An Application of the Finite Element Approximation Method to Find the Complex Zeros of the Modified Bessel Function $K_n(z)$

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Abstract. Using a finite element approximation, an iterative optimization scheme is described to find the z zeros of $K_n(z)$ for fixed order n. Two computer programs have been implemented to find the complex zeros with a computational accuracy of either 13 or 27 significant digits. The optimization scheme described in the paper may also be readily applied to find real and complex zeros of an arbitrary function with real and complex coefficients. Neither its accuracy nor its efficiency is affected by the number of the roots of the function.

1. Introduction. In investigation of wave propagation and scattering in an elastic medium, the modified Bessel functions of the second kind $K_n(z)$ are used to describe the potentials for outgoing radiation waves which decay with distance from their source. If scattering problems are studied by use of integral transforms, it becomes necessary to determine the z zeros of $K_n(z)$ in order to locate the poles required for inversion of the transform.

Luke [7] evaluated the zeros of Bessel functions by means of rational approximations. Such approximations have proven useful, both as first approximations of the zeros and as the starting point for iterative schemes that use higher-order rational approximations to yield more accurate estimates of the zeros. The error in the rational approximations for $K_n(z)$ is treated by Fields [3] and Luke [8], [9].

Other methods have also been employed successfully [12]. Olver [10] evaluated zeros of Bessel functions of large order using uniform asymptotic expansions. For the case of Hankel functions, this work has been extended by Cochran and Hoffspiegel [1]. Based on the McMahon and Olver expansions, Döring [2] derived a method for the evaluation of complex zeros of cylinder functions.

By tracing the argument of $K_n(z)$ along the four sides of a square, and using a double linear interpolation, Parnes [12] has given an iterative scheme to obtain the complex z zeros of $K_n(z)$ for fixed integer orders $n = 2, 3, \ldots, 10$. The scheme consists of generating a sequence of squares whose sides are reduced by a reduction factor of 0.1 at each iteration. If the double linear interpolation could ensure that a complex

zero would always be within these squares, each reduction in the size of the square would yield a further significant figure in the location of the zeros.

In the following section a finite element method for finding the complex z zeros of $K_n(z)$ is proposed. The method compares favorably with Parnes's iterative scheme insofar as its rate of convergence, computational accuracy and efficiency are concerned. It also compares favorably with other iterative methods such as Ward's downhill method [14] and Frank's quadratic approximation method [4].

2. Formulas and Method. The modified Bessel function of the second kind is defined as follows:

$$K_n(z) = \frac{1}{2} \sum_{r=0}^{n-1} (-1)^r \frac{(n-r-1)!}{r!} \left(\frac{2}{z}\right)^{n-2r}$$

(1)

$$+ (-1)^{n+1} \sum_{r=0}^{\infty} \frac{1}{r!(n+r)!} \left(\frac{z}{2}\right)^{n+2r} \left\{ \ln\left(\frac{z}{2}\right) - \frac{1}{2} \left[\Psi(r+1) + \Psi(n+r+1) \right] \right\},$$

where

$$\Psi(n+r+1) = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n+r} - \gamma \quad \text{and} \quad \Psi(1) = -\gamma$$

with

$$\gamma = \lim_{m \to \infty} \left[\sum_{k=1}^{m} \frac{1}{k} - \ln(m) \right]$$

$$= 0.57721\ 56649\ 01532\ 86060\ 65120\ 90082\ 40243\ 10421\ \ldots \quad [13].$$

Let

(2) $$F(x_1, x_2) = [R(x_1, x_2)]^2 + [I(x_1, x_2)]^2 \geqslant 0,$$

where $R(x_1, x_2)$ and $I(x_1, x_2)$ are, respectively, the real and imaginary parts of $K_n(z)$ with $z = x_1 + ix_2$.

The problem of finding the z zeros of $K_n(z)$ may be reduced to determination of x_1 and x_2 to minimize $F(x_1, x_2)$. The proposed method of finding the minimum of $F(x_1, x_2)$ is described in Appendix I. This method starts with an arbitrarily chosen initial point $(x_1^0\ x_2^0)$ and generates a sequence of further points $(x_1^1, x_2^1), \ldots,$ $(x_1^n, x_2^n), \ldots,$ that converges to a point where $F(x_1, x_2)$ is minimal. At each iteration $F(x_1, x_2)$ is approximated by a quadratic function $F^*(x_1, x_2)$, and the next point of the sequence is chosen as the point where $F^*(x_1, x_2)$ is minimal.

