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Retraction

Retracted: The Rational Third-Kind Chebyshev Pseudospectral Method for the Solution of the Thomas-Fermi Equation over Infinite Interval

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The paper titled "The Rational Third-Kind Chebyshev Pseudospectral Method for the Solution of the Thomas-Fermi Equation over Infinite Interval" [1] has been retracted as it was found to contain a substantial amount of material, without referencing, from the following published papers: "On the rational second kind Chebyshev pseudospectral method for the solution of the Thomas-Fermi equation over an infinite interval," published in Journal of Computational and Applied Mathematics (Volume 257, February 2014, Pages 79–85), and "Rational Chebyshev pseudospectral approach for solving Thomas-Fermi equation," published in Physics Letters A (Volume 373, Issue 2, 5 January 2009, Pages 210–213).

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[1] M. Tavassoli Kajani, A. Kılıçman, and M. Maleki, "The rational third-kind Chebyshev pseudospectral method for the solution of the Thomas-Fermi equation over infinite interval," *Mathematical Problems in Engineering*, vol. 2013, Article ID 537810, 6 pages, 2013.

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Research Article

The Rational Third-Kind Chebyshev Pseudospectral Method for the Solution of the Thomas-Fermi Equation over Infinite Interval

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We propose a pseudospectral method for solving the Thomas-Fermi equation which is a nonlinear ordinary differential equation on semi-infinite interval. This approach is based on the rational third-kind Chebyshev pseudospectral method that is indeed a combination of Tau and collocation methods. This method reduces the solution of this problem to the solution of a system of algebraic equations. Comparison with some numerical solutions shows that the present solution is highly accurate.

1. Introduction

Many science and engineering problems of current interest are set in unbounded domains. We can apply different spectral methods that are used to solve problems in semi-infinite domains. The first approach is using the Laguerre polynomials [1–4]. The second approach is replacing semi-infinite domain with $[0, L]$ interval by choosing L, sufficiently large. This method is named domain truncation [5]. The third approach is reformulating original problem in semi-infinite domain to singular problem in bounded domain by variable transformation and then using the Jacobi polynomials to approximate the resulting singular problem [6]. The fourth approach of spectral method is based on rational orthogonal functions. Boyd [7] defined a new spectral basis, named the rational Chebyshev functions on the semi-infinite interval, by mapping to the Chebyshev polynomials. Guo et al. [8] introduced a new set of the rational Legendre functions which are mutually orthogonal in $L^2(0, +\infty)$. They applied a spectral scheme using the rational Legendre functions for solving the Korteweg-de Vries equation on the half line. Boyd et al. [9] applied pseudospectral methods on a semi-infinite interval and compared the rational Chebyshev, Laguerre, and mapped Fourier-sine methods.

The authors of [10–12] applied spectral method to solve nonlinear ordinary differential equations on semi-infinite intervals. Their approach was based on a rational Tau method. They obtained the operational matrices of the derivative and the product of the rational Chebyshev and Legendre functions and then they applied these matrices together with the Tau method to reduce the solution of these problems to the solution of system of algebraic equations. Furthermore, the authors of [13, 14] introduced the rational second- and third-kind Chebyshev-Tau method for solving the Lane-Emden equation and Volterra's population model as nonlinear differential equations over infinite interval.

One of the most important nonlinear singular ordinary differential equations that occurs in semi-infinite interval is the Thomas-Fermi equation, which is given as follows [15, 16]:

