

AN IMPROVED LOWER BOUND FOR THE DE BRUIJN-NEWMAN CONSTANT

YANNICK SAOUTER, XAVIER GOURDON, AND PATRICK DEMICHEL

ABSTRACT. In this article, we report on computations that led to the discovery of a new Lehmer pair of zeros for the Riemann ζ function. Given this new close pair of zeros, we improve the known lower bound for de Bruijn-Newman constant Λ . The Riemann hypothesis is equivalent to the assertion $\Lambda \leq 0$. In this article, we establish that in fact we have $\Lambda > -1.14541 \times 10^{-11}$. This new bound confirms the belief that if the Riemann hypothesis is true, it is barely true.

1. INTRODUCTION

The Riemann hypothesis is a long standing conjecture in mathematics. It asserts that the non-trivial zeros of the Riemann ζ function all have a real part equal to $1/2$. Many attempts have been made to prove it. To this end, Pólya considered a family of trigonometric integrals H_λ , defined by

$$H_\lambda(x) = \int_0^\infty e^{tu^2} \Phi(u) \cos(xu) du \quad (\lambda \in \mathbb{R}, x \in \mathbb{C}),$$

where

$$\Phi(u) = \sum_{n=1}^\infty (2\pi^2 n^4 e^{9u} - 3\pi n^2 e^{5u}) \exp(-\pi n^2 e^{4u}) \quad (0 \leq u < \infty).$$

With this definition, we have [Tit86, p. 255] $H_0(x) = \Xi(x/2)/8$, where Ξ is the classic Riemann function defined by

$$\begin{aligned} \Xi(x) &= -\frac{1}{2}\left(x^2 + \frac{1}{4}\right)\xi\left(\frac{1}{2} + ix\right), \\ \xi(s) &= \frac{1}{2}s(s-1)\pi^{-s/2}\Gamma\left(\frac{1}{2}s\right)\zeta(s). \end{aligned}$$

The Riemann hypothesis is then equivalent to the fact that the functions Ξ and H_0 have only real zeros. Pólya hoped to prove this property for the integral functions H_λ , and to deduce the Riemann hypothesis as a corollary. In the general case, results were obtained by de Bruijn and Newman. In fact, de Bruijn [dB50] showed that H_λ has only real zeros if $\lambda \geq 1/2$. Moreover, if λ is such that H_λ has only real zeros, then it also holds for any λ' with $\lambda' \geq \lambda$. On the other hand, Newman [New76] showed that there is at least one value for λ such that the corresponding H_λ function has at least one non-real zero. Thus the following definition makes sense.

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Definition 1.1. There exists a finite real value Λ such that H_λ has only real zeros if and only if $\lambda \geq \Lambda$. The value Λ is called the *de Bruijn-Newman constant*.

With this definition, the Riemann hypothesis is equivalent to the assertion $\Lambda \leq 0$. Recently, Kai *et al.* [KKL09] have shown that $\Lambda < 1/2$. Much work has been done to obtain lower bounds for Λ [CNV88, tR91, NRV92, CRV91]. These were based on the search of non-real zeros for Jensen polynomials, except for [CRV91], which involves the computation of the Laguerre difference for functions H_λ . Then, Csordas *et al.* [CSV94] made studies on the law of motion for the zeros of functions H_λ when λ is varying. They obtained a new lower bound for Λ by considering a close pair of zeros for the function ζ . Such pairs, whose difference is unusually small, are called *Lehmer pairs*. Then successive computations of zeros for ζ gave improved lower bounds for Λ [CSV94, COSV93, Odl00]. In [Odl00], Odlyzko obtained the best lower bound, prior to the work related here, by establishing that $\Lambda > -2.7 \times 10^{-9}$.

