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LETTER TO THE EDITOR

A symmetric matrix method for Schrödinger eigenstates

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Abstract. It is shown how the one-dimensional Schrödinger eigenvalue equation can be transformed into a *symmetric generalised matrix eigenproblem* with a local truncation error of only δ^4, where δ is the step size, as in the Numerov algorithm. Standard *sparse matrix* library packages are available for the solution and it is demonstrated that groups of eigenvalues and their associated eigenvectors (wavefunctions) can be determined simultaneously with high precision and speed.

In many branches of physics there is a need for the accurate determination of eigenvalues and eigenfunctions of the one-dimensional Schrödinger equation. This may be an end in itself or merely the starting point for, for example, a many-body calculation.

If a large number of eigenfunctions is required then the conventional techniques are very inconvenient. These are usually 'shooting methods' based either on the Numerov-Cooley algorithm [1] or on the Pruefer transformation to a phase function [2]. Ixaru and Rizea [3] have recently shown how to adapt the Numerov-Cooley method specifically to the Schrödinger equation and Eckart [4] has developed an extrapolation technique to improve the accuracy of the eigenvalue and has also shown how (with considerable difficulty) the method can be applied in two dimensions. Such methods work on one eigenstate at a time and in many algorithms† the step size, which determines the coordinates at which the eigenfunction is evaluated, is generated internally. This means that different eigenfunctions are determined at different sets of coordinates, making the calculations of matrix elements inconvenient.

One solution to this problem was presented by Cooney *et al* [5]. Their method was to use the standard second-order finite difference expression [6] for the second derivative and thus replace the differential equation

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x)+V(x)\Psi(x)=E\Psi(x) \tag{1}$$

by the difference equation

$$\frac{-\hbar^2}{2m}\left(\frac{\Psi_{n+1}+\Psi_{n-1}-2\Psi_n}{\delta^2}\right)+V_n\Psi_n=E\Psi_n \tag{2}$$

where $\Psi_n=\Psi(x_n)$, $V_n=V(x_n)$ and $\delta=x_{n+1}-x_n$ is the step size. The set of linear equations can then be solved as a *symmetric matrix eigenvalue problem* [7].

† The NAG algorithm D02KEF which uses a scaled Prufer phase function transformation is an example.

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One advantage of this simple technique is that the eigenfunctions are determined at a common set of coordinate values, thus facilitating the calculation of matrix elements. Another advantage is the availability of many 'off the shelf' high-quality subroutines from such matrix libraries as EISPACK [8], NAG [9] and Harwell [10].

A *disadvantage* is that the difference equation (2) is not a very good representation of the Schrödinger equation (1), the error in the representation relative to $(2mE/\hbar^2)\Psi_n$ being

$$\tfrac{1}{12}\delta^2\Psi_n^{(4)}. \tag{3}$$

In order to overcome this problem the Numerov-Cooley algorithm replaces (2) by the second-order difference equation

$$\frac{-\hbar^2}{2m}\left(\frac{\Psi_{n+1}+\Psi_{n-1}-2\Psi_n}{\delta^2}\right)=\tfrac{5}{6}(E-V_n)\Psi_n+\tfrac{1}{12}(E-V_{n+1})\Psi_{n+1}+\tfrac{1}{12}(E-V_{n-1})\Psi_{n-1}. \tag{4}$$

The relative error in the representation is then reduced to

$$\tfrac{29}{300}\delta^4\Psi_n^{(6)}. \tag{5}$$

Unfortunately this leads to an *asymmetric* matrix equation and, whilst techniques exist for such problems, they are not nearly as efficient as those for the *symmetric* case.

We set out to improve the simple algorithm represented by equation (2) but to *force* the resulting difference equation into the *symmetric* form

$$\mathbf{A}\Psi = E\,\mathbf{a}\Psi \tag{6}$$

where Ψ is a column vector and $\mathbf{A}$ and $\mathbf{a}$ are *symmetric tridiagonal* $N\times N$ matrices. The only non-zero elements of $\mathbf{A}$ and $\mathbf{a}$ are denoted by

$$\begin{aligned} &A_{nn}=A_n \\ &a_{nn}=a_n \qquad n=1,\ldots,N \\ &A_{n\,n+1}=A_{n+1\,n}=B_n \\ &a_{n\,n+1}=a_{n+1\,n}=b_n \qquad n=1,\ldots,N-1. \end{aligned} \tag{7}$$

The values of these parameters which minimise the error in the representation of the differential equation are

$$\begin{aligned} &a_n=\frac{5}{6}-\frac{m\delta^2}{6\hbar}(V_n-\bar{V}) \qquad b_n=\tfrac{1}{12} \\ &A_n=\frac{\hbar^2}{m\delta^2}+\frac{\bar{V}+4V_n}{6}+\frac{m\delta^2}{6\hbar^2}V_n(V_n-\bar{V}) \\ &B_n=\frac{-\hbar^2}{2m\delta^2}+\frac{V_{n+1}+V_n-\bar{V}}{12} \end{aligned} \tag{8}$$

where $\bar{V}$ is some 'average' potential.

As δ tends to zero these reduce to the Numerov-Cooley expressions. The relative error in the representation is

$$\tfrac{1}{144}\delta^4(V_n-\bar{V})\Psi_n^{(4)}+\tfrac{1}{240}\delta^4\Psi_n^{(6)} \tag{9}$$

which is of the same order in δ as the Numerov-Cooley algorithm (although involving a lower-order derivative). $\bar{V}$ may be chosen to further reduce this error.

The solutions for A_n and a_n do not (necessarily) apply at the boundaries. We denote the boundaries by $x = \alpha$ and $x = \beta$ and we consider only two types of boundary condition

$$\Psi(\alpha) = 0 \qquad \text{or} \qquad \Psi^{(1)}(\alpha) = 0$$

and

$$\Psi(\beta) = 0 \qquad \text{or} \qquad \Psi^{(1)}(\beta) = 0.$$

For the lower boundary, if Ψ vanishes then $x_1 = \alpha + \delta$ and the equation (8) is valid for A_1 and a_1. If the derivative $\Psi^{(1)}$ vanishes then $x_1 = \delta$ and A_1 and a_1 are precisely *one-half* the values given by equation (8). Similar results hold for the upper boundary.

Equation (6) represents a *symmetric generalized eigenvalue problem* and the well-known matrix subroutine libraries (EISPACK, NAG, Harwell) all contain procedures for its solution. See also Parlett [7] for a general discussion of the most recent methods for the *symmetric eigenvalue problem* and for the *symmetric generalised eigenvalue problem.* Kaufmann [11] has presented methods for the solution of equation (6) on *vector* machines.

In order to demonstrate the effectiveness of the procedure, we have applied it to the one-dimensional harmonic oscillator using the NAG routines F02FJF and F04LEF. In dimensionless form this Schrödinger equation is

$$-\frac{d^2}{dx^2}\Psi + x^2\Psi = E\Psi \tag{10}$$

and the exact eigenvalues and (unnormalised) eigenfunctions are

$$E_\nu = (2\nu + 1) \qquad \Psi_\nu = \exp(-x^2/2)H_\nu(x) \tag{11}$$

where H_ν is a Hermite polynomial.

Table 1 shows the eigenvalues and the RMS errors in the first eight odd eigenfunctions calculated using the present algorithm and the simple algorithm (2). In both cases the values of N and δ were taken to be 100 and 0.08 respectively. The results show clearly the improved accuracy that has been obtained.

The simple algorithm is somewhat quicker. The CPU times for the present method and the simple method to determine these eight eigenfunctions using an Amdahl 5870 were respectively 0.72 s and 0.56 s.

Table 1. Eigenvalues E_ν and RMS errors in the first eight odd eigenfunctions, calculated using the present algorithm compared with those using the simple algorithm.

	Present Algorithm		Simple Algorithm	
ν	E_ν	RMS eigenfunction error	E_ν	RMS eigenfunction error
1	2.999 997	8.99×10^{-7}	2.998	8.38×10^{-4}
3	6.999 98	3.84×10^{-6}	6.989	2.38×10^{-3}
5	10.999 95	1.98×10^{-5}	10.98	6.32×10^{-3}
7	14.999 87	4.80×10^{-5}	14.95	1.13×10^{-2}
9	18.999 7	9.54×10^{-5}	18.93	1.78×10^{-2}
11	22.999 6	1.68×10^{-4}	22.89	2.59×10^{-2}
13	26.999 3	2.70×10^{-4}	26.85	3.55×10^{-2}
15	30.998 9	4.07×10^{-4}	30.81	4.67×10^{-2}

Table 2. As for table 1 but demonstrating the poorer accuracy of the simple algorithm.

	Present algorithm $N = 100$ $\delta = 0.08$ Time = 0.72 s		Simple algorithm $N = 1050$ $\delta = 7.619 \times 10^{-3}$ Time = 4.92 s	
ν	E_ν	RMS eigenfunction error	E_ν	RMS eigenfunction error
1	2.999 97	8.99×10^{-7}	2.999 98	7.59×10^{-6}
3	6.999 98	3.84×10^{-6}	6.999 91	2.58×10^{-5}
5	10.999 95	1.98×10^{-5}	10.999 8	5.81×10^{-5}
7	14.999 87	4.80×10^{-5}	14.999 6	1.02×10^{-4}
9	18.999 7	9.54×10^{-5}	18.999 3	1.61×10^{-4}
11	22.999 6	1.68×10^{-4}	22.999 0	2.33×10^{-4}
13	26.999 3	2.70×10^{-4}	26.998 7	3.19×10^{-4}
15	30.998 9	4.07×10^{-4}	30.998	4.19×10^{-4}

However, this slight increase in speed does not compensate for the poorer accuracy. To demonstrate this we have progressively reduced the step size (and correspondingly increased the size of the matrix) for the simple algorithm so as to produce approximately the same accuracy as is achieved with $\delta = 0.8$, $N = 100$ for our present method. The results are shown in table 2.

Quite clearly the algorithm we have presented provides a rapid and accurate method of determining simultaneously a group of eigenvalues and their eigenvectors.

Although the results presented refer only to the harmonic oscillator, the method is quite general. The only restriction is that the potential is non-singular (except at the boundaries).

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