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Implementation of New Iterative Techniques for Solutions of Thomas–Fermi and Emden–Fowler Equations

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Results of computational trials of recently developed iterative techniques for finding positive solutions of boundary-value problems for the Thomas–Fermi and generalized Emden–Fowler equations are presented. Proofs of convergence of iterative techniques have been established in other papers by the authors. The proofs, and therefore the iterative techniques, are based upon solutions of linear Sturm–Liouville problems related to the original nonlinear problems.

1. INTRODUCTION

Iterative techniques for finding positive solutions of boundary-value problems for Thomas–Fermi and generalized Emden–Fowler equations have recently been developed by two of the authors [11–14]. It is the purpose of this article to present results of our computational implementation of the mathematical techniques developed in [11–14].

In Section 2 the iteration scheme for the Thomas–Fermi equation is described and the convergence results proved in [11, 12] are stated. In Section 3 the iteration scheme for the generalized Emden–Fowler equation is described and the convergence results proved in [13, 14] are stated. In Section 4, the implementational technique is described and the computational results which were obtained when the iteration schemes were applied to various examples are presented.

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2. The Thomas–Fermi Equation

In appropriate units the Thomas–Fermi equation, used in atomic calculations, may be written

$$y''(x) = x^{-1/2}(y(x))^{3/2}, \qquad x > 0. \tag{1}$$

There are three sets of boundary values of interest for this equation: the neutral atom with Bohr radius $b > 0$

$$y(0) = 1, \qquad by'(b) = y(b); \tag{1a}$$

the isolated neutral atom

$$y(0) = 1, \qquad \lim_{x \to +\infty} y(x) = 0; \tag{1b}$$

and the ionized atom

$$y(0) = 1, \qquad y(a) = 0, \qquad a > 0. \tag{1c}$$

The importance of the Thomas–Fermi equation in physics may be inferred from the review articles [9, 16]. Because of this importance, solution techniques for the boundary-value problems (1a), (1b), and (1c) and other mathematical aspects of Eq. (1), with or without the boundary conditions, have been and continue to be subjects of research. Briefly, the solution history is as follows: Thomas used Adam's method of numerical integration of the differential equation to obtain approximate solutions to problem (1b), while Fermi used graphical methods. In fact, Fermi obtained the approximation for small x of

$$y(x) \doteq 1 - 1.58x + (4/3)x^{3/2} + \cdots.$$

Baker [2] later improved this result to

$$y(x) = 1 + b_2 x + b_3 x^{3/2} + \cdots$$

with $b_2 = -1.588588\ldots$. At about the same time, Sommerfeld [23] developed an approximate solution to (1b):

$$y(x) = y_1(x)\{1 + [y_1(x)]^{\lambda_1/3}\}^{\lambda_2/3},$$

where λ_1, λ_2 are zeros of the polynomial $\lambda^2 + 7\lambda - 6$, $\lambda_1 > 0 > \lambda_2$, and

$$y_1(x) = 144/x^3.$$

Sommerfeld's approximation is quite accurate for large x but underestimates the solution near the origin [7]. Analogue computers have been used to find numerical solutions [6]. More recently Ramnath [19] has used a technique known as multiple scales to obtain an approximate solution for (1b).

Since all three problems (1a), (1b), and (1c) have the same boundary conditions at zero, much computational use has been made of the series expension

$$y(x) = 1 + b_2 x + b_3 x^{3/2} + \cdots + b_k x^{k/2} + \cdots$$

which is regarded as semiconvergent [8]. The value of b_2, the slope of y at the origin, falls into three classes: $b_2 < -1.588...$, $b_2 = -1.588...$, and $b_2 > -1.588...$ which correspond respectively to solutions of problem (1a), (1b), and (1c). Hille [10] answers questions concerning the convergence of this latter series.

