are given by(Jafari & Tajadodi, 2016)

$$C^T \phi_m(t)\phi_m(t)^T = \phi_m(t)^T \widehat{C}, \tag{4.24}$$

where $\widehat{C}$ is $(m+1) \times (m+1)$ matrix. So we have

$$\begin{aligned}
C^T \phi_m(t)\phi_m(t)^T &= C^T \phi_m(t) \left( T_m(t)^T A^T \right) \\
&= \left[ C^T \phi_m(t), t(C^T \phi_m(t)), \cdots, t^m (C^T \phi_m(t)) \right] A^T \\
&= \left[ \sum_{i=0}^{n} c_i B_{i,m}(t), \sum_{i=0}^{n} c_i t B_{i,m}(t), \cdots, \sum_{i=0}^{n} c_i t^m B_{i,m}(t) \right] A^T.
\end{aligned} \tag{4.25}$$

Now, we approximate all functions $t^k B_{i,m}(t)$ in terms of $\{B_{i,m}\}_{i=0}^{m}$ for $i, k = 0, 1, \cdots, m$. From (4.12), we have

$$t^k B_{i,m}(t) \simeq e_{k,i}^T \phi_m(t), \tag{4.26}$$

where $e_{k,i} = \left[e^0_{k,i}, e^1_{k,i}, \cdots, e^m_{k,i}\right]^T$, and we obtain the components of the vector of $e_{k,i}$ where

$$\begin{aligned} e^j_{k,i} &= Q^{-1}\left(\int_0^1 t^k B_{i,m}(t)\phi_m(t)dt\right) \\ &= Q^{-1}\left[\int_0^1 t^k B_{i,m}(t)B_{0,m}(t)dt, \int_0^1 t^k B_{i,m}(t)B_{1,m}(t)dt, \cdots, \int_0^1 t^k B_{i,m}(t)B_{m,m}(t)dt\right]^T \\ &= \frac{Q^{-1}}{2m+k+1}\left[\frac{\binom{m}{0}}{\binom{2m+k}{i+k}}, \frac{\binom{m}{1}}{\binom{2m+k}{i+k+1}}, \cdots, \frac{\binom{m}{m}}{\binom{2m+k}{i+k+m}}\right]^T \quad i,k = 0,1,\cdots,m. \end{aligned}$$

Thus, we obtain

$$\begin{aligned} \sum_{i=0}^n c_i t^k B_{i,m}(t) &= \sum_{i=0}^n c_i\left(\sum_{j=0}^n e^j_{k,i} B_{j,m}(t)\right) \\ &= \sum_{j=0}^n B_{j,m}(t)\left(\sum_{i=0}^n c_i e^j_{k,i}\right) \\ &= \phi_m(t)^T\left[\sum_{i=0}^n c_i e^0_{k,i}, \sum_{i=0}^n c_i e^1_{k,i}, \cdots, \sum_{i=0}^n c_i e^m_{k,i}\right]^T \\ &= \phi_m(t)^T\left[e_{k,0}, e_{k,1}, \cdots, e_{k,m}\right] C \\ &= \phi_m(t)^T V_{k+1} C, \end{aligned} \tag{4.27}$$

where $V_{k+1}(k = 0,1,\cdots,m)$ is an $(m+1)\times(m+1)$ matrix that has vectors $e_{k,i}(i = 0,1,\cdots,m)$ given for each column. If we choose an $(m+1)\times(m+1)$ matrix $\overline{C} = \left[V_0 c, V_1 c, \cdots, V_{m+1} c\right]$, then from (3.25) and (3.26) we can write

$$C^T \phi_m(t)\phi_m(t)^T \simeq \phi_m(t)^T \overline{C} A^T, \tag{4.28}$$

and therefore we obtain the operational matrix of product,

$$\widehat{C} = \overline{C} A^T. \tag{4.29}$$

When $m = 2$, we have

$$\widehat{C} = \overline{C}A^T = \begin{bmatrix} 2.6857c_0 & 2.2143c_1 & 5.7857c_2 \\ 6.0571c_0 & 5.5429c_1 & 16.6571c_2 \\ 10.7143c_0 & 10.2857c_1 & 32.7143c_2 \end{bmatrix} \begin{bmatrix} 1 & -2 & 1 \\ 0 & 2 & -2 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2.6857c_0 & -0.9429c_1 & 4.0429c_2 \\ 6.0571c_0 & -1.0286c_1 & 11.6286c_2 \\ 10.7143c_0 & -0.8571c_1 & 22.8571c_2 \end{bmatrix}.$$