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

which appears in the problem of determining the effective nuclear charge in heavy atoms. Boundary conditions for this equation are given as follows:

$$y(0) = 1, \quad \lim_{x \to \infty} y(x) = 0. \tag{2}$$

The Thomas-Fermi equation is useful for calculating the form factors and for obtaining effective potentials which can be used as initial trial potentials in self-consistent field calculations. The problem has been solved by different techniques. [17–19] used perturbative approach to determine analytic solutions for The studies in Thomas-Fermi equation. Bender et al. [17] replaced the right-hand side of a this equation by one which contains the parameter δ, that is, $y''(x) = y(x)(y(x)/x)^{\delta}$; the potential is then expanded in a power series in δ as follows:

$$y = y_0 + \delta y_1 + \delta^2 y_2 + \delta^3 y_3 + \cdots. \tag{3}$$

This procedure reduced (1) into a set of linear equations with associated boundary conditions. Laurenzi [19] applied perturbative method by combining it with an alternate choice of the nonlinear term of (1) to produce a rapidly converging analytic solution. Cedillo [18] wrote (1) in terms of density, and then the δ-expansion was employed to obtain an absolute converging series of equations. Adomian [20] applied the decomposition method for solving the Thomas-Fermi equation, and then Wazwaz [21] proposed a nonperturbative approximate solution to this equation by using the modified decomposition method in a direct manner without any need for a perturbative expansion or restrictive assumptions. He combined the series obtained with the Padé approximation which provided a promising tool to handle problems on an unbounded domain. Liao [22] solved the Thomas-Fermi equation by the homotopy analysis method. This method provided a convenient way to control the convergence of approximation series and adjusted convergence regions when necessary, which was a fundamental qualitative difference in analysis between the homotopy analysis method and all other reported analytic techniques. Khan and Xu [23] used the homotopy analysis method (HAM) with a new and better transformation which improved the results in comparison with Liao's work. In [24], the quasilinearization approach was applied for solving (1). This method approximated the solution of a nonlinear differential equation by treating the nonlinear terms as a perturbation about the linear ones, and, unlike perturbation theories it is not based on the existence of some kind of a small parameter. Ramos [25] presented two piecewise quasilinearization methods for the numerical solution of (1). Both methods were based on the piecewise linearization of ordinary differential equations. The first method (C1-linearization) provided global smooth solutions, whereas the second one (C0-linearization) provided continuous solutions. Recently, Boyd [26] solved the Thomas-Fermi equation using the rational first-kind Chebyshev collocation method with very high accuracy. He showed that the singularity of the Thomas-Fermi function at the origin, which would otherwise degrade convergence of the rational Chebyshev series to fourth order, can be eliminated by a simple transformation of the coordinate and the unknown coefficients to reach a convergence slightly larger than that of the tenth order.

In this paper, we introduce the rational third-kind Chebyshev (RTC) functions, and, for the first time, we derive the operational matrix of the derivatives of RTC functions. We then introduce a combination of Tau and pseudospectral methods based on RTC functions to illustrate its efficiency in solving differential equations on a semi-infinite interval. The proposed method requires the definition of RTC functions, the operational matrix of the derivative, and the rational third-kind Chebyshev-Gauss collocation points and weights. The application of the method to the Thomas-Fermi equation leads to a nonlinear algebraic system. High accurate results for $y'(0)$ are obtained with moderate number of collocation points. We employ this method to the Thomas-Fermi equation because, first, this equation is nonlinear singular, second, the proposed method is easy to apply and numerically achieve spectral convergence, and, because of singularity in this equation, this method can handle this problem, third, the limit of the RTC functions at infinity is computable, and thus the boundary conditions at infinity can be easily handled.

This paper is arranged as follows. In Section 2, we describe the formulation and some properties of the rational third-kind Chebyshev functions required for our subsequent development. Section 3 summarizes the application of this method for solving the Thomas-Fermi equation, and a comparison is made with existing methods in the literature. The results show preference of this method in comparison with the others. The conclusions are described in the final section.

2. Properties of RTC Functions

In this section, we present some properties of the rational third-kind Chebyshev functions and introduce the rational third-kind Chebyshev pseudospectral approach.

