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On an iteration method for eigenvalue problems

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Abstract
We discuss a recently proposed asymptotic iteration method for eigenvalue problems. We analyse its rate of convergence, the use of adjustable parameters to improve it and the relationship with an alternative method based on the same ideas.

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1. Introduction

In a recent paper Ciftci *et al* [1] developed an interesting asymptotic iteration method (AIM) for eigenvalue problems. They showed that the AIM yielded the correct answer for exactly solvable models and gave reasonably approximate results for some nontrivial one-dimensional problems such as anharmonic oscillators and singular potentials. Unfortunately, the authors did not show the rate of convergence of their calculations and simply mentioned the number of iterations necessary to obtain their results. Also, they did not compare the performance of the AIM with other existing methods.

The purpose of this paper is to fill that gap and to investigate the AIM somewhat further. First, we derive some of the AIM equations in a different way, second, we review one of the exactly solvable models considered by Ciftci *et al* [1], third, we carry out calculations of order considerably greater than those of Ciftci *et al* [1] in order to test the rate of convergence of the method numerically, fourth, we explore the use of adjustable parameters to improve the rate of convergence, fifth, we compare the AIM with a closely related method, and, finally, we try to draw some conclusions about the performance of the AIM.

2. The asymptotic iteration method

Ciftci *et al* [1] proposed the AIM to solve second-order differential equations of the form

$$y''(x) = \lambda_0(x)y'(x) + s_0(x)y(x). \tag{1}$$

They found that the general solution to this equation is

$$y(x) = \exp\left[-\int^x \alpha(x')\,\mathrm{d}x'\right]\left\{C_2 + C_1\int^x \exp\left[\int^{x'}\{\lambda_0(x'') + 2\alpha(x'')\}\,\mathrm{d}x''\right]\mathrm{d}x'\right\} \tag{2}$$

where C_1 and C_2 are arbitrary integration constants, and showed that one can obtain $\alpha(x)$ as the limit of a sequence of quotients $s_n(x)/\lambda_n(x)$ where the numerator $s_n(x)$ and denominator $\lambda_n(x)$ are given by

$$\begin{aligned} s_n &= s'_{n-1} + s_0\lambda_{n-1} \\ \lambda_n &= \lambda'_{n-1} + \lambda_0\lambda_{n-1} + s_{n-1} \qquad n = 1, 2, \ldots. \end{aligned} \tag{3}$$

In some trivial cases one may obtain the exact result after a finite number of iterations, for example

$$\frac{s_n}{\lambda_n} = \frac{s_{n-1}}{\lambda_{n-1}} = \alpha. \tag{4}$$

Note that we can also start the recurrence relations (3) from $n = 0$ with the initial conditions $\lambda_{-1} = 1$ and $s_{-1} = 0$.

Ciftci *et al* [1] showed that equation (4) is exact for some exactly solvable problems, and approximate for all nontrivial cases, where it is supposed to give a reasonable approximation for sufficiently great values of n. In the case of eigenvalue problems Ciftci *et al* [1] conjectured that one may obtain approximate eigenvalues from the roots of

$$\lambda_{n+1}s_n - s_{n+1}\lambda_n = 0. \tag{5}$$

This equation depends only on the eigenvalue if the problem is exactly solvable. In nontrivial cases, on the other hand, equation (5) depends also on x so that one has to choose an appropriate value of the latter in order to obtain the former [1]. The chosen value of x is arbitrary in principle, and affects the rate of convergence of the method.

Before discussing the performance of the AIM we first develop some of its equations in a different way in order to gain further insight, and also to have an idea of other methods that may be worth comparing with it. Note that we can factor the differential equation (1) as

$$\left[\frac{\mathrm{d}}{\mathrm{d}x} + a(x)\right]\left[\frac{\mathrm{d}}{\mathrm{d}x} + b(x)\right]y(x) = 0 \tag{6}$$

where $a = -\lambda_0 - b$ and b is a solution of the Riccati equation

$$b' - b^2 - \lambda_0 b + s_0 = 0. \tag{7}$$

By straightforward integration of equation (6) we obtain

$$y(x) = \exp\left[-\int^x b(x')\,\mathrm{d}x'\right]\left\{C_2 + C_1\int^x \exp\left[\int^{x'}\{\lambda_0(x'') + 2b(x'')\}\,\mathrm{d}x''\right]\mathrm{d}x'\right\} \tag{8}$$

which is identical to equation (2) if $b(x) = \alpha(x)$. We have arrived at the well-known result that the general solution to the second-order differential equation (1) can be expressed in terms of a solution of the Riccati equation (7). Note that the logarithmic derivative $-y'(x)/y(x)$ satisfies the Riccati equation (7).