Other mathematical work that has been done includes the early work of Mambriani [15] and Scorza-Dragoni [22] in which the existence and uniqueness of the solution to problem (1b) was established, and the more recent work of Reid [20] and Reid and Depuy [21]. The work of Ramnath [19], Reid [20], and Reid and Depuy [21] also applies to the more general Emden-type equations. Most recently Mooney [17, 18] has shown how to transform the Thomas–Fermi problems to problems amenable to solution by monotone iterations of Picard and Newton type.

In our approach we consider the nonlinear eigenvalue problem

$$u''(x) = \lambda x^{-1/2} u^{3/2}(x), \qquad 0 < x < 1, \tag{2}$$

with either of the boundary conditions

$$-au(0) + u'(0) = 0, \qquad -u(1) + u'(1) = 0, \tag{2a}$$

$$-au(0) + u'(0) = 0, \qquad u(1) = 0 \tag{2b}$$

and where the solution is normalized by $u(0) = 1$. For the case of the neutral atom with Bohr radius b, we have the result [11, Theorem 1]:

THEOREM. *For* $\alpha \geqslant -1$, *let* $u_0(x) = 1 + \alpha x$ *and* $f_0(x) = u_0^{1/2}(x)$. *For each* $k = 1, 2,...,$ *let* (u_k, λ_k) *denote the positive solution of*

$$\begin{aligned} u''(x) - \lambda x^{-1/2} f_{k-1}(x)\, u(x) &= 0, \qquad 0 < x < 1, \\ -au(0) + u'(0) &= 0, \qquad -u(1) + u'(1) = 0, \end{aligned} \tag{3}$$

where $u_k(x)$ *is normalized by* $u_k(0) = 1$ *and* $f_k(x) = u_k^{1/2}(x)$. *Then* $u_0(x) < u_k(x)$, $0 < x < 1$, $k = 1, 2,...,$ *and*

$$\lambda_2 < \lambda_4 < \cdots < \lambda_{2k+2} < \lambda_{2k+1} < \cdots < \lambda_3 < \lambda_1,$$

$$u_2(x) < u_4(x) < \cdots < u_{2k+2}(x) < u_{2k+1}(x) < \cdots < u_3(x) < u_1(x), \qquad 0 < x < 1.$$

Moreover, there is a positive solution (λ, u) of (2a) such that as $k \to \infty$, $\lambda_k \to \lambda$ and $u_k(x) \to u(x)$ uniformly on $[0, 1]$. In addition, by means of the substitution $y(x) = u(\lambda^{-2/3}x)$, $b = \lambda^{2/3}$, y is a solution of (1) and (1a).

For the ionized atom case (1c) we have the result [12, Theorem 1]:

THEOREM. *For $\alpha < -1$, let $u_0(x) = X_I(x)(1 + \alpha x)$, $0 < x < 1$, where $I = [0, -\alpha^{-1}]$ and $X_I(x)$ is the characteristic function of I. Let $\rho_0 = 1 - u_0^{1/2}$. For $n \geqslant 1$ let (u_n, v_n) be the unique positive solution of*

$$\begin{aligned} u''(x) - \lambda^2 x^{-1/2} u(x) + v x^{-1/2} \rho_{n-1}(x)\, u(x) = 0, \\ -\alpha u(0) + u'(0) = 0, \qquad u(1) = 0, \end{aligned} \tag{4}$$

where u_n is normalized by $u_n(0) = 1$, λ is chosen so that $v_n = \lambda^2$, and $\rho_n = 1 - u_n^{1/2}$. (Thus for each $n \geqslant 1$, $u_n'' = v_n x^{-1/2} u_{n-1}^{1/2}(x)\, u_n(x)$, $0 < x < 1$.) Then

$$0 < v_2 < v_4 < \cdots < v_{2k+2} < \cdots < v_{2k+1} < \cdots < v_3 < v_1$$

and

$$u_0(x) < u_2(x) < u_4(x) < \cdots < u_{2k+2}(x) < \cdots < u_{2k+1}(x) < \cdots < u_3(x) < u_1(x).$$

Moreover, there is a positive solution solution (v, u) of (2b) such that as $n \to +\infty$, $v_n \to v$ and $u_n(x) \to u(x)$ uniformly in $[0, 1]$. In addition, by means of the substitution $y(x) = u(v^{-2/3}x)$, $a = v^{2/3}$, $y(x)$ is a solution of (1c).

