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A comparison between pre-Newton and post-Newton approaches for solving a physical singular second-order boundary problem in the semi-infinite interval

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In this paper, two numerical approaches based on the Newton iteration method with spectral algorithms are introduced to solve the Thomas-Fermi equation. That Thomas-Fermi equation is a nonlinear singular ordinary differential equation (ODE) with a boundary condition in infinite. In these schemes, the Newton method is combined with a spectral method where in one of those, by the Newton method we convert nonlinear ODE to a sequence of linear ODE and then, solve them using the spectral method. In another one, by the spectral method, the nonlinear ODE is converted to a system of nonlinear algebraic equations, then, this system is solved by the Newton method. In both approaches, the spectral method is based on the fractional order of rational Gegenbauer functions. Finally, the obtained results of the two introduced schemes are compared to each other in accuracy, runtime, and iteration number. Numerical experiments are presented showing that our methods are as accurate as the best results obtained until now. **Copyright © 2022 Shahid Beheshti University.**

Keywords: Pre-Newton method; Post-Newton method; Fractional order of rational Gegenbauer functions; Thomas-Fermi equation; Spectral method.

1. Introduction

Nonlinear problems arise in various fields of research such as biology, cognitive sciences, engineering, finance, etc. One of the branches of nonlinear problems is nonlinear ODEs which have unbounded domains. Since these problems are significant, many researchers developed different numerical schemes to solve them. There are various numerical algorithms to compute the solution of nonlinear problems over the semi-infinite domains such as the Adomian decomposition method [1–4], finite difference and finite element methods [5–7], Hermite collocation [8], meshless methods [9–11], etc. In this work, two different approaches based on the combination of spectral methods and Newton family algorithms are introduced. As the first one, we can refer to the pre-Newton. In the pre-Newton approach, a linearization method is done directly on the nonlinear ODE; then, nonlinear ODE is converted to a sequence of linear ODE which can be solved by different numerical algorithms such as spectral methods. The second approach is the post-Newton. In the post-Newton approach, by using a numerical method the nonlinear ODE is converted to a system of nonlinear algebraic equations, and then, this system is solved using various Newton-type algorithms. To show the efficiency of these approaches and compare them to each other, we consider a nonlinear ODE called the Thomas-Fermi equation which arises in theoretical physics as a test problem. This model has two significant roles in mathematical physics for two reasons: Thomas-Fermi equation was enhanced to model the effective nuclear charge in heavy atoms, and was investigated to analyze the potentials and charge densities of atoms having numerous electrons [12].

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Table 1. Different forms of Thomas-Fermi equation

Equation	Boundary conditions	Unknown	coordinate
$\frac{d^2y}{dx^2} - \frac{1}{\sqrt{x}}y^{\frac{3}{2}}(x) = 0$	$y(0) = 1, y(\infty) = 0$	y	$x \in [0, \infty]$
$z\{y\frac{d^2y}{dz^2} + \frac{dy}{dz}\} - y\frac{dy}{dz} - 2z^2y^3 = 0$	$y(0) = 1, y(\infty) = 0$	$\sqrt{y}$	$z = \sqrt{x}$
$z\frac{d^2y}{dz^2} - \frac{dy}{dz} - 4z^2y^{\frac{3}{2}} = 0$	$y(0) = 1, y(\infty) = 0$	y	$z = \sqrt{x}$

In this paper, pre-Newton and post-Newton approaches based on the fractional order of rational Gegenbauer (FRG) functions are used to solve the Thomas-Fermi equation in the semi-infinite interval. The main aim of this paper is to present a kind of collocation method based on FRG for the solving Thomas-Fermi equation which can obtain the most accurate results which are reported until now. In this paper, we are going to compute $y'(0)$. The obtained value for $y'(0)$ is as follows:

$$-1.588071022611375312718684509423950109452746621674825616765677.$$

This value is obtained in [37] using 600 basis functions. But in this paper, we will obtain this value by using only 200 basis functions The main advantage of the presented method is highly convergence rate of it. On the other hand, it has a good time efficiency. The main idea behind this paper is to use the linearization method to overcome the non-linearity of the Thomas-Fermi equation and we have used fractional order of rational Gegenbauer functions for the first time for solving the Thomas-Fermi equation. Moreover, the main advantage of our algorithm is the reduction of the essential basis function which is needed for obtaining the best possible accuracy. The organization of the paper is expressed as follows: Thomas-Fermi equation is introduced in Section 2, and the Gegenbauer polynomials and FRG functions are introduced in Section 3. Section 4 contains the Newton-Kantorovich method and the application of spectral methods. Results and discussion of the proposed methods are shown in Section 4. Finally, a conclusion is provided in Section 5.