If we try a rational solution to the Riccati equation (7)

$$b(x) = \frac{A(x)}{B(x)} \tag{9}$$

the functions $A(x)$ and $B(x)$ satisfy

$$\frac{A}{B} = \frac{(A' + s_0 B)}{(B' + A + \lambda_0 B)}. \tag{10}$$

Note that if the sequences s_n and λ_n converged towards some functions s and λ, respectively, then the latter would satisfy an equation identical to equation (10) with $A = s$ and $B = \lambda$. However, we should point out that the AIM does not require convergence of the sequences s_n and λ_n but of their ratio.

3. An exactly solvable problem

Before discussing nontrivial applications of the AIM we first consider an exactly solvable example that is slightly more general than the one treated by Ciftci *et al* [1]. If both λ_0 and s_0 are independent of x then b is independent of x and satisfies the quadratic equation $b^2 + \lambda_0 b - s_0 = 0$ with roots

$$r_1 = -\frac{\lambda_0 + \Delta}{2} \qquad r_2 = -\frac{\lambda_0 - \Delta}{2} \qquad \Delta = \sqrt{\lambda_0^2 + 4s_0}. \tag{11}$$

On the other hand, the sequences (3) become $s_n = s_0\lambda_{n-1}$, and $\lambda_n = \lambda_0\lambda_{n-1} + s_{n-1}$, so that

$$\frac{s_n}{\lambda_n}\frac{s_{n-1}}{\lambda_{n-1}} + \lambda_0\frac{s_n}{\lambda_n} - s_0 = 0. \tag{12}$$

If we assume that

$$\lim_{n\to\infty}\frac{s_n}{\lambda_n} = \alpha \tag{13}$$

then we conclude that α and b are solutions of the same quadratic equation as expected.

If we substitute one of the recurrence relations into the other we obtain $\lambda_n - \lambda_0\lambda_{n-1} - s_0\lambda_{n-2} = 0$. The general solution to this difference equation is $\lambda_n = c_1\rho_1^n + c_2\rho_2^n$, where $\rho_1 = -r_1$ and $\rho_2 = -r_2$. Taking into account the initial conditions we obtain

$$\lambda_n = \frac{1}{\Delta}\left(\rho_1^{n+2} - \rho_2^{n+2}\right) \qquad s_n = \frac{s_0}{\Delta}\left(\rho_1^{n+1} - \rho_2^{n+1}\right). \tag{14}$$

If $|\rho_1| > |\rho_2|$ we find that

$$\lim_{n\to\infty}\frac{s_n}{\lambda_n} = \frac{s_0}{\rho_1} = -\rho_2 = r_2 \tag{15}$$

which is one of the roots of the quadratic equation for b or α.

This simple example reveals two important features of the AIM. First, the ratio s_n/λ_n converges although the numerator and denominator may not. Second, the limit of the ratio s_n/λ_n is just one of the solutions; in this particular case the root with smaller absolute value.