For the isolated neutral atom case (1b) we have the result [12, Sect. 4]:

As $a \to -\infty$, the eigenvalues v from (3) increase to $+\infty$. Since $a = v^{2/3}$, $a \to +\infty$ and the scheme for solving (1c) furnishes a solution scheme for (1b). In particular, denoting the solution of (1c) as $y_a(x)$, $y_a(x)$ converves uniformly on $[0, +\infty)$ to $y_\infty(x)$, the solution of (1b).

We note that the iterative techniques require solution of a sequence of linear Sturm–Liouville problems, with the weight function changing at each stage of the iteration. This makes our technique slower than Picard- or Newton-type methods. This is also characteristic of our iterative technique for the generalized Emden–Fowler equations which is now presented.

3. Generalized Emden–Fowler Equations

The Emden–Fowler equation is

$$(x^\rho v'(x))' + x^\sigma v^\gamma(x) = 0, \qquad x \geqslant 0, \tag{5}$$

when $\gamma > 0$, and ρ, σ, γ are real numbers. For instance (5) with $\rho = 2$, $\sigma = 2$, and $\gamma = 1.5$ or 2.5 yields the Lane–Emden equation. The theory of (5) was developed by Fowler in a series of papers bridging the years 1914 to 1931. For more historical comments one should consult the review article by Wong [24].

The generalized Emden–Fowler equation is

$$(p(x)\, v'(x))' + q(x)\, v^\gamma(x) = 0,$$

where $p(x)$ is absolutely continuous and positive and $q(x)$ continuous and nonnegative. This equation may, in turn, by reduced by means of a Liouville transformation to

$$y''(x) + a(x)\, y^{v}(x) = 0. \tag{6}$$

The problem we consider is

$$\begin{aligned} u''(x) + \lambda a(x)\, u^{v}(x) &= 0, \qquad x \in (0, 1), \\ \alpha u(0) - \beta u'(0) &= 0, \\ \gamma u(1) + \delta u'(1) &= 0, \end{aligned} \tag{7}$$

where $v \neq 0$ and $v \neq 1$. If u is a solution of (7), then $y(x) = \lambda^{-1/(1-v)} u(x)$ is a solution of

$$\begin{aligned} y''(x) + a(x)\, y^{v}(x) &= 0, \qquad x \in (0, 1), \\ \alpha y(0) - \beta y'(0) &= 0, \\ \gamma y(1) + \delta y'(1) &= 0. \end{aligned} \tag{8}$$

Thus the study of the eigenvalue problem (7) yields information about the boundary-value problem (8).

The Emden–Fowler equation arises in various applications in mechanics, nuclear physics, gasdynamics, stellar structures, and chemically reacting systems. Recently, the eigenvalue problem (7) has arisen in the study of cross-field diffusion in toroidal multipole plasmas [3, 4]. In this instance λ corresponds to a separation constant and $a(x)$ to the geometry of the problem. In [4] Berryman has used an iterative technique of (essentially) Picard type which has worked well for cases of interest. Attempts to apply monotonic methods have not met with success (a unified account of monotone methods is available in Amann [1]).

Our results for (7) differ depending on whether $v > 1$ (called the superlinear case) or $v < 1$ (called the sublinear case). In both cases we require:

(1) $a(x)$ is positive and continuous on $(0, 1)$,

(2) $\gamma\beta + \gamma\alpha + \alpha\delta \neq 0$,

(3) (a) $\alpha, \beta, \gamma, \delta \geqslant 0$, or

(b) $\alpha > 0, \beta > 0, \delta > 0, 0 < \gamma < -\alpha\delta/(\alpha + \beta)$, or

(c) $\beta > 0, \gamma > 0, \delta > 0, 0 < \alpha < -\gamma\beta(\gamma + \delta)$.

