Numerical Solutions of Fractional Chemical Kinetics System

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Abstract: The aim of this paper was to investigate a fractional model of chemical kinetics system. The numerical solution of this fractional model is obtained by Bernstein polynomials. The basic idea is to apply operational matrices of fractional integration and multiplication of Bernstein polynomials. The important point to note here is the given problem turns into a set of algebraic equations by expanding the solution as Bernstein polynomials with unknown coefficients. Then, by solving algebraic equations, the numerical solutions are obtained. This result may be explained by the fact that the suggested technique is computationally efficient.

1 Introduction

One of the most significant current subjects in pure and applied mathematics is fractional calculus. Many applications have appeared in different areas of applied sciences such as physics and engineering [1–3]. 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. A chemical kinetics system is represented by a nonlinear system of ordinary differential equations.

Consider this model of a chemical process consisting of three species, which are denoted by A, B and C. The three reactions are:

$$A \longrightarrow B, \tag{1}$$

$$B + C \longrightarrow A + C, \tag{2}$$

$$B + B \longrightarrow C. \tag{3}$$

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We assume that the concentrations of A, B and C are indicated by ζ, η, and κ, respectively. We suppose that these concentrations are scaled so that the sum of three concentrations is one and that all of three constituent reactions are added with the concentration of some of the species accurately at the rate of the corresponding values of the reactants. We denote by θ_1 the the reaction rate of equation (1) . It indicates that the rate at which ζ decreases, and the rate at which η increases, because of this reaction, are equivalent to $\theta_1\zeta$. In the reaction showed by equation (2), C acts as a catalyst for the configuration of species A from B. The reaction rate is represented by using the symbol θ_2 which means the increase in the concentration ζ and the decrease in the concentration κ; this reaction has a rate and is equivalent to the product $\theta_2\eta\kappa$. Lastly, the formation of C from B has a constant rate equivalent to θ_3, which means the rate at which the mentioned reaction is occurring has to be equivalent to the product $\theta_3\eta^2$. We find the system of differential equations for the variation with time of the three concentrations to be:

$$\begin{aligned}
\frac{d\zeta}{dt} &= -\theta_1\zeta(t) + \theta_2\eta(t)\kappa(t), \\
\frac{d\eta}{dt} &= \theta_1\zeta(t) - \theta_2\eta(t)\kappa(t) - \theta_3\eta^2(t), \\
\frac{d\kappa}{dt} &= \theta_3\eta^2(t).
\end{aligned} \tag{4}$$

Since various materials and dynamical processes with memory and hereditary effects can be modeled by fractional order models better than integer-order models, we repleace the time-derivative in equation (4) by the Caputo fractional derivative:

$$\begin{aligned}
{}_0D_t^\gamma\zeta(t) &= -\theta_1\zeta(t) + \theta_2\eta(t)\kappa(t), \\
{}_0D_t^\gamma\eta(t) &= \theta_1\zeta(t) - \theta_2\eta(t)\kappa(t) - \theta_3\eta^2(t), \\
{}_0D_t^\gamma\kappa(t) &= \theta_3\eta^2(t),
\end{aligned} \tag{5}$$

with the initial conditions $\zeta(0) = 1$, $\eta(0) = 0$, $\kappa(0) = 0$.

In 2011, Aminikhah obtained the analytical approximation of chemical kinetics system using a homotopy perturbation method [4]. Two years later, Khader derived numerical solutions of this system using the Picard-Padé technique [5]. In 2017, Singh and co-workers considered the analysis of chemical kinetics system with a fractional derivative with the Mittag-Leffler type kernel [6] and numerous papers have been published on the analytical and numerical methods for solving nonlinear fractional differential equations such as [7–20]. In this paper, we apply Bernstein polynomials (Bps) for solving fractional chemical kinetics system. Here, we use operational matrices of fractional integration and multiplication of Bps. In equation (5), $D^\gamma\zeta(t)$ is indicated to be the Caputo fractional derivative of order γ which is defined as [1,3]:

$$D_t^\gamma\zeta(t) = \begin{cases} \frac{1}{\Gamma(n-\gamma)}\int_0^t \frac{\zeta(\tau)}{(t-\tau)^{1+\gamma-n}}d\tau, & n-1 < \gamma < n, \quad n \in I\!\!N, \\[2mm] \frac{d^n\zeta(t)}{dt^n}, & \gamma = n. \end{cases} \tag{6}$$

