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A new lower bound for the de Bruijn-Newman constant

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Abstract

A new lower bound, -5, is presented for the so-called de Bruijn-Newman constant. This constant is related to the Riemann hypothesis. The new bound is established by the high-precision computation (with an accuracy of 250 decimal digits) of i) the coefficients of a so-called Jensen polynomial of degree 406, and ii) the so-called Sturm sequence of this polynomial which shows that it has two complex zeros. These complex zeros are given explicitly.

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1 Introduction

Recently, Csordas et al. [2] have introduced the so-called *de Bruijn-Newman constant* Λ as follows. Let the function $H_\lambda(x), \lambda \in \mathcal{R}$, be defined by

$$H_\lambda(x) := \int_0^\infty e^{\lambda t^2} \Phi(t) \cos(xt) dt, \tag{1}$$

where

$$\Phi(t) = \sum_{n=1}^{\infty} (2n^4\pi^2 e^{9t} - 3n^2\pi e^{5t}) \exp(-n^2\pi e^{4t}). \tag{2}$$

The function Φ satisfies the following properties:

i) $\Phi(z)$ is analytic in the strip $-\pi/8 < \Im z < \pi/8$;
ii) $\Phi(t) = \Phi(-t)$, and $\Phi(t) > 0 (t \in \mathcal{R})$;
iii) for any $\epsilon > 0, \lim_{t\to\infty} \Phi^{(n)}(t) \exp[(\pi - \epsilon)e^{4t}] = 0$, for each $n = 0, 1, 2, \ldots$.

The function H_λ is an entire function of order one, and $H_\lambda(x)$ is real for real x. From results of de Bruijn [1] it follows that if the Riemann hypothesis is true, then $H_\lambda(x)$ must possess only real zeros for any $\lambda \geq 0$. Newman has shown [6] that there exists a real number $\Lambda, -\infty < \Lambda \leq \frac{1}{2}$, such that

i) $H_\lambda(x)$ has only real zeros when $\lambda \geq \Lambda$, and
ii) $H_\lambda(x)$ has some non-real zeros when $\lambda < \Lambda$.

This number Λ was baptized the *de Bruijn-Newman constant* in [2]. The truth of the Riemann hypothesis would imply that $\Lambda \leq 0$, whereas Newman [6] conjectures that $\Lambda \geq 0$. In [2] it was proved that $\Lambda > -50$.

In this note we will describe high-precision computations which establish $\Lambda > -5$. Moreover, our computations suggest that trying to improve upon this result would be a formidable task, unless the algorithm used could be improved substantially.

The computations were carried out on the CDC Cyber 995 (about 2 hours CPU time for testing), and on the CDC Cyber 205 (about 30 hours CPU time for 'production') of SARA (The Academic Computer Centre Amsterdam). Brent's MP package was an indispensable tool for the high-precision floating point computations. Since this package has not been vectorized, we used the Cyber 205 just as an extremely fast scalar machine.

This note will rely heavily on [2]. We assume the reader to have a copy of [2] at hand.

2 Algorithm and results

If we expand the cosine in (1) in its Taylor series, we obtain

$$H_\lambda(x) = \sum_{m=0}^{\infty} \frac{(-1)^m b_m(\lambda) x^{2m}}{(2m)!}, \tag{3}$$

where

$$b_m(\lambda) = \int_0^\infty t^{2m} e^{\lambda t^2} \Phi(t) dt,$$

$m = 0, 1, 2, \ldots; \lambda \in \mathcal{R}$. The n-th degree Jensen polynomial $G_n(t;\lambda)$ associated with H_λ is defined by

$$G_n(t;\lambda) := \sum_{k=0}^{n} \binom{n}{k} \frac{k! b_k(\lambda)}{(2k)!} t^k, \tag{4}$$

and it is shown in [2] that if there exists a positive integer m and a real number $\hat{\lambda}$ such that $G_m(t;\hat{\lambda})$ possesses a non-real zero, then $\hat{\lambda} < \Lambda$. The problem is to find m, given $\hat{\lambda}$.