For the superlinear case we have the result [13]:

THEOREM. *Let $a(x)$ be in $L^1(0, 1)$ and $u_0(x) = |\alpha x + \beta|$. Define the sequence (λ_k, u_k), $k = 1, 2,...,$ as the positive eigenpair of*

$$\begin{aligned} u''(x) + \lambda a(x)\, u_{k-1}^{p-1}(x)\, u(x) &= 0, \qquad 0 < x < 1, \\ \alpha u(0) - \beta u'(0) &= 0, \\ \gamma u(1) + \delta u'(1) &= 0 \end{aligned} \tag{9}$$

normalized by $\beta u_k(0) + \alpha u_k'(0) = \operatorname{sign} \beta(\alpha^2 + \beta^2)$. ($\operatorname{sign} \beta = 1$ if $\beta \geqslant 0$, -1 if $\beta < 0$.) There is a positive solution (λ, u) of (9) such that as $k \to +\infty$, $\lambda_k \to \lambda$ and $u_k \to u$ uniformly on $[0, 1]$. Moreover, the convergence is monotone:

$$0 < \lambda_1 < \lambda_2 < \cdots < \lambda_k < \cdots \lambda,$$

$$u_0(x) > u_1(x) > \cdots > u_k(x) > \cdots > u(x) > 0, \not\equiv 0, \qquad 0 < x < 1.$$

For the sublinear case we have [14]:

THEOREM. *Let $a(x)$ be such that for some $\varepsilon > 0$*

$$\int_0^{\epsilon} x^{p-1} a(x)\, dx < \infty,$$

$$\int_{\epsilon}^1 (1 - x)^{p-1} a(x)\, dx < \infty,$$

and let $u_0(x) = |\alpha x + \beta|$. Define the sequence (λ_k, u_k), $k = 1, 2,...,$ as the positive eigenpair of

$$\begin{aligned} u''(x) + \lambda a(x)\, u_{k-1}^{p-1}(x)\, u(x) &= 0, \qquad 0 < x < 1, \\ \alpha u(0) - \beta u'(0) &= 0, \\ \gamma u(1) + \delta u'(1) &= 0 \end{aligned}$$

normalized by $\beta u_k(0) + \alpha u_k'(0) = \operatorname{sign} \beta(\alpha^2 + \beta^2)$. ($\operatorname{sign} \beta = 1$ if $\beta \geqslant 0$, -1 if $\beta < 0$.) There is a positive solution (λ, u) of (9) such that as $k \to +\infty$, $\lambda_k \to \lambda$ and $u_k \to u$ uniformly on $[0, 1]$. Moreover the convergence is alternating monotone in that

$$0 < \lambda_2 < \lambda_4 < \cdots < \lambda < \cdots < \lambda_3 < \lambda_1$$

and

$$u_0(x) > u_2(x) > \cdots > u(x) > \cdots > u_3(x) > u_1(x) > 0, \qquad 0 < x < 1.$$

4. Implementation

In each technique, we are required to calculate in each iterative step a solution of a Sturm–Liouville problem where the weight function is determined by the solution in the previous iterative step. This solution is calculated using the SLEIGN Code [3]. At each step the calculated solution is approximated by a polynomial to a sufficient degree of accuracy, so that it may be input, in the weight function at the next step, in SLEIGN.