Chapter 5

# RESULT AND DISCUSSION

## 5.1 Fractional Model of Nonlinear Chemical Kinetics System

Consider the model of a chemical process consisting of four species, which are denoted by $P$, $X$, $Y$ and $Z$ where $P$ is reactant, $Z$ is product and $X$ and $Y$ are the intermediates. We can define the three reactions as:

$$P + X \xrightarrow{\theta_1} X + X, \tag{5.1}$$

$$X + Y \xrightarrow{\theta_2} Y + Y, \tag{5.2}$$

$$Y \xrightarrow{\theta_3} Z. \tag{5.3}$$

where $\theta_1$, $\theta_2$ and $\theta_3$ are the constant chemical reaction rates. Assume that the concetrations of all four species of $P$, $X$, $Y$ and $Z$ are denoted by $\zeta$, $\eta$, $\kappa$ and $\mu$, respectively. We suppose that these concentrations are scaled so that the sum of four concentrations is one and that all of four constituent reactions are added with the concentration of some of the species accurately at the rate of the corresponding values of the reactants. That means, $\frac{d(P+X+Y+Z)}{dt} = 0$, so that the sum of $P + X + Y + Z$ is one. The concentrations of the species as functions of time $t$ are denoted by $\zeta(t)$, $\eta(t)$, $\kappa(t)$ and $\mu(t)$. In chemistry, the law of mass action says that the rate of the chemical reaction is directly proportional to the product of the activities or concentrations of the reactants.

Then we find the system of differential equations for the variation with time of the four concentrations to be:

$$\begin{aligned}
\frac{d\zeta}{dt} &= -\theta_1\zeta(t)\eta(t),\\
\frac{d\eta}{dt} &= \theta_1\zeta(t)\eta(t) - \theta_2\eta(t)\kappa(t),\\
\frac{d\kappa}{dt} &= \theta_2\eta(t)\kappa(t) - \theta_3\kappa(t),\\
\frac{d\mu}{dt} &= \theta_3\kappa(t).
\end{aligned} \tag{5.4}$$

with initial condition $\zeta(0) = 0.5$, $\eta(0) = 0.3$, $\kappa(0) = 0.2$ and $\mu(0) = 0$.

The main target of this section is converted above integer order chemical kinetics problem into fractional order chemical kinetics problem. In the fields of dynamical systems and control theory, a fractional-order system is a dynamical system that can be modeled by a fractional differential equation containing derivatives of non-integer order. The nature of many systems makes that they can be more precisely modeled using fractional differential equations. Fractional differential equations are generalized from classical integer order ones, which are obtained by replacing integer-order derivatives by fractional ones. Their advantages comparing with integer-order differential equations are the capability of simulating natural physical process and dynamic system more accurately. Thus we replace the time-derivative in equation (5.4) by the Caputo fractional derivative and the fractional model of chemical kinetics problem is presented as :

$$\begin{aligned}
D_t^{\gamma}\zeta(t) &= -\theta_1\zeta(t)\eta(t),\\
D_t^{\gamma}\eta(t) &= \theta_1\zeta(t)\eta(t) - \theta_2\eta(t)\kappa(t),\\
D_t^{\gamma}\kappa(t) &= \theta_2\eta(t)\kappa(t) - \theta_3\kappa(t),\\
D_t^{\gamma}\mu(t) &= \theta_3\kappa(t)
\end{aligned} \tag{5.5}$$

with initial condition $\zeta(0) = 0.5$, $\eta(0) = 0.3$, $\kappa(0) = 0.2$ and $\mu(0) = 0$. The above system is representing a nonlnear chemical reaction.

## 5.2 Numerical Results

In this section, we estimate the numerical results for the fractional model of chemical kinetics system (5.5) by using the operational matrix of fractional integration and multiplication of Bernstein polynomials. For solving equation (5.5), we expand the fractional derivative by

the Bernstein polynomials as, say:

$$\begin{cases} D_t^{\gamma}\zeta(t) = Z^T\phi_m(t), \\ D_t^{\gamma}\eta(t) = N^T\phi_m(t), \\ D_t^{\gamma}\kappa(t) = K^T\phi_m(t), \\ D_t^{\gamma}\mu(t) = M^T\phi_m(t) \end{cases} \tag{5.6}$$

where,

$$Z^T = [\zeta_0, \zeta_1, \cdots, \zeta_m], \qquad N^T = [\eta_0, \eta_1, \cdots, \eta_m]$$

$$K^T = [\kappa_0, \kappa_1, \cdots, \kappa_m], \qquad M^T = [\mu_0, \mu_1, \cdots, \mu_m]$$

are unknown vectors and

$$\phi_m(t) = \left[B_{0,m}, B_{1,m}, \cdots, B_{m,m}\right]^T,$$

is Bernstein polynomials of degree $m$.