2.1. RTC Functions. The third-kind Chebyshev polynomials are orthogonal in the interval $[-1, 1]$ with respect to the weight function

$$\rho(x) = \sqrt{\frac{1+x}{1-x}}, \tag{4}$$

and we find that $V_n(x)$ satisfies the recurrence relation

$$\begin{gathered} V_0(x) = 1, \qquad V_1(x) = 2x - 1, \\ V_n(x) = 2xV_{n-1}(x) - V_{n-2}(x), \quad n \geq 2. \end{gathered} \tag{5}$$

The RTC functions are defined by

$$R_n(x) = V_n\left(\frac{x-L}{x+L}\right). \tag{6}$$

Thus, RTC functions satisfy

$$\begin{gathered} R_0(x) = 1, \qquad R_1(x) = 2\left(\frac{x-L}{x+L}\right) - 1, \\ R_n(x) = 2\left(\frac{x-L}{x+L}\right) R_{n-1}(x) - R_{n-2}(x), \quad n \geq 2. \end{gathered} \tag{7}$$

2.2. Function Approximation. Let $w(x) = 2\sqrt{Lx}/(x+L)^2$ denote a nonnegative, integrable, real-valued function over the interval $I = [0, +\infty)$. We define

$$L_w^2(I) = \{y : I \longrightarrow \mathbb{R} \mid y \text{ is measurable and } \|y\|_w < \infty\}, \tag{8}$$

where

$$\|y\|_w = \left(\int_0^\infty |y(x)|^2 w(x)\, dx\right)^{1/2} \tag{9}$$

is the norm induced by the scalar product

$$\langle y, z\rangle_w = \int_0^\infty y(x)\, z(x)\, w(x)\, dx. \tag{10}$$

Thus, $\{R_n(x)\}_{n\ge 0}$ denote a system which is mutually orthogonal under (10), that is,

$$\int_0^\infty R_n(x)\, R_m(x)\, w(x)\;\, dx = \pi\delta_{nm}, \tag{11}$$

where δ_{nm} is the Kronecker delta function. This system is complete in $L_w^2(I)$; as a result, any function $y \in L_w^2(I)$ can be expanded as follows:

$$y(x) = \sum_{k=0}^{\infty} a_k R_k(x), \tag{12}$$

with

$$a_k = \frac{1}{\pi}\langle y, R_k\rangle_w. \tag{13}$$

The a_k's are the expansion coefficients associated with the family $\{R_k(x)\}$. If the infinite series in (12) is truncated, then it can be written as

$$y(x) \simeq \sum_{k=0}^{N} a_k R_k(x) = A^T R(x), \tag{14}$$

where

$$A = [a_0, a_1, \ldots, a_N]^T, \qquad R(x) = [R_0(x), R_1(x), \ldots, R_N(x)]^T. \tag{15}$$

Moreover, from recurrence relation in (7), we have

$$R(0) = \left[1, -3, 5, \ldots, (-1)^N (2N+1)\right]^T = \mathbf{e}_1, \qquad \lim_{x\to\infty} R(x) = [1, 1, \ldots, 1]^T = \mathbf{e}_2. \tag{16}$$

2.3. Operational Matrix of Derivative. The derivative of the vector $R(x)$ defined in (14) can be approximated by

$$R'(x) \simeq DR(x), \tag{17}$$

where D is the $n \times n$ operational matrix for the derivative. Differentiating (7), we get

$$\begin{aligned} R_0'(x) &= 0, \\ R_1'(x) &= \frac{1}{2}R_0(x) - \frac{3}{4}R_1(x) + \frac{1}{4}R_2(x), \\ R_n'(x) &= \left(R_1(x)\, R_{n-1}(x)\right)' \\ &\quad + R_{n-1}'(x) - R_{n-2}'(x), \quad n \ge 2. \end{aligned} \tag{18}$$