In [2] a lower bound for Λ was constructively obtained as follows. For suitable values of λ and N the moments $b_m(\lambda), m = 0, 1, \ldots, N$ were computed with a known precision, by means of Romberg quadrature. For the corresponding Jensen polynomial *all* its zeros were computed by means of the Jenkins algorithm. A theorem of Ostrowski was then invoked to find an upper bound for the error made by using approximate rather than exact coefficients in the Jensen polynomial. This error was small enough to guarantee that the complex zero found by high-precision computation indeed was an approximation of a complex zero of the Jensen polynomial. The sensibility of the zeros of polynomials for errors in their coefficients required that the computations were performed in very high precision. Csordas et al. [2] used 110 digits of precision for their proof that $-50 < \Lambda$. As a partial check, we repeated their computations in double precision on a CDC Cyber 995 (which means an accuracy of about 28 decimal digits) and could reproduce the complex zero of $G_{16}(t;-50)$ with an accuracy of about 20 decimal digits. This illustrates the enormous amount of extra work needed to provide a *proof* of the existence of complex zeros of the Jensen polynomials $G_n(t;\lambda)$.

In order to improve the result of Csordas et al., we realized that the degree of the Jensen polynomial $G_n(t;\lambda)$ which possesses complex zeros, might grow very fast with λ. Consequently, finding *all* the zeros of $G_n, n = 1, 2, \ldots$ (in order to prove the existence of complex ones) might become very expensive. Therefore, we decided to use so-called *Sturm sequences* [4] to determine whether the given Jensen polynomial has any complex zeros (which is all we need to know, in principle). This is computationally much simpler than finding all the zeros of a polynomial. A Sturm sequence associated with a given polynomial $p_0(x)$ of degree m is a sequence of polynomials $p_0(x), p_1(x), \ldots$ of strictly decreasing degree which can be defined as follows:

$$p_1(x) := p_0'(x),$$

$$p_{i-1}(x) := q_i(x)p_i(x) - p_{i+1}(x), i = 1, 2, \ldots,$$

where $q_i(x)$ is found by the Euclidean algorithm, such that the degree of $p_{i+1}(x)$ is less than the degree of $p_i(x)$. If $p_0(x)$ has only simple zeros, $p_i(x)$ has degree $m-i$, and the Sturm sequence consists of $m+1$ polynomials $p_0(x), \ldots, p_m(x)$. Let $v(a)$ be the number of sign changes in the sequence $\{p_i(a)\}_{i=0}^{m}$ (where zero values are skipped). Then $v(a) - v(b)$ is the number of real zeros of the polynomial $p_0(x)$ on the interval $[a, b]$.

Our algorithm now works as follows. Suppose we know λ_0 and $m = m(\lambda_0)$ is the smallest value for which $G_m(t; \lambda_0)$ has complex zeros (to start with, we take $\lambda_0 = -50$ and $m = 16$ from [2]). Then for a new value of λ which is somewhat larger than λ_0 we compute $\beta_i(\lambda), i = 0, 1, \ldots$, and for each new β_i we compute the associated Jensen polynomial, and, by means of the associated Sturm sequence, its number of real zeros on the interval $[-A, 0]$, where $A > 0$ is suitably chosen. This is continued until we have found n for which $g_n(t; \lambda)$ should have complex zeros. Then, as a check, we compute a complex zero of this polynomial by means of the Newton process, where the starting value is chosen as follows. Let $z = z(\lambda_0)$ be the known complex zero of $g_m(t; \lambda_0)$. We tabulate the values of the Jensen polynomial $g_n(t; \lambda)$ and its derivative, for some values of t *around* $\Re(z)$, and we look for a local *positive minimum*, or a local *negative maximum*. In our experience, such a minimum, or maximum, is easy to find if λ is not too far away from λ_0. Then we take $a + bi$ as starting value for the Newton process where a is the value of t for which $g_n(t; \lambda)$ assumes its local minimum or maximum, and where $b = \Im(z)$.

In this way we found complex zeros of $g_n(t; \lambda)$ for $\lambda = -50(1) - 40, -30, -20, -10, -5$. Table 1 presents the values of λ for which we have determined the Jensen polynomial of smallest degree with complex roots by means of the associated Sturm sequence. This degree is denoted by $m = m(\lambda)$. In all cases this Jensen polynomial has $m(\lambda) - 2$ *real* roots. Table 1 also lists the complex zeros found, truncated to 10 decimal digits, and the accuracy used. For λ close to -50, the degree of the Jensen polynomial with complex zeros does not increase too quickly with λ. However, from $\lambda \approx -20$ this pattern changes drastically, as Table 1 shows. As λ increases, the imaginary parts of the complex zeros found seem to tend to zero.