3. Results and Observations. All calculations were undertaken on a CDC 6400 computer. A Fortran program, using double-precision arithmetic, was able to perform the calculations to an accuracy of 27 significant figures. However, as complex double-precision operations are not available in standard programming languages, the real and

imaginary parts of $K_n(z)$ had to be evaluated by the following formulas:

Real:

$$R(z) = \frac{1}{2} \sum_{r=0}^{n-1} (-1)^r \frac{(n-r-1)!}{r!} \left(\frac{\rho}{z}\right)^{2r-n} \cos(2r-n)\theta$$

$$+ (-1)^{n+1} \sum_{r=0}^{\infty} \frac{1}{r!(r+n)!} \left(\frac{\rho}{2}\right)^{2r+n}$$

$$\cdot \left\{ \left[\ln\left(\frac{\rho}{2}\right) - \frac{\psi(r+1)}{2} - \frac{\psi(r+n+1)}{2} \right] \cos(2r+n)\theta - \theta \sin(2r+n)\theta \right\},$$

Imaginary:

$$I(z) = \frac{1}{2} \sum_{r=0}^{n-1} (-1)^r \frac{(n-r-1)!}{r!} \left(\frac{\rho}{2}\right)^{2r-n} \sin(2r-n)\theta$$

$$+ (-1)^{n+1} \sum_{r=0}^{\infty} \frac{1}{r!(r+n)!} \left(\frac{\rho}{2}\right)^{2r+n}$$

$$\cdot \left\{ \left[\ln\left(\frac{\rho}{2}\right) - \frac{\psi(r+1)}{2} - \frac{\psi(r+n+1)}{2} \right] \sin(2r+n)\theta + \theta \cos(2r+n)\theta \right\},$$

where ρ and θ are the modulus and argument of z, respectively. The complex zeros of $K_n(z)$ were determined for integer order $n = 2(1)10$ and are shown in Table II. At these zeros, $F(x_1, x_2)$, as defined by (2), is of the order of 10^{-55}.

TABLE I

Coordinates of the nodes, and the values of α_0, α_1, α_2 at these nodes

$Q^{(i,j)}$	$x_1^{(i,j)}$	$x_2^{(i,j)}$	$\alpha_0^{(i,j)}$	$\alpha_1^{(i,j)}$	$\alpha_2^{(i,j)}$
$Q^{(0,0)}$	$x_1^{(0,0)} = x_1^r - \frac{1}{3}h^r$	$x_2^{(0,0)} = x_2^r - \frac{1}{3}h^r$	1	0	0
$Q^{(1,1)}$	$x_1^{(1,1)} = x_1^{(0,0)} + h^r$	$x_2^{(1,1)} = x_2^{(0,0)}$	0	1	0
$Q^{(2,2)}$	$x_1^{(2,2)} = x_1^{(0,0)}$	$x_2^{(2,2)} = x_2^{(0,0)} + h^r$	0	0	1
$Q^{(0,1)}$	$x_1^{(0,1)} = x_1^{(0,0)} + \frac{1}{2}h^r$	$x_2^{(0,1)} = x_2^{(0,0)}$	$\frac{1}{2}$	$\frac{1}{2}$	0
$Q^{(0,2)}$	$x_1^{(0,2)} = x_1^{(0,0)}$	$x_2^{(0,2)} = x_2^{(0,0)} + \frac{1}{2}h^r$	$\frac{1}{2}$	0	$\frac{1}{2}$
$Q^{(1,2)}$	$x_1^{(1,2)} = x_1^{(0,0)} + \frac{1}{2}h^r$	$x_2^{(1,2)} = x_2^{(0,0)} + \frac{1}{2}h^r$	0	$\frac{1}{2}$	$\frac{1}{2}$

It appears that the required number of iterations, and hence the amount of CPU time required to obtain the zeros of $K_n(z)$, is very sensitive to changes in the reduction factor λ of the size of the finite elements. Starting from an initially chosen point where $x_1 = -1.3$ and $x_2 = 0.5$, and with values of the reduction factor chosen as