When we apply Riemann-Liouville fractional integral operator on the both sides of equation (5.6) and substituting the initial condition, we can obtain the following result:

$$\begin{aligned} \zeta(t) &= Z^T I_t^{\gamma}\phi_m(t) + \zeta(0) \approx Z^T\mathbf{I}_t^{\gamma}\phi_m(t) + a^T\phi_m(t) = G_1^T\phi_m(t), \\ \eta(t) &= N^T I_t^{\gamma}\phi_m(t) + \eta(0) \approx N^T\mathbf{I}_t^{\gamma}\phi_m(t) + b^T\phi_m(t) = G_2^T\phi_m(t), \\ \kappa(t) &= K^T I_t^{\gamma}\phi_m(t) + \kappa(0) \approx K^T\mathbf{I}_t^{\gamma}\phi_m(t) + c^T\phi_m(t) = G_3^T\phi_m(t), \\ \mu(t) &= M^T I_t^{\gamma}\phi_m(t) + \mu(0) \approx M^T\mathbf{I}_t^{\gamma}\phi_m(t) = G_4^T\phi_m(t) \end{aligned} \tag{5.7}$$

where $Z^T\mathbf{I}_t^{\gamma} + a^T = G_1^T$, $N^T\mathbf{I}_t^{\gamma} + b^T = G_2^T$, $K^T\mathbf{I}_t^{\gamma} + c^T = G_3^T$, $M^T\mathbf{I}_t^{\gamma} = G_4^T$ and $\mathbf{I}^{\gamma}$ is the fractional integration of operational matrix of order $\gamma$ and

$$a^T = [\zeta(0), \zeta(0), \cdots, \zeta(0)], \quad b^T = [\eta(0), \eta(0), \cdots, \eta(0)], c^T = [\kappa(0), \kappa(0), \cdots, \kappa(0)].$$

Now substituting equation (5.6) and equation (5.7) into equation (5.5), we obtain:

$$\begin{aligned} Z^T\phi_m(t) &= -\theta_1 G_1^T\phi_m(t)G_2^T\phi_m(t), \\ N^T\phi_m(t) &= \theta_1 G_1^T\phi_m(t)G_2^T\phi_m(t) - \theta_2 G_2^T\phi_m(t)G_3^T\phi_m(t), \\ K^T\phi_m(t) &= \theta_2 G_2^T\phi_m(t)G_3^T\phi_m(t) - \theta_3 G_3^T\phi_m(t), \\ M^T\phi_m(t) &= \theta_3 G_3^T\phi_m(t). \end{aligned} \tag{5.8}$$

Then by applying the operational matrix of multiplication of equation (4.24) into equation (5.8), we have

$$\begin{aligned} Z^T\phi_m(t) &= -\theta_1 G_1^T \widehat{G}_2^T \phi_m(t), \\ N^T\phi_m(t) &= \theta_1 G_1^T \widehat{G}_2^T \phi_m(t) - \theta_2 G_2^T \widehat{G}_3^T \phi_m(t) \\ K^T\phi_m(t) &= \theta_2 G_2^T \widehat{G}_3^T \phi_m(t) - \theta_3 G_3^T \phi_m(t), \\ M^T\phi_m(t) &= \theta_3 G_3^T \phi_m(t) \end{aligned} \tag{5.9}$$

and which yields the system

$$\begin{aligned} (Z^T + \theta_1 G_1^T \widehat{G}_2^T)\phi_m(t) &= 0, \\ (N^T - \theta_1 G_1^T \widehat{G}_2^T + \theta_2 G_2^T \widehat{G}_3^T)\phi_m(t) &= 0 \\ (K^T - \theta_2 G_2^T \widehat{G}_3^T + \theta_3 G_3^T)\phi_m(t) &= 0, \\ (M^T - \theta_3 G_3^T)\phi_m(t) &= 0. \end{aligned} \tag{5.10}$$

Using the independent property of Bernstein polynomials on to equation (5.10), we get the following set of nonlinear algebraic equations as:

$$\begin{aligned} Z^T + \theta_1 G_1^T \widehat{G}_2^T &= 0, \\ N^T - \theta_1 G_1^T \widehat{G}_2^T + \theta_2 G_2^T \widehat{G}_3^T &= 0, \\ K^T - \theta_2 G_2^T \widehat{G}_3^T + \theta_3 G_3^T &= 0, \\ M^T - \theta_3 G_3^T &= 0 \end{aligned} \tag{5.11}$$

where $\widehat{G}_2^T$ is an operational matrix of product.