2. Thomas-Fermi equation

The Thomas-Fermi theorem illustrates how the energy of an electronic system, E, and the electronic density, ρ, are connected to each other by the following formula [14]:

$$E[\rho] = \frac{9}{10B}\int \rho(r)d\tau + \frac{1}{2}\int \frac{\rho(r)\rho(r')}{|r-r'|}d\tau' d\tau + \int \rho(r)\nu(r)d\tau, \tag{1}$$

where $\nu(r)$ is the external potential and $B = 3(3\pi)^{-\frac{2}{3}}$. In order to obtain the density the energy functional should be minimized with respect to ρ and subject to the normalization restriction $\int \rho(r)d\tau = N$ where N is the number of electrons

$$\frac{3}{2B}\rho(r)^{\frac{3}{2}} + \int \frac{\rho(r')}{|r-r'|}d\tau' + \nu(r) = \mu, \tag{2}$$

where μ is the Lagrange multiplier related to the normalization restriction [13, 14]. By using Poisson's equation to remove the density and a change of variables Thomas-Fermi equation is obtained as below:

$$\frac{d^2y}{dx^2} = \frac{1}{\sqrt{x}}y^{\frac{3}{2}}(x), \tag{3}$$

with the following boundary conditions:

$$y(0) = 1, \qquad \lim_{x\to\infty} y(x) = 0. \tag{4}$$

This equation describes the charge density in atoms of high atomic number and appears in the problem of determining the effect of nuclear charge in heavy atoms [14–16].

As the solution of the Thomas-Fermi equation is effective in theoretical physics, many scientists have studied this model. Moreover, this equation has three different forms which can be effective on the rate of convergence of the using numerical algorithm [37]. These three forms of the Thomas-Fermi equation are listed in Table 1.

One special parameter in the Thomas-Fermi equation is the first derivative of the unknown function at the region $y'(0)$. This importance is because of some reasons, as the first one, we can refer to the expansion of y about the region, the expansion of y about the region is as follows [17]:

$$y(x) = 1 + \lambda x + \frac{4}{3}x^{\frac{3}{2}} + \frac{2\lambda}{5}x^{\frac{5}{2}} + \frac{1}{3}x^3 + \frac{3\lambda^2}{70}x^{\frac{7}{2}} + \dots, \tag{5}$$

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Table 2. A brief bibliography on Thomas-Fermi equation

Years	Description
1930–1970	In these years, scientists studied the singularity and convergence of the Thomas-Fermi equation, found an analytical solution [17], and investigate the asymptotic behavior of $y(x)$ [19].
1970–2000	Researchers found an alternate analytical solution for the Thomas-Fermi equation using perturbative procedure [18], solved the Thomas-Fermi equation by standard decomposition method [1], Adomian decomposition method and Padé approximation [2, 4].
2000-2010	In this decade, scientists proposed various approaches for approximating the solution of the Thomas-Fermi equation such as a combination of a semi-inverse scheme and the Ritz method [20], piecewise quasilinearization technique [21], an iterative approach and the sweep method [22], computing the potential slope at the origin by exploiting integral properties of the Thomas-Fermi equation [23], rational Chebyshev collocation method [24].
2010–2015	Scientists used semi-analytical and numerical approaches to solve the Thomas-Fermi equation with high accuracy. These techniques are improved Adomian decomposition method [25], optimal parametric iteration method [26], combination of three schemes based on Taylor series, Padé approximates and conformal mappings [27], the Hankel-Padé method [28], an adaptive finite element method based on moving mesh [12], Homotopy analysis method and Padé approximates [29], Newton-Kantorovich iteration and collocation approach based on rational Chebyshev functions [30], Sinc-collocation method [14], Rational second-kind Chebyshev pseudospectral technique [31], collocation method on Hermite polynomials [8]
2015–2018	Recently, researchers proposed fractional order of rational orthogonal [32,33] and non-orthogonal functions [34, 35] for approximating Thomas-Fermi equation. In 2018, Sabir et al suggest an artificial neural network [36] to solve that. Moreover, some other researchers study coordinate transformations [37] for approximating the Thomas-Fermi equation and found a highly accurate solution to 60 decimal places for $y'(0)$

