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AUTOMATIC COMPUTATION OF ZEROS OF BESSEL FUNCTIONS AND OTHER SPECIAL FUNCTIONS*

JAMES S. BALL†

Abstract. An efficient algorithm is developed for the automatic calculation of the zeros of Bessel functions of arbitrary order, Coulomb wave functions, and other special functions. Remarkably, this can be done without any actual functional evaluations. Limitations and generalizations are discussed.

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1. Introduction. Bessel functions have many applications in the solution of partial differential equations. They are the radial eigenfunctions obtained in cylindrical and spherical geometry when one uses the method of separation of variables on the wave equation, the diffusion equation, and the Poisson equation. The zeros of these functions are required for matching boundary conditions and forming sets of orthogonal functions for application to these problems.

Determining the zeros of Bessel functions has been thoroughly studied for nearly two centuries, and Watson's 1944 *Treatise* [1] remains the standard reference on Bessel functions. For numerical applications, the fact that approximate formulas for the zeros exist can be used with Newton's method to obtain any zero. On the other hand, the methods described in this paper produce an algorithm that consists of only a few lines of code that automatically evaluates the first N zeros (user specified) of a Bessel function of arbitrary real order greater than -2 without any actual functional evaluations. The general technique can be used to determine the zeros of a more general class of special functions.

Section 2 of this paper will outline the basic procedure and necessary conditions for success. The following section will treat Bessel functions specifically. Other applications will be discussed in section 4.

2. Derivation of method for determination of the zeros of special functions. The first requirement for this method is that the special function satisfy a three-term recurrence formula of the form

$$g(x)f_n(x) = A_n f_{n+1}(x) + B_n f_n(x) + C_n f_{n-1}(x), \tag{2.1}$$

where $g(x)$ must have an analytic inverse $g^{-1}(g(x)) = x$ and be independent of n. If we change the normalization of $f_n(x)$ as follows,

$$\gamma_n \phi_n(x) = f_n(x), \tag{2.2}$$

γ_n can be chosen so that $\phi_n(x)$ satisfies the following recurrence formula:

$$g(x)\phi_n(x) = \alpha_n \phi_{n+1}(x) + \beta_n \phi_n(x) + \alpha_{n-1}\phi_{n-1}(x), \tag{2.3}$$

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†Physics Department, University of Utah, Salt Lake City, UT 84112 (ball@physics.utah.edu).

where $\alpha_n = \sqrt{A_n C_{n+1}}$ and $\beta_n = B_n$.

If the first $N+1$ terms generated by this recurrence formula are arranged in matrix form, we obtain the equation

$$g(x)\Phi_N(x) = T_N\Phi_N(x) + r_N(x), \tag{2.4}$$

where

$$\Phi_N(x) = \begin{pmatrix} \phi_0(x) \\ \phi_1(x) \\ \phi_2(x) \\ . \\ . \\ . \\ . \\ \phi_N(x) \end{pmatrix}, \quad r_N(x) = \begin{pmatrix} \alpha_{-1}\phi_{-1}(x) \\ 0 \\ 0 \\ . \\ . \\ . \\ . \\ \alpha_N\phi_{N+1}(x) \end{pmatrix} \tag{2.5}$$

$$\text{and } T_N = \begin{pmatrix} \beta_0 & \alpha_0 & 0 & 0 & \cdots & 0 \\ \alpha_0 & \beta_1 & \alpha_1 & 0 & \cdots & 0 \\ 0 & \alpha_1 & \beta_2 & \alpha_2 & \cdots & 0 \\ . & . & . & . & \cdots & . \\ . & . & . & . & \cdots & . \\ . & . & . & . & \cdots & . \\ . & . & . & . & \cdots & \alpha_{N-1} \\ 0 & 0 & 0 & \cdots & \alpha_{N-1} & \beta_N \end{pmatrix}.$$

Note that the matrix of recurrence coefficients is a symmetric tridiagonal matrix. If $r_N(x) = 0$, then $\Phi_N(x)$ is an eigenvector of T_N with eigenvalue $g(x)$. If, for some reason, one of the two elements of $r_N(x)$ is identically zero, the eigenvalues of T_N can be directly related to the zeros of the other element of $r_N(x)$. For orthogonal polynomials, $\phi_{-1}(x) \equiv 0$, and $\phi_{N+1}(x) = 0$ has $n+1$ roots. This fact is the basis of the well-known method for the computation of the zeros of orthogonal polynomials [2]. In this case $g(x) = x$. These arguments do not follow in the case of Bessel and other special functions because there are no trivial ones, but as we will show that this formulation provides a useful computational technique in those cases as well.

A simple example of these results is provided by letting $\phi_{n-1}(x) = \sin(nx)$, which satisfies the requirements because $\phi_{-1} = 0$. In this case $g(x) = \cos(x)$, $\alpha_i = \frac{1}{2}$, and $\beta_i = 0$. Since the zeros of $\sin[(N+2)x]$ are $x_i = i\pi/(N+2)$, the eigenvalues of the matrix are $\cos[i\pi/(N+2)]$ and the eigenvectors, u_i, are

$$u_i = \left[\sin\left(\frac{i\pi}{N+2}\right), \sin\left(\frac{2i\pi}{N+2}\right), \ldots, \sin\left(\frac{Ni\pi}{N+2}\right)\right]. \tag{2.6}$$

It should be noted that the zeros at 0 and at π are trivial in that the eigenvectors are identically zero. If one recalls that the Chebyshev polynomial, $U_n(x)$, can be written as

$$U_n(cos(\theta)) = \frac{\sin[(n+1)\theta]}{\sin(\theta)}, \tag{2.7}$$

it is not surprising that the eigenvalues obtained above are just the nodes of the Gaussian quadrature based on these polynomials and that the weights for this quadrature can be calculated analytically from the eigenvectors given above.

3. The zeros of Bessel functions. The starting point for this calculation is the well-known recurrence formula for Bessel functions:

$$\frac{1}{x}J_\nu(x) = \frac{1}{2\nu}[J_{\nu+1}(x) + J_{\nu-1}(x)]. \tag{3.1}$$

For reasons that will become clear later, it is useful to iterate this relation once obtaining

$$\frac{1}{x^2}J_\nu(x) = \frac{1}{2\nu}\left[\frac{1}{x}J_{\nu+1}(x) + \frac{1}{x}J_{\nu-1}(x)\right]$$
$$= \frac{1}{2\nu}\left[\frac{1}{2(\nu+1)}J_{\nu+2}(x) + \left(\frac{1}{2(\nu+1)} + \frac{1}{2(\nu-1)}\right)J_\nu(x) + \frac{1}{2(\nu-1)}J_{\nu-2}(x)\right].$$

This is now a three-term recurrence formula for Bessel functions with order spaced by 2. If the functions $\phi_n(x)$ are defined as

$$\phi_n(x) = \sqrt{2n+2+\nu}J_{2n+2+\nu}(x), \tag{3.2}$$

the functions $\phi_n(x)$ satisfy the three-term recurrence formula given in (2.3) with $g(x) = 1/x^2$,

$$\alpha_n = \frac{1}{4(2n+3+\nu)\sqrt{(2n+2+\nu)(2n+4+\nu)}}, \tag{3.3}$$

and

$$\beta_n = \frac{1}{2}\left(\frac{1}{2n+3+\nu} \times \frac{1}{2n+1+\nu}\right). \tag{3.4}$$

This provides the matrix T_N defined in (2.5). If we now restrict $\nu > -2$, T_N is real and therefore self-adjoint. This guarantees that its eigenvalues are real and its eigenvectors are orthogonal.

The two endpoint terms that make up the nonzero elements of $r_N(x)$ are

$$\alpha_{-1}\phi_{-1}(x) = \frac{1}{4(\nu+1)\sqrt{\nu+2}}J_\nu(x) \tag{3.5}$$

and

$$\alpha_N\phi_{N+1}(x) = \frac{1}{4(2N+\nu+3)\sqrt{2N+\nu+2}}J_{2N+4+\nu}(x). \tag{3.6}$$

In the limit $N \to \infty$ with x fixed, $\alpha_N\phi_{N+1}(x) \to 0$, and the eigenvalues of T_N converge to $1/j_{\nu,i}^2$, where $j_{\nu,i}$ is the ith root of $J_\nu(x)$. For large but finite N, $\alpha_N\phi_{N+1}(x)$ is small but nonzero. If the eigenvalues of T_N, denoted λ_i, are arranged in decreasing order (i.e., in increasing order for the roots of $J_\nu(x)$), what one obtains is the following: the small roots are obtained to machine accuracy, but for some value of i the values determined from λ_i begin to differ from $1/j_{\nu,i}^2$. This error grows rapidly with increasing i. Since this error limits the range of i for a given N, for which this method can be used to determine the roots of $J_\nu(x)$, we will investigate the source of this error in the limit that $\alpha_N\phi_{N+1}(x)$ is small. In this limit, first order perturbation theory can be

used to obtain the relation between the eigenvalues λ_i and $1/j_{\nu,i}^2$ at large but finite N. Using the fact that the eigenvectors of T_N are orthogonal, we obtain from (2.4)

$$1/j_{\nu,i}^2 = \lambda_i + \frac{\alpha_N \phi_N(j_{\nu,i})\phi_{N+1}(j_{\nu,i})}{\sum_{n=0}^{N}(\phi_n(j_{\nu,i})^2}. \tag{3.7}$$

Here we have assumed that the error term

$$R = \frac{\alpha_N \phi_N(j_{\nu,i})\phi_{N+1}(j_{\nu,i})}{\sum_{n=0}^{N}\phi_n(j_{\nu,i})^2} \tag{3.8}$$

is small and for lowest order the eigenvectors of T_N are given by Φ_N. The function R can be evaluated using Debye's asymptotic expansion for Bessel functions of large μ and fixed $z < 1$:

$$J_\mu(\mu z) = \frac{1}{\sqrt{2\pi\mu}}\left(\frac{ze^{\sqrt{1-z^2}}}{1+\sqrt{1-z^2}}\right)^{\mu}(1-z^2)^{-\frac{1}{4}}(1+O(1/\mu)). \tag{3.9}$$

Finally, we use the fact that

$$S(x) = \frac{x^2}{4}(J_{\nu-1}^2(x) - J_\nu(x)J_{\nu-2}(x)) = \sum_{n=0}^{\infty}(2n+\nu)J_{2n+\nu}(x)^2 = \sum_{n=-1}^{\infty}\phi_n^2(x). \tag{3.10}$$

If $\phi_N(j_{\nu,i})$ is small as is required for R to be small, $S(j_{\nu,i})$ is approximately equal to the sum in (3.8). In the limit $j_{\nu,i} >> \nu$, $S(x_i) \approx j_{\nu,i}/2\pi$. For $z_i = j_{\nu,i}/(2N+3+\nu)$ the relative error in the eigenvalue (twice the error in $j_{\nu,i}$) introduced by R is

$$\epsilon = j_{\nu,i}^2 * R_i \approx \frac{1}{4(2N+3+\nu)}\frac{z_i}{\sqrt{1-z_i^2}}\left(\frac{z_i e^{\sqrt{1-z_i^2}}}{(1+\sqrt{1-z_i^2})}\right)^{4N+6+2\nu}. \tag{3.11}$$

Clearly for small z and large N, ϵ is vanishingly small. If we use the fact that the large zeros of $J_\nu(x)$ are approximately given by $j_{\nu,i} = (i + \frac{1}{2}\nu - \frac{1}{4})\pi$, we see that

$$\left(2i + \nu - \frac{1}{2}\right) < \frac{2}{\pi}(2N+3+\nu) \tag{3.12}$$

for $z_M < 1$. Consider as an example $\nu = 0$ and $N = 100$. For $i = 56$ we obtain from (3.11) $\epsilon = 2 \times 10^{-12}$; ϵ increases at $i = 58$ to 2×10^{-9} and is unacceptably large at $i = 64$, the value for which $z_i = 1$. When this experiment is performed numerically in double precision, the zeros agree to 14 significant figures with tabulated values for the first 55 zeros. The 56th zero has 12 figure accuracy, falling to 9 figures at 58. The accuracy deteriorates rapidly at larger i. The time required by this calculation on an IBM RS6000-370 workstation was 0.02sec.

The reason is now clear for using the second recurrence formula rather than the first. Using the first would have found both the positive and negative roots, thereby duplicating the effort and would have required a matrix twice as large as that required for the second recurrence formula to produce the same number of zeros.

For $\nu > -2$, T_N is self-adjoint because it is a real symmetric tridiagonal matrix. (See appendix for the Bessel function code to be used with EISPACK TQL2.) For $\nu < -2$, T_N has one pair of symmetric imaginary elements and therefore requires a more general (and slower) code to determine the eigenvalues. The error analysis which

used the fact that the eigenvectors of a self-adjoint matrix with differing eigenvalues are orthogonal may also need to be modified for this range of ν.

This technique can be used to determine the zeros of Bessel functions of any real order excluding the negative integer values. Since $J_n(x) = (-1)^n J_{-n}(x)$, these special points are of no interest. This method and the code are very simple when $\nu > -2$.

4. Zeros of other special functions. In this section the method described above will be applied to two other sets of special functions that satisfy three-term recurrence formulas. These will provide examples of two different ways in which the requirements on the nonzero elements of $r_N(x)$ can be treated.

