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A NUMERICAL APPROACH FOR SOLVING A CLASS OF SINGULAR BOUNDARY VALUE PROBLEMS ARISING IN PHYSIOLOGY

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Abstract. In this paper, two numerical schemes for finding approximate solutions of singular two-point boundary value problems arising in physiology are presented. While the main ingredient of both approaches is the employment of cubic B-splines, the obstacle of singularity has to be removed first. In the first approach, L'Hopital's rule is used to remove the singularity due to the boundary condition (BC) $y'(0) = 0$. In the second approach, the economized Chebyshev polynomial is implemented in the vicinity of the singular point due to the BC $y(0) = A$, where A is a constant. Numerical examples are presented to demonstrate the applicability and efficiency of the methods on one hand and to confirm the second order convergence on the other hand.

Key words. Boundary value problems; Chebyshev polynomial; B-spline; Singularities

1. Introduction

Many numerical treatments for singular boundary value problems have emerged in recent years. To mention few, Pandey and Singh [14] applied a finite difference method on a uniform mesh for a class of singular boundary value problem (BVP), Kanth and Bhattacharya [12] employed B-spline functions after reducing the nonlinear problem into a sequence of linear problems by using quesilinearization techniques, and then modifying the resulting sets of differential equations around the singular point. For a homogenous and linear singular BVP, Kadalbajoo and Aggarwal [11] started by finding a series solution in the vicinity of the singularity and then applying a cubic spline method for the remaining part of the interval. The reader may also see [6] and [7] for extra readings.

In this paper, we will consider a more general nonlinear singular BVP of the form

$$(p(x)y')' = p(x)f(x,y), \quad x \in (0,1] \tag{1}$$

with boundary conditions (BC)

$$y'(0) = 0, \quad \alpha y(1) + \beta y'(1) = \gamma \tag{2}$$

or

$$y(0) = A, \quad \alpha y(1) + \beta y'(1) = \gamma \tag{3}$$

where

$$p(x) = x^b g(x), \ x \in [0,1] \tag{4}$$

here $\alpha > 0$, $\beta \geq 0$ and A and γ are finite constants. Also, the following restrictions are imposed on $p(x)$ and $f(x,y)$.

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(I) $p(x) > 0$ on $[0,1]$, $p(x) \in C^1(0,1]$, and $1/g(x)$ is analytic in $\{z \text{ s.t. } |z| < r\}$ for some $r > 1$.

(II) $f(x,y) \in [0,1] \times R$, is continuous, $\partial f/\partial y$ exists, continuos, and nonnegative for all $(x,y) \in [0,1] \times R$.

The existence-uniqueness of (1) has been established for BCs $y(0) = A$ and $y(1) = B$ with $0 \leq b < 1$, and BCs $y'(0) = 0$ and $y(1) = B$ with $b \geq 0$, provided that xp'/p is analytic in $\{z \text{ s.t. } |z| < r\}$ for some $r > 1$ [15–17].

The BVP (1) with BC (3) arises in the study of tumor growth problems [1–3, 10] where $b = 0, 1, 2$, $g(x) = 1$, and $f(x,y)$ is either linear or nonlinear of the form

$$f(x,y) = \frac{\theta y}{y + \kappa}, \qquad \theta, \kappa > 0. \tag{5}$$

and also arises in the study of a steady-state oxygen diffusion in a cell with Michaleis-Menten uptake kinetics when $b = 2$ and $g(x) = 1$ [13].

Also, a similar problem arises in the study of the distribution of heat sources in the human head [8, 9] where $b = 2$, $g(x) = 1$, and

$$f(x,y) = -\delta e^{-\theta y}, \qquad \theta, \delta > 0. \tag{6}$$

In this paper, we propose two numerical schemes to find approximate solutions for (1) with BC (2), and for (1) with BC (3) for a wider range of b and for the case where $f(x,y)$ is nonlinear. The paper is outlined as follows: In section 2, we describe the two methods for the two sets of boundary conditions (2) and (3). In section 3, two applications to physiology are presented and the results are compared to those obtained by [14], also the second-order of convergence will be verified as was established by Ahlberg and Ito [4]. Some concluding remarks are summarized in section 4.

2. Description of the method

Substituting the value of $p(x)$ in (4) into (1), and algebraic manipulations yields

$$y'' + \left(\frac{b}{x} + \frac{g'(x)}{g(x)}\right) y' = f(x,y) \tag{7}$$

Each set of boundary conditions (2) and (3) will be treated separately.