During the computation of Sturm sequences, it is easy to check when the accuracy used becomes insufficient: in that case the sequence of signs $\{p_i(a)\}_{i=0}^{m}$, associated with g_m, deviates in a chaotic way from the previous sequence of signs (associated with g_{m-1}).

Table 1 Minimal degrees $m(\lambda)$ of Jensen polynomials with complex roots

λ	$m(\lambda)$	complex zeros of $g_m(t;\lambda)$ $\Re$	$\pm\Im$	accuracy used
-50	16	-220.9191117	7.092565255	28D
-49	16	-217.9076244	5.773253615	28D
-48	16	-214.9084360	4.111013736	28D
-47	16	-211.9217860	1.006843660	28D
-46	17	-202.2196553	5.677704348	28D
-45	17	-199.3211883	3.991036911	28D
-44	17	-196.4360833	0.462709708	28D
-43	18	-187.4386728	4.830351149	28D
-42	18	-184.6425759	2.749091911	28D
-41	19	-176.2289375	4.969975476	28D
-40	19	-173.5216696	3.024436421	28D and 40D
-30	27	-116.8258164	2.400595686	28D and 50D
-20	41	-111.0654985	1.322239430	50D
-10	97	-45.53019819	0.156978360	75D
-5	406	-24.34071458	0.031926616	250D

3 Some computational details

In this section we shall explain some details of how we computed $\beta_m(\lambda)$ and the Sturm sequences of $g_n(t;\lambda)$.

We write $b_m(\lambda)$ as the sum

$$b_m(\lambda) = \int_0^a t^{2m} e^{\lambda t^2} \Phi(t)dt + \int_a^\infty t^{2m} e^{\lambda t^2} \Phi(t)dt \tag{5}$$

(Csordas et al. used $a = 1$). An upper bound for the second integral of (5) is found as follows. The function $t^{2m}e^{\lambda t^2}$ has maximum value $\exp[m(-1+\log \frac{m}{-\lambda})]$ (for $t = (-m/\lambda)^{1/2}$), so that

$$\int_a^\infty t^{2m} e^{\lambda t^2} \Phi(t)dt < \exp[m(-1 + \log \frac{m}{-\lambda})] \int_a^\infty \Phi(t)dt$$

$$< \frac{\pi}{2} \exp[m(-1 + \log \frac{m}{-\lambda}) + 5a - \pi e^{4a}]$$

(cf. [3, ineq. (3.7)]). This bound is used, for given λ and m, to choose a such that the contribution of the second integral in (5) to the value of $b_m(\lambda)$ is negligible, in view of the precision used. E.g., for $\lambda = -5$, we chose $a = 1.65$. For $m = 406$, this yields an upper bound of 10^{-400} on the value of the second integral in (5). The smallest $b_m(-5)$ we found is $b_{344}(-5) = 1.46822\ldots \times 10^{-73}$. Since we worked with a precision of 250 decimal digits, it follows that the contribution of the second integral in (5) to $\{b_m(-5)\}_{m=0}^{406}$ is indeed negligible.

Let $\Phi_N(t)$ denote the sum of the first N terms of (2), then we have (cf. [3, eq. (4.6)])

$$0 < \Phi(t) - \Phi_N(t) < \pi N^3 \exp(5t - \pi N^2 e^{4t})(0 \leq t < \infty).$$

Given t, the number N is chosen such that the right hand side is less than 10^{-A} where A is the number of decimal digits of precision employed in the computations *plus* $\{-\log_{10}(\text{first term of } \Phi(t))\}$ (since this first term determines the size of $\Phi(t)$). Since the N in the exp is dominating, it is sufficient (most of the time) to choose N to be the smallest integer larger than $\sqrt{(}e^{-4t}(A \log 10 + 5t)/\pi)$.