Note that

$$(i) \; {}_0D_t^\gamma\lambda = 0, \qquad (\lambda \; is \; a \; constant),$$

$$(ii) \qquad {}_0D_t^\gamma t^\delta = \begin{cases} 0, & \delta \in I\!N_0, \ \delta < \gamma, \\ \\ \frac{\Gamma(\delta+1)}{\Gamma(1+\delta-\gamma)}t^{\delta-\gamma}, & Otherwise, \end{cases} \qquad (7)$$

$$(iii) \qquad {}_0I_t^\gamma {}_0D_t^\gamma \zeta(t) = \zeta(t) - \sum_{l=0}^{n-1} \zeta^{(l)}(0^+)\frac{t^l}{l!}, \qquad n-1 < \gamma \le n. \qquad (8)$$

In equation (8) the fractional Riemann-Liouville integral I_t^γ is described as [1,3]:

$$ {}_0I_t^\gamma \zeta(t) = \frac{1}{\Gamma(\gamma)} \int_0^t \frac{\zeta(\tau)}{(t-\tau)^{1-\gamma}}d\tau, \qquad \gamma > 0. \qquad (9)$$

The rest part of the present paper is organized as follows. The second section of this paper will impart Bernstein polynomials and approximation of function. Section 3 gives a brief overview of the operational matrix for fractional integration and multiplication of Bps. The suggested approach is used to approximate the fractional chemical kinetics system in the next Section 4. In Section 5, we assess the proposed technique with two examples. In the last section, conclusion is summarised.

2   Bernstein Polynomials and Approximation of Function

2.1   Definition of Bernstein polynomials

The Bernstein polynomials of the n-th degree on $[0,1]$ are presented as [21]:

$$\begin{aligned} B_{l,n}(t) &= \binom{n}{l}t^l(1-t)^{n-l} = \sum_{j=0}^{n-l}(-1)^j \binom{n}{l}\binom{n-l}{j}t^{l+j} \\ &= \sum_{j=l}^{n}(-1)^{j-l}\binom{n}{l}\binom{n-l}{j-l}t^j, \qquad l = 0,1,\ldots,n. \end{aligned} \qquad (10)$$

We can demonstrate $\phi(t) = \Lambda T_n(t)$, where $\phi(t) = [B_{0,n}(t), B_{1,n}(t), \cdots, B_{n,n}(t)]^T$, $T_n(t) = [1, t, \cdots, t^n]^T$ and $\Lambda = (\lambda_{l,j})_{l,j=1}^{n+1}$ is a matrix of order $(n+1)$ given in the form:

$$\lambda_{l+1,j+1} = \begin{cases} (-1)^{j-l}\binom{n}{l}\binom{n-l}{j-l}, & l \le j, \\ & \qquad\qquad l,j = 0,1,\cdots,n, \\ 0, & l > j. \end{cases} \qquad (11)$$

2.2   Approximation of function

The set of Bernstein polynomials $\{B_{0,n}(t), B_{1,n}(t), \ldots, B_{n,n}(t)\}$ in Hilbert space $L^2[0,1]$ is a complete basis [22]. In consequence, we can indicate any function by BPs:

$$\zeta(t) = \sum_{l=0}^{n} z_l B_{l,n}(t) = Z^T \phi(t), \qquad (12)$$

where $Z^T = [z_0, z_1, \ldots, z_n]$. Then, we can find Z^T as below:

$$Z^T = \left(\int_0^1 \zeta(t)\phi(t)^T dt\right) Q^{-1}. \qquad (13)$$

In equation (13), Q is called the dual matrix of $\phi(t)$ and the Q is derived such that

$$Q = \int_0^1 \phi(t)\phi(t)^T dt. \tag{14}$$

3   Operational Matrix for Fractional Integration based on BPs

In this subsection, we want to investigate an operational matrix of fractional integration for Bps. Therefore, by fractional integration of the vector $\phi(t)$ as below, we get

$$_0I_t^\gamma \phi(t) \simeq \mathbf{I}^\gamma \phi(t), \tag{15}$$

where $\mathbf{I}^\gamma$ is the $(n+1) \times (n+1)$ Riemann-Liouville fractional operational matrix of integration for BPs. Instead of using $\phi(t)$ we can substitute $\Lambda T_n(t)$, in consequence we get to:

$$
\begin{aligned}
_0I_t^\gamma \phi(t) &= {}_0I_t^\gamma \Lambda T_n(t) = \Lambda \, _0I_t^\gamma T_n(t) = \Lambda \left[_0I_t^\gamma 1, _0I_t^\gamma t, \dots, _0I_t^\gamma t^n \right]^T \\
&= \Lambda \left[\frac{0!}{\Gamma(\gamma+1)} t^\gamma, \frac{1!}{\Gamma(\gamma+2)} t^{\gamma+1}, \dots, \frac{n!}{\Gamma(\gamma+n+1)} t^{\gamma+n} \right]^T = \Lambda \Theta \overline{T}_n(t),
\end{aligned} \tag{16}
$$

where Θ, being an $(n+1) \times (n+1)$ matrix, and $\overline{T}_n(t)$ are given by

$$\Theta_{i,j} = \begin{cases} \frac{i!}{\Gamma(\gamma+i+1)}, & i = j, \\ \\ 0, & i \neq j. \end{cases} \qquad i,j = 0 \cdots, n, \qquad \overline{T}_n = \left[t^\gamma, t^{\gamma+1}, \cdots, t^{\gamma+n} \right]^T. \tag{17}$$

In the same way as in Subsection 2.2, we approximate $t^{l+\alpha}$ as follows:

$$t^{\gamma+l} \simeq w_l^T \phi(t), \qquad l = 0, \cdots, n. \tag{18}$$

Therefore we have

$$
\begin{aligned}
w_l &= Q^{-1} \left(\int_0^1 t^{\gamma+l} \phi(t) dt \right) \\
&= Q^{-1} \left[\int_0^1 t^{\gamma+l} B_{0,n}(t) dt, \int_0^1 t^{\gamma+l} B_{1,n}(t) dt, \dots, \int_0^1 t^{\gamma+l} B_{n,n}(t) dt \right]^T = Q^{-1} \overline{w}_l,
\end{aligned} \tag{19}
$$

where $\overline{w}_l = [\overline{w}_{l,0}, \overline{w}_{l,1}, \dots, \overline{w}_{l,n}]^T$ and

$$\overline{w}_{l,k} = \int_0^1 t^{\gamma+l} B_{k,n}(t) dt = \frac{n! \Gamma(l+k+\gamma+1)}{k! \Gamma(l+n+\gamma+2)}, \qquad l, k = 0, 1, \dots, n, \tag{20}$$

where $w = [w_0, w_1, \cdots, w_n]^T$ is an $(n+1) \times (n+1)$ matrix that has vector $Q^{-1} \overline{w}_l$ for the i-th columns. Therefore, we can write

$$_0I_t^\gamma \phi(t) \simeq \mathbf{I}^\gamma \phi(t) = \Lambda \Theta w^T \phi(t), \tag{21}$$

where $\mathbf{I}^\gamma = \Lambda \Theta w^T$ is called the fractional integration within the operational matrix.

4 Convergence Analysis

In the current section, we compute the error bounds of the operational matrices of fractional integrals for obtaining the convergence of the numerical approach introduced in the previous section.

Theorem 4.1 *Suppose that H is a Hilbert space and Y is a closed subspace of H such that $dim Y < \infty$ and $\{y_1, y_2, \ldots, y_n\}$ is any basis for Y. Let x be an arbitrary element in H and y_0 be the unique best approximation to x out of Y. Then*

$$\|x - y_0\|^2 = \frac{G(x, y_1, y_2, \ldots, y_n)}{G(y_1, y_2, \ldots, y_n)}, \tag{22}$$

where

$$G(x, y_1, y_2, \ldots, y_n) = \begin{vmatrix} \langle x, x \rangle & \langle x, y_1 \rangle & \ldots & \langle x, y_n \rangle \\ \langle y_1, x \rangle & \langle y_1, y_2 \rangle & \ldots & \langle y_1, y_n \rangle \\ \vdots & \vdots & & \vdots \\ \langle y_n, x \rangle & \langle y_n, y_1 \rangle & \ldots & \langle y_n, y_n \rangle \end{vmatrix}.$$

Proof. See Kreyszig, 1978 [22].

Theorem 4.2 *Suppose that function $f \in L^2[0, 1]$ and $Y = Span\{B_{0,n}(t), B_{1,n}(t), \ldots, B_{n,n}(t)\}$, if $f(t)$ is approximated by*

$$f_n(t) = \sum_{l=0}^{n} c_l B_l(t) = C^T \phi(t), \tag{23}$$

where f_n is the best approximation of f out of Y.
Consider

$$L_n(f) = \int_0^1 [f(t) - f_n(t)]^2 dt,$$

then we have

$$\lim_{n \longrightarrow \infty} L_n(t) = 0.$$

Proof. For the proof see [19].