By using (18), the matrix D can be calculated. The matrix D is a lower Hessenberg matrix and can be expressed as $D = D_1 + D_2$, where D_1 is a tridiagonal matrix which is obtained from

$$D_1 = \begin{bmatrix} 0 & 0 & & & & \\ \frac{1}{2} & -\frac{3}{4} & \frac{1}{4} & & & \\ & \frac{9}{4} & -\frac{7}{4} & \frac{1}{2} & & \\ & & 4 & \ddots & \ddots & \\ & & & \ddots & & \\ & & & & & \frac{N-1}{4} \\ & & & & \frac{7N-5}{4} & \frac{1-4N}{4} \end{bmatrix} \tag{19}$$

and the matrix D_2 is obtained from

$$D_2 = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & -3 & 0 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ (-1)^{N-1} & (-1)^N 3 & (-1)^{N+1} 5 & \cdots & 0 & 0 & 0 & 0 \\ (-1)^N & (-1)^{N+1} 3 & (-1)^{N+2} 5 & \cdots & -(2N-5) & 0 & 0 & 0 \\ (-1)^{N+1} & (-1)^{N+2} 3 & (-1)^{N+3} 5 & \cdots & (2N-5) & -(2N-3) & 0 & 0 \end{bmatrix}. \tag{20}$$

2.4. RTC Collocation Points and Weights

Theorem 1. *Consider the interpolatory quadrature formula*

$$\int_{-1}^{1} f(x)\rho(x)\,dx = \sum_{i=0}^{N}\omega_i f(\tau_i) + E_N(f). \quad (21)$$

If nodes τ_i *zeros of the* $(N+1)$*th-degree Chebyshev polynomial of the third kind* V_{N+1} *and the corresponding weights* ω_i *are given by*

$$\omega_i = \frac{4\sin((2i+1)\pi/(2N+3))}{(N+3/2)\rho(\tau_i)} \times \sum_{k=0}^{[(N+1)/2]} \frac{\sin((2k+1)(2i+1)\pi/(2N+3))}{2k+1}, \quad i = 0,1,\ldots,N, \quad (22)$$

then $E_N(f) = 0$ *for all* $f \in \mathbb{P}_{2N+1}$.

Proof (see [29]). Abramowitz and Stegun [30] introduced the rational third-kind Chebyshev-Gauss points. Let

$$\mathscr{R}_N = \operatorname{span}\{R_0, R_1, \ldots, R_N\}, \quad \tau_i = \cos\left(\frac{(2i+1)\pi}{2N+3}\right), \quad i = 0,1,\ldots,N, \quad (23)$$

Be the $N+1$ third-kind Chebyshev-Gauss points; thus, we define

$$x_i = L\frac{1+\tau_i}{1-\tau_i}, \quad i = 0,1,\ldots,N, \quad (24)$$

which are named the rational third-kind Chebyshev-Gauss nodes. Boyd [31] offered guidelines for optimizing the map parameter L. The relations between the rational third-kind Chebyshev orthogonal systems and the rational third-kind Gauss integration are given as follows:

$$\int_0^\infty y(x)w(x)\,dx = \int_{-1}^{1} y\left(L\frac{1+t}{1-t}\right)\rho(t)\,dt = \sum_{i=0}^{N} y(x_j)\,w_j, \quad \forall y \in \mathscr{R}_{2N+1}. \quad (25)$$

□

3. Numerical Solution of the Thomas-Fermi Equation

In this phase, at first, we rewrite the Thomas-Fermi equation introduced in (1) and (2) as

$$\sqrt{x}y''(x) - y^{3/2}(x) = 0, \quad y(0) = 1, \quad \lim_{x\to\infty} y(x) = 0. \quad (26)$$

By applying (14) and (17) on (26), we define

$$\operatorname{Res}(x) = \sqrt{x}A^T D^2 R(x) - \left(A^T R(x)\right)^{3/2}. \quad (27)$$

Table 1: Approximations of $y'(0)$ for the present method.