4. The Schrödinger equation

The Schrödinger equation for one-dimensional and central-field models can be written as

$$\psi''(x) = [V(x) - E]\psi(x) \tag{16}$$

where $\psi(x \to \pm\infty) = 0$ in the former and $\psi(0) = \psi(x \to \infty) = 0$ in the latter. Straightforward application of the AIM to this eigenvalue equation does not give reasonable results. For that reason we transform the solution according to $\psi(x) = g(x)y(x)$ that leads to a more convenient differential equation for $y(x)$

$$y'' = -\frac{2g'}{g}y' + \left(V - E - \frac{g''}{g}\right)y. \tag{17}$$

Ciftci *et al* [1] showed that the AIM gave the correct answer for several exactly solvable models; one of them being the harmonic oscillator. Here we concentrate only on nontrivial

Table 1. Ground state of the anharmonic oscillators by means of the AIM and nearly optimum values of β.

n	$k = 2,\ \beta = 5$	$k = 3,\ \beta = 9$	$k = 4,\ \beta = 12$
10	1.325 073 435	1.802 796 295	
15	1.147 766 154	1.421 665 204	1.809 765 257
20	1.072 223 000	1.193 157 512	1.388 298 227
25	1.062 711 298	1.151 776 895	1.265 435 601
30	1.060 482 716	1.143 861 469	1.217 197 329
35	1.060 372 025	1.144 668 302	1.221 967 230
40	1.060 362 059	1.144 837 075	1.226 994 501
45	1.060 362 077	1.144 798 326	1.226 106 604
50	1.060 362 091	1.144 802 367	1.225 633 738
55	1.060 362 091	1.144 802 992	1.225 851 219
60	1.060 362 090	1.144 802 347	1.225 830 628
65	1.060 362 090	1.144 802 468	1.225 801 249
70	1.060 362 090	1.144 802 452	1.225 826 262
75	"	1.144 802 452	1.225 821 973
80	"	1.144 802 454	1.225 818 670
85	"	1.144 802 454	1.225 821 060
90	"	1.144 802 454	1.225 819 794

problems. One of such problems successfully treated by Ciftci *et al* [1] is the anharmonic oscillator $V(x) = x^2 + 0.1x^4$. However, in order to determine the performance of the AIM we prefer the much more demanding family of anharmonic oscillators

$$V(x) = x^{2k} \qquad k = 2, 3, \ldots . \tag{18}$$

On setting $g(x) = \exp(-\beta x^2/2)$ we obtain

$$y'' = 2\beta x y' + (x^{2k} - \beta^2 x^2 + \beta - E)y. \tag{19}$$

For obvious symmetry reasons we follow Ciftci *et al* [1] and arbitrarily set $x = 0$ in order to obtain the energy from equation (5). We expect the rate of convergence to decrease as k increases because the oscillator becomes 'more anharmonic'.

Numerical investigation shows that the AIM converges for the ground states of the oscillators with $k = 2, 3, 4$, and that the rate of convergence depends on the value of β. The optimum value of β appears in all cases to be far from that given by the variational method with the trial function $\varphi = \exp(-\beta x^2/2)$ (namely $\beta = [4k^2\Gamma(k + 1/2)^2/\pi]^{1/(2k+2)}$). We did not attempt to determine the optimum value of β exactly; we simply tried a set of values $\beta = 1, 2, \ldots$ and kept the one that appeared to yield the best convergence rate (to 10 exact digits in this case). For example, in the case of the $k = 2$ oscillator and $n \leqslant 90$ we did not obtain convergence for $\beta = 1$ or $\beta > 8$. For $\beta = 2, 3, 4, 5, 6, 7$ and 8 convergence seems to take place at $n = 72, 60, 46, 44, 48, 60$ and 78, respectively. Therefore, in this case we chose $\beta = 5$. Proceeding in the same way with other anharmonic oscillators we thus obtained the results in table 1 which show the rate of convergence for the chosen values of β. It seems clear that the AIM converges for the first three values of k considered, and that the rate of convergence decreases with k as expected.

An interesting feature of the AIM is that the optimum value of β seems to be almost the same for all states. For example, table 2 shows the energies of some excited states of the $k = 2$ oscillator and reveals that convergence decreases as the quantum number v increases.