2. THE DE BRUIJN-NEWMAN CONSTANT AND LEHMER PAIRS

The basic tool that we will use in this article is the main theorem of [CSV94] (Theorem A, below). As we will see, this theorem enables us to obtain only negative lower bounds for Λ . Thus, without explicit mention to the contrary, in this paper, we always suppose that the Riemann hypothesis holds. If it is not the case, then we have $\Lambda > 0$ and thus any negative lower bound we might obtain for Λ is trivially correct. Likewise, an eventual multiple zero for H_0 would immediately prove that $\Lambda \geq 0$ [CSV94]. Thus, we also suppose that the zeros of H_0 are all real and simple. Note that if x is a zero, then $-x$ is also a zero. Therefore, we number the positive zeros of H_0 in increasing order:

$$0 < x_1 \leq x_2 \leq x_3 \leq x_4 \leq \dots$$

and we extend our numbering to negative zeros by putting

$$x_{-j} = -x_j \quad (j = 1, 2, \dots),$$

with x_0 undefined. With the definition of H_0 , we note that the zeros of the Riemann ζ function are exactly $1/2 + ix_j/2$ for $j \in \mathbb{Z} - 0$. Given this, following [CSV94], we define Lehmer pairs of zeros.

Definition A. Let k be a positive integer such that x_k and x_{k+1} are successive simple zeros of H_0 . Then (x_k, x_{k+1}) is a *Lehmer pair of zeros* for H_0 if we have $(x_{k+1} - x_k)^2 \cdot G_k < 4/5$ with

$$(2.1) \quad G_k = \sum_{j \neq 0, k, k+1} \left\{ \frac{1}{(x_k - x_j)^2} + \frac{1}{(x_{k+1} - x_j)^2} \right\}.$$

We can now state the main theorem from [CSV94].

Theorem A. Let (x_k, x_{k+1}) be a Lehmer pair of zeros for H_0 . Set

$$(2.2) \quad \lambda_k = \frac{(1 - \frac{5}{4}(x_{k+1} - x_k)^2 \cdot G_k)^{4/5} - 1}{8G_k}$$

so that $-1/(8G_k) < \lambda_k < 0$. Then the de Bruijn-Newman constant Λ satisfies the inequality $\Lambda \geq \lambda_k$.

The Taylor expansion for λ_k shows that, provided that G_k is not too large, λ_k is close to $-(x_{k+1} - x_k)^2/8$. In this case, the closer a Lehmer pair, the better the lower bound.

TABLE 1. Close pairs of zeros for the function $\zeta(1/2+it)$, according to Gourdon and Demichel [GD04].

| t_1 | t_2 | $t_2 - t_1$ |
|---------------------------|---------------------------|--------------------------|
| 7954022502373.43289015387 | 7954022502373.43289494012 | 4.7863×10^{-6} |
| 18580341990011.1593414105 | 18580341990011.1593364110 | 4.9995×10^{-6} |
| 18523741991636.3643689901 | 18523741991636.3643759580 | 6.9679×10^{-6} |
| 4307762397492.0712366929 | 4307762397492.0712295734 | 7.1195×10^{-6} |
| 16671318581127.6545668867 | 16671318581127.6545740724 | 7.1857×10^{-6} |
| 8847150598019.2235982778 | 8847150598019.2236059816 | 7.7038×10^{-6} |
| 10123949469608.2309097616 | 10123949469608.2309189455 | 9.1839×10^{-6} |
| 20825125156965.3882387859 | 20825125156965.3882484837 | 9.6978×10^{-6} |
| 17335277232221.2458033031 | 17335277232221.2457934935 | 9.8096×10^{-6} |
| 5907264585921.6903635665 | 5907264585921.6903535057 | 1.00608×10^{-5} |
| 21285800773585.4550406956 | 21285800773585.4550510671 | 1.03715×10^{-5} |

3. NUMERICAL VERIFICATION OF THE RIEMANN HYPOTHESIS

Much work has been done on the numerical verification of the Riemann hypothesis. For what we are concerned with here, those computations are useful to obtain Lehmer pairs of zeros. However, from a more general point of view, those computations can be used, for instance, to improve bounds on Chebyshev functions or to broaden zero free regions for ζ . The largest systematic verification with an official announcement was performed in 2001 by van de Lune [vdL01]. He claimed that the first 10^{10} zeros of the function ζ lie on the critical line and they are all simple. The verification performed was systematic up to height $T = 3293531632.415$. These numerical values will be used in what follows.