First, consider regular Coulomb wave functions. In the notations of [3], the Coulomb wave function $F_L(\eta, \rho)$ satisfies the following recurrence formula:

$$\frac{1}{\rho}F_L(\eta,\rho) = \frac{\sqrt{(L+1)^2+\eta^2}}{(2L+1)(L+1)}F_{L+1}(\eta,\rho) - \frac{\eta}{L(L+1)}F_L(\eta,\rho) + \frac{\sqrt{L^2+\eta^2}}{L(2L+1)}F_{L-1}(\eta,\rho). \tag{4.1}$$

If $\phi_L(\rho)$ is defined to be

$$\phi_L(\rho) = \sqrt{2L+1}F_L(\eta,\rho), \tag{4.2}$$

a three-term recurrence formula, as given in (2.3), is obtained with $g(\rho) = 1/\rho$,

$$\alpha_L = \frac{\sqrt{(L+1)^2+\eta^2}}{(L+1)\sqrt{(2L+1)(2L+3)}}, \tag{4.3}$$

and

$$\beta_L = -\frac{\eta}{L(L+1)}. \tag{4.4}$$

For large L the Coulomb wave function behavior is similar to that of the Bessel function,

$$F_L(\eta,\rho) \to \frac{e^{-\frac{\eta\pi}{2}-1}}{\sqrt{2}\left(\frac{e\rho}{2L}\right)^{L+1}}. \tag{4.5}$$

The procedure for obtaining the zeros of $F_{L_0}(\eta,\rho)$ is as follows: Form the matrix of α's and β's starting with $L = L_0 + 1$ and ending with L_{max} which must be large enough so that the endpoint error is negligible for the range of zeros to be calculated. The eigenvalues of this matrix with large magnitude will be the reciprocal of the zeros of $F_{L_0}(\eta,\rho)$. This differs from the Bessel function in that the negative and positive zeros are not related by symmetry. In practice it appears that $L_{max} = 100$ produces 50 accurate zeros of $F_0(\eta,\rho)$ with essentially the same computing time as was needed for the Bessel function case.

A second example of this technique is provided by associated Legendre functions. These functions satisfy the following three-term recurrence formula:

$$xP_\nu^{-\mu}(x) = \frac{\nu+\mu+1}{2\nu+1}P_{\nu+1}^{-\mu}(x) + \frac{\nu-\mu}{2\nu+1}P_{\nu-1}^{-\mu}(x). \tag{4.6}$$

If we choose $\nu = \mu + n$ and define $\phi_n = \gamma_n P_{\mu+n}^{-\mu}(x)$, we obtain the recurrence formula of (2.3) with

$$\alpha_n = \sqrt{\frac{(n+1)(2\mu+n+1)}{4(\mu+n+1)^2-1}} \tag{4.7}$$

and $\beta_n = 0$. The fact that α_{-1} is zero means that the only extra term in (2.5) is at the upper end. This means that like the case of $\sin(nx)$ the eigenvalues of the matrix will be the zeros of $P_{\mu+N+1}^{-\mu}(x)$. This result will be valid for any $N > 0$.

5. Conclusions. A very simple and relatively efficient algorithm for obtaining the zeros of certain special functions has been derived and applied to several different special functions. The required programming has very few lines of code, and changing from one special function to another only requires changing three to four lines.

The applications to these particular functions are examples of this method and are not meant to be an exhaustive list. There are no doubt other special functions which satisfy the basic requirements for this approach to succeed.

6. Appendix. The following is the code for use with the EISPACK routine for evaluation of the eigenvalues and eigenvectors of a tridiagonal matrix (TQL2). Since the eigenvectors are not needed and the sorting will produce the zeros in wrong order, both of these operations should be removed from TQL2.

```
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSIONE(400),D(400)
c     nt number of zeros, a is Bessel fn  order
      read(5,*)nt,a
      nmax=2*nt
      do 10 i=1,nmax
         fl=dfloat(i)+.5d0*a+.5d0
         d(i)=.125d0/fl/(fl-1.d0)
         e(i+1)=.125d0/fl/dsqrt(4.d0*fl**2-1.d0)
 10   continue
c     input e(i)=alpha, d(i)= beta; tql2 returns eigenvalues
c     of symmetric tridiagonal matrix in d(i); unsorted
      call tql2(d,e,nmax,ierr)
c     form zeros by inverse of g(x)
      do 20 i=1,nmax
         d(i)=1.d0/dsqrt(d(i))
 20   continue
c     sort zeros
      do 30 i=1,nmax
         a1=d(i)
         do 25 j=i+1,nmax
            if(d(j).lt.a1)then
               aa=d(j)
               d(J)=a1
               a1=aa
            endif
 25      continue
         d(i)=a1
 30   continue
```

```
      do 40 i=1,nt
         write(6,*)i,d(i)
 40   continue
      stop
      end
```

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