2.1. L'Hopital's rule and cubic B-splines. In this section, we discuss a method for solving BVP (1) with BCs (2), which is analogous to, but more general than, that introduced in [5].

To overcome the singularity at $x = 0$, we apply L'Hopital's rule as x approaches zero to the term $\frac{b}{x} y'$ in (7). So we obtain the boundary value problem

$$y'' + \left(\frac{\mu}{x} + \eta \frac{g'(x)}{g(x)}\right) y' = F(x,y) \tag{8}$$

where

$$F(x,y) = \begin{cases} f(x,y), & x \neq 0 \\ \dfrac{1}{b+1} f(0,y), & x = 0 \end{cases} \tag{9}$$

and

$$\begin{cases} \mu = b \text{ and } \eta = 1, & x \neq 0 \\ \mu = 0 \text{ and } \eta = \frac{1}{b+1}, & x = 0 \end{cases} \tag{10}$$

Now we describe the B-spline collocation method to obtain an approximate solution for problem (8) with BC (2). Consider the nodal points x_i on the interval $[a, b]$ where

$$a = x_0 < x_1 < ... < x_{n-1} < x_n = b$$

Note that, if the nodal points are equidistant from each other, then we have $x_i = ih, \quad i = 0, 1, 2, ..., n$ where $h = \dfrac{b-a}{n}$ on the interval $[a, b]$. Let $\psi(t)$ be an approximate solution that satisfies the two boundary conditions (3) and written as a linear combination of $n + 3$ shape functions given by

$$\psi(t) = \sum_{i=-3}^{n-1} A_i \psi_i(t) \tag{11}$$

where A_i, $i = -3, -2, \cdots, n-1$ are unknown real coefficients and the $\psi_i(x)$ are the cubic B-splines functions defined as follows:

(12)

$$\psi_i(x) = \frac{1}{h^3} \begin{cases} (x - x_i)^3, & [x_i, x_{i+1}] \\ h^3 + 3h^2(x - x_{i+1}) + 3h(x - x_{i+1})^2 - 3(x - x_{i+1})^3, & [x_{i+1}, x_{i+2}] \\ h^3 + 3h^2(x_{i+3} - x) + 3h(x_{i+3} - x)^2 - 3(x_{i+3} - x)^3, & [x_{i+2}, x_{i+3}] \\ (x_{i+4} - x)^3, & [x_{i+3}, x_{i+4}] \\ 0, & \text{otherwise} \end{cases}$$

in which $h = x_{j+1} - x_j$ for all j.

From (12), the values of ψ_i, ψ_i' and ψ_i'' at the nodal points $x_i = ih$ are given in Table 1.

Table 1
ψ_i, ψ_i', and ψ_i''evaluated at nodal points

Nodes	ψ_i	ψ_i'	ψ_i''
x_i	0	0	0
x_{i+1}	1	$\frac{3}{h}$	$\frac{6}{h^2}$
x_{i+2}	4	0	$\frac{-12}{h^2}$
x_{i+3}	1	$\frac{-3}{h}$	$\frac{6}{h^2}$
x_{i+4}	0	0	0

Substituting the approximate solution (11) into equation (1) yields

$$\sum_{i=-3}^{n-1} A_i \psi_i''(x_j) + \left(\frac{\mu}{x_j} + \eta \frac{g'(x_j)}{g(x_j)}\right) \sum_{i=-3}^{n-1} A_i \psi_i'(x_j) = F\left(x_j, \sum_{i=-3}^{n-1} A_i \psi_i(x_j)\right) \tag{13}$$

$$j = 0, 1, 2, ..., n$$

or equivalently

$$\sum_{i=-3}^{n-1} A_i \left[\psi_i''(x_j) + \left(\frac{\mu}{x_j} + \eta\frac{g'(x_j)}{g(x_j)}\right)\psi_i'(x_j)\right] = F\left(x_j, \sum_{i=-3}^{n-1} A_i\psi_i(x_j)\right) \tag{14}$$

$$j = 0, 1, 2, ..., n$$

Note that we have $\frac{\mu}{x_0} = 0$. The system (14) consists of $n+1$ equations in $n+3$ unknowns. Using expansion (4), the two boundary conditions in (2), respectively, take on the forms

$$\sum_{i=-3}^{n-1} A_i\psi_i'(x_0) = 0 \tag{15}$$

and

$$\sum_{i=-3}^{n-1} A_i\left(\alpha\psi_i(x_n) + \beta\psi_i'(x_n)\right) = \gamma \tag{16}$$