where $\lambda = y'(0) < 0$. On the other hand, $y'(0)$ can be used to obtain the energy of a neutral atom by the following formula:

$$E = \frac{6}{7}(\frac{4\pi}{3})^{\frac{2}{3}} Z^{\frac{7}{3}} y'(0), \tag{6}$$

where Z is the nuclear charge [18].

As mentioned above Thomas-Fermi equation has special significance in theoretical physics and thanks to this importance many researchers develop various numerical algorithms to approximate the solution of the Thomas-Fermi equation. We summarize some previous works in the literature in Table 2.

3. Fractional order of rational Gegenbauer (FRG) functions

There are various types of orthogonal polynomials, which have different behaviors and properties. Choosing a good orthogonal function as a basis that behaves as same as the behavior of the exact solution is a challenging problem in spectral methods because we have no exact solution. But in some problems such as the Thomas-Fermi equation, although we have no exact solution we have some information about the behavior of the solution.

As mentioned in Eq. (5), $y(x)$ can be expanded by a power series of $x^{\frac{1}{2}}$ [33]. So if we choose fractional functions as a basis it can be fitted to the Baker expansion. Moreover, the Thomas-Fermi equation is defined in the semi-infinite domain. One choice for the semi-infinite domains is rational functions. Therefore, we select the fractional order of rational Gegenbauer functions as a basis. In this section, we introduce Gegenbauer polynomials and FRG functions, then we explain how to use the FRG function for function approximating.

3.1. Gegenbauer polynomials

In this paper, we use the fractional order of the rational Gegenbauer function, where this function is obtained from Gegenbauer polynomials. The Gegenbauer polynomial of degree n, $G_n^a(x)$, and order $a > -\frac{1}{2}$ is solution of following differential equation:

$$(1-x^2)\frac{d^2y}{dx^2} - (2a+1)x\frac{dy}{dx} + n(n+2a)y = 0, \tag{7}$$

where n is a positive integer.

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The standard Gegenbauer polynomial $G_n^a(x)$, is defined as follows:

$$G_n^a(x) = \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j \frac{\Gamma(n+a-j)}{j!(n-2j)!\Gamma(a)} (2x)^{n-2j}, \tag{8}$$

where $\Gamma(.)$ is the Gamma function.
The Gegenbauer polynomials are orthogonal over the interval $[-1, 1]$ with the weight function $w(x) = (1-x^2)^{a-\frac{1}{2}}$ which means:

$$\int_{-1}^{1} G_n^a(x) G_m^a(x) w(x) dx = \frac{\pi 2^{1-2a} \Gamma(n+2a)}{n!(n+a)(\Gamma(a))^2} \delta_{nm}, \tag{9}$$

where δ_{nm} is the Kronecker delta function.

In addition, Gegenbauer polynomials can be obtained by the following recursive formula:

$$G_0^a(x) = 1, \qquad G_1^a(x) = 2ax, \tag{10}$$

$$G_{n+1}^a(x) = \frac{1}{n+1}[2x(n+a)G_n^a(x) - (n+2a-1)G_{n-1}^a(x)], \quad n \geq 1 \tag{11}$$