We assume that the values of the three reaction rates are: $\theta_1 = 0.1$, $\theta_2 = 0.02$ and $\theta_3 = 0.009$ as given in Aminikhah (Aminikhah, 2011). From equation (5.11) we obtained $4(m+1)$ nonlinear algebraic equations which can be solved by Newton iteration method. Then, after solving this nonlinear algebraic equations we obtain the results for vector $Z$, $N$, $K$ and $M$. Finally, we substitute these vector results into system (5.7) in order to get the approximate solution of $\zeta(t)$, $\eta(t)$, $\kappa(t)$ and $\mu(t)$.

The above procedure will be clear and illustrated by the following numerical example given in the next section.

## 5.3 Numerical Example

In this section, we will give one illustrative example in order to illustrate the above scheme and the results obtained using this scheme will be compared with the analytical solution.

**Example 1:**

In this example we will compare the exact solution and the numerical results obtained by proposed technique for $\zeta(t)$, $\eta(t)$, $\kappa(t)$, $\mu(t)$ when $\gamma = 0.97$ and $m = 2$. Since $m = 2$, so we use Bernstein polynomials of degree 2 in order to find approximate solution from equation (5.11).

To find approximate solution we use the following matrix which is already computed in chapter three.

$$G_1^T = \begin{bmatrix} 1.9194\zeta_0 + 1.6842\zeta_1 + 0.1733\zeta_2 + 0.5 \\ 4.7664\zeta_0 + 4.8419\zeta_1 + 0.5203\zeta_2 + 0.5 \\ 8.8027\zeta_0 + 9.4731\zeta_1 + 1.0408\zeta_2 + 0.5 \end{bmatrix}^T,$$

$$\widehat{G}_2^T = \begin{bmatrix} 2.6857\eta_0 & -0.9429\eta_1 & 4.0429\eta_2 \\ 6.0571\eta_0 & -1.0286\eta_1 & 11.6286\eta_2 \\ 10.7143\eta_0 & -0.8571\eta_1 & 22.8571\eta_2 \end{bmatrix}^T,$$

$$G_3^T = \begin{bmatrix} 1.9194\kappa_0 + 1.6842\kappa_1 + 0.1733\kappa_2 + 0.2 \\ 4.7664\kappa_0 + 4.8419\kappa_1 + 0.5203\kappa_2 + 0.2 \\ 8.8027\kappa_0 + 9.4731\kappa_1 + 1.0408\kappa_2 + 0.2 \end{bmatrix}^T$$

and

$$G_4^T = \begin{bmatrix} 1.9194\mu_0 + 1.6842\mu_1 + 0.1733\mu_2 \\ 4.7664\mu_0 + 4.8419\mu_1 + 0.5203\mu_2 \\ 8.8027\mu_0 + 9.4731\mu_1 + 1.0408\mu_2 \end{bmatrix}^T.$$

By putting the above matrix in equation (5.11), we get the following nonlinear algebraic equations:

$$\zeta_0+0.5155\zeta_0\eta_0+0.4523\zeta_1\eta_0+0.0465\zeta_2\eta_0+0.1343\eta_0-0.4451\zeta_0\eta_1-0.4565\zeta_1\eta_1-0.0491\zeta_2\eta_1-0.0472\eta_1 + 3.5588\zeta_0\eta_2 + 3.8301\zeta_1\eta_2 + 0.4208\zeta_2\eta_2 + 0.2022\eta_2 = 0$$

$$\zeta_1+1.1626\zeta_0\eta_0+1.0201\zeta_1\eta_0+0.1049\zeta_2\eta_0+0.3028\eta_0-0.4923\zeta_0\eta_1-0.498\zeta_1\eta_1-0.0535\zeta_2\eta_1-0.0514\eta_1 + 10.2363\zeta_0\eta_2 + 11.0160\zeta_1\eta_2 + 1.2103\zeta_2\eta_2 + 0.5814\eta_2 = 0$$

$$\zeta_2+2.0565\zeta_0\eta_0+1.8045\zeta_1\eta_0+0.1857\zeta_2\eta_0+0.5357\eta_0-0.4102\zeta_0\eta_1-0.4149\zeta_1\eta_1-0.0446\zeta_2\eta_1-0.0428\eta_1 + 20.1204\zeta_0\eta_2 + 21.6527\zeta_1\eta_2 + 2.3789\zeta_2\eta_2 + 1.1429\eta_2 = 0$$

