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The Topological Degree Theory for the Localization and Computation of Complex Zeros of Bessel Functions

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Abstract

We study the complex zeros of Bessel functions of real order of the first and second kind and their first derivatives. The notion of the topological degree is employed for the calculation of the exact number of these zeros within an open and bounded region of the complex plane, as well as for localization of these zeros. First, we prove that the value of the topological degree provides the total number of complex roots within this region. Subsequently, these roots are computed by a generalized bisection method. The method presented here computes complex zeros of Bessel functions, requiring only the algebraic signs of the real and imaginary part of these functions. It has been implemented and tested, and performance results are presented.

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Keywords: Bessel functions, complex zeros, topological degree, localization of zeros, computation of roots, generalized method of bisection.

1. Introduction

Many scientists are interested in finding the zeros of Bessel functions of first and second kind:

$$J_\nu(z) = z^\nu \sum_{m=0}^{\infty} \frac{(-1)^m \, z^{2m}}{2^{2m+\nu} \, m! \, \Gamma(\nu+m+1)}, \tag{1.1}$$

and

$$Y_\nu(z) = \begin{cases} \dfrac{J_\nu(z) \, \cos \nu\pi - J_{-\nu}(z)}{\sin \nu\pi}, & \nu \text{ nonintegral}, \\[2ex] \lim\limits_{n\to\nu} \dfrac{J_n(z) \, \cos n\pi - J_{-n}(z)}{\sin n\pi}, & \nu = 0,1,2,\ldots . \end{cases} \tag{1.2}$$

Most of the results obtained refer to upper and/or lower bounds of the real zeros, or regions of existence or non–existence in the complex plane, for the complex zeros.

In previous communications of ours [20,22,23] the localization and computation of the real zeros of Bessel and Bessel related functions have been treated.

In the present paper we tackle the complex roots. We use the notion of the topological degree, to compute the total number of complex zeros of a Bessel function within a given region. The numerical calculation of these roots is subsequently performed utilising a generalized bisection method and the characteristic polyhedron criterion. The methods implemented here require only the algebraic signs of the functions involved.

2. The topological degree for the computation of the total number of zeros

Consider the equation $F_n(x) = \mathcal{O}_n$ ($\mathcal{O}_n = (0,\dots,0)$ denotes the origin of $\mathbb{R}^n$), where $F_n = (f_1,\dots,f_n)^\top : \mathcal{D}_n \subset \mathbb{R}^n \to \mathbb{R}^n$ is a function defined and twice continuously differentiable in a bounded domain $\mathcal{D}_n$ of $\mathbb{R}^n$ with boundary $\mathrm{b}(\mathcal{D}_n)$, whose zeros are simple and not located on $\mathrm{b}(\mathcal{D}_n)$. Then the *topological degree of F_n at $\mathcal{O}_n$ relative to $\mathcal{D}_n$* is defined by the following sum [2,9]:

$$\deg[F_n, \mathcal{D}_n, \mathcal{O}_n] = \sum_{X \in F_n^{-1}(\mathcal{O}_n)} \operatorname{sgn} \mathcal{J}(X), \tag{2.1}$$

where, $\mathcal{J}$ stands for the Jacobian determinant and sgn denotes the sign function.

The topological degree can be represented by the Kronecker integral as follows [8]:

$$\deg[F_n, \mathcal{D}_n, \mathcal{O}_n] = \frac{\Gamma(n/2)}{2\pi^{n/2}} \int\!\!\int_{b(\mathcal{D}_n)}\!\!\cdots\int \frac{\sum_{k=1}^{n} A_k dx_1 \cdots dx_{k-1} dx_{k+1} \cdots dx_n}{({f_1}^2 + {f_2}^2 + \cdots + {f_n}^2)^{n/2}}, \tag{2.2}$$

where the A_k are the following determinants:

$$A_k = (-1)^{n(k-1)} \left| F_n \quad \frac{\partial F_n}{\partial x_1} \quad \cdots \quad \frac{\partial F_n}{\partial x_{k-1}} \quad \frac{\partial F_n}{\partial x_{k+1}} \quad \cdots \quad \frac{\partial F_n}{\partial x_n} \right|. \tag{2.3}$$

In the literature there are several numerical methods for the computation of the topological degree [1,5,6,10–13].

Since $\deg[F_n, \mathcal{D}_n, \mathcal{O}_n]$ is equal to the number of simple solutions of $F_n(x) = \mathcal{O}_n$ which give positive Jacobian, minus the number of simple solutions which give negative Jacobian, the total number $\mathcal{N}^r$ of the roots of F_n can be obtained by the value of $\deg[F_n, \mathcal{D}_n, \mathcal{O}_n]$, if the Jacobian possesses the same sign at these roots.