Now, by using these theorems, we compute the error upper bound of the operational matrix of the fractional integration $\mathbf{I}^\gamma$ based on Bernstein polynomials in the interval $[0, 1]$. Consider $E_\mathbf{I}^\gamma$ as the error vector of the operational matrix of fractional integration as

$$E_\mathbf{I}^\gamma = \mathbf{I}^\gamma \phi(t) - {}_0 I_t^\gamma \phi(t), \tag{24}$$

where $E_\mathbf{I}^\gamma = \left[E_{\mathbf{I},0}^\gamma, E_{\mathbf{I},1}^\gamma, \cdots, E_{\mathbf{I},n}^\gamma \right]^T$.

The fractional integral of any Bernstein polynomial $B_{l,n}$ is given by

$$
\begin{aligned}
_0I_t^\gamma B_{l,n} &= \sum_{j=l}^n (-1)^{j-l} \binom{n}{l}\binom{n-l}{j-l} {}_0I_t^\gamma t^j \\
&= \sum_{j=l}^n (-1)^{j-l} \binom{n}{l}\binom{n-l}{j-l} {}_0I_t^\gamma \frac{t^{j+\gamma}\Gamma(j+1)}{\Gamma(j+\gamma+1)} \\
&= \sum_{j=l}^n (-1)^{j-l} \frac{n!j!}{l!(j-l)!(n-2l-j)!\Gamma(j+\gamma+1)} t^{j+\gamma} = \sum_{j=l}^n b_{l,j} t^{j+\gamma}.
\end{aligned}
\tag{25}
$$

By virtue of (15), (24) and (25), we have

$$
\begin{aligned}
\parallel E_{\mathbf{I},l}^\gamma \parallel_2 &= \parallel \mathbf{I}^\gamma B_{l,n}(t) - \sum_{k=0}^n \Big(\sum_{j=l}^n b_{l,j} c_{j,k}\Big) B_{k,n}(t) \parallel \\
&\leq \sum_{j=l}^n (-1)^{j-l} \frac{n!j!}{l!(j-l)!(n-2l-j)!\Gamma(j+\gamma+1)} \parallel t^{j+\gamma} - \sum_{k=0}^n c_{j,k} B_{k,n}(t) \parallel \\
&\leq \sum_{j=l}^n b_{l,n} \left(\frac{G(t^{j+\gamma}, B_{0,n}(t), B_{1,n}(t),\ldots,B_{n,n}(t))}{G(B_{0,n}(t), B_{1,n}(t),\ldots,B_{n,n}(t))} \right)^{\frac{1}{2}}.
\end{aligned}
\tag{26}
$$

We can conclude by Theorem 2 and equation (26) that by increasing the number of Bernstein bases, the error vector $E_{\mathbf{I},l}^\gamma$ tends to zero.

5 Numerical Results

In this section, we estimate the numerical results for the fractional chemical kinetics model for various values of γ by using the operational matrix of fractional integration and multiplication of Bps. For solving equation (5), we expand fractional derivatives by Bernstein polynomials as, say,

$$
D_t^\gamma \zeta(t) = Z^T \phi(t), \qquad D_t^\gamma \eta(t) = N^T \phi(t), \qquad D_t^\gamma \kappa(t) = K^T \phi(t),
\tag{27}
$$

where

$$
Z^T = [\zeta_0,\zeta_1,\cdots,\zeta_n]^T, \qquad N^T = [\eta_0,\eta_1,\cdots,\eta_n]^T, \qquad K^T = [\kappa_0,\kappa_1,\cdots,\kappa_n]^T.
$$

Applying the fractional integral operator on the both sides of equation (27) and by replacing the initial condition in equation (28), then with the aid of equation (12) and equation (21) we can obtain the following result:

$$
\begin{aligned}
\zeta(t) &= Z^T {}_0I_t^\gamma \phi(t) + \zeta(0) = Z^T \mathbf{I}^\gamma \phi(t) + d^T \phi(t) = G_1^T \phi(t), \\
\eta(t) &= N^T {}_0I_t^\gamma \phi(t) + \eta(0) = N^T \mathbf{I}^\gamma \phi(t) = G_2^T \phi(t), \\
\kappa(t) &= K^T {}_0I_t^\gamma \phi(t) + \kappa(0) = K^T \mathbf{I}^\gamma \phi(t) = G_3^T \phi(t).
\end{aligned}
\tag{28}
$$