3.2. Fractional order of rational Gegenbauer (FRG) functions

Scientists have been proposing the fractional order of rational functions such as rational Chebyshev [33], rational Jacobi [32], rational Euler [35], etc. to solve some ODEs. A fractional order of the rational Gegenbauer (FRG) function is defined as follows:

$$FRG_n^a(L, \alpha, x) = G_n^a(\frac{x^\alpha - L}{x^\alpha + L}), \tag{12}$$

in which L and α are real positive numbers. FRG functions are orthogonal functions in semi-infinite intervals same as Eq. (9) according to the weight function $w(x) = (1 - (\frac{x^\alpha - L}{x^\alpha + L}))^{a-\frac{1}{2}} \frac{2\alpha L x^{\alpha-1}}{(x^\alpha + L)^2}$:

$$\int_0^\infty FRG_n^a(L, \alpha, x) FRG_m^a(L, \alpha, x) w(x) dx = \frac{\pi 2^{1-2a} \Gamma(n+2a)}{n!(n+a)(\Gamma(a))^2} \delta_{nm}. \tag{13}$$

For more information about fractional order functions, interested readers can see [38–41].

3.3. Approximation of functions

Definition 1 *Consider* $\Gamma = \{x | 0 \leq x \leq \infty\}$ *and* $L_w^2(\Gamma) = \{f : \Gamma \longrightarrow \Re | f$ *is measurable and* $||f||_w < \infty\}$ *where,*

$$w(x) = (1 - (\frac{x^\alpha - L}{x^\alpha + L}))^{a-\frac{1}{2}} \frac{2\alpha L x^{\alpha-1}}{(x^\alpha + L)^2},$$

and

$$||f(x)||_w = \left(\int_0^\infty f^2(x) w(x) dx \right)^{\frac{1}{2}},$$

is the norm induced by the inner product of the space

$$\langle f(x), g(x) \rangle_w = \int_0^\infty f(x) g(x) w(x) dx.$$

Any function $y(x) \in C(0, \infty)$ can be expanded as the follows:

$$y(x) = \sum_{n=0}^{\infty} a_n FRG_n^a(L, \alpha, x), \tag{14}$$

where

$$a_i = \langle y(x), FRG_i^a(L, \alpha, x) \rangle = \langle \sum_{n=0}^{\infty} a_n FRG_n^a(L, \alpha, x), FRG_i^a(L, \alpha, x) \rangle, \tag{15}$$

that is,

$$a_n = \frac{n!(n+a)(\Gamma(a))^2}{\pi 2^{1-2a} \Gamma(n+2a)} \int_0^\infty FRG_n^a(L, \alpha, x) y(x) w(x) dx, \tag{16}$$

Now let assume

$$V_m = span\{FRG_0^a(L, \alpha, x), FRG_1^a(L, \alpha, x), \ldots, FRG_m^a(L, \alpha, x)\},$$

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is a finite dimensional subspace, therefore V_m is a complete subspace of $L^2_w(\Gamma)$ [33, 42, 43]. Let define the $L^2_w(\Gamma)$-orthogonal projection $\Pi_{N,w} : L^2_w(\Gamma) \to V_m$, that for any function $y \in L^2_w(\Gamma)$:

$$\langle \Pi_{N,w} y - y, v \rangle = 0, \quad \forall v \in V_m. \tag{17}$$

It is clear that $\Pi_{N,w} y$ is the best approximation of $y(x)$ in V_m and can be expanded as [44]:

$$\Pi_{N,w} y = y_m(x) = \sum_{i=0}^{m} a_i FRG_i^a(L, \alpha, x). \tag{18}$$

4. Application of the methods

In this section, two approaches based on the Newton method and spectral collocation algorithm are explained to approximate the solution of the Thomas-Fermi equation. In one of them, we use the Newton method to linearize the Thomas-Fermi equation and then solve the several linear ODEs by a spectral method that we call this method pre-Newton method. In the other method, we convert the Thomas-Fermi equation to a nonlinear system of algebraic equations by using a spectral algorithm, then, solve this nonlinear system by using the classical Newton method which we call this method post-Newton. These two schemes are illustrated as follows.

4.1. Pre-Newton approach for Thomas-Fermi equation

Solving a system of nonlinear algebraic equations by using traditional Newton-type solvers have three major practical difficulties. The first one is selecting the start point which yields the convergence of the iterations. The second one is computing the Jacobian matrix of the system of equations at each iteration which has a lot of computational load on the algorithm. The last one is inverting a Jacobian matrix at each iteration which is the most expensive step of the algorithm. In the post-Newton approaches for solving nonlinear ODEs, we should overcome these difficulties [42]. In order to avoid these difficulties, we can apply the Newton method directly to the nonlinear ODE. In the next part, a famous Newton-type algorithm is described which converts nonlinear ODEs to a sequence of linear differential equations.

