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’s fixed point equation in the local potential approximation, a Riccati equation, and the Thomas–Fermi equation. We consider two models where the approach does not apply in order to show the limitations of our Padé–Hankel approach.
1 Introduction

Some time ago Fernández et al [1–9] 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 Riccati–Padé, 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

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

(1)

about $x = 0$, where $\alpha$ and $\beta$ 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 the following section.

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

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

(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 [1–9]

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

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 Hankel sequence for short. If such convergent sequence is monotonously increasing or decreasing we assume that it yields a lower or upper bound, respectively. Such bounds where 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 recently by Boisseau et al by means of a most interesting algebraic approach [10]. We first consider the field equation determining the vortex profile in a Ginzburg–Landau effective theory [10] (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

\[
\begin{align*}
f_1 &= -\frac{f_0}{8}, \\
f_2 &= \frac{f_0}{192} + \frac{f_0^3}{24}, \\
f_3 &= -\frac{f_0}{9216} - \frac{5f_0^3}{576}, \ldots
\end{align*} \tag{5}
\]

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: $0.58318949586060 < f_0 < 0.58318949586061$.

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 $n = 2, 3, 4$.

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

$$2 f''(x) - 4 f(x)f'(x) - 5xf'(x) + f(x) = 0, \quad x > 0.$$  \hspace{1cm} (6)

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

$$f_1 = \frac{f_0}{3} + \frac{f_0^2}{3}, \quad f_2 = \frac{7f_0}{60} + \frac{f_0^2}{4} + \frac{2f_0^3}{15}, \ldots.$$  \hspace{1cm} (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. Fig. 1 displays the great rate of convergence of these sequences as $\Delta = |f_0(D, d = 0) - f_0(D, d = 1)|, \quad D = 2, 3, \ldots$, from which we obtain the accurate bounds $-1.22859820243702192438 < f_0 < -1.22859820243702192437$.

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

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

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

$$f_1 = -\frac{f_0}{3} - \frac{f_0^2}{3}, \quad f_2 = \frac{f_0}{60} + \frac{2f_0^2}{15} + \frac{7f_0^3}{60}, \ldots.$$  \hspace{1cm} (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).

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 know yet the reason for the failure of the method in this case.

Present approach has earlier proved suitable for the treatment of the Riccati equation derived from the Schrödinger equation [1–9]. Consider, for example, the following Riccati equation

\[ f'(x) - f(x)^2 + x^2 = 0, \quad x > 0. \]  

(10)

The solution can be expanded as in equation (11) with \( \alpha = \beta = 1 \); the first coefficients are

\[ f_1 = f_2^0, \quad f_2 = f_3^0, \quad f_3 = -\frac{1}{3} + f_4^0, \ldots \]

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 \( f(0) = f_{0c} \). 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 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 the Thomas–Fermi equation [11–13] (and references therein)

\[ \Phi''(x) = x^{-1/2}\Phi(x)^{3/2}, \quad x > 0 \]  

(11)

that provides a semiclassical description of the charge density in atoms of high atomic number. It poses the problem of finding the slope at origin \( \Phi'(0) \) so that \( \Phi(0) = 1 \) and \( \Phi(x \to \infty) = 0 \). The change of variables \( t = x^{1/2} \) leads to a more tractable equation

\[ t\xi''(t) - \xi'(t) - 4t^2\xi(t)^{3/2}, \quad t > 0 \]  

(12)

where \( \xi(t) = \Phi(t^2) \). We can expand the solution to this equation in a Taylor series: \( \xi(t) = 1 + a_2 t^2 + 4t^3/3 + 2a_2 t^5/5 + \ldots \) and the unknown slope is given by the unknown coefficient: \( \Phi'(0) = a_2 \). One easily derives a recurrence relation for the coefficients of this expansion [13]. Although the treatment
of equation (12) is straightforward, we find it more convenient to define the function \( f(t) = \xi(t)^{1/2} \) that is a solution to
\[
 t \left[ f(t)f''(t) + f'(t)^2 \right] - f(t)f'(t) - 2t^2 f(t)^3 = 0.
\] (13)
The function \( f(t) \) satisfies a series like (1) with \( \alpha = 0 \) and \( \beta = 1 \). The first coefficients are
\[
f_1 = 0, \ f_3 = \frac{2}{3}, \ f_4 = -\frac{f_2^2}{2}, \ f_5 = -\frac{4f_2}{15}, \ldots \quad (14)
\]
We expect that a Hankel sequence will converge towards \( f_2 = f''(0)/2 = \Phi'(0)/2 \). Since \( f_4 \) is the first nonzero coefficient that depends on \( f_2 \) we choose \( d \geq 4 \) in the Hankel determinant. Table 6 shows that the Hankel sequence with \( d = 4 \) converges rapidly giving a most accurate value of the slope at origin \( \Phi'(0) \).

Finally, we consider two examples discussed by Bender et al [14]; the first of them is the instanton equation
\[
f''(x) + f(x) - f(x)^3 = 0 \quad (15)
\]
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
\[
f_1 = -\frac{f_0}{6}, \ f_3 = -\frac{f_0(6f_0^2 + 1)}{120}, \ f_5 = -\frac{f_0(66f_0^2 + 1)}{5040}, \ldots, \quad (16)
\]
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 [14]
\[
2y''(x) + y(x)y''(x) = 0 \quad (17)
\]
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
\[
f_1 = -\frac{f_0^2}{60}, \ f_2 = \frac{11f_0^3}{20160}, \ldots \quad (18)
\]
Since, in general, \( f_j \propto f_0^{j+1} \), then the only root of the Hankel determinants is \( f_0 = 0 \) that 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.