$$\eta_0-0.5155\zeta_0\eta_0-0.4523\zeta_1\eta_0-0.0465\zeta_2\eta_0-0.1343\eta_0+0.4451\zeta_0\eta_1+0.4565\zeta_1\eta_1+0.0491\zeta_2\eta_1+0.0472\eta_1 - 3.5588\zeta_0\eta_2 - 3.8301\zeta_1\eta_2 - 0.4208\zeta_2\eta_2 - 0.2022\eta_2 + 0.1031\kappa_0\eta_0 + 0.0905\kappa_1\eta_0 + 0.0093\kappa_2\eta_0 + 0.0026\eta_0 - 0.0903\kappa_0\eta_1 - 0.0913\kappa_1\eta_1 - 0.0098\kappa_2\eta_1 - 0.0094\eta_1 + 0.7117\kappa_0\eta_2 + 0.7660\kappa_1\eta_2 + 0.0842\kappa_2\eta_2 + 0.0404\eta_2 = 0$$

$\eta_1 - 1.1626\zeta_0\eta_0 - 1.0201\zeta_1\eta_0 - 0.1049\zeta_2\eta_0 - 0.3028\eta_0 + 0.4923\zeta_0\eta_1 + 0.498\zeta_1\eta_1 + 0.0535\zeta_2\eta_1 + 0.0514\eta_1 - 10.2363\zeta_0\eta_2 - 11.0160\zeta_1\eta_2 - 1.2103\zeta_2\eta_2 - 0.5814\eta_2 + 0.2325\kappa_0\eta_0 + 0.2040\kappa_1\eta_0 + 0.0209\kappa_2\eta_0 + 0.0606\eta_0 - 0.0985\kappa_0\eta_1 - 0.0996\kappa_1\eta_1 - 0.0107\kappa_2\eta_1 - 0.0128\eta_1 + 2.0472\kappa_0\eta_2 + 2.2032\kappa_1\eta_2 + 0.2421\kappa_2\eta_2 + 0.1163\eta_2 = 0$

$\eta_2 - 2.0565\zeta_0\eta_0 - 1.8045\zeta_1\eta_0 - 0.1857\zeta_2\eta_0 - 0.5357\eta_0 + 0.4102\zeta_0\eta_1 + 0.4149\zeta_1\eta_1 + 0.0446\zeta_2\eta_1 + 0.0428\eta_1 - 20.1204\zeta_0\eta_2 - 21.6527\zeta_1\eta_2 - 2.3789\zeta_2\eta_2 - 1.1429\eta_2 + 0.4113\kappa_0\eta_0 + 0.3609\kappa_1\eta_0 + 0.0371\kappa_2\eta_0 + 0.1071\eta_0 - 0.0820\kappa_0\eta_1 - 0.0829\kappa_1\eta_1 - 0.0089\kappa_2\eta_1 - 0.0085\eta_1 + 4.0241\kappa_0\eta_2 + 4.3305\kappa_1\eta_2 + 0.4757\kappa_2\eta_2 + 0.2285\eta_2 = 0$

$\kappa_0 - 0.1031\kappa_0\eta_0 - 0.0905\kappa_1\eta_0 - 0.0093\kappa_2\eta_0 - 0.0026\eta_0 + 0.0903\kappa_0\eta_1 + 0.0913\kappa_1\eta_1 + 0.0098\kappa_2\eta_1 + 0.0094\eta_1 - 0.7117\kappa_0\eta_2 - 0.7660\kappa_1\eta_2 - 0.0842\kappa_2\eta_2 - 0.0404\eta_2 + 0.0173\kappa_0 + 0.0152\kappa_1 + 0.0016\kappa_2 + 0.0045 = 0$

$\kappa_1 - 0.2325\kappa_0\eta_0 - 0.2040\kappa_1\eta_0 - 0.0209\kappa_2\eta_0 - 0.0606\eta_0 + 0.0985\kappa_0\eta_1 + 0.0996\kappa_1\eta_1 + 0.0107\kappa_2\eta_1 + 0.0128\eta_1 - 2.0472\kappa_0\eta_2 - 2.2032\kappa_1\eta_2 - 0.2421\kappa_2\eta_2 - 0.1163\eta_2 + 0.0431\kappa_0 + 0.0436\kappa_1 + 0.0046\kappa_2 + 0.0045 = 0$

$\kappa_2 - 0.4113\kappa_0\eta_0 - 0.3609\kappa_1\eta_0 - 0.0371\kappa_2\eta_0 - 0.1071\eta_0 + 0.0820\kappa_0\eta_1 + 0.0829\kappa_1\eta_1 + 0.0089\kappa_2\eta_1 + 0.0085\eta_1 - 4.0241\kappa_0\eta_2 - 4.3305\kappa_1\eta_2 - 0.4757\kappa_2\eta_2 - 0.2285\eta_2 + 0.0792\kappa_0 + 0.0852\kappa_1 + 0.0094\kappa_2 + 0.0045 = 0$