TABLE II

The real parts $R(z)$ and imaginary parts $I(z)$ of
the complex zeros of $K_n(z)$ with $n = 2(1)10$

n	R(z)	±I(z)
2	-1.2813737976560964788484347943	4.2948496520871968779577284110
3	-1.6817888047458454647221805246	1.3080120322739490396502284389
4	-1.9781618634659070241700412324	2.2043719815468711802301895462
4	-2.6286711679571242189239356978	4.3269664862177846518524769588
5	-2.2186262746398760466991398972	3.1130829449859484932024599078
5	-3.1351328447046434221402224695	1.3038823977137057333868902412
6	-2.4234043880011252372669320326	4.0309615812693082518160866112
6	-3.5510979040000786787689256194	2.1834951775778858208942180135
6	-3.9615580702543404860650878072	4.3334540861473783228197493649
7	-2.6031262658681676073605916898	4.9559696065385237377946547292
7	-3.9081257398031834786414725236	3.0708717702488955667126782799
7	-4.5126267774997091289243634516	1.3027788416202445155997188405
8	-2.7641429773113422214747067049	5.8867128822557099755500071045
8	-4.2231522789550338555580428982	3.9650659693874916655430042023
8	-4.9882787925531101790986431543	2.1770827464789907589102679543
8	-5.2907612925994479853857895222	4.3357769522400748475850727130
9	-2.9105824231361973641127863752	6.8221903314329512927258712281
9	-4.5064659455202975444947754224	4.8652071432637217649541918277
9	-5.4097474475400236316635820253	3.0565442393434597827549120928
9	-5.8665514666851772591442131577	1.3023283269981807534615329324
10	-3.0452934989589489096726573840	7.7616556708745682219592817911
10	-4.7648453733729039927675961572	5.7705555987099768475527429057
10	-5.7900271641796772769369101588	3.9409726157692468366207406587
10	-6.3783949707941569023306522990	2.1742485862026654802191073802
10	-6.6184818847079360692456212008	4.3368620578620986460836833209

0.5, 0.25, 0.025, and 0.0001, a zero of $K_n(z)$ is found after 45, 23, 13, and 7 iterations, respectively. The effects of the reduction factor λ on the number of iterations and CPU time are shown in Figures II and III.
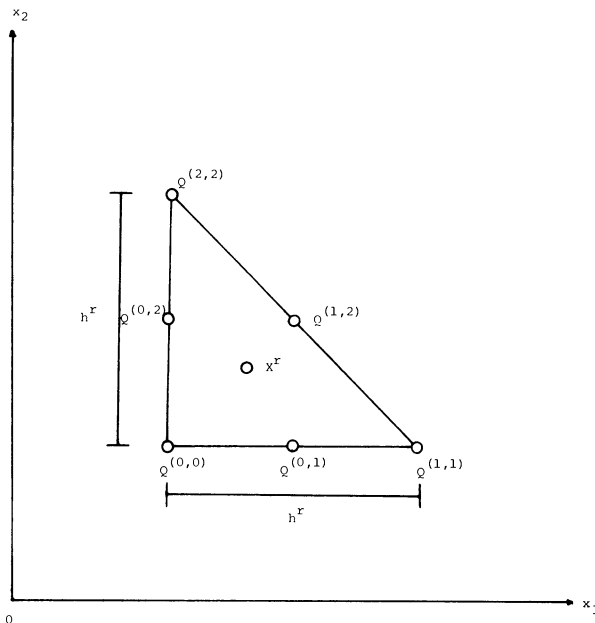