Two other larger verifications have been performed but neither obtained an official certification. The first one was managed by Wedeniwski [Wed05], and involved distributed computations over more than ten thousands computers. After four years of computation, the project was ended and Wedeniwski announced that the first 10^{11} zeros of the Riemann ζ function lie on the critical line. Computations were based on the Riemann-Siegel formula. The second verification was by Gourdon and Demichel [GD04]. Using the fast multiple evaluation algorithm of Odlyzko [OS88], in 2004, they verified that the first 10^{13} zeros lie on the critical line. Moreover, Demichel continued computing and reached the 10^{14} -th zero. They obtained many pairs of close zeros (see Table 1).

However, neither of these verifications was validated by the American Mathematical Society. The reason seems to be, in Wedeniwski's case, that there was no evidence that all zeros were computed. Also, the verification of Gourdon and Demichel had not been checked independently. In this paper, we refer to close zeros obtained by Gourdon and Demichel. Thus, in order to formally establish our new lower bound, we will have to verify their calculations, at least near the close pair of zeros we will consider.

4. AN UPPER BOUND FOR G_K

In order to establish the new lower bound, we will use Theorem A with the first close pair of Table 1. In the following, we denote the rank of appearance of this

TABLE 2. A close pair of zeros for ζ , with adjacent zeros.

| Gram blocks | Zeros |
|--|--|
| $[g_{34011300784333}, g_{34011300784335})$ | $t_{K-2} = 7954022502373.0094352194$ $t_{K-1} = 7954022502373.1219461606$ |
| $[g_{34011300784335}, g_{34011300784337})$ | $t_K = 7954022502373.43289015387$ $t_{K+1} = 7954022502373.43289494012$ |
| $[g_{34011300784337}, g_{34011300784338})$ | $t_{K+2} = 7954022502373.7336782379$ |

pair as K . This means that $x_K = 2t_1$ and $x_{K+1} = 2t_2$ where the values t_1 and t_2 refer to the champion pair of Table 1. We will then have to verify that this pair of zeros is indeed a Lehmer pair. The purpose of this part is to obtain an upper bound for G_K that only depends on x_{K-1} , x_K , x_{K+1} and x_{K+2} .

The main theorem that we will use to validate our new lower bound is the following (see [COSV93]).

Theorem B. *If $K > 10^{10}$, then*

$$(4.1) \quad G_K \leq \frac{2 \log(x_{K+1})}{(x_{K+1} - x_{K+2})^2} + \frac{2 \log(x_K)}{(x_K - x_{K-1})^2} + (\log(x_K) + \log(x_{K+1})) \frac{\pi^2}{12} + \frac{4 \times 10^{10}}{(x_K - 2T)^2} + 4.$$

Proof. Analytical computations related to the proof of this theorem can be found in [COSV93]. The major difference here, concerns K , which is treated as an unknown in Theorem B, while it has a fixed value in [COSV93]. \square

5. A NEW BOUND FOR THE DE BRUIJN-NEWMAN CONSTANT

With Theorem B, for a given close pair of zeros (t_K, t_{K+1}) of ζ , it is possible to compute an upper bound for G_K if we also have numerical values for the two adjacent zeros t_{K-1} and t_{K+2} . Computations performed by Gourdon and Demichel give us these values for the specific close pair we are considering (see Table 2). It is then eventually possible to compute a lower bound for Λ , provided that conditions of Theorem A are satisfied. Checking that the zeros are simple is not necessary as stated in Section 2. The only remaining problem is to check that computed values for t_{K-1} , t_K , t_{K+1} and t_{K+2} are correct, that is to say that no intermediate zero is missing. This point is implicit in computational verifications of the Riemann hypothesis but here an independent verification is necessary, since Gourdon and Demichel's computations are not officially certified.

Modern computational verifications of the Riemann hypothesis have been greatly simplified by Turing's approach to the problem [Tur53], although some errors of detail were later corrected by Lehman [Leh70]. The main interest of this method is that it only involves evaluations of ζ on the critical line.

First, let us recall some classical definitions. For $t > 0$, we define the functions $\theta(t)$ and $Z(t)$ by $\theta(t) = \text{Arg}\{\Gamma(\frac{1}{4} + \frac{1}{2}it)\} - \frac{t}{2} \log \pi$ and $Z(t) = \exp(i\theta(t))\zeta(\frac{1}{2} + it)$.