$\mu_0 - 0.0173\kappa_0 - 0.0152\kappa_1 - 0.0016\kappa_2 - 0.0045 = 0$

$\mu_1 - 0.0431\kappa_0 - 0.0436\kappa_1 - 0.0046\kappa_2 - 0.0045 = 0$

$\mu_2 - 0.0792\kappa_0 - 0.0852\kappa_1 - 0.0094\kappa_2 - 0.0045 = 0$

To solve the above equations we use Newton iteration method and Matlab toolbox. Then after solving this equations we will get the following coefficient result:

$\zeta_0 = -0.0022, \zeta_1 = 0.0376, \zeta_2 = 0.0972, \eta_0 = 0.0626, \eta_1 = 0.1528, \eta_2 = 0.2841,$

$\kappa_0 = -0.0636, \kappa_1 = -0.1825, \kappa_2 = -0.3618, \mu_0 = 0.0000, \mu_1 = -0.0079$ and $\mu_2 = -0.0195.$

Again, by substituting the above values into equation (5.7), we get the approximate solutions. That is:

$$\begin{aligned}
\zeta(t) &= G_1^T \phi_2(t) \\
&= \begin{bmatrix} 1.9194\zeta_0 + 1.6842\zeta_1 + 0.1733\zeta_2 + 0.5 \\ 4.7664\zeta_0 + 4.8419\zeta_1 + 0.5203\zeta_2 + 0.5 \\ 8.8027\zeta_0 + 9.4731\zeta_1 + 1.0408\zeta_2 + 0.5 \end{bmatrix}^T \begin{bmatrix} 1 - 2t + t^2 \\ 2t - 2t^2 \\ t^2 \end{bmatrix} \\
&= -0.002t^2 - 0.013t + 0.5 = 0.
\end{aligned}$$

In similar manner will get the approximate solutions of:

$$\zeta(t) = -0.002t^2 - 0.013t + 0.5 = 0,$$

$$\eta(t) = 0.0009t^2 + 0.013t + 0.3004 = 0,$$

$$\kappa(t) = -0.0001t^2 - 0.0005t + 0.2 = 0$$

and

$$\mu(t) = 0.0001t^2 + 0.0017t + 0.00002 = 0.$$

Finally we compare the exact solution with approximate solution by plotting the graph and to sketch the graph we will use Mathematica software (See Appendix C).

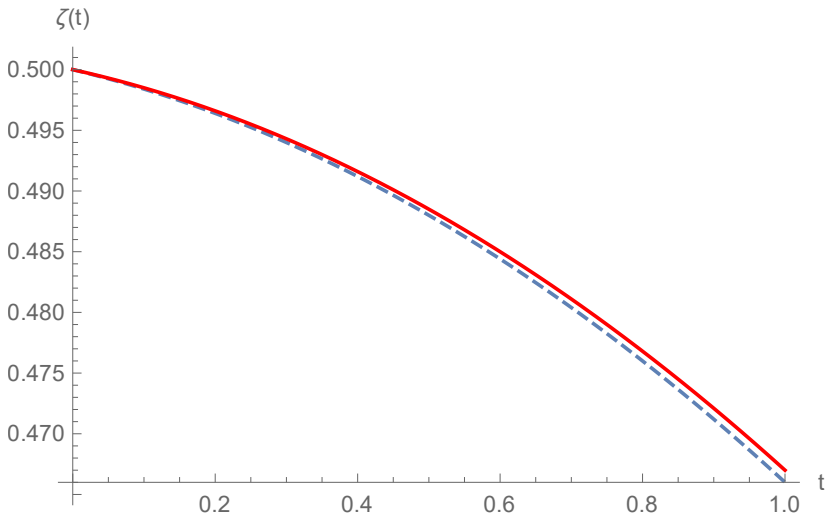


Figure 5.1: The exact solution: (Red line) and the approximation solutions of $\zeta(t)$ for $\gamma = 0.97$ when $m = 2$ (Dashed)