N	L	$y'(0)$	Absolute error
5	0.149599864	−1.5880710242	1.57×10^{-9}
7	0.07732831999	−1.588071022646	3.51×10^{-11}
8	0.0849432650716649	−1.588071022611374	1.78×10^{-15}

Boyd result [26]: $y'(0) = -1.588071022611375312718684 5$.

As in a typical Tau method and using (10), we can write

$$\langle \operatorname{Re} s(x), R_k(x)\rangle_w = \int_0^\infty \operatorname{Re} s(x)R_k(x)w(x)\,dx = 0, \quad k = 0,1,\ldots,N-2. \quad (28)$$

Now, a pseudospectral method is defined by applying (25) on (28) to generate $(N-2)$ algebraic equations as follows:

$$\sum_{i=0}^{N} \operatorname{Re} s(x_i)R_k(x_i)w_i = 0, \quad k = 0,1,\ldots,N-2. \quad (29)$$

In addition, using (14)–(16), the boundary conditions in (26) can be approximated as

$$A^T\mathbf{e}_1 = 1, \qquad A^T\mathbf{e}_2 = 0. \quad (30)$$

Solving the system of $N+1$ nonlinear equations in (29) and (30) using Newton's method for the unknown coefficients a_j and substituting the obtained results in (14) and (17), the values of $y(x)$ and $y'(0)$ can be approximated.

The importance of the initial slope $y'(0)$ is that it plays a major role in determining the energy of a neutral atom in the Thomas-Fermi approximation

$$E = \frac{6}{7}\left(\frac{4\pi}{3}\right)^{2/3} Z^{7/3}y'(0), \quad (31)$$

where Z is the nuclear charge.

The initial slope $y'(0)$ of the Thomas-Fermi equation is calculated by Kobayashi et al. [32] as $y'(0) = -1.588071$. Boyd [26] obtained $y'(0) = -1.588071022611375312718684 5$, correct to 25 decimal places; however, he obtained this accuracy with $N = 600$ and $L = 64$. In fact, he overcame the singularity of the problem by a change of variable and, increasing N. The proposed method in this paper has the ability that it provides high accurate values for $y'(0)$ by moderate number of collocation points and by obtaining suitable mapping parameter $L > 0$. This method overcame the singularity by employing the Tau method and, obtaining suitable L. As Boyd stated, the constant L is a user-choosable map parameter, which sets the length scale of the mapping. Although there are sophisticated ways to estimate the best choice of L [31], in practice, it is usual to begin with an L according to the physical properties of the problem, and then experiment. The criterion for optimum is rate of convergence. In general, there is no way to avoid a small amount of trial and error in choosing L when solving problems on an

Table 2: Comparison between methods in [22, 23, 27] and the present method for $y'(0)$.

N	Padé	Liao [22]	Khan and Xu [23]	Yao [27]	Present method
7	[20, 20]	−1.58281	−1.582901807	−1.585148733	−1.588071022646
8	[30, 30]	−1.58606	−1.586494973	−1.588004950	−1.588071022611374

Table 3: Approximations of $y(x)$ for the present method, [23, 28].

x	Khan and Xu [23]	Liao [28]	Present method
0.25	0.776191000	0.755202000	0.755455402
0.50	0.615917000	0.606987000	0.602998554
0.75	0.505380000	0.502347000	0.494347872
1.00	0.423772000	0.424008000	0.416399658
1.25	0.362935000	0.363202000	0.358770806
1.50	0.314490000	0.314778000	0.314761643
1.75	0.275154000	0.275451000	0.280179962
2.00	0.242718000	0.243009000	0.252344355
2.25	0.215630000	0.215895000	0.229482688
2.50	0.192795000	0.192984000	0.210384924
2.75	0.173364000	0.173441000	0.194199930
3.00	0.156719000	0.156633000	0.180313058
3.25	0.142371000	0.142070000	0.168270054
3.50	0.129937000	0.129370000	0.157728304
3.75	0.119108000	0.118229000	0.148424721
4.00	0.109632000	0.108404000	0.140154047
4.25	0.101303000	0.099697900	0.132753853
4.50	0.093950400	0.091948200	0.126093968
4.75	0.087432000	0.085021800	0.120068868
5.00	0.081629600	0.078807800	0.114592127
6.00	0.063816200	0.059423000	0.096904158
7.00	0.051800500	0.046097800	0.083941323
8.00	0.043285900	0.036587300	0.074034822
9.00	0.037002300	0.029590900	0.066218399
10.0	0.032208100	0.024314300	0.059894055
15.0	0.019184300	0.010805400	0.040533524
20.0	0.013493700	0.005784940	0.030630632
25.0	0.010357000	0.003473750	0.024616163
50.0	0.004730890	0.000632255	0.012420906
75.0	0.003052460	0.000218210	0.008305908
100	0.002251000	0.000100243	0.006238954