The system of equations in (14)-(16) is expressed in the matrix equation

$$\mathbf{C}\,\mathbf{d} = \mathbf{b} \tag{17}$$

where

$$\mathbf{C} = \begin{bmatrix} -\frac{3}{h} & 0 & \frac{3}{h} & 0 & 0 & ... & 0 \\ p_0 & q_0 & r_0 & 0 & 0 & ... & 0 \\ 0 & p_1 & q_1 & r_1 & 0 & ... & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & ... & p_n & q_n & r_n \\ 0 & 0 & 0 & ... & \alpha - \frac{3\beta}{h} & 4\alpha & \alpha + \frac{3\beta}{h} \end{bmatrix}$$

in which

$$p_i = \frac{6 - 3hG_i}{h^2}, \qquad q_i = \frac{-12}{h^2} \qquad r_i = \frac{6 + 3hG_i}{h^2}$$

where

$$G_i = G(x_i) = \frac{\mu}{x_i} + \eta\frac{g'(x_i)}{g(x_i)}, \quad i = 0, 1, \cdots, n$$

$$\mathbf{b} = \begin{bmatrix} 0 \\ F\left(x_0,\ A_{-3}+4A_{-2}+A_{-1}\right) \\ F\left(x_1,\ A_{-2}+4A_{-1}+A_0\right) \\ F\left(x_2,\ A_{-1}+4A_0+A_1\right) \\ \cdot \\ \cdot \\ \cdot \\ F\left(x_{n-1},\ A_{n-4}+4A_{n-3}+A_{n-2}\right) \\ F\left(x_n,\ A_{n-3}+4A_{n-2}+A_{n-1}\right) \\ \gamma \end{bmatrix}$$

$$\mathbf{d}^T = [A_{-3},\ A_{-2},\ A_{-1},\ A_0,\ \cdots,\ A_{n-3},\ A_{n-2},\ A_{n-1}\ ]$$

2.2. Economized Chebyshev polynomial and cubic B-splines. In this section, we discuss the method for solving BVP (1) with BCs (3).

To apply Chebyshev approximation, we begin by finding a linear approximation for $f(x, y)$, on the right hand side of (1), near the singularity

$$f(x, y) = f(x, y_0) + f_y(x, y_0)(y - y_0) \tag{18}$$

where $y_0 = y(0) = A$. Notice that the condition $y_0 = y(0) = A$ is crucial to obtain very accurate approximation for y close to y_0.

Substitute (18) into (1) gives

$$(p(x)y')' - yp(x)f_y(x, y_0) = p(x)f(x, y_0) - y_0 p(x)f_y(x, y_0) \tag{19}$$

Because of the singularity at $x = 0$, the solution of (19) is given in the form

$$y(x) = \sum_{k=0}^{\infty} a_k x^{k+p}, \quad a_0 \neq 0. \tag{20}$$

Substituting (20) in (19) gives the general solution

$$y(x) = \sum_{i=1}^{m} \alpha_i S_i(x), \quad m = 1, 2,$$

where S_1 and S_2 are two linearly independent solutions of (18). To expedite the convergence of the series over $\Omega = (0, 1)$, we choose δ sufficiently close to the singularity, and then employ Chebyshev economized expansion over the interval $\Omega_1 = (0, \delta)$. Over the interval $\Omega_2 = (\delta, 1)$, we apply a cubic B-spline approximation.

Assume that $S_1(x)$ and $S_2(x)$ are equal to $S(x)$ for different indicial values so that the general solution is

$$y(x) = (\alpha_1 x^{m_1} + \alpha_2 x^{m_2})\, S(x) \tag{21}$$

where m_1, $m_2 \geq 0$ are the roots of the indicial equation. Now we assume that the economized expansion, $P_N(x) = \sum_{k=0}^{N} p_k x^k$, of $S(x)$ satisfies the equation

$$(p(x)y')' - yp(x)f_y(x, y_0) = p(x)f(x, y_0) - y_0 p(x)f_y(x, y_0) + \tau T_M\left(\frac{2x}{\delta} - 1\right) \tag{22}$$

where $T_M\left(\frac{2x}{\delta} - 1\right)$ is the shifted Chebyshev polynomial in the interval Ω_1. It is required, here, that $P_N(0) = y_0 = y(0) = A$. The coefficients p_k and τ can be found from equation (22) with the modified BC at $x = \delta$

$$ay(\delta) + by'(\delta) = c \tag{23}$$

where

$$\begin{aligned} a &= R_2'(\delta)R_1(0) - R_1'(\delta)R_2(0) \\ b &= R_1(\delta)R_2(0) - R_2(\delta)R_1(0) \\ c &= A\left(R_1(\delta)R_2'(\delta) - R_2(\delta)R_1'(\delta)\right) \end{aligned}$$

in which $R_i(x) = x^{m_i} P_N(x), i = 1, 2$ (see [11] for details).