FIGURE I

Finite right-angled triangular element Δ^r associated with $X^r = (x_1^r, x_2^r)$
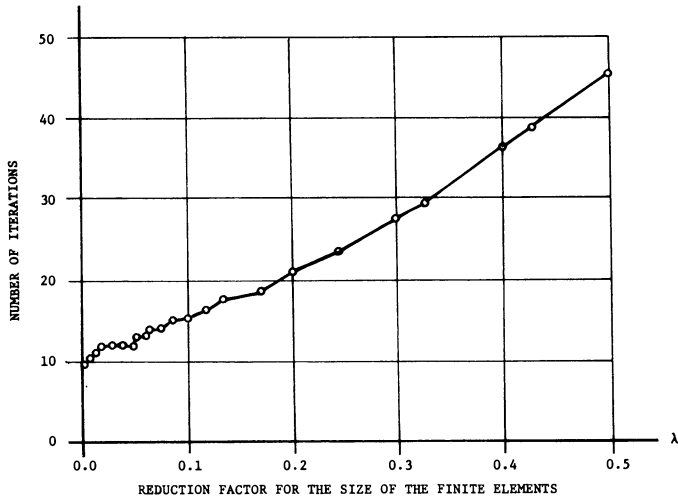
FIGURE II

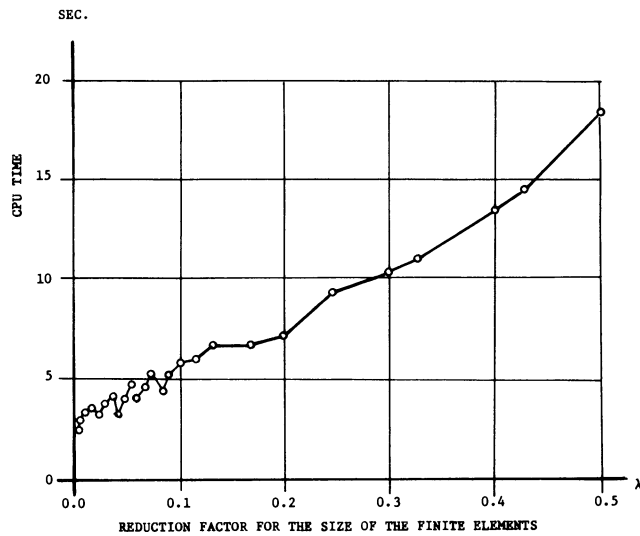*Dependence of number of iterations on the reduction factor for the step size of the finite element*

FIGURE III

Dependence of CPU time on the reduction factor for the step size of the finite element

A second computer program, also written in Fortran, but using single-precision arithmetic has been tested. This program, which is four times faster than the previous version, provides computations to only 13 significant digits.

Appendix I

The Finite Element Algorithm. The algorithm described here is based on a sequence of quadratic surface-fitting problems. At each stage of minimization, the objective function $F(x_1, x_2)$ is approximated by a quadratic form over the finite element region about the current minimum point. Zlámal [16] has proved the existence and uniqueness of such a quadratic polynomial. Each finite element is a right-angle triangle, with nodes at the vertices and midpoints of each side. Ghaderpanah [5] has generalized this technique and applied it in higher-dimensional minimization problems.

Iteration Steps. 1. Set $r = 0$. A starting point $X^0 = (x_1^0, x_2^0)$ and a step size h^0 are given.

2. Select the vertices $Q^{(i,i)}$, $i = 0, 1, 2$, for the right-angle triangle Δ^r according to the following scheme:

$$Q^{(0,0)} = X^r - \left(\frac{h^r}{3}, \frac{h^r}{3} \right),$$

$$Q^{(1,1)} = (q_1^{(0,0)} + h^r, q_2^{(0,0)}),$$

$$Q^{(2,2)} = (q_1^{(0,0)}, q_2^{(0,0)} + h^r)$$

and determine the side midpoints as follows:

$$Q^{(1,k)} = \frac{1}{2} [Q^{(1,1)} + Q^{(k,k)}], \quad 0 \leqslant 1 < k < 2.$$

Figure I illustrates the construction of the element about the point X^r.

3. Compute the nodal values $F^{(i,j)}$ at the six nodes $Q^{(i,j)}$, i.e.,

$$F^{(i,j)} = F(Q^{(i,j)}), \quad 0 \leqslant i \leqslant j \leqslant 2.$$

4. Approximate F by the quadratic F^* given by

$$F^*(X) = \sum_{i=0}^{2} \sum_{j=i}^{2} F^{(i,j)} S^{(i,j)}(\alpha_i, \alpha_j),$$

where $S^{(i,j)}$, $0 < i \leqslant j \leqslant 2$, are the quadratic shape functions defined by

$$S^{(i,j)}(\alpha_i, \alpha_j) = 2(2 - \delta_{ij})\alpha_i\alpha_j - \frac{1}{2}\delta_{ij}(\alpha_i + \alpha_j)$$

and δ_{ij} is the Kronecker delta. The functions α_i are the coordinate functions defined by

$$\alpha_i(X) = \frac{1}{h^r} (x_i - q_i^{(0,0)}), \quad i = 1, 2, \quad \text{and} \quad \alpha_0 = 1 - \alpha_1 - \alpha_2.$$