The problem of finding complex zeros of a Bessel function $\mathcal{B}_\nu(z)$, where $\mathcal{B}_\nu$ stands for J_ν, J'_ν, Y_ν or Y'_ν, in a given domain $\mathcal{D}_2$, amounts to finding points $z^\star = z_1^\star + i\, z_2^\star \in \mathcal{D}_2$ which satisfy the following system of equations:

$$\begin{aligned} \Re\{\mathcal{B}_\nu(z^\star)\} &= 0, \\ \Im\{\mathcal{B}_\nu(z^\star)\} &= 0, \end{aligned} \tag{2.4}$$

where $\Re\{\mathcal{B}_\nu(z^\star)\}$ and $\Im\{\mathcal{B}_\nu(z^\star)\}$ indicate the real and imaginary part of $\mathcal{B}_\nu(z^\star)$ respectively. Obviously, the problem of finding such points is equivalent to solving the following system:

$$F_2(X) = (f_1(X), f_2(X))^\top = \mathcal{O}_2, \tag{2.5}$$

where $X = (x_1, x_2)^\top$ and

$$\begin{aligned} f_1(X) &= \Re\{B_\nu(x_1 + i\, x_2)\} = 0, \\ f_2(X) &= \Im\{B_\nu(x_1 + i\, x_2)\} = 0. \end{aligned} \tag{2.6}$$

The following theorem characterizes the total number of complex zeros of Bessel functions in an open bounded region $\mathcal{D}_2$.

Theorem 2.1 *The total number $\mathcal{N}^r$ of complex zeros of the Bessel function $\mathcal{B}_\nu(z)$, where $\mathcal{B}_\nu(z)$ is $J_\nu(z)$, $J'_\nu(z)$, $Y_\nu(z)$ or $Y'_\nu(z)$, in an open bounded region $\mathcal{D}_2$ is equal to the value of the topological degree of F_2 at $\mathcal{O}_2$ relative to $\mathcal{D}_2$ where:*

$$F_2(X) = (f_1(X), f_2(X))^\top = \Big(\Re\{\mathcal{B}_\nu(x_1 + i\,x_2)\}, \Im\{\mathcal{B}_\nu(x_1 + i\,x_2)\}\Big)^\top. \tag{2.7}$$

Proof. Since $\mathcal{B}_\nu$ is an analytic function in the complex plane, the Cauchy–Riemann equations are satisfied. In particular, if $F_2(x_1 + i\,x_2) = f_1 + i\,f_2$, then the following hold:

$$\frac{\partial f_1}{\partial x_1} = \frac{\partial f_2}{\partial x_2} \qquad \text{and} \qquad \frac{\partial f_1}{\partial x_2} = -\frac{\partial f_2}{\partial x_1}.$$

So, the Jacobian of F_2 is:

$$\begin{vmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} \\ \dfrac{\partial f_2}{\partial x_1} & \dfrac{\partial f_2}{\partial x_2} \end{vmatrix} = \begin{vmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} \\ -\dfrac{\partial f_1}{\partial x_2} & \dfrac{\partial f_1}{\partial x_1} \end{vmatrix} = \left[\frac{\partial f_1}{\partial x_1}\right]^2 + \left[\frac{\partial f_1}{\partial x_2}\right]^2. \tag{2.8}$$

As it is known [24, p.479], the zeros of $J_\nu(z)$ and $Y_\nu(z)$ are all simple. Now, if z_0 is a multiple zero of $J'_\nu(z)$ or $Y'_\nu(z)$, then the Bessel equation

$$z^2 y''(z) + zy'(z) + (z^2 - \nu^2)y(z) = 0$$

implies that z_0 must satisfy the relation $z_0^2 - \nu^2 = 0$. Therefore, for real values of ν, $J'_\nu(z)$ and $Y'_\nu(z)$ have no multiple complex zeros. Thus, the Jacobian determinant of F_2 is positive at the zeros of $\mathcal{B}_\nu$. Consequently, the total number $\mathcal{N}^r$ of solutions of $F_2(X) = \mathcal{O}_2$ can be obtained by the value of $\deg[F_2, \mathcal{D}_2, \mathcal{O}_2]$. Thus the theorem is proved. □

We could use any one of the degree computation methods (see for example [1,5,6,10–13]) to determine the total number of complex zeros. Here we use Kearfott's method [5–7] which is briefly described in the sequel.