3. Numerical examples

In this section, we employ the two proposed methods to solve a singular two-point boundary value problem that arise in physiology [14]. Analysis of error shows that both methods converge with order 2.

Example 1. *Consider the boundary value problem*

$$\begin{aligned} &(p(x)y')' = p(x)f(x, y), \quad x \in [0, 1] \\ &p(x) = x^b g(x), g(x) = e^x, f(x, y) = \tfrac{5x^3\left(5x^5 e^y - x - b - 4\right)}{4 + x^5} \\ &y'(0) = 0, \ y(1) + 5y'(1) = -5 - \ln 5 \end{aligned} \tag{24}$$

whose analytic solution is $y = -\ln(x^5 + 4)$ for all $b \in R$. This problem is an application of oxygen diffusion corresponding to (1), (2), and (5) with $p(x) = x^2$, $\theta = 0.76129$, $\kappa = 0.03119$, $\alpha = 5$, $\beta = 1$, $\gamma = 5$.

Applying L'Hopital's rule, to overcome the singularity at $x = 0$, and then the modified spline approach as described in section 2.1, the approximate and exact solutions for $b = 0.5$ with 8 grid points are shown in Figure 1.

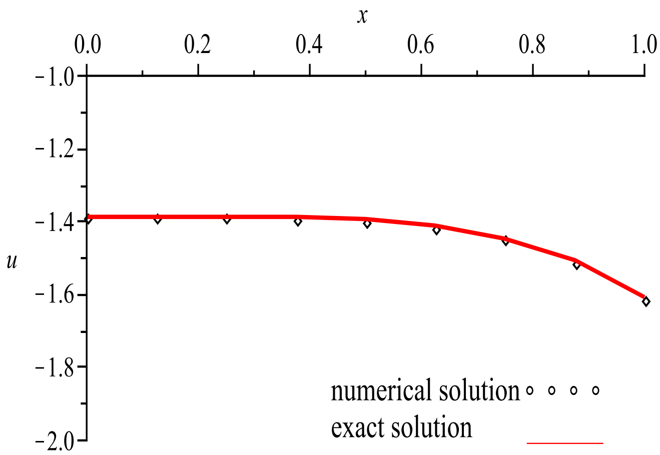

Figure 1: The exact and approximate solution for (24) with $b = 0.5$ and $N = 8$.

For further illustration, Figure 2 shows the log of the error of the approximate solution of (24) for different numbers of mesh points using $b = 0.5$.

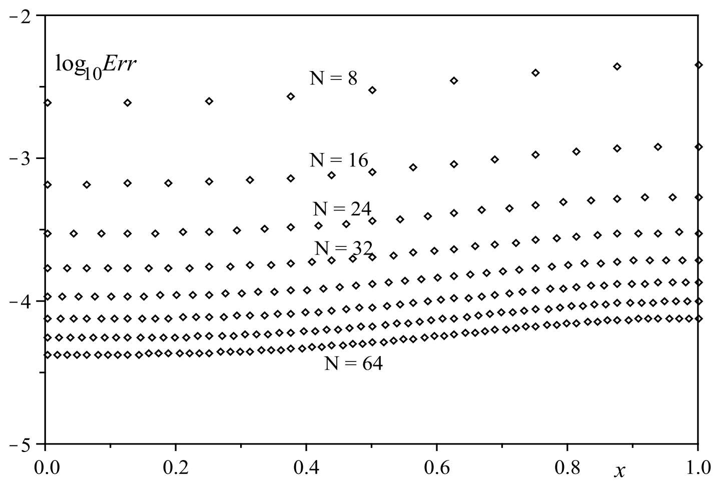

Figure 2: Log of the errorof the approximate solution of (24) with $b = 0.5$.

To examine the error of the approximation, let $E(h) = \max_{0 \le i \le N} |y(x_i) - y_i|$, where $hN = 1$. It is known that for large N, if M is the order of convergence of the method, then

$$E(h) \simeq K\, |h|^M \tag{25}$$

where K is the error constant. Following the generalized algorithm for the order verification of numerical methods given in [18], we can find M and K from the line $y = Mx + \log K$ that best fits the equation

$$\log E(h) = \log K + M \log h. \tag{26}$$

Applying this algorithm for Example 1, the best fit line whose graph is shown in Figure 3 is given by

$$y = -0.545 + 1.97x \tag{27}$$

where $x = \log h$ and $y = \log E(h)$. From equation (27), we conclude that the order of convergence $M \simeq 2$ with error constant $K = 10^{-0.545} \simeq 0.285$.

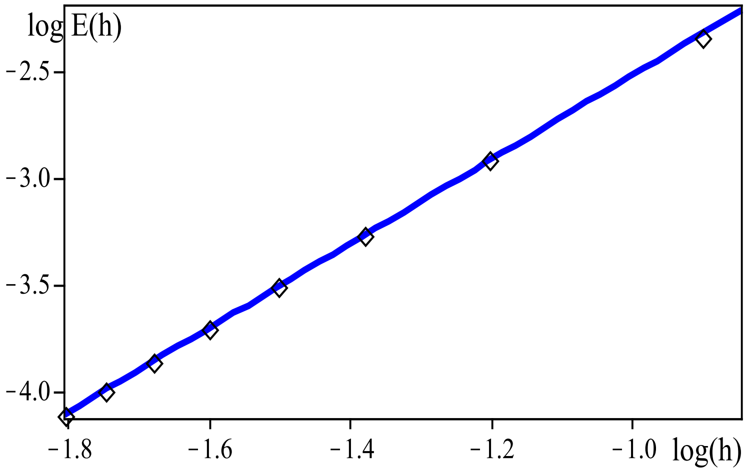

Figure 3: The best fit line for the order of convergence of (24).

In Table 2, we show a comparison between the maximum error obtained by our proposed method and the maximum error obtained by a finite difference approach suggested by Pandey and Singh [14].

Table 2
Maximum error for BVP (24)

	$b = 0.25$		$b = 1.0$		$b = 8.0$	
N	our method	Pandey's	our method	Pandey's	our method	Pandey's
16	7.79(−4)	1.17(−3)	7.79(−4)	1.46(−3)	2.52(−3)	4.11(−3)
32	1.98(−4)	3.04(−4)	1.98(−4)	3.68(−4)	6.30(−4)	9.76(−4)
64	4.98(−5)	7.67(−5)	4.98(−5)	9.20(−5)	1.57(−4)	2.38(−4)

The proposed method superiority is evident here when compared to the finite difference method [14] for each mesh size.

Example 2. *The boundary value problem (24) is reconsidered again but with the change in the first boundary condition.*

$$\begin{aligned} &(p(x)y')' = p(x)f(x,y), \quad x \in [0,1] \\ &p(x) = x^b g(x), g(x) = e^x, f(x,y) = \frac{5x^3\left(5x^5 e^y - x - b - 4\right)}{4+x^5} \\ &y(0) = -\ln 4, \ \ y(1) + 5y'(1) = -5 - \ln 5 \end{aligned} \tag{28}$$

This problem is an application of nonlinear heat conduction model of the human head corresponding to equations (1), (3), and (6) with $p(x) = x^2$, $\delta = \theta = 1$, and $\gamma = 0$.

As described in section 2.2, we start with formulating a Chebyshev polynomial around a small neighborhood of the singularity and then apply the spline functions over the rest of the boundary interval. With $\delta = 0.1$, $N = 9$, and $M = 6$, we derived the economized Chebyshev polynomial over the interval $\Omega_1 = [0, \delta]$ for $b = 0.5$

$$P_9(x) = -2.94178 \times 10^{-8}x^2 + 8.48013 \times 10^{-6}x^3 - 5.31338 \times 10^{-4}x^4 \\ - 0.23585x^5 - 0.18700x^6 + 1.216372x^7 - 3.15430x^8 + 0.32986x^9$$

Here the roots of the indicial equation of the associated homogeneous form of (28) are $m_1 = 0$ and $m_2 = 1 - b$. Hence for $b = 0.5$, the solution over $\Omega_1$takes on the form

$$y(x) = (\alpha_1 + \alpha_2 x^{0.5})P_9(x)$$

and over the interval $\Omega_2 = [\delta, 1]$, we apply a B-spline collocation method using the modified BC obtained by (23), that is

$$3.03871y(\delta) - 0.60773y'(\delta) = -4.21248.$$

It is to be noted, here, that when $b \geq 1$, the condition $y(0) = P_N(0) = A$ holds only when the approximate solution over $\Omega_1$is $y(x) \simeq P_N(x)$, and hence the modified BC at δ may be taken as $y(\delta) = P_N(\delta)$.

The exact, approximate spline, and Chebyshev approximation using $N = 10$ and $b = 0.5$ are shown in Figure 4.

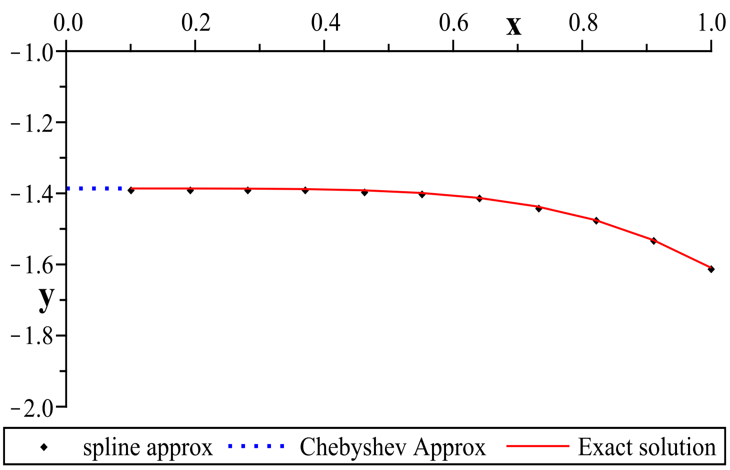

Figure 4: Exact and approximate solutions for BVP (28) with $b = 0.5$ and $N = 10$.

The illustration, in Figure 5, shows the logarithm of the error of the approximate solution of BVP (28) using $b = 0.5$ for various mesh sizes.

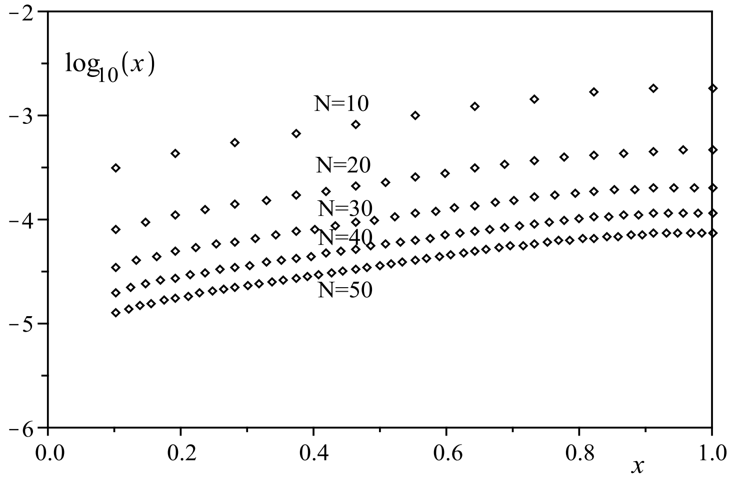

Figure 5: The log of the error of the approximate solution of BVP (28).

The order of convergence can be estimated using formula (26). The best fit line is found to be

$$y = -0.643 + 1.99x$$

from which we conclude that the method converges approximately with order 2.

The effect of b is analyzed in Table 3, where the maximum errors of the approximation for various values of b and different mesh sizes are considered.

Table 3
Maximum error for the approx. solution of BVP (28) for different values of b

N/b	0.25	0.5	0.75	1.0	2.0
16	5.60(−4)	7.84(−4)	1.04(−3)	1.01(−3)	1.77(−3)
32	1.41(−4)	1.88(−4)	2.61(−4)	2.51(−4)	4.36(−4)
48	6.28(−5)	8.37(−5)	1.16(−4)	1.12(−4)	1.94(−4)
64	3.54(−5)	4.71(−5)	6.53(−5)	6.29(−5)	1.09(−4)

4. Conclusion

Cubic B-spline functions were employed to solve a class of singular two-point boundary value problems. The removal of the singularity was achieved by using L'Hopital's rule when the BC $y'(0) = 0$ is present, and Chebyshev polynomial around δ, the vicinity of the singularity, in the presence of the BC $y(0) = A$. After removing the singularity, a cubic B-spline collocation approach was used to approximate the solution over the rest of the interval, namely $[\delta, 1]$. Both approaches were applied to singular two-point BVP that arise in physiology. The results were compared to a finite difference technique applied by Pandey's [14] and shown to be more accurate and of second order accuracy. Another advantage of our proposed methods that the solution can be estimated within the boundary interval whereas, the finite difference approach approximates the solution solely at the nodal points.

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