More specifically, consider the implementation for the superlinear generalized Emden–Fowler problem (other implementations are almost the same). All necessary parameters $\alpha, \beta, \gamma, \delta, \nu$ and parameters for SLEIGN are input and $a(x)$ is entered as a subroutine or as tabulated data on cards. In this latter case $a(x)$ is approximated by Legendre polynomials on $[0, 1]$. Since $\alpha x + \beta$ is of one sign, $u_0(x)$ is calculated as $\alpha x + \beta$ or $-\alpha x - \beta$. SLEIGN then calculates the solution to

$$u''(x) + \lambda a(x)\, u_0^{\nu-1}(x)\, u(x) = 0,$$
$$\alpha u(0) - \beta u'(0) = 0,$$
$$\gamma u(1) + \delta u'(1) = 0.$$

The calculated solution $u_1(x)$ is given by SLEIGN at a specified number of points in $[0, 1]$. We used 100 equally spaced points. After $u_1(x)$ has been calculated, it is normalized by our normalization

$$\beta u_1(0) + \alpha u_1'(0) = \operatorname{sign} \beta(\alpha^2 + \beta^2).$$

(Note: SLEIGN returns $u_1'(0)$.) Then $u_1(x)$ is approximated by Legendre polynomials and SLEIGN is used to calculate the solution to

$$u'' + \lambda a(x)\, u_1^{\nu-1}(x)\, u(x) = 0,$$
$$\alpha u(0) = \beta u'(0) = 0,$$
$$\gamma u(1) + \delta u'(1) = 0;$$

calling this solution $u_2(x)$, we proceed as before with $u_1(x)$; we obtain $u_3(x)$, $u_4(x)$,..., similarly.

When the convergence is alternating montone, the error in approximation to the true solution may be found a posteriori by subtracting the two most recent solutions. This is illustrated in the examples. For the strictly monotone convergence our stopping criterion was based upon maximum difference of successive iterates. In the examples below all calculations were made in double precision arithmetic on the Amdahl 470/V6 at Texas A&M University.

Example 1. Thomas–Fermi (neutral atom). Note that α is simply the initial slope of $u_k(x)$ for $k = 1, 2,\ldots$. We compare our results with those of Baker [1] for the

calculation of the minimal ordinate. With an initial slope of $\alpha = -0.62221$ Baker calculates the minimal ordinate as 0.97950 occurring at $x \approx 1.0$. We found a minimal value of 0.980076 at $x = 1.0$. Similarly, for $\alpha = -0.65170$ we agree with Baker that the minimal ordinate occurs at 1.1. Our value for the minimal ordinate is 0.977474 and Baker's is 0.97636.

To illustrate the alternating monotonicity we list λ_k, $y_k(0.495)$, and $y_k(1)$ for the solution of (2) when $\alpha = 0$.

Iteration (k)	λ_k	$y_k(0.495)$	$y_k(1)$
1	0.9024	1.4379	2.3878
1	0.7325	1.3617	2.1977
3	0.7518	1.3699	2.2168
4	0.7497	1.3690	2.2149
5	0.74993	1.36912	2.2152
6	0.74991	1.36911	2.2151

EXAMPLE 2. Thomas–Fermi (ionized atom). We list the solution values for $\alpha = -2$. The alternating monotonicity in the iterations is the same as in Example 2, so we omit illustration of that.

$\lambda = 1.11274$

x	$y(x)$
0	1
0.1	0.845949
0.2	0.720035
0.3	0.610595
0.4	0.512327
0.5	0.421051
0.6	0.333707
0.7	0.248356
0.8	0.164177
0.9	0.018473
1.0	0

The maximum error as determined a posteriori is 1×10^{-6}. This was achieved with eight iterations.

EXAMPLE 3. Generalized Emden–Fowler (superlinear case).

$$y''(x) + \lambda y^3(x) = 0,$$

$$y(0) = y(1) = 0.$$

The actual solution of this problem involves an elliptic sine function, whose values can be calculated using tables. The initial function is $u_0(x) = x$. Our normalized results for 18 iterations (11.27 secs) are tabulated below. The solution is symmetric about $x = 1/2$.

x	Computed Solution	Actual Solution
0	0	0
0.1	0.09636	0.09961
0.2	0.19981	0.19790
0.3	0.29201	0.28879
0.4	0.35465	0.35498
0.5	0.37675	0.38025

$$\lambda = 95.107$$

To illustrate the monotonicity we trace some calculated values of λ_k and $y_k(0.3)$