Table 2. Excited-state energies with quantum number v for the $k = 2$ oscillator by means of the AIM and $\beta = 5$.

n	$v = 2$	$v = 4$	$v = 6$	$v = 8$	$v = 10$
10	–	–	–	–	–
15	–	–	26.671 517 05	37.930 200 16	–
20	7.497 990 251	16.781 882 47	–	38.399 282 84	–
25	7.457 160 839	16.311 203 72	–	–	–
30	7.455 587 976	16.258 694 66	26.493 612 10	37.810 294 71	50.619 031 36
35	7.455 705 021	16.261 874 34	26.525 570 04	37.859 901 83	–
40	7.455 697 770	16.261 828 37	26.528 738 41	37.928 838 58	50.309 144 16
45	7.455 697 902	16.261 823 77	26.528 411 15	37.922 343 40	50.257 077 53
50	7.455 697 939	16.261 826 13	26.528 474 83	37.923 054 22	50.256 273 80
55	7.455 697 938	16.261 826 00	26.528 470 89	37.923 002 93	50.256 436 32
60	7.455 697 938	16.261 826 02	26.528 471 21	37.923 001 22	50.256 244 29
65	"	16.261 826 02	26.528 471 18	37.923 001 12	50.256 258 20
70	"	"	26.528 471 18	37.923 001 03	50.256 254 30
75	"	"	"	37.923 001 03	50.256 254 58
80	"	"	"	"	50.256 254 51
85	"	"	"	"	50.256 254 52
90	"	"	"	"	50.256 254 52

We carried out the present calculations by means of the computer algebra system Maple [2] that allows analytical calculation of the functions s_n and λ_n and unlimited precision when solving equation (5) numerically.

Ciftci *et al* [1] also considered singular potentials of the form

$$V(x) = x^2 + \frac{L(L+1)}{x^2} + \frac{\xi}{x^v} \tag{20}$$

where $\xi, v > 0$ and $L \geqslant -1$ may in some particular cases be related to the number of spatial dimensions and the angular momentum quantum number [1]. If we choose $g = x^{\gamma+1}\exp(-x^2/2)$ we obtain

$$y'' = 2\left(x - \frac{\gamma+1}{x}\right)y' + \left[\frac{\xi}{x^v} + \frac{L(L+1) - \gamma(\gamma+1)}{x^2} + 2\gamma + 3 - E\right]y. \tag{21}$$

The value of γ is arbitrary, and we may choose the most convenient one. For example, $\gamma = -1$ gives us the equation considered by Ciftci *et al* [1], and $\gamma = L$ also appears to be a reasonable candidate. In addition to that, we may vary γ in order to improve convergence. For simplicity, we follow Ciftci *et al* [1] and choose the minimum of $x^2 + \xi/x^v$ in the equation for the energy (5).

In particular we consider one of the examples chosen by Ciftci *et al* [1], namely, the ground state of the model with $L = 0$ and $v = 1.9$. Table 3 shows a root of equation (5) for $\xi = 10$, $\gamma = -1$ and $5 \leqslant n \leqslant 50$ (in this case $x_0 = 1.78$). The sequence appears to converge when $n < \approx 30$ but then starts to oscillate as n increases. We increased the precision of the calculation in order to make round-off errors as small as possible, and we believe that this is not the cause of the apparent divergence. In this case we may obtain a reasonably accurate eigenvalue by truncation of the sequence at an appropriate stage as one commonly does in the case of asymptotic divergent series. Other values of γ made the calculation more time consuming and did not appear to improve convergence considerably.

The most interesting singular potentials are those with small values of ξ because they are almost negligible everywhere except at the origin where they rise sharply. Unfortunately,

Table 3. Ground state of the singular potential with $\xi = 10$ and $\nu = 1.9$.

n	E_0
5	8.572 3354
10	8.564 4218
15	8.564 3628
20	8.564 3569
25	8.564 3573
30	8.564 3478
35	8.564 4691
40	8.561 8325
45	8.658 2906
50	7.324 7696

Table 4. Ground-state energies of the anharmonic oscillators by means of the Riccati–Padé method and Hankel determinants of dimension D.

D	$k = 2$	$k = 3$	$k = 4$
2	1.050 229 315	–	–
3	1.060 234 468	1.136 053 454	–
4	1.060 360 577	1.145 233 319	1.219 052 324
5	1.060 362 073	1.144 790 196	1.226 659 815
6	1.060 362 090	1.144 802 855	1.225 667 864
7	1.060 362 090	1.144 802 441	1.225 821 874
8	"	1.144 802 454	1.225 821 878
9	"	1.144 802 454	1.225 820 097
10	"	"	1.225 820 119
11	"	"	1.225 820 113
12	"	"	1.225 820 114
13	"	"	1.225 820 114

it seems that the present version of the AIM does not apply to such 'stiff' cases, even for moderately small values of ξ such as $\xi = 1$. We could not obtain reasonable results no matter which values of γ we tried.