Suppose that $S^{n-1} = \langle x_1, x_2, \dots, x_n \rangle$ is an $(n-1)$-simplex in $\mathbb{R}^n$ [5,6,11] and assume $F_n = (f_1, f_2, \dots, f_n)^\top : S^{n-1} \to \mathbb{R}^n$ is continuous. Then the *range simplex associated with S^{n-1} and F_n*, denoted by $\mathcal{R}(S^{n-1}, F_n)$, is an $n \times n$ matrix with elements a_{kl}, $1 \le k, l \le n$ given by:

$$a_{kl} = \begin{cases} 1, & \text{if} \quad f_l(x_k) \ge 0\,, \\ -1, & \text{if} \quad f_l(x_k) < 0\,. \end{cases} \tag{2.9}$$

$\mathcal{R}(S^{n-1}, F_n)$ is called *usable* if one of the following conditions holds:

(a) the elements a_{kl} of $\mathcal{R}(S^{n-1}, F_n)$, are:

$$a_{kl} = \begin{cases} 1, & \text{if} \quad k \ge l\,, \\ -1, & \text{if} \quad l = k+1\,. \end{cases} \tag{2.10}$$

(b) $\mathcal{R}(S^{n-1}, F_n)$ can be put into this form by a permutation of its rows.

When $\mathcal{R}(S^{n-1}, F_n)$ is usable, then the $\mathrm{Par}\big(\mathcal{R}(S^{n-1}, F_n)\big)$ is defined to be 1, if the number of the permutations of the rows required to put $\mathcal{R}(S^{n-1}, F_n)$ into the form (a) is even. If this number is odd then $\mathrm{Par}\big(\mathcal{R}(S^{n-1}, F_n)\big)$ is defined to be -1. For all other cases, we set $\mathrm{Par}\big(\mathcal{R}(S^{n-1}, F_n)\big) = 0$. Then the value of the topological degree of F_n at $\mathcal{O}_n$ relative to an n-dimensional polyhedron P^n can be obtained, under suitable assumptions referring to the boundary of P^n [5,6], by the following relation:

$$\deg[F_n, P^n, \mathcal{O}_n] = \sum_{i=1}^{m} \mathrm{Par}\Big(\mathcal{R}(S^{n-1}, F_n)\Big). \tag{2.11}$$

Obviously, this degree computational method requires only the algebraic signs of the function F_n to be known.

3. The CP–criterion and a generalized bisection

We now give a topological degree based criterion for the existence of a zero of a continuous mapping $F_n = (f_1, f_2, \dots, f_n)^\top : P^n \subset \mathbb{R}^n \to \mathbb{R}^n$ within a predetermined domain. This criterion, called the CP–criterion, is based on the construction of an n–dimensional polyhedron within a scaled translation of the unit cube, which we call "a characteristic polyhedron". The theoretical development of the concepts employed here can be found in [15,21]. Furthermore, a generalized bisection method will be briefly described for the computation of the solutions of $F_n(x) = \mathcal{O}_n$.

To define a characteristic n-polyhedron we construct the $2^n \times n$ matrices $\mathcal{M}_n$ whose rows are formed by all possible combinations of -1, 1. For example for $n = 1, 2$ we have:

$$\mathcal{M}_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}, \qquad \mathcal{M}_2 = \begin{bmatrix} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}. \tag{3.1}$$

Suppose now that $P^n = \langle \Upsilon_1, \Upsilon_2, \dots, \Upsilon_{2^n} \rangle$ is an oriented n–dimensional polyhedron with 2^n vertices, $\Upsilon_k \in \mathbb{R}^n$ (i.e. an orientation has been assigned to its vertices). Then we call the *matrix of signs associated with F_n and P^n*, denoted by $\mathcal{S}(F_n;\, P^n)$, the $2^n \times n$ matrix whose entries in the kth row are the corresponding coordinates of the vector:

$$\mathrm{sgn}\, F_n(\Upsilon_k) = \Big(\mathrm{sgn}\, f_1(\Upsilon_k), \mathrm{sgn}\, f_2(\Upsilon_k), \dots, \mathrm{sgn}\, f_n(\Upsilon_k)\Big). \tag{3.2}$$

In the case $n = 2$, we consider the polyhedron $P^2 = \langle \Upsilon_1, \Upsilon_2, \Upsilon_3, \Upsilon_4 \rangle$. Then the matrix of signs associated with F_2 and P^2 will have the form:

$$\mathcal{S}(F_2;\, P^2) = \begin{bmatrix} \mathrm{sgn}\, f_1(\Upsilon_1) & \mathrm{sgn}\, f_2(\Upsilon_1) \\ \mathrm{sgn}\, f_1(\Upsilon_2) & \mathrm{sgn}\, f_2(\Upsilon_2) \\ \mathrm{sgn}\, f_1(\Upsilon_3) & \mathrm{sgn}\, f_2(\Upsilon_3) \\ \mathrm{sgn}\, f_1(\Upsilon_4) & \mathrm{sgn}\, f_2(\Upsilon_4) \end{bmatrix}. \tag{3.3}$$