Inserting equations (27) and (28) in equation (5), we have

$$
\begin{aligned}
Z^T \phi(t) &= -\theta_1 G_1^T \phi(t) + \theta_2 G_3^T \hat{G}_2^T \phi(t), \\
N^T \phi(t) &= \theta_1 G_1^T \phi(t) - \theta_2 G_3^T \hat{G}_2^T \phi(t) - \theta_3 G_2^T \hat{G}_2^T \phi(t), \\
K^T \phi(t) &= \theta_3 G_2^T \hat{G}_2^T \phi(t),
\end{aligned}
\tag{29}
$$

where $\hat{G}_2$ is an operational matrix of product. For more information about an operational matrix of product, refer to [11]. Finally, we get the following set of algebraic equations as:

$$Z^T + \theta_1 G_1^T - \theta_2 G_3^T \hat{G}_2^{\ T} = 0,$$
$$N^T - \theta_1 G_1^T + \theta_2 G_3^T \hat{G}_2^{\ T} + \theta_3 G_2^T \hat{G}_2^{\ T} = 0, \qquad (30)$$
$$K^T - \theta_3 G_2^T \hat{G}_2^{\ T} = 0.$$

By solving this system for the vectors ζ, η, κ, we can approximate $\zeta(t), \eta(t)$ and $\kappa(t)$ from (28). We have taken the values of parameters as $\theta_1 = 0.1$, $\theta_2 = 0.02$, and $\theta_3 = 0.009$. Comparisons between the exact solution and the numerical results obtained by this technique for $m = 6$ and different values of γ for $\zeta(t), \eta(t), \kappa(t)$ are shown in Fig. 1 respectively. Fig. 2 presents comparison between the exact and approximate solutions obtained by the help of BPs for $\zeta(t), \eta(t), \kappa(t)$ when $\gamma = 0.97$ and $m = 2, 3, 6$.
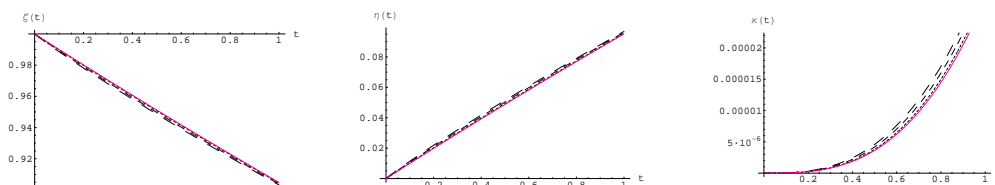
Figure 1: The exact solution: (red line) and approximation solutions $\zeta(t), \eta(t), \kappa(t)$ for $m = 6$ when $\gamma = 0.99$ (dotted), $\gamma = 0.97$ (dashed), $\gamma = 0.95$ (long-dashed).
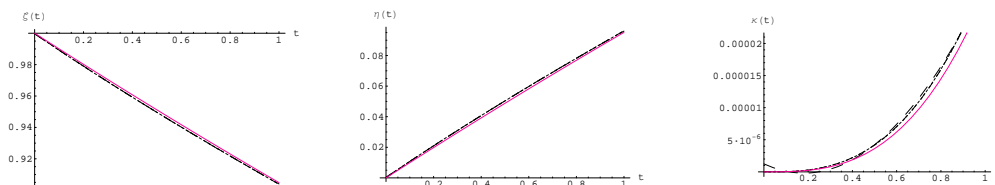
Figure 2: The exact solution: (red line) and approximation solutions $\zeta(t), \eta(t), \kappa(t)$ for $\gamma = 0.97$ when $m = 6$ (dotted), $m = 3$ (dashed), $m = 2$ (long-dashed).

6 Concluding Remarks and Discussion

In this work we have presented a numerical solution of the fractional chemical kinetics model using the operational matrices of fractional integration and multiplication based on BPs. The main advantage of this method is that the main problem reduces into a system of nonlinear algebraic equations. The obtained results demonstrate that only a small number of Bernstein polynomials bases is needed to obtain the accurate approximate solution via the present method. For the accuracy of the scheme we have given an example which shows that the results are much better.

The numerical simulations were carried out by Mathematica.

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