4.1.1. Newton–Kantorovich method

Newton–Kantorovich method is a well-known and strong approach to converting nonlinear ODEs to linear ones which was introduced by Bellman and Kalaba [45–47]. This approach obtains the solution of a nonlinear ODE by solving a sequence of linear differential equations [48]. In fact, approximating the solution of a nonlinear equation is more complicated than a linear one; therefore, by using Newton–Kantorovich method, the solution of the sequence of the linear differential equations converges to the solution of the original nonlinear ODE [45, 49, 50]. This method is based on approximating a nonlinear function by using the linear part of the Taylor expansion of that function.

This fact can be extended to linearize a nonlinear ODE. In order to show how Newton–Kantorovich method works we consider a n-th order nonlinear ODE over the interval $[0, b]$ as follows [50]:

$$L^{(n)} y(x) = f(y(x), y^{(1)}(x), \ldots, y^{(n-1)}(x), x), \tag{19}$$

with the following boundary conditions:

$$B_k(y(0), y^{(1)}(0), \ldots, y^{(n-1)}(0)) = 0 \quad k = 1, 2, \ldots, l, \tag{20}$$

and

$$B_k(y(b), y^{(1)}(b), \ldots, y^{(n-1)}(b)) = 0 \quad k = l+1, l+2, \ldots, n, \tag{21}$$

where $L^{(n)}$ is a linear n-th order ordinary differential operator and f and $B_1, B_2, \ldots, B_n$ are nonlinear functions of $y(x)$ and its $n-1$ derivatives $y^{(s)}, s = 1, 2, \ldots, n-1$. If we apply Newton–Kantorovich method on Eq. (19) the $(r+1)$-th iterative approximation of $y(x)$ is obtained by solving follow linear ODE,

$$\begin{aligned} &L^{(n)} y_{r+1}(x) = f(y_r(x), y_r^{(1)}(x), \ldots, y_r^{(n-1)}(x), x) + \\ &\sum_{s=0}^{n} \left(y_{r+1}^{(s)}(x) - y_r^{(s)}(x)\right) f_{y^{(s)}}(y_r(x), y_r^{(1)}(x), \ldots, y_r^{(n-1)}(x), x), \end{aligned} \tag{22}$$

where $y_r^0(x)$ is a notation for $y_r(x)$. Also, the linearized boundary conditions are obtained as follows:

$$\sum_{s=0}^{n-1} \left(y_{r+1}^{(s)}(0) - y_r^{(s)}(0)\right) B_{ky^{(s)}}(y_r(0), y_r^{(1)}(0), \ldots, y_r^{(n-1)}(0), 0) = 0, \qquad k = 1, \ldots, l, \tag{23}$$

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and

$$\sum_{s=0}^{n-1} \left(y_{r+1}^{(s)}(b) - y_r^{(s)}(b)\right) B_{ky^{(s)}}(y_r(b), y_r^{(1)}(b), \ldots, y_r^{(n-1)}(v), b) = 0, \qquad k = 1, \ldots, l. \tag{24}$$

It is worth to mention that in the above formulas $f_{y^{(s)}} = \frac{\partial f}{\partial y^{(s)}}$ and $B_{ky^{(s)}} = \frac{\partial B_k}{\partial y^{(s)}}$ for $s = 0, 1, \ldots, n-1$

By implementing Newton–Kantorovich method on Eq. (3), the $(i+1) - th$ iteration linear ODE for approximating the solution of Thomas-Fermi equation is as follows ($i = 0, 1, 2, \ldots$):

$$\sqrt{x} y''_{i+1}(x) - \frac{3}{2}\left(y_i(x)\right)^{\frac{1}{2}} y_{i+1}(x) = \frac{-1}{2}\left(y_i(x)\right)^{\frac{3}{2}}, \tag{25}$$

with the following boundary conditions:

$$y_{i+1}(0) = 1, \qquad \lim_{x\to\infty} y_{i+1}(x) = 0. \tag{26}$$

An initial guess $y_0(x)$ is required for the first step of the Newton–Kantorovich method. It is proved that when the initial guess satisfies one of the boundary conditions, the Newton–Kantorovich method will be convergent [45]. Thus, we consider $y_0(x)$=1.