Iteration	λ_k	$y_k(0.3)$
1	76.962	0.2999551
5	92.871	0.2926361
10	95.029	0.2920336
15	95.105	0.2920146
17	95.107	0.2920139
18	95.107	0.2920138

EXAMPLE 4. Generalized Emden–Fowler (sublinear case).

$$y'' + \lambda[x(1-x)]^4 y^{-2} = 0,$$
$$y(0) - 2y'(0) = 0,$$
$$y(1) - 4y'(1) = 0.$$

The calculated solution, obtained in six iterations (10.7 secs) was, with our normalization:

$$\lambda = 1096.6781 \text{ with } |\text{error}| < 0.0012$$

x	$y(x)$
0	2.
0.1	2.099710
0.2	2.199992
0.3	2.298103
0.4	2.391715
0.5	2.479489
0.6	2.561077
0.7	2.637117
0.8	2.709237
0.9	2.780052
1.0	2.853167

The maximum error in the values for y is 2×10^{-7}. To illustrate the alternating character of the iteration we trace the calculated values of λ_k and $y_k(0.3)$.

Iteration	λ_k	$y_k(0.3)$
1	1129.6870	2.29801532
2	1096.0188	2.29814055
3	1096.8602	2.29810146
4	1096.6715	2.29810326
5	1096.6792	2.29810302
6	1096.6781	2.29810303

REFERENCES

1. H. AMANN, *SIAM Rev.* **18** (1976), 620.
2. E. B. BAKER, *Phys. Rev.* **36** (1930), 630.
3. P. B. BAILEY, M. K. GORDON, AND L. F. SHAMPINE, Sandia Laboratories Report SAND 76-0560, 1976.
4. J. G. BERRYMAN, *J. Mathematical Phys.* **18** (1977), 2108.
5. J. G. BERRYMAN AND C. J. HOLLAND, *J. Mathematical Phys.* **19** (1978), 2476.
6. V. BUSH AND S. H. CALDWELL, *Phys. Rev.* **38** (1931), 1898–1901.
7. H. T. DAVIS, "Introduction to Nonlinear Differential and Integral Equations," Dover, New York, 1962.
8. R. P. FEYMAN, N. METROPOLIS, AND E. TELLER, *Phys. Rev.* **75** (1949), 1561–1573.
9. P. GOMBÁS, "Die statistische Theorie des Atoms," Springer, Berlin, 1948.
10. E. HILLE, *J. Analyse Math.* **23** (1970), 147–170.
11. C. D. LUNING, *SIAM J. Math. Anal.* **9** (1978), 515.
12. C. D. LUNING AND W. L. PERRY, *Quart. Appl. Math.* **35** (1977), 257.
13. C. D. LUNING AND W. L. PERRY, *J. Differential Equations*, in press.
14. C. D. LUNING AND W. L. PERRY, preprint.
15. A. MAMBRIANI, *Rend. Accad. Naz. Lincei* **9** (1929), 620–622.
16. N. H. MARCH, *Advances in Phys.* **6** (1957), 1.
17. J. W. MOONEY, *Quart. Appl. Math.* **36** (1978), 305.
18. J. W. MONEY, *J. Nonlinear Anal.* **3** (1979), 449–465.
19. R. V. RAMNATH, *J. Math. Anal. Appl.* **31** (1970), 285–296.
20. J. L. REID, *Rend. Accad. Naz. Lincei* **53** (1972), 376–379.
21. J. L. REID AND R. J. DEPUY, *Atti. Accad. Naz. Lincei* **54** (1973), 529.
22. G. SCORZA-DRAGONI, *Rend. Accad. Naz. Lincei* **9** (1929), 623–625.
23. A. SOMMERFELD, *Z. Physik* **78** (1932), 283–308.
24. J. S. W. WONG, *SIAM Rev.* **17** (1975), 339.