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 [14]. However, our procedure is much simpler and more straightforward and may be a suitable alternative for the treatment of this kind of problems. Besides, if our approach converges, it yields remarkably accurate results as shown in the examples above. For example, it gives us the slope of the electrostatic potential of the Thomas–Fermi theory with unprecedented accuracy.

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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       | 0.5829      |
| 4   | 0.58324     | 0.58315     |
| 5   | 0.58320     | 0.583183    |
| 6   | 0.583192    | 0.583187    |
| 7   | 0.583190    | 0.5831890   |
| 8   | 0.5831897   | 0.5831893   |
| 9   | 0.58318954  | 0.58318946  |
| 10  | 0.58318952  | 0.58318948  |
| 11  | 0.58318951  | 0.583189491 |
| 12  | 0.583189498 | 0.583189494 |
| 13  | 0.5831894964| 0.5831894953|
| 14  | 0.5831894961| 0.5831894956|
| 15  | 0.5831894960| 0.5831894957|
| 16  | 0.58318949590| 0.58318949583|
| 17  | 0.58318949588| 0.58318949584|
| 18  | 0.583189495867| 0.583189495854|
| 19  | 0.583189495864| 0.583189495857|
| 20  | 0.583189495862| 0.5831894958591|
| 21  | 0.5831894958609| 0.5831894958598|
| 22  | 0.5831894958607| 0.5831894958601|
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   | 0.1528  | 0.154   |
| 5   | 0.15310 | 0.1530  |
| 6   | 0.15309 | 0.15311 |
| 7   | 0.153098| 0.15310 |
| 8   | 0.153097| 0.15310 |
| 9   | 0.1530991| 0.153099|
| 10  | 0.15309914| 0.1530989|
| 11  | 0.15309912| 0.153099095|
| 12  | 0.15309917| 0.153099091|
| 13  | 0.153099105| 0.153099097|
| 14  | 0.1530991021| 0.15309911|
| 15  | 0.15309910272| 0.153099102|
| 16  | 0.153099102697| 0.153099103|
| 17  | 0.153099102782| 0.15309910292|
| 18  | 0.153099103124| 0.15309910293|
| 19  | 0.153099102857| 0.15309910289|
| 20  | 0.153099102864| 0.15309910278|
| 21  | 0.15309910286136| 0.153099102860|
| 22  | 0.15309910286142| 0.153099102858|

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

| $n$ | $D_{\text{max}}$ | $f_0$ |
|-----|------------------|------|
| 2   | 21               | 0.15309910286 |
| 3   | 21               | 0.0261834207  |
| 4   | 26               | 0.0033271734  |
Table 4: Convergence of the Hankel sequences for the Wegner–Houghton connection parameter

| $D$ | $d = 0$          | $d = 1$          |
|-----|-----------------|-----------------|
| 3   | -0.3013652092   | -0.4190129312   |
| 4   | -0.5405112824   | -0.4696457170   |
| 5   | -0.4552012493   | -0.4604796926   |
| 6   | -0.4624525979   | -0.4616935821   |
| 7   | -0.4613759926   | -0.4615091717   |
| 8   | -0.4615571129   | -0.4615373393   |
| 9   | -0.4615303767   | -0.4615331535   |
| 10  | -0.4615342975   | -0.4615338165   |
| 11  | -0.461536147    | -0.461537043    |
| 12  | -0.461537357    | -0.461537227    |
| 13  | -0.461537173    | -0.461537196    |
| 14  | -0.461537207    | -0.461537202    |
| 15  | -0.461537200    | -0.461537201    |
| 16  | -0.4615372013   | -0.46153720119  |
| 17  | -0.46153720113  | -0.461537201157 |
| 18  | -0.461537201168 | -0.461537201163 |
| 19  | -0.461537201161 | -0.461537201162 |
| 20  | -0.461537201162 |                 |
Table 5: Convergence of the Hankel sequences with $d = 0$ for the Riccati equation.

| $D$ | $f_0$     |
|-----|-----------|
| 4   | 0.6762    |
| 5   | 0.675970  |
| 6   | 0.6759785 |
| 7   | 0.67597823|
| 8   | 0.6759782403 |
| 9   | 0.675978240059 |
| 10  | 0.6759782400675 |
| 11  | 0.675978240067277 |
| 12  | 0.6759782400672850 |
| 13  | 0.675978240067284722 |
| 14  | 0.675978240067284729 |
| 15  | 0.67597824006728472899 |
| 16  | 0.67597824006728472900 |
| 17  | 0.67597824006728472900 |

Figure 1: $\Delta = |f_0(D, d = 0) - f_0(D, d = 1)|$ for Wilson’s renormalization
Table 6: Convergence of the Hankel sequences with $d = 4$ for the Thomas–Fermi equation

| $D$  | $2f_2$                  |
|------|-------------------------|
| 10   | -1.5880709              |
| 11   | -1.5880706              |
| 12   | -1.58807103             |
| 13   | -1.588071024            |
| 14   | -1.5880710227           |
| 15   | -1.58807102264          |
| 16   | -1.588071022609         |
| 17   | -1.588071022609         |
| 18   | -1.5880710226116        |
| 19   | -1.5880710226115        |
| 20   | -1.58807102261139       |
| 21   | -1.58807102261138       |
| 22   | -1.58807102261137       |
| 23   | -1.58807102261137       |
| 24   | -1.5880710226113756     |
| 25   | -1.58807102261137537    |
| 26   | -1.58807102261137532    |
| 27   | -1.5880710226113753154  |
| 28   | -1.5880710226113753152  |
| 29   | -1.5880710226113753154  |
| 30   | -1.5880710226113753137  |