JOURNAL OF COMPUTATIONAL PHYSICS 19, 236–240 (1975)

Note

Extrapolation of Finite Difference Approximations for Bound State Equations

A common technique for approximating the discrete eigenvalues of Sturm–Liouville eigenvalue problems of the type

$$\frac{-d^2y}{dx^2} + q(x)\,y(x) = \lambda y(x), \qquad 0 < x < \infty, \tag{1}$$

with $y(0) = 0$ and $y(x) \to 0$ as $x \to \infty$, is to replace infinity by some suitably large number $b > 0$ and then treat the problem over the interval $[0, b]$ with the added boundary condition $y(b) = 0$ by using either the central difference or Numerov finite difference methods. A discussion of various implementations and applications of these methods can be found in, for example, Cooley [2], Keller [6], Truhlar [9], Dickinson [3], Guest [5], and Shore [8]. The purpose of this note is to present experimentally observed convergence rates for the standard matrix implementation of these methods and to show the effects of Richardson and Padé extrapolation for typical potentials $q(x)$. These extrapolation techniques have been recently examined for numerical integration problems by Chisolm, Genz, and Rowlands [1]. Guest and Shore also examined convergence rates for eigenvalues computed by central difference and Numerov methods. Guest treats Richardson extrapolation while the paper by Shore is a comprehensive review of many approximation methods.

Let $\Delta_n:\ 0 = x_0 < x_1 < \cdots < x_{n+1} = b$ be a partition of $(0, b)$ with $x_i - x_{i-1} = b/(n+1) = h$ for $i = 1,\ldots, n+1$. The central difference method approximates the eigenvalues of (1) with the eigenvalues of the matrix problem

$$\begin{gathered} -[(y_{i-1} - 2y_i + y_{i+1})/h^2] + q(x_i)\,y_i = \lambda y_i\,, \qquad i = 1,\ldots, n, \\ y_0 = 0, \qquad y_{n+1} = 0. \end{gathered} \tag{2}$$

The Numerov method approximates the eigenvalues of (1) with the eigenvalues of the matrix problem

$$\begin{gathered} \left(\frac{1}{h^2} - \frac{q_{i-1}}{12}\right) y_{i-1} + \left(\frac{-2}{h^2} + \frac{5q_i}{6}\right) y_i + \left(\frac{1}{h^2} - \frac{q_{i+1}}{12}\right) y_{i+1} \\ = \lambda \left(\frac{1}{12} y_{i-1} + \frac{5}{6} y_i + \frac{1}{12} y_{i+1}\right), \qquad i = 1,\ldots, n, \\ y_0 = 0, \qquad y_{n+1} = 0. \end{gathered} \tag{3}$$

The approximate eigenvalues λ are functions of the mesh size h. Extrapolation procedures combine, via an approximation of this function, a sequence of computed eigenvalues for different values of h to obtain an extrapolated and hopefully improved answer. Besides the well-known Richardson technique [6], we wish to test two other extrapolation procedures on the eigenvalue problem based on Padé approximants [1], namely type I Padé approximants (P.A.) and type II P.A.

The type I formula is used in the following way. From a sequence of computed eigenvalues $\lambda(h_1)$, $\lambda(h_2)$, $\lambda(h_3)$,..., one forms a series

$$\Lambda(g) = \lambda(h_1) + g(\lambda(h_2) - \lambda(h_1)) + g^2(\lambda(h_3) - \lambda(h_2)) + \cdots.$$

From this series, which terminates with either an odd or even power of g, one forms either a diagonal P.A., $\Lambda(g)^{[N/N]}$ ($2N + 1$ terms in the series), or an off-diagonal P.A., $\Lambda(g)^{[N+1,N]}$ ($2N + 2$ terms in the series). One then evaluates these sequences of P.A. at $g = 1$. Details of this procedure may be found in the article by Chisholm *et al.*

The type II or fixed-point P.A. for the central difference method is based on the assumption that

$$\lambda(h) = \frac{A + Bh^2 + Ch^4 + \cdots}{1 + Dh^2 + Eh^4 + \cdots}.$$

This form is fitted to the fixed points $\lambda(h_1)$, $\lambda(h_2)$,... with A then being the extrapolated result. This function is motivated by a consideration of the Taylor's series expansion for the truncation error. With the Numerov technique, it is not as clear what functional form to assume. In those cases where the potential is singular, the above form for $\lambda(h)$ is adequate as the Numerov appears to converge like h^2. However, if the potential is smooth (or can be made smooth by appropriate scale change) then a more appropriate form is

$$\lambda(h) = \frac{A + Bh^4 + Ch^8 + \cdots}{1 + Dh^4 + Eh^8 + \cdots}.$$

In Tables I–VI, we present the results of numerical experiments in the case of two different central potentials. The eigenvalues λ_0 refer to the ground state energies and λ_{I}, λ_{II}, and λ_{III} are three different extrapolated results. The eigenvalue λ_{I} is the extrapolated result obtained by using type I Padé approximants on the sequence of eigenvalues $\lambda(h_i)$, and λ_{II} is the result using type II or fixed-point Padé approximants. The results of Richardson extrapolation are given by λ_{III}. The number β is the exponent of the leading power of h in the computed extrapolation rates for the eigenvalue λ. On both of these examples the endpoint was chosen to be $x_N = 16$ and λ_0 is the exact eigenvalue.