5. Comparison with a closely related method

As argued in section 2 the AIM appears to be based on a rational approximation to the logarithmic derivative of the solution to the differential equation. Another approach based on the same idea is the Riccati–Padé method (RPM) [3, 4] where one approximates a Taylor expansion of a sort of regularized logarithmic derivative of the solution by means of a Padé approximant. When the approximant is forced to give one more coefficient of the Taylor expansion one obtains an expression for the energy as a root of a Hankel determinant. As the dimension of the determinant increases the roots approach the actual eigenvalues of the problem. This method has been extensively discussed elsewhere [3, 4] and will not be developed here.

Tables 4 and 5 show the rate of convergence of the RPM for the ground and excited states of the anharmonic oscillators discussed above. We clearly appreciate that the RPM converges

Table 5. Excited-state energies with quantum number v for the $k = 2$ oscillator by means of the Riccati–Padé method and Hankel determinants of dimension D.

D	$v = 2$	$v = 4$	$v = 6$	$v = 8$	$v = 10$
3	7.361 589 045	–	–	–	–
4	7.454 596 870	15.473 545 91	–	–	–
5	7.455 685 333	16.253 827 02	–	–	–
6	7.455 697 797	16.261 736 50	26.474 373 08	–	–
7	7.455 697 936	16.261 825 03	26.527 879 28	37.555 839 15	–
8	7.455 697 938	16.261 826 01	26.528 464 72	37.919 234 53	–
9	7.455 697 938	16.261 826 02	26.528 471 11	37.922 960 24	50.232 807 89
10	"	16.261 826 02	26.528 471 18	37.923 000 59	50.256 003 14
11	"	"	26.528 471 18	37.923 001 02	50.256 251 82
12	"	"	"	37.923 001 03	50.256 254 49
13	"	"	"	37.923 001 03	50.256 254 52
14	"	"	"	"	50.256 254 52

much faster and more smoothly than the AIM. Moreover, in some cases the RPM even yields tight upper and lower bounds to the eigenvalues [3, 4].

6. Conclusions

Throughout this paper we investigated the convergence rate of the AIM by means of numerical calculations. According to our results the AIM appears to converge for the eigenvalues of anharmonic oscillators and the appropriate choice of adjustable parameters improves the convergence properties remarkably. On the other hand, the AIM does not seem to apply to singular potentials in spite of attempts to tune adjustable parameters. In particular, the AIM fails badly in the most interesting cases of singular potentials that rise sharply at origin. It is true that Ciftci *et al* [1] gave results for a singular potential with $\nu = 4$ and ξ as small as 0.001. However, in those examples they chose $L \geqslant 3$ and the 'centrifugal' term $L(L+1)/x^2$, which does not rise so sharply at origin, appears to mask the behaviour of the singular term. For such large values of L other standard approaches yield more accurate results than the AIM. We mention, for example, the $1/N$ expansions [5–7] and other polynomial approximations [7, 8]. In spite of this failure we believe that the AIM is an interesting approach that is worth further scrutinity with the purpose of improvement. In particular it may not be unlikely that a more judicious choice of the function $g(x)$ and of adjustable parameters (including the coordinate point at which one solves equation (5) could improve the convergence properties of the method in these difficult cases.

We have shown that the AIM converges much more slowly than the RPM which is based on a similar idea [3, 4]. In addition to it, the RPM yields upper and lower bounds to the eigenvalues of certain models [3, 4], and even the energies of metastable states [9]. However, the AIM is in certain sense more general because it does not require a Taylor expansion of the logarithmic derivative of the wavefunction. Note, for example, that it is not possible to apply the RPM to the singular potentials discussed above. It is because of this somewhat greater generality that we believe that the AIM is worth further investigation.

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