P^n is called a *characteristic n-polyhedron relative to* F_n, if $\mathcal{S}(F_n;\, P^n)$ agrees with the matrix $\mathcal{M}_n$ up to a permutation of the rows. Then, under suitable assumptions on the boundary of P^n [5,6],

$$\deg[F_n, P^n, \mathcal{O}_n] = \pm 1 \neq 0, \tag{3.4}$$

which implies, by Kronecker's theorem [9, p.161], the existence of a zero inside P^n [21]. For a detailed description of how to construct a characteristic n-polyhedron to locate a desired zero, see [15,16].

The CP–criterion is a generalization of Bolzano's existence criterion [17].

Next, we turn to the description of a generalized bisection method for computing zeros of any continuous function and at any desired accuracy. This method is used in combination with the CP–criterion, and it is called *characteristic bisection.*

Table 1

Function	a_1	b_1	a_2	b_2	$\mathcal{N}^r$
$J_{-3.5}$	-2.0	2.0	-3.0	3.0	6
	0.5	2.0	-3.0	3.0	2
	-2.0	2.0	0.5	3.0	3
$J_{-4.5}$	-4.0	4.0	-4.0	4.0	8
	0.5	4.0	-4.0	4.0	4
	-4.0	4.0	0.5	4.0	4
$J_{-5.5}$	-4.0	4.0	-4.0	4.0	10
	0.5	4.0	-4.0	4.0	4
	-4.0	4.0	0.5	4.0	5
$Y_{6.2}$	-5.5	5.5	-4.5	4.5	12
	0.5	5.5	-4.5	4.5	6
	-5.5	5.5	0.5	4.5	6
$Y_{6.7}$	-9.0	9.0	-5.0	5.0	14
	0.5	9.0	-5.0	5.0	6
	-9.0	9.0	0.5	5.0	7

Bisection methods for finding solutions of systems of equations depend on a criterion which guarantees that a solution lies within a given region. Then this region is subdivided in such a way that the criterion can again be applied to the new subregion [4–6,14–16]. The method used here has all the advantages of the one-dimensional bisection, it always converges within the initially specified domain and has been successfully applied to various difficult problems [3,18,19]. The only information required is the algebraic signs of the components of the considered function.

In the literature, several bisection methods are available [4–6,14] that require the computation of the topological degree to secure its nonzero value. However, the present characteristic bisection method avoids this computation by ensuring that the topological degree retains a nonzero value at every iteration. To this end, we bisect a characteristic n-polyhedron P^n in such a way that the new refined one is also characteristic. For this purpose the midpoint of a proper 1-simplex (edge) of P^n is used to replace that vertex of P^n for which the signs of the function components are identical.

The number of bisections of the proper 1-simplexes of the initial characteristic polyhedron P^n required to obtain a new refined characteristic polyhedron $P^n_\star$ such that the length of its longest edge $\Delta(P^n_\star)$ satisfies $\Delta(P^n_\star) \leq \varepsilon$, for some $\varepsilon \in (0,1)$, is given by:

$$\zeta = \left\lceil \log_2(\Delta(P^n)\varepsilon^{-1}) \right\rceil , \tag{3.5}$$

(see [21] for a proof) where $\lceil \cdot \rceil$ denotes the smallest integer not less than the real argument.

The CP-criterion combined with knowledge of the total number of zeros can be used to isolate each of the zeros by considering suitable subregions. Once this has been accomplished, generalized bisection can be employed to compute them.

The signs of the real and imaginary parts of Bessel functions can be determined by adding a few dominant terms of the respective series, so that the magnitude of the first neglected term is too small to affect the sign of the summation.