4.1.2. Collocation method in the pre-Newton method

The spectral collocation method based on FRG functions is applied to Eq. (25) at each iteration. According to the boundary conditions in Eq. (26), we approximate $y_{i+1}(x)$ in $(i+1) - th$ iteration as:

$$y_{i+1}(x) \simeq y_{i+1}^N(x) = 1 + x \sum_{j=0}^{N-1} a_j^{i+1} FRG_j^a(L, \alpha, x). \tag{27}$$

where a_j^{i+1} is the $j - th$ unknown coefficient in $(i+1) - th$ iteration. Equation (27) satisfies the boundary condition $y(0) = 1$. To satisfy the other boundary condition, we choose a sufficiently large number K and consider $y_{i+1}(K) = 0$. The Eq. (27) is replaced in Eq. (25); afterwards, the residual function is obtained:

$$Res_{i+1}(x) = \sqrt{x} y''^N_{i+1}(x) - \frac{3}{2}\left(y_i^N(x)\right)^{\frac{1}{2}} y_{i+1}^N(x) + \frac{1}{2}\left(y_i^N(x)\right)^{\frac{3}{2}}, \tag{28}$$

The roots of $FRG_N^a(L, \alpha, x)$ are considered as the collocation points which are collocated in Eq. (28) and a system of linear algebraic equations is established. By solving this system at each iteration, $y(x)$ is approximated.

$$Res_{i+1}(x_j) = 0, \quad j = 0, \ldots, N-1. \tag{29}$$

4.2. Post-Newton approach for Thomas-Fermi equation

In the post-Newton approach for solving the Thomas-Fermi equation, we use a fully spectral technique same collocation method to solve the nonlinear equation Eq. (3) without any linearization method. In this method, by using the spectral collocation method based on the fractional order of rational Gegenbauer functions, we convert the nonlinear Thomas-Fermi equation Eq. (3) to a system of nonlinear algebraic equations. In this method, the unknown solution $y(x)$ of Thomas-Fermi is approximated by the following series:

$$y(x) \simeq y_N(x) = 1 + x \sum_{j=0}^{N-1} a_j FRG_j^a(L, \alpha, x). \tag{30}$$

Then by substitution $y^N(x)$ instead of $y(x)$ in Eq. (3) the residual function is constructed as follows:

$$Res(x) = \sqrt{x} y''^N(x) - \frac{1}{\sqrt{x}}\left(y^N(x)\right)^{\frac{3}{2}}. \tag{31}$$

Now, there are N unknown coefficients $a_i, i = 0, 1, \ldots, N-1$, to find these unknowns we need N equations. By using the collocation technique and roots of the fractional order of rational Gegenbauer function of order N, and by substitution of these nodes in the residual function we construct N nonlinear equations as follows:

$$F_i = Res(x_i) = 0, \quad i = 0, 1, \ldots, N-2,$$

to satisfy the boundary condition in infinite we set $F_{N-1} = y_N(L) = 0$ for sufficient large L.

So, $F : \mathbb{R}^N \to \mathbb{R}^N$ is a nonlinear function, and therefore, finding the solution of Eq. (3) has been transformed to find the solution of the nonlinear system of equations:

$$F(A) = 0, \qquad A = [a_0, a_1, \ldots, a_{N-1}]^T,$$

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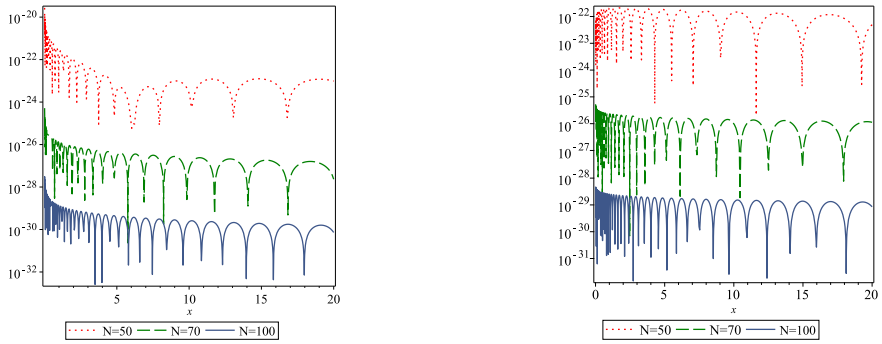

(a) (b)

Figure 1. Graph of the logarithm of the absolute residual errors for different N for (a) pre-Newton and (b) post-Newton.