infinite domain. Note that our experiments show that (i) for obtaining accurate results for $y'(0)$ using the present method optimum L is less than 1 and (ii) the number of decimal places of L and the number of correct values of $y'(0)$ are almost the same. The reason that such a value of L provides high accurate initial slope is that it essentially moves collocation points associated with large values of x to the left. Because the exact solution changes slowly when x is large, this leftward movement of the collocation points is beneficial since more collocation points are situated where the solution is changing most rapidly. For this particular reason, very accurate approximations of $y'(0)$ are obtained with moderate number of collocation points. We point out that the scheme

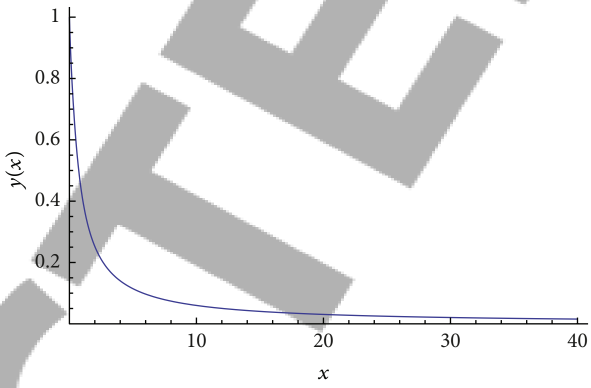

Figure 1: Thomas-Fermi graph obtained by the present method.

of Boyd [26] is based on collocation, and for approximating $y'(0)$ it needs very large number of collocation points and a large value for L, while our scheme is based on the Tau method and the Chebyshev-Gauss quadrature that needs few collocation points and small L.

The approximations of $y'(0)$ computed by the present method and their relative errors are shown in Table 1. Obviously, this method is convergent by increasing the number of points and obtaining suitable L. The comparison of the initial slope $y'(0)$ calculated by the present paper with values obtained by Liao [22], Khan and Xu [23], and Yao [27] is given in Table 2, which shows that the present solution is highly accurate. Table 3 shows the approximations of $y(x)$ obtained by the method proposed in this paper for $N = 8$ and $L = 0.0849432650716649$ and those obtained by Khan and Xu [23] and Liao [28]. Figure 1 shows the resulting graph of the Thomas-Fermi equation for $N = 8$ which tends to zero as x increases by the boundary condition $\lim_{x\to\infty} y(x) = 0$.

4. Conclusion

The fundamental goal of this paper has been to construct an approximation to the solution of the nonlinear Thomas-Fermi equation in a semi-infinite interval which has singularity at $x = 0$ and whose boundary condition occurs in infinity. In the above discussion, the pseudospectral method with RTC functions, which have the property of orthogonality, is employed to achieve this goal. Advantages of this method are that we do not reform the problem to a finite domain and that with a small N very accurate results are obtained. There is a good agreement between the obtained results, and exact values which demonstrates the validity of the present method for this type of problems and gives the method a wider applicability. Comparing the computed results by this method with the others shows that this method provides more accurate and numerically stable solutions than those obtained by other methods.

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