Table 2

Function	$\Re\{z_\nu^*\}$	$\Im\{z_\nu^*\}$
$J_{-3.5}$	0.00000000000000	−2.51821469985976
	−1.86866736701277	−2.04810004956751
	1.86866736701277	−2.04810004956751
	−1.86866736701277	2.04810004956751
	1.86866736701277	2.04810004956751
	0.00000000000000	2.51821469985976
$J_{-4.5}$	−0.90624416289284	−3.09287420339388
	0.90624416289284	−3.09287420339388
	−2.80266861329756	−2.31961612178580
	2.80266861329756	−2.31961612178580
	−2.80266861329756	2.31961612178580
	2.80266861329756	2.31961612178580
	−0.90624416289284	3.09287420339388
	0.90624416289284	3.09287420339388
$J_{-5.5}$	0.00000000000000	−3.84131610077643
	−1.80928426210063	−3.55080092521796
	1.80928426210063	−3.55080092521796
	−3.74122352456633	−2.54691956902185
	3.74122352456633	−2.54691956902185
	−3.74122352456633	2.54691956902185
	3.74122352456633	2.54691956902185
	−1.80928426210063	3.55080092521796
	1.80928426210063	3.55080092521796
	0.00000000000000	3.84131610077643
$Y_{6.2}$	0.62649520528882	−4.27391799602890
	−1.16553459156468	−4.19771702352715
	2.44269288905019	−3.82723553123862
	−3.00555785660360	−3.57433283616921
	4.40075330264958	−2.68766359398660
	−5.07431004353783	−2.12169468594545
	−5.07431004353783	2.12169468594545
	4.40075330264958	2.68766359398660
	−3.00555785660360	3.57433283616921
	2.44269288905019	3.82723553123862
	−1.16553459156468	4.19771702352715
	0.62649520528882	4.27391799602890
$Y_{6.7}$	−0.71454322875555	−4.59849659381814
	1.07287087406319	−4.55152621181362
	−2.52500911890794	−4.16156082248494
	2.89617438090860	−4.00812035260413
	−4.45195609774797	−3.10318047432551
	4.87301234219963	−2.78095055769101
	−7.13134306218891	−0.67166558082952
	−7.13134306218891	0.67166558082952
	4.87301234219963	2.78095055769101
	−4.45195609774797	3.10318047432551
	2.89617438090859	4.00812035260413
	−2.52500911890794	4.16156082248493
	1.07287087406319	4.55152621181362
	−0.71454322875555	4.59849659381814

4. Applications and concluding remarks

We have tried our method with several random regions of the complex plane, and our experience is that it behaves predictably and accurately.

Let us, for instance, locate and compute some complex zeros $z_\nu = (\Re\{z_\nu\}, \Im\{z_\nu\})$ of (1.1) for various ν. We have considered $J_{-4.5}(z)$ and the polyhedron:

$$P^2 = [-4, 4] \times [-4, 4].$$

Using Kearfott's method, we have found that the value of the topological degree relative to P^2 is equal to eight. Thus, by Theorem 2.1, this value is the total number of complex zeros of the above function in P^2. On the other hand, according to Hurwitz Theorem [24, p.483] this function has a total of eight complex zeros in the whole complex plane. Therefore, we have managed to localize all of these zeros in a specific bounded region around the origin. Also, we have considered several other randomly chosen polyhedra and we have obtained similar results. For example, by taking the polyhedron:

$$P^2 = [0.5, 3] \times [0.5, 3],$$

we have found that there exists one single complex zero within it. Employing the CP–criterion and the generalized method of bisection described previously, we have computed this zero, which is:

$$z^\star_{-4.5} = \left(\Re\{z^\star_{-4.5}\}, \Im\{z^\star_{-4.5}\}\right) = (2.80266861329756, 2.31961612178580),$$

within an accuracy of 10^{-15}.

Using the same process we have been able to isolate and compute all the complex zeros of the above function, and they are exhibited in Table 2. Since Kearfott's method depends on a heuristic parameter, we have had to ensure that the estimated number of zeros is correct. For this reason we have used several values of the parameter and, besides, we have tested the results by subdividing the initial polyhedron into smaller regions and calculating the topological degree of the subregions so obtained.

Analogous results have been extracted for $J_{-5.5}(z)$. We have found that it has ten complex zeros, two of which are purely imaginary, and this accords with Hurwitz theorem. All of them lie also within the polyhedron:

$$P^2 = [-4, 4] \times [-4, 4].$$

They have been isolated and computed and are presented in Table 2.

Further results regarding other Bessel functions and starting regions are exhibited in Tables 1 & 2.

In the first table we give the total number $\mathcal{N}^r$ of roots of various Bessel functions existing within several regions. In the second table we display, giving fifteen significant digits, the corresponding complex roots $z^\star_\nu = (\Re\{z^\star_\nu\}, \Im\{z^\star_\nu\})$ of these functions.

It is worth noticing that the nonzero value of the topological degree relative to a polyhedron P^2 ensures, by virtue of Kronecker's existence theorem [9, p.161], the existence of at least one zero within P^2. In such a case, employing the CP–criterion and the generalized bisection method, we are able to isolate and compute these zeros one by one.

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