Now, we have transformed solving the nonlinear differential equation to finding the root of a nonlinear $\mathbb{R}^N \to \mathbb{R}^N$ function.

One of the best methods to solve a nonlinear system is the classical Newton iterative method, that by using Tylor expansion:

$$F(x_{n+1}) = F(x_n) + (x_n - x_{n+1})F'(x_n), \tag{32}$$

presuppose x_{n+1} be root of $F(x)$, $F(x_{n+1}) = 0$:

$$F(x_n) + (x_{n+1} - x_n)F'(x_n) = 0, \tag{33}$$

$$\Rightarrow x_{n+1} = x_n - F'(x_n)^{-1}F(x_n), \tag{34}$$

$F'(x) = J(x)$ is the $n \times n$ Jacobian matrix and is defined as follows:

$$J_{ij} = \left(\frac{\partial f_i}{\partial x_j}\right), \tag{35}$$

therefore:

$$x_{n+1} = x_n - J(x_n)^{-1}F(x_n). \tag{36}$$

In fact, in each iteration, a linear system must be solved:

$$\begin{cases} x_{n+1} = x_n + \delta x_n \\ \\ J(x_n)\delta x_n = F(x_n). \end{cases} \tag{37}$$

In this paper, we use LU method to solve linear system $J(x_n)\delta x_n = F(x_n)$ in each iteration of Newton method. The initial guess of the post-Newton method is the simple vector $x_0 = (1, 1, \ldots, 1)^T$.

5. Numerical results and discussion

According to Boyd's book [42], L can be chosen by "The experimental trial-and-error method"; so, we consider $L = 3$ in pre-Newton and $L = 2.828$ in post-Newton, also we consider $\alpha = \frac{1}{2}$, $a = \frac{1}{2}$ in the both and report the results. It is worth mentioning that all the computations are done by Maple, in a personal computer with the following hardware configuration: desktop 64-bit Intel Core i5 CPU, 8GB of RAM, 64-bit Operating System. In [37], Zhang and Boyd calculated an approximate solution for $y'(0)$ with high accuracy; thus, the results of this study are compared with [37] and found that the obtained results are as accurate as [37]. The logarithm of absolute residual error for the Thomas-Fermi equation in the best iteration is represented in Fig. 1. This figure shows when the number of collocation points increases, the residual error tends to zero. The value of $y'(0)$ is presented in Table 3 and compared with the obtained solution by state-of-the-art methods. Table 4 contains the values of $y(x)$ and $y'(x)$ for different values of x.

Table 3. Comparison of the obtained values of $y'(0)$ by some researchers

Author/Authors	Year	Obtained value of $y'(0)$
Boyd [30]	(2013)	-1.588071022611375312718684509423950109
Parand et al [32]	(2017)	-1.588071022611375312718684509423950109
Parand and Delkhosh (N=300) [33]	(2017)	-1.588071022611375312718684509423950109 51
Zhang and Boyd (N=600) [37]	(2018)	-1.588071022611375312718684509423950109452746621674825616765677
pre-Newton (N=100)		-1.588071022611375312718684509423950109452746621674825616765677
post-Newton (N=200)		-1.588071022611375312718684509423950109452746621674825616765677

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Table 5. Runtime for the proposed methods with the different values of N and iteration

N	Iteration	Runtime for pre-Newton (s)	Runtime for post-Newton (s)
50	20	39.901	32.392
	30	60.626	48.688
	40	80.361	56.359
70	20	104.191	76.690
	30	172.292	111.274
	40	211.721	136.428
100	20	343.672	208.404
	30	469.262	304.123
	40	622.255	392.937

