Rational Approximation to the Solutions of Two-Point Boundary Value Problems

P. Amore, F. M. Fernández

Abstract

We propose a method for the treatment of two-point boundary value problems given by nonlinear ordinary differential equations. The approach leads to sequences of roots of Hankel determinants that converge rapidly towards the unknown parameter of the problem. We treat several problems of physical interest: the field equation determining the vortex profile in a Ginzburg-Landau effective theory, the fixed-point equation for Wilson's exact renormalization group, a suitably modified Wegner-Houghton fixed point equation in the local potential approximation, and a Riccati equation. We consider two models where the approach does not apply in order to show the limitations of our Padé-Hankel approach.

Keywords: nonlinear differential equations, Ginzburg-Landau, Wilson's renormalization, Wegner-Houghton, Riccati equation, Padé-Hankel method.

1 Introduction

Some time ago Fernández et al [1–3,5,6,4,7–9] developed a method for the accurate calculation of eigenfunctions and eigenvalues for bound states and resonances of the Schrödinger equation. This approach is based on the Taylor expansion of a regularized logarithmic derivative of the eigenfunction. The physical eigenvalue is given by a sequence of roots of Hankel determinants constructed from the coefficients of that series. One merit of this approach, called the Riccati-Padé method, is the great convergence rate in most cases and that the same equation applies to bound states and resonances. Besides, in some cases it yields upper and lower bounds to the eigenvalues [1].

The logarithmic derivative satisfies a Riccati equation, and one may wonder if the method applies to other nonlinear ordinary differential equations. The purpose of this paper is to investigate whether a kind of Padé-Hankel method may be useful for two-point boundary value problems given by nonlinear ordinary differential equations.

In Section 2 we outline the method, in Section 3 we apply it to several problems of physical interest, and in Section 4 we discuss the relative merits of the approach.

2 Method

It is our purpose to propose a method for the treatment of two-point boundary value problems. We suppose that the solution $f(x)$ of a nonlinear ordinary differential equation can be expanded as

$$f(x) = x^{\alpha} \sum_{j=0}^{\infty} f_j x^{\beta j} \tag{1}$$

about $x = 0$, where α and β are real numbers, and $\beta > 0$. We also assume that we can calculate sufficient coefficients f_j in terms of one of them that should be determined by the boundary condition at the other point; for example, at infinity. We show several illustrative examples in section 3.

We try a rational approximation to $x^{-\alpha} f(x)$ of the form

$$[M,N](z) = \frac{\sum_{j=0}^{M} a_j z^j}{\sum_{j=0}^{N} b_j z^j}. \tag{2}$$

where $z = x^{\beta}$. The Taylor expansion of the usual Padé approximant yields $M + N + 1$ coefficients of the series (1) [11]; but in the present case we require that the rational approximation (2) gives us one more coefficient, that is to say, $M + N + 2$. If $M = N + d$, $N = 1, 2, \ldots$, $d = 0, 1, \ldots$, this requirement leads to the equation [1–3,5,6,4,7–9]

$$H_D^d = |f_{i+j+d+1}|_{i,j=0,1,\ldots N} = 0, \tag{3}$$

where $D = N + 1 = 2, 3, \ldots$ is the dimension of the Hankel determinant H_D^d.

In general, equation (3) exhibits many roots and one expects to find a sequence, for $D = 2, 3, \ldots$ and fixed d, that converges towards the required value of the unknown coefficient. From now on we call it the Hankel sequence for short. If such a convergent sequence is monotonously increasing or decreasing we assume that it yields a lower or upper bound, respectively. Such bounds have been proved rigorously for some eigenvalue problems [1].

3 Examples

In order to test the performance of the Padé-Hankel method, in this section we consider the examples treated by Boisseau et al [10] by means of a most interesting algebraic approach. We first consider the field equation determining the vortex profile in a Ginzburg-Landau effective theory (and references therein)

$$f''(r) + \frac{1}{r}f'(r) + \left(1 - \frac{n^2}{r^2}\right) f(r) - f(r)^3 = 0, \quad r > 0. \tag{4}$$

The solution $f(r)$ satisfies the expansion (1) with $x = r$, $\alpha = n = 1, 2, \ldots$, and $\beta = 2$. If we substitute this series into the differential equation and solve for the coefficients f_j, we obtain them in terms of the only unknown f_0 that is determined by the boundary condition at infinity: $f(r \to \infty) = 1$ [10] (and references therein). The coefficients f_j, and therefore the Hankel determinant H_D^d, are polynomial functions of f_0. For example, for $n = 1$ we have

$$f_1 = -\frac{f_0}{8}, \; f_2 = \frac{f_0}{192} + \frac{f_0^3}{24}, \quad f_3 = -\frac{f_0}{9216} - \frac{5f_0^3}{576}, \ldots \tag{5}$$

Tables 1 and 2 show two Hankel sequences with $d = 0$ and $d = 1$ that converge rapidly towards the result of the accurate shooting method [10] for $n = 1$ and $n = 2$, respectively. We appreciate that in the case $n = 1$ the sequences with $d = 0$ and $d = 1$ give upper and lower bounds, respectively, that tightly bracket the exact value of the unknown parameter of the theory: $0.583\,189\,495\,860\,60 < f_0 < 0.583\,189\,495\,860\,61$.