Using the same notation as in [2], we now have to compute the integral

$$b_m^{(2)}(\lambda) = \int_0^a t^{2m} e^{\lambda t^2} \Phi_N(t) dt \tag{6}$$

to sufficient accuracy. In [2] this was done by Romberg quadrature. However, by inspecting the Romberg table for $b_m^{(2)}(\lambda)$, we noticed that when going from left to right, i.e. when comparing T_{ij} with $T_{i,j+1}$, the accuracy did *decrease* (rather than increase, as one would expect: cf., e.g., [7, p.141]). Moreover, the most accurate results were found in the first column of the Romberg table (just the trapezoidal rule results for step $a, a/2, a/4, \ldots$), and the convergence in this column was much faster than quadratic. An explanation is given by the fact that the integrand in $b_m(\lambda)$ is an *even* function, and under certain conditions given in Theorem 2.2 of [5] the convergence of the trapezoidal rule for such functions is exponential. The integrand $b_m(\lambda)$ happens to satisfy these conditions. Therefore, it is unnecessary to apply Romberg quadrature. We just applied the composite quadrature rule with step $a, a/2, a/4, \ldots$, until a sufficiently small correction was obtained. For the computation of $b_m(-5)$ we never needed to work with a step less than $a/1024$. Before applying the trapezoidal rule, a table of values of $e^{\lambda t^2}\Phi(t)$ was precomputed for $t = ja/1024, j = 0, \ldots, 1024$ since (a selection of) these values are needed for each $b_m(\lambda)$. In the final steps, we usually observed a doubling of the number of correct digits upon halving the step.

The Sturm sequence associated with the polynomial $g_m(t;\lambda)$ was computed as follows. Let $p_0(x) := g_m(t;\lambda)$ and let

$$p_i(x) := \sum_{j=0}^{m-i} c_{ij} x^{m-i-j}, i = 0, 1, \ldots, m.$$

The coefficients c_{0j} of p_0 are computed from the $b_j(\lambda)$ by (3), and since $p_1(x) = p_0'(x)$ we have $c_{1j} = (m-j)c_{0j}, j = 0, \ldots, m-1$. Let $q_i(x) := q_{i0}x + q_{i1}, i =$

$1, \ldots, m-1$. Then, by applying the definition of a Sturm sequence given in §2, for $i = 1, 2, \ldots, m-1$ we find q_{i0} and q_{i1} from

$$q_{i0}c_{i0} - c_{i-1,0} = 0,$$

$$q_{i0}c_{i1} + q_{i1}c_{i0} - c_{i-1,1} = 0,$$

and $c_{i+1,j}, j = 0, \ldots, m-i-2$ from

$$c_{i+1,j} = q_{i0}c_{i,j+2} + q_{i1}c_{i,j+1} - c_{i-1,j+2}$$

and $c_{i+1,m-i-1}$ from

$$c_{i+1,m-i-1} = q_{i1}c_{i,m-i} - c_{i-1,m-i+1}.$$

Now we have to estimate an interval $[a, b]$ which covers all the real zeros of $g_m(t; \lambda)$. It is known that the real zeros are negative. For $\lambda = -49$ we took $[a, b] = [-1000, 0]$ which covers all the real zeros of $g_{16}(t; -50)$, according to [2]. This interval turned out to cover all the real zeros of $\{g_m(t; -49)\}_{m=1}^{16}$. The same interval was chosen for the cases $\lambda = -48, \lambda = -47, \ldots$ until by the Sturm sequence mechanism we did not find sufficiently many real zeros, nor did we find any complex zeros in the way as described in §2. In that case, the interval $[a, b]$ was enlarged (by decreasing a). For $\lambda = -5$ it was sufficient to take $[a, b] = [-5000, 0]$. In some instances, going from g_m to g_{m+1} the difference $v(a) - v(b)$ (which counts the number of real zeros) dropped down from m sharply. It turned out that this was caused always by insufficient precision used in the computation of the Sturm sequence of g_{m+1}. By increasing the accuracy, the normal pattern (i.e., finding $v(a) - v(b) = m+1$, or $m-1$) could be restored easily. By means of this strategy one avoids the need to extend the precision for the application of the theorem of Ostrowski, as Csordas et al. did. The explicit computation of the complex zeros by finding a local positive minimum or a negative maximum may be considered as an extra check.

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