Then the function $Z(t)$, called the *Hardy function*, is real and $\zeta(1/2 + it) = 0$ if and only if $Z(t) = 0$. The Riemann-Siegel formula gives a practical way to compute $Z(t)$. The function $\theta(t)$ is computed by its asymptotic expansion for large t . For $n \geq 0$, the n -th *Gram point* is defined to be the unique solution greater than 7 of $\theta(g_n) = n\pi$. A Gram point g_n is said to be *regular* if $(-1)^n Z(g_n) > 0$, and *irregular*

otherwise. A *Gram block* is an interval $[g_n, g_{n+k})$ with $k \geq 1$ such that g_n and g_{n+k} are regular Gram points, while the Gram points $g_{n+k'}$ are irregular for all k' with $1 \leq k' < k$. Corresponding to the points g_n , we define a companion sequence h_n of real numbers such that

- h_n can be positive, zero or negative;
- if g_n is a regular Gram point, then $h_n = 0$;
- the property $(-1)^n Z(g_n + h_n) > 0$ holds for all n ;
- the series $g_n + h_n$ is monotonically increasing.

Finally, we denote by $N(T)$ as usual the number of solutions to $\zeta(\sigma + it) = 0$ with $0 \leq t < T$, and $0 < \sigma < 1$. We then have the following.

Theorem C. *Let n be a positive integer such that g_n is a regular Gram point. If there exist integers $k, k' > 0$ such that $g_{n-k} > 168\pi$ and*

$$\frac{2.30 + 0.128 \log\left(\frac{g_n}{2\pi}\right) + \sum_{j=1}^{k-1} h_{n-j}}{g_n - g_{n-k}} < 1,$$

$$\frac{2.30 + 0.128 \log\left(\frac{g_{n+k'}}{2\pi}\right) + \sum_{j=1}^{k'-1} h_{n+j}}{g_{n+k'} - g_n} < 1,$$

then we have $N(g_n) = n + 1$.

Proof. This theorem is proved for the general case of Dirichlet L -series in [Rum93, Prop. 3]. \square

Thus, Theorem C can be used to determine exactly the number of solutions to $\zeta(\sigma + it) = 0$ with $0 \leq t < g_n$ and $0 < \sigma < 1$, provided that g_n is a regular Gram point and that a companion series h_m has been computed for $n - k + 1 \leq m \leq n + k' - 1$. To apply Theorem C, the values k and k' can be arbitrary, i.e., no hypothesis is required on the eventual regularity of either the Gram points g_{n-k} or $g_{n+k'}$, or for any intermediate Gram points (except g_n).

It has also to be noted that numerical values 2.30 and 0.128 involved in Theorem C can be improved. Recently, Trudgian [Tru09] claimed that they can be replaced by 1.41 and 0.0054, respectively. However, this improvement, from a computational point of view, leads to only a minor decrease in complexity. Indeed, when checking the Riemann hypothesis, most of the time is spent evaluating the function Z at various points in order to locate changes of signs. Thus, in such computations, the impact of Trudgian's result is quite limited.

Saouter made an independent verification of the computed values for zeros in an interval of 200 Gram points around the critical pair (t_K, t_{K+1}) . Since few zeros had to be checked, the Riemann-Siegel formula was used (see [BBC00]), unlike in Gourdon's and Demichel's work. To ensure great precision in computed zeros, three correcting terms were also used. Computations were made by the MPFR [FHL+07] multiprecision package. Computed values for zeros in this second verification were in complete agreement with those computed by Gourdon and Demichel. A companion series h_n was computed and, setting $k = k' = 35$ in Theorem C, computations showed that Turing's condition holds at least for all Gram points in the interval $[g_{K-65}, g_{K+65}]$. Thus, no zero is missing in Table 2.

Reminding ourselves that we have $x_n = 2t_n$ for all $n \geq 0$, we can now use Theorem B. We obtain $G_K \leq 379.1995$ and $(x_{K+1} - x_K)^2 \times G_K \leq 3.47471 \times 10^{-8}$. Thus, (x_K, x_{K+1}) is a Lehmer pair and Theorem A gives $\lambda_K > -1.14541 \times 10^{-11}$.

TABLE 3. Probability of appearance of Lehmer pairs.

| Lower bound