On the other hand, the appropriate Hankel sequences are oscillatory when $n \geq 2$ and their rate of convergence decreases with n. Table 3 shows the best estimates of f_0 for $n = 2, 3, 4$.

Table 1: Convergence of the Hankel series for the connection parameters of the global vortex for $n = 1$

D	$d = 0$	$d = 1$
2	0.595	0.578
3	0.584	0.582 9
4	0.583 24	0.583 15
5	0.583 20	0.583 183
6	0.583 192	0.583 187
7	0.583 190	0.583 189 0
8	0.583 189 7	0.583 189 3
9	0.583 189 54	0.583 189 46
10	0.583 189 52	0.583 189 48
11	0.583 189 51	0.583 189 491
12	0.583 189 498	0.583 189 494
13	0.583 189 496 4	0.583 189 495 3
14	0.583 189 496 1	0.583 189 495 6
15	0.583 189 496 0	0.583 189 495 7
16	0.583 189 495 90	0.583 189 495 83
17	0.583 189 495 88	0.583 189 495 84
18	0.583 189 495 867	0.583 189 495 854
19	0.583 189 495 864	0.583 189 495 857
20	0.583 189 495 862	0.583 189 495 859 1
21	0.583 189 495 860 9	0.583 189 495 859 8
22	0.583 189 495 860 7	0.583 189 495 860 1

Table 2: Convergence of the Hankel series for the connection parameters of the global vortex for $n = 2$

D	$d = 0$	$d = 1$
3	0.156	0.151
4	0.152 8	0.154
5	0.153 10	0.153 0
6	0.153 09	0.153 11
7	0.153 098	0.153 10
8	0.153 099 7	0.153 10
9	0.153 099 1	0.153 099
10	0.153 099 14	0.153 098 9
11	0.153 099 12	0.153 099 095
12	0.153 099 17	0.153 099 091
13	0.153 099 105	0.153 099 097
14	0.153 099 102 1	0.153 099 11
15	0.153 099 102 72	0.153 099 102
16	0.153 099 102 697	0.153 099 103
17	0.153 099 102 782	0.153 099 102 92
18	0.153 099 103 124	0.153 099 102 93
19	0.153 099 102 857	0.153 099 102 89
20	0.153 099 102 864	0.153 099 102 78
21	0.153 099 102 861 36	0.153 099 102 860
22	0.153 099 102 861 42	0.153 099 102 858

Table 3: Best estimates of the connection parameters of the global vortex for $n = 2, 3, 4$ by means of Hankel sequences with $D \leq D_{max}$

n	D_{max}	f_0
2	21	0.153 099 102 86
3	21	0.026 183 420 7
4	26	0.003 327 173 4

Our second example is the fixed-point equation for Wilson's exact renormalization group [10] (and references therein)

$$2f''(x) - 4f(x)f'(x) - 5xf'(x) + f(x) = 0, \quad x > 0. \tag{6}$$

The solution to this equation can be expanded as in equation (1) with $\alpha = 1$ and $\beta = 2$. The first coefficients are

$$f_1 = \frac{f_0}{3} + \frac{f_0^2}{3},\ f_2 = \frac{7f_0}{60} + \frac{f_0^2}{4} + \frac{2f_0^3}{15}, \ldots \tag{7}$$

For large values of x the physical solution should behave as $f(x) = ax^{1/5} + a^2/(5x^{3/5}) + \ldots$ The Hankel sequences with $d = 0$ and $d = 1$ converge towards the numerical result [10] (and references therein) from above and below, respectively. Figure 1 displays the great rate of convergence of these sequences as $\Delta = |f_0(D, d = 0) - f_0(D, d = 1)|$, $D = 2, 3, \ldots$, from which we obtain the accurate bounds $-1.228\,598\,202\,437\,021\,924\,38 < f_0 < -1.228\,598\,202\,437\,021\,924\,37$.