It is easy to verify that the functions $S^{(i,j)}$ and α_i satisfy the respective properties of shape functions and natural coordinate functions given in [15]. The values of α_i at each node are explicitly shown in Table I. It may be shown that the quadratic F^* is continuous and interpolates F at the six nodes $Q^{i,j}$, i.e.,

$$F^*(Q^{(i,j)}) = F(Q^{(i,j)}), \quad 0 \leqslant i \leqslant j \leqslant 2.$$

Moreover, the first and second partial derivatives of F and F^* at $Q^{(0,0)}$ are identical. Therefore, the approximation is of second order over the triangular region, thus

$$|F(X) - F^*(X)| \approx O((h^r)^3)$$

for all X in Δ^r.

    5. Determine the new approximation to the local minimum X^{r+1} as follows:

$$x_i^{r+1} = q_i^{(0,0)} + \alpha_i^r h^r, \quad i = 1, 2,$$

where $(\alpha_0^r, \alpha_1^r, \alpha_2^r)$ is a stationary of F^* in the natural coordinate system obtained by solving the system of algebraic equations in the unknowns α_0^r, α_1^r and α_2^r given by

$$\frac{\partial F^*}{\partial \alpha_1^r} = 0, \quad \frac{\partial F^*}{\partial \alpha_2^r} = 0, \quad \alpha_0^r + \alpha_1^r + \alpha_2^r = 1.$$

The solution of this system is given by:

$$\alpha_1^r = (B_1 A_{22} - B_2 A_{12})/D, \quad \alpha_2^r = (B_2 A_{11} - B_1 A_{21})/D$$

and $\alpha_0^r = 1 - \alpha_1^r - \alpha_2^r$, where $D = A_{11}A_{22} - A_{12}A_{21}$ and

$$\begin{cases} A_{11} = F^{(0,0)} - 2F^{(0,1)} + F^{(1,1)}, \\ A_{22} = F^{(0,0)} - 2F^{(0,2)} + F^{(2,2)}, \\ A_{12} = A_{21} = F^{(0,0)} - F^{(0,1)} - F^{(0,2)} + F^{(1,2)}, \\ B_1 = \tfrac{3}{4}F^{(0,0)} - F^{(0,1)} + \tfrac{1}{4}F^{(1,1)}, \\ B_2 = \tfrac{3}{4}F^{(0,0)} - F^{(0,2)} + \tfrac{1}{4}F^{(2,2)}. \end{cases}$$

Let δ^r be the distance between the solution $\bar{X} = (\bar{x}_1, \bar{x}_2)$ and the point $X^r = (x_1^r, x_2^r)$, i.e., $\delta^r = \|X^r - \bar{X}\|$. It may be shown by use of the Taylor series expansion of F that for sufficiently small δ^r, δ^{r+1} is reduced to $O((\delta^r)^2)$.

    6. *Termination Criterion and Convergence.* Let $0 < \lambda < 1$, be a predetermined reduction factor for the step size. Define the step size h^{r+1} for the next iteration as follows:

$$h^{r+1} = \begin{cases} \lambda h^r & \text{if } X^r \text{ is inside } \Delta^r, \text{ i.e., } 0 \leqslant \alpha_0^r, \alpha_1^r, \alpha_2^r \leqslant 1, \\ h^r & \text{if otherwise.} \end{cases}$$

Terminate the process if $h^{r+1} < \epsilon_1$ or

$$F(X^{r+1}) - F(X^r) < \epsilon_2 \quad \text{and} \quad \|X^{r+1} - X^r\| < \epsilon_3,$$

where the nonzero scalars ϵ_1, ϵ_2 and ϵ_3 are predetermined minimal improvement, minimal step length and minimal step size, respectively. Otherwise, accept the new point X^{r+1}, set $r = r + 1$ and repeat from step 2.

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