TABLE I

Central Difference Method for $V = -2/x$; $\lambda_0 = -1$

h	$-\lambda_0 + \lambda$	β	$-\lambda_0 + \lambda_{\mathrm{I}}$	$-\lambda_0 + \lambda_{\mathrm{II}}$	$-\lambda_0 + \lambda_{\mathrm{III}}$
1/2	0.05572809	—	0.05572809	0.05572809	0.05572809
1/4	0.01515450	1.88	0.01515500	0.00163063	0.00163063
1/8	0.00387602	1.97	−0.00046666	0.00000327	0.00001542
1/16	0.00097466	1.99	−0.00003015	0.00000001	0.00000004
1/32	0.00024402	2.00	0.00000029	0.00000000+	0.00000000+

TABLE II

Numerov Method for $V = -2/x$: $\lambda_0 = -1$

h	$-\lambda_0 + \lambda$	β	$-\lambda_0 + \lambda_{\mathrm{I}}$	$-\lambda_0 + \lambda_{\mathrm{II}}$	$-\lambda_0 + \lambda_{\mathrm{III}}$
1/2	0.09358441	—	0.09358441	0.09358441	0.09358441
1/4	0.03124154	1.58	0.03124154	0.01046571	0.01046572
1/8	0.00906178	1.79	−0.00319147	0.00080949	0.00108207
1/16	0.00243485	1.90	−0.00038886	0.00008897	0.00011457
1/32	0.00063010	1.95	0.00001956	0.00000983	0.00001315

TABLE III

Central Difference Method for $V = x^2$; $\lambda_0 = 3$

h	$\lambda_0 - \lambda$	β	$\lambda_0 - \lambda_{\mathrm{I}}$	$\lambda_0 - \lambda_{\mathrm{II}}$	$\lambda_0 - \lambda_{\mathrm{III}}$
1/2	0.08051590	—	0.08051590	0.08051590	0.08051590
1/4	0.01967134	2.03	0.01967134	−0.00061018	−0.00061018
1/8	0.00459144	2.10	0.00014929	0.00000198	0.00000312
1/16	0.00122124	1.91	0.00000876	0.00000000+	0.00000000+
1/32	0.00030521	2.00	0.00000005	0.00000000+	0.00000000+

TABLE IV

Numerov Method for $V = x^2$; $\lambda_0 = 3$

h	$\lambda_0 - \lambda$	β	$\lambda_0 - \lambda_{\rm I}$	$\lambda_0 - \lambda_{\rm II}$	$\lambda_0 - \lambda_{\rm III}$
1/2	0.00358114	—	0.00358114	0.00358114	0.00358114
1/4	0.00021586	4.05	0.00021586	−0.00090590	−0.00090590
1/8	0.00001334	4.04	0.00000381	0.00000068	0.00000262
1/16	0.00000083	4.01	0.00000000+	0.00000000+	0.00000000+
1/32	0.00000005	4.05	0.00000000+	0.00000000+	0.00000000+

TABLE V

Convergence Rate of Extrapolated h^2 Behavior for Finite Difference Method; $V = -2/x$; $\lambda_0 = -1$

(h_1, h_2)	$\lambda_{\rm EX} - \lambda_0$	β
(1/2, 1/4)	0.00163063	—
(1/4, 1/8)	0.00011637	3.81
(1/8, 1/16)	0.00000754	3.95
(1/16, 1/32)	0.00000048	3.99

TABLE VI

Convergence Rate of Extrapolated h^2 Behavior for Numerov Method; $V = -2/x$; $\lambda_0 = -1$

(h_1, h_2)	$\lambda_{\rm EX} - \lambda_0$	β
(1/2, 1/4)	0.01046572	—
(1/4, 1/8)	0.00166855	2.65
(1/8, 1/16)	0.00022586	2.89
(1/16, 1/32)	0.000028515	2.99

The last two tables give the convergence rate of the Richardson extrapolated values for the case of a singular Coulomb potential. The extrapolated eigenvalue is $\lambda_{\rm EX}$.

As expected, the finite difference method gives a convergence rate on the order of h^2 for both the singular $(-2/x)$ and smooth (x^2) potentials. The Numerov technique, although it has order h^4 truncation error, gives a convergence rate of order h^2 for the singular potential. For the smooth potential, its convergence rate is of order h^4 as verified also in Guest [5] and Shore [8]. The extrapolated h^2 behavior of the finite difference method convergences like h^4 while the extrapolated h^2 Numerov behavior for singular potentials converges like h^3. In every case, type II Padé and Richardson extrapolation on the eigenvalue are superior to the type I Padé technique. Type II Padé approximants appear to be consistently and significantly better than the Richardson technique. We obtained essentially the same results using other examples of smooth and singular potentials.

For the case of a singular potential of, for example, the Coulomb type, it is possible to make a change of variables as in Froese [4] to eliminate the singularity. The Numerov method will then achieve order h^4 convergence when applied to the new problem, but we found it difficult to choose the truncation points of the interval to compare the results fairly. As $[0, \infty)$ for the radial problem will be mapped into $(-\infty, \infty)$ by this change of variables, both $-\infty$ and ∞ have to be replaced by finite numbers. Although it is possible to do this so that excellent numerical results are then obtained, we feel it is simpler to apply the methods directly to the problem in radial form and apply type II Padé extrapolation. Padé approximations have recently been used by Lavine [7], but in a different context. There, an integral equation formulation of (1) is used and then the kernel is replaced by a Padé approximant. A matrix approximation is then defined by numerical quadrature.

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Received: August 15, 1973; revised April 8, 1975

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Printed in Belgium