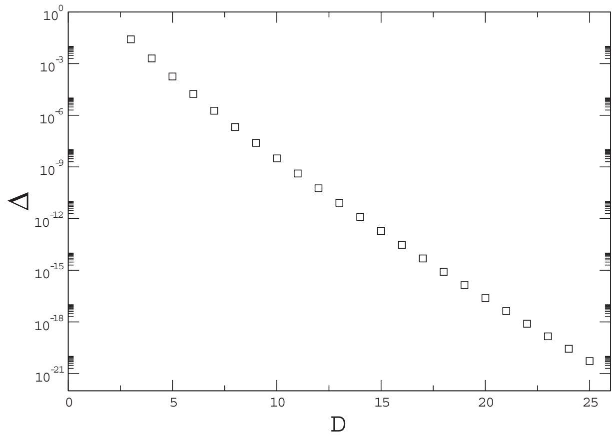

Fig. 1: $\Delta = |f_0(D, d = 0) - f_0(D, d = 1)|$ for Wilson's renormalization

The third example comes from a suitably modified Wegner-Houghton's fixed point equation in the local potential approximation [10] (and references therein)

$$2f''(x) + [1 + f'(x)][5f(x) - xf'(x)] = 0, \quad x > 0. \tag{8}$$

The solution satisfies the series (1) with $\alpha = 1$ and $\beta = 2$, and the first coefficients are

$$f_1 = -\frac{f_0}{3} - \frac{f_0^2}{3},\ f_2 = \frac{f_0}{60} + \frac{2f_0^2}{15} + \frac{7f_0^3}{60}, \ldots \tag{9}$$

On the other hand, the acceptable solution should behave as $f(x) = ax^5 - 4/(3x) + \ldots$ when $x \gg 1$.

Table 4 shows Hankel sequences with $d = 0$ and $d = 1$ that clearly converge towards the numerical value of f_0 [10] (and references therein).

Table 4: Convergence of the Hankel sequences for the Wegner-Houghton connection parameter

D	$d = 0$	$d = 1$
3	$-0.301\,365\,209\,2$	$-0.419\,012\,931\,2$
4	$-0.540\,511\,282\,4$	$-0.469\,645\,717\,0$
5	$-0.455\,201\,249\,3$	$-0.460\,479\,692\,6$
6	$-0.462\,452\,597\,9$	$-0.461\,693\,582\,1$
7	$-0.461\,375\,992\,6$	$-0.461\,509\,171\,7$
8	$-0.461\,557\,112\,9$	$-0.461\,537\,339\,3$
9	$-0.461\,530\,376\,7$	$-0.461\,533\,153\,5$
10	$-0.461\,534\,297\,5$	$-0.461\,533\,816\,5$
11	$-0.461\,533\,614\,7$	$-0.461\,533\,704\,3$
12	$-0.461\,533\,735\,7$	$-0.461\,533\,722\,7$
13	$-0.461\,533\,717\,3$	$-0.461\,533\,719\,6$
14	$-0.461\,533\,720\,7$	$-0.461\,533\,720\,2$
15	$-0.461\,533\,720\,0$	$-0.461\,533\,720\,1$
16	$-0.461\,533\,720\,13$	$-0.461\,533\,720\,119$
17	$-0.461\,533\,720\,113$	$-0.461\,533\,720\,115\,7$
18	$-0.461\,533\,720\,116\,8$	$-0.461\,533\,720\,116\,3$
19	$-0.461\,533\,720\,116\,1$	$-0.461\,533\,720\,116\,2$
20	$-0.461\,533\,720\,116\,2$	

We have also applied our approach to the ordinary differential equation for the spherically symmetric skyrmion field [10] (and references therein) but we could not obtain convergent Hankel sequences. We do not yet know the reason for the failure of the method in this case.

The present approach has earlier proved suitable for the treatment of the Riccati equation derived from the Schrödinger equation [1–3, 5, 6, 4, 7–9]. Consider, for example, the following Riccati equation

$$f'(x) - f(x)^2 + x^2 = 0, \quad x > 0. \tag{10}$$

The solution can be expanded as in equation (1) with $\alpha = \beta = 1$; the first coefficients are

$$f_1 = f_0^2,\ f_2 = f_0^3,\ f_3 = -\frac{1}{3} + f_0^4, \ldots$$

There is a critical value f_{0c} of $f(0) = f_0$ such that $f(x) \sim -x$ at large x if $f(0) < f_{0c}$, $f(x)$ develops a singular point if $f(0) > f_{0c}$, and $f(x) \sim x$ at large x if $f(0) = f_{0c}$. The present Padé-Hankel method yields the value of f_{0c} with remarkable accuracy, as shown in Table 5. The rate of convergence of the Hankel sequence for this problem is considerably greater than for the preceding ones.