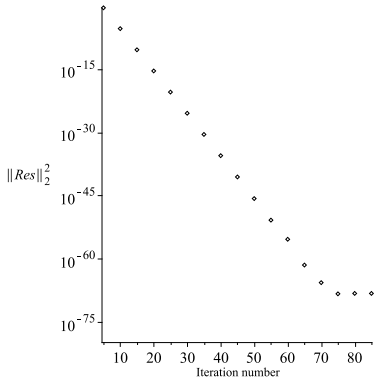

Figure 2. Graph of the $\log(||Res||_2^2)$ for the post-Newton method with $N = 200$ at different iterations.

Table 4. Values of $y(x)$ and $y'(x)$ obtained by the presented methods for the various values of x

$y(x)$ and $y'(x)$	x	pre-Newton (N=100 and iteration=40)	post-Newton (N=200 and iteration=85)
$y(x)$	0.5	0.60698638335597990949444607017402210170 49	0.60698638335597990949444607017408423784 63
	3	0.15663267321649584133981344047753661254 33	0.15663267321649584133981344047791183027 83
	10	0.02431429298868086419011038817329136955 53	0.02431429298868086419011038817630496836 85
	50	0.00063225478298490472677977872873020555 60	0.00063225478298490472677977874278866581 14
	200	0.00001450180349694576468039866296234326 65	0.00001450180349694576468039876872769291 18
	5000	0.00000000113092670634308480760211255593 61	0.00000000113092670634308482638551787878 50
$y'(x)$	0.5	-0.48941161257453808864700584756117431236 09	-0.48941161257453808864700584755734628873 37
	3	-0.06245713085412097622870489999415819898 93	-0.06245713085412097622870489999952179737 89
	10	-0.00460288187126925450254351185548730813 22	-0.00460288187126925450254351185158861542 32
	50	-0.00003249890204825881462420066924767616 11	-0.00003249890204825881462420068023960976 50
	200	-0.00000020575323164752689260570438551149 49	-0.00000020575323164752689260568583630017 42
	5000	-0.00000000000067533971216388346597961193 95	-0.00000000000067533971216388351445037449 57

One of the advantages of the post-Newton approach is its computational speed. This approach is much faster than pre-Newton; as the iterations can be increased to 85 with an acceptable runtime. In Table 5, pre-Newton and post-Newton methods are compared in runtime with the different number of collocation points and iterations. It is derived that post-Newton is much faster than the other approach; therefore, we can consider a larger number of iterations for the post-Newton than pre-Newton. The logarithm of $||Res||^2$ at different iterations of the post-Newton method for the Thomas-Fermi equation by using 200 points is represented in Fig. 2.

6. Conclusion

In this paper, we introduced and compared two points of view to solve nonlinear boundary problems over the semi-infinite interval. These two approaches are called the pre-Newton method and post-Newton method, respectively. The pre-Newton method is based on applying Newton–Kantorovich algorithm to the nonlinear ODE and solving the obtained linear ODEs from Newton–Kantorovich method by using the collocation algorithm. The post-Newton method is based on applying the collocation algorithm directly to the nonlinear ODE and then solving the obtained nonlinear system of algebraic equations by the classical iterative Newton method. The collocation algorithm which is used is based on orthogonal functions in the interval $[0, \infty)$ which are called the fractional order of the rational Gegenbauer. Since the significance of the Thomas-Fermi equation, here, we consider

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it as a test problem. In the Thomas-Fermi equation, the value of $y'(0)$ has important information in physics and scientists attempt to approximate that precisely. Therefore, we compare the approximation solution in $y'(0)$ with the other numerical methods and realize that our proposed method is effective. The approximate solutions for $y(x)$ and $y'(x)$ for various values of x are represented. Additionally, the suggested methods are compared in runtime to find out which method is more efficient. According to the results, the post-Newton approach is faster and more accurate than the pre-Newton approach. It is worth mentioning that one of the limitations of the proposed algorithms is the ill-posedness of systems of algebraic equations. This limitation causes we can not increase the number of collocation points. Moreover, the basis functions are too complex, and finding their roots as the collocation points is very time-consuming.

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