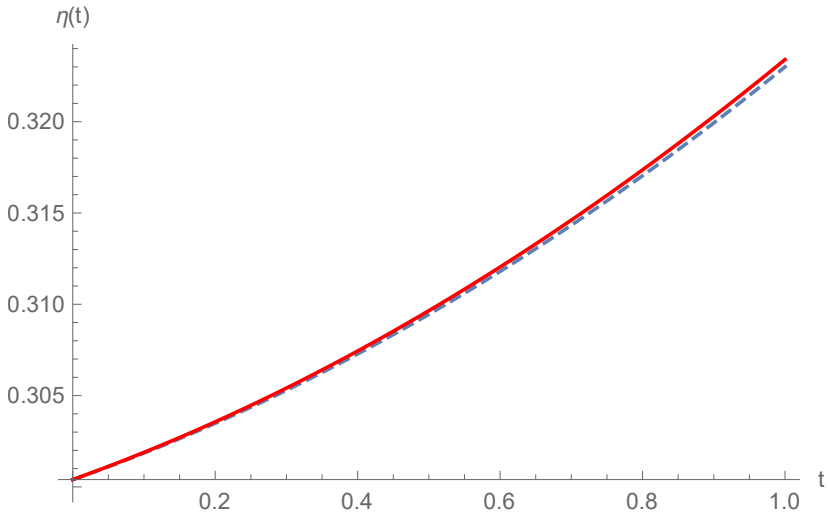


Figure 5.2: The exact solution: (Red line) and the approximation solutions of $\eta(t)$ for $\gamma$ = 0.97 when $m$ = 2 (Dashed)

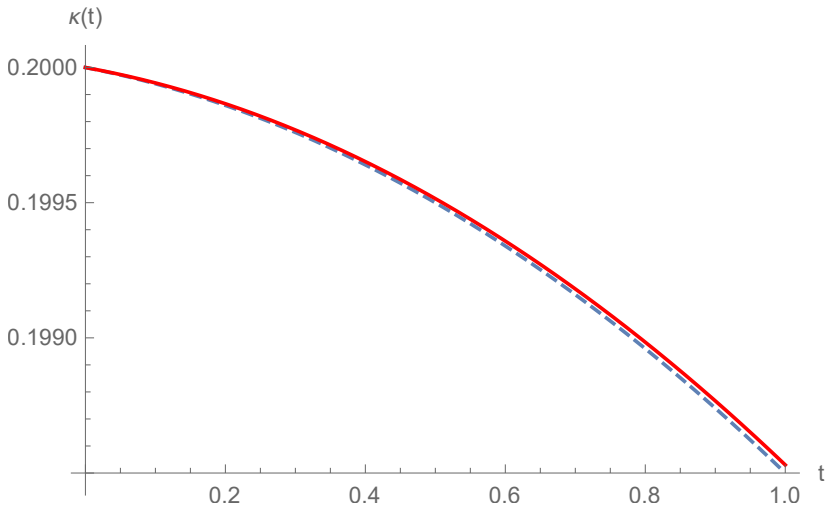


Figure 5.3: The exact solution: (Red line) and the approximation solutions of $\kappa(t)$ for $\gamma$ = 0.97 when $m$ = 2 (Dashed)

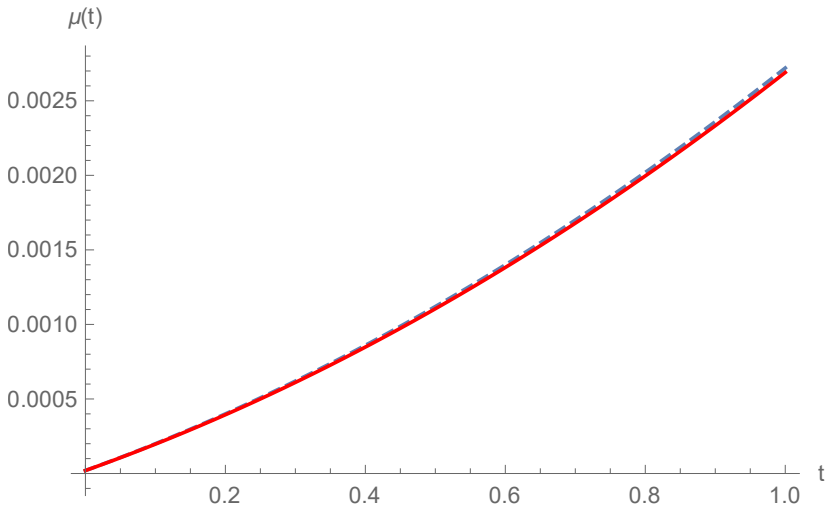


Figure 5.4: The exact solution: (Red line) and the approximation solutions of $\mu(t)$ for $\gamma$ = 0.97 when $m$ = 2 (Dashed)

## 5.4 Discussions

We used Bernstein polynomials method to solve a fractional model of nonlinear chemical kinetics system. First, we derived the corresponding nonlinear algebraic equations using this method. Then after solving this nonlinear algberaic equation we obtained the approximate solution. We compare the solution obtained by using Bernstein polynomials method with exact solution graphically. A solution obtained through Bernstein polynomials method is very close to the exact solution. This analysis shows that Bernstein polynomials technique has helpful method for solving fractional model of nonlinear chemical kinetics system.

# Conclusion and Recommendation

## Conclusion

In this thesis we have presented an approximate solution of a fractional model of nonlinear chemical kinetics system using the operational matrices of fractional integration and multiplication based on Bernstein polynomials method. The advantage of this method is to reduces nonlinear chemical kinetics system into a system of nonlinear algebraic equations. Then, this equations can be solved by using Newton iteration method in order to get approximate solution. One of the most important properties of this method is that when the result of equation is in the form of a polynomial of degree $\leq m$, the exact solution is obtained. In order to achieve our goal, we presented one illustrative example which demonstrate the Bernstein polynomials method is an efficient technique. Therefore this technique is a helpful tool for solving a fractional model of nonlinear chemical kinetics system. Mathematica has been used for computations and programming in this study.

## Recommendation

This thesis specifically focused on application of Bernstein polynomials to solve a fractional model of nonlinear chemical kinetics system. The proposed method is very interesting and easy to find approximate solution of nonlinear differential equations. But finding solution on large systems are so hard. Hence, we recommended that, one can use this method to solve more complicated model in chemical kinetics reaction. Future researchers should try to compare suggested method with other method to generalize the efficiency of this method. Also, one can go through application of the proposed method on nonlinear ordinary differential equations and partial differential equations.

## Future work

In this thesis, we have developed a fractional model of chemical kinetics system. But, the convergece analysis and stability of the problem is not addressed in this thesis. This will be addressed in the future.

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# Appendix A

# (Mathematica coding for Bernstein basis polynomial of degree 1)

```
BernsteinB[0, n_, 0] := 1
BernsteinB[n_, n_, t_] := t^n
BernsteinB[i_, n_, t_] := Binomial[n, i] t^i (1 - t)^(n - i);
Show[GraphicsArray[Partition[Table[Plot[
Evaluate[Table[BernsteinB[i, n, t], {i, 0, n}], {t, 0, 1},
AxesLabel ->
TraditionalForm /@ {t, Subscript[B, Sequence[i, n]][t]},
Ticks -> {Range[0, 1, .5], Range[0, 1, .5]},
PlotRange -> {{-.1, 1.1}, {-.1, 1.1}},
PlotStyle -> {Black, Red, Yellow, Green, Blue, Violet},
DisplayFunction -> Identity,
Epilog -> {{Arrow[{{0.6, 0.86}, {0.7, 0.7}}],
Text["\!\(\*SubscriptBox[\(B\), \(0, 1\)]\)(t)", {0.63,
0.9}], Arrow[{{0.9, 0.6}, {0.8, 0.2}}],
Text["\!\(\*SubscriptBox[\(B\), \(1, 1\)]\)(t)", {0.9,
0.63}]}}]], {n, 1, 2}], 1]]]
```

# Appendix B

# (Mathematica coding for Bernstein basis polynomial of degree 2)

```
BernsteinB[0, n_, 0] := 1
BernsteinB[n_, n_, t_] := t^n
BernsteinB[i_, n_, t_] := Binomial[n, i] t^i (1 - t)^(n - i);
Show[GraphicsArray[Partition[Table[Plot[
Evaluate[Table[BernsteinB[i, n, t], {i, 0, n}], {t, 0, 1},
AxesLabel ->
TraditionalForm /@ {t, Subscript[B, Sequence[i, n]][t]},
Ticks -> {Range[0, 1, .5], Range[0, 1, .5]},
PlotRange -> {{-.1, 1.1}, {-.1, 1.1}},
PlotStyle -> {Black, Red, Yellow, Green, Blue, Violet},
DisplayFunction -> Identity,
Epilog -> {{Arrow[{{0.6, 0.9}, {0.78, 0.6}}],
Text["\!\(\*SubscriptBox[\(B\), \(0, 2\)]\)(t)", {0.55,
0.64}], Arrow[{{0.5, 0.6}, {0.4, 0.34}}],
Text["\!\(\*SubscriptBox[\(B\), \(2, 2\)]\)(t)", {0.63,
0.94}], Arrow[{{0.9, 0.6}, {0.8, 0.3}}],
Text["\!\(\*SubscriptBox[\(B\), \(1, 2\)]\)(t)", {0.9,
0.63}]}}]], {n, 1, 2}], 1]]]
```