If we substitute $f(x) = -y'(x)/y(x)$ into equation (10), then the function $y(x)$ satisfies the Schrödinger equation for a harmonic oscillator with zero energy

Table 5: Convergence of the Hankel sequences with $d = 0$ for the Riccati equation

D	f_0
4	0.676 2
5	0.675 970
6	0.675 978 5
7	0.675 978 23
8	0.675 978 240 3
9	0.675 978 240 059
10	0.675 978 240 067 5
11	0.675 978 240 067 277
12	0.675 978 240 067 285 0
13	0.675 978 240 067 284 722
14	0.675 978 240 067 284 729
15	0.675 978 240 067 284 728 99
16	0.675 978 240 067 284 729 00
17	0.675 978 240 067 284 729 00

Table 6: Convergence of the Hankel sequences with $d = 4$ for the Thomas-Fermi equation

D	$2f_2$
10	−1.588 070 9
11	−1.588 070 6
12	−1.588 071 03
13	−1.588 071 024
14	−1.588 071 022 7
15	−1.588 071 022 64
16	−1.588 071 022 609
17	−1.588 071 022 609
18	−1.588 071 022 611 6
19	−1.588 071 022 611 5
20	−1.588 071 022 611 39
21	−1.588 071 022 611 38
22	−1.588 071 022 611 37
23	−1.588 071 022 611 37
24	−1.588 071 022 611 375 6
25	−1.588 071 022 611 375 37
26	−1.588 071 022 611 375 32
27	−1.588 071 022 611 375 315 4
28	−1.588 071 022 611 375 315 2
29	−1.588 071 022 611 375 315 4
30	−1.588 071 022 611 375 313 7

on the half line: $y''(x) - x^2 y(x) = 0$, and the problem solved above is equivalent to finding the logarithmic derivative at origin $y'(0)/y(0)$ so that $y(x)$ behaves as $\exp(-x^2/2)$ at infinity. Obviously, any approach for linear differential equations is suitable for this problem.

Finally, we consider two examples discussed by Bender et al [12]; the first of them is the instanton equation

$$f''(x) + f(x) - f(x)^3 = 0 \tag{11}$$

with the boundary conditions $f(0) = 0$, $f(\infty) = 1$. The solution to this equation is $f(x) = \tanh\left(x/\sqrt{2}\right)$. The expansion of $f(x)$ is a particular case of equation (1) with $\alpha = 1$ and $\beta = 2$; its first coefficients being

$$\begin{aligned} f_1 &= -\frac{f_0}{6},\ \frac{f_0\left(6f_0^2+1\right)}{120}, \\ f_3 &= -\frac{f_0\left(66f_0^2+1\right)}{5\,040}, \ldots, \end{aligned} \tag{12}$$

where $f_0 = f'(0)$ is the unknown. The Hankel series with $d = 0$ and $d = 1$ converge rapidly giving upper and lower bounds, respectively, to the exact result $f_0 = 1/\sqrt{2}$.

The second example is the well known Blasius equation [12]

$$2y'''(x) + y(x)y''(x) = 0 \tag{13}$$

with the boundary conditions $y(0) = y'(0) = 0$, $y'(\infty) = 1$. The expansion of the solution in a Taylor series about $x = 0$ is a particular case of equation (1) with $\alpha = 2$ and $\beta = 3$; its first coefficients are

$$f_1 = -\frac{f_0^2}{60},\ f_2 = \frac{11f_0^3}{20160}, \ldots \tag{14}$$

Since, in general, $f_j \propto f_0^{j+1}$, then the only root of the Hankel determinants is $f_0 = 0$, which leads to the trivial solution $y(x) \equiv 0$. We thus see another case where the Padé-Hankel method does not apply.

4 Conclusions

We have presented a simple method for the treatment of two-point boundary value problems. If there is a suitable series for the solution about one point, we construct a Hankel matrix with the expansion coefficients and obtain the physical value of the undetermined coefficient from the roots of a sequence of determinants. The value of this coefficient given by a convergent Hankel sequence is exactly the one that produces the correct asymptotic behaviour at the other point. We cannot prove this assumption rigorously, but it seems that if there is a convergent sequence, it yields the correct answer. Moreover, in some cases the Hankel sequences produce upper and lower bounds bracketing the exact result tightly.

The present Padé-Hankel approach is not as general as the one proposed by Boisseau et al [10], as we have already seen that the former does not apparently apply to the skyrmion problem or to the Blasius equation [12]. However, our procedure is much simpler and more straightforward and may be a suitable alternative for treating problems of this kind. Besides, if our approach converges, it yields remarkably accurate results, as shown in the examples above.

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Paolo Amore
E-mail: paolo@cgic.ucol.mx
Facultad de Ciencias
Universidad de Colima
Bernal Díaz del Castillo 340, Colima, Colima, Mexico

Francisco M. Fernández
E-mail: fernande@quimica.unlp.edu.ar
INIFTA (Conicet,UNLP), Diag. 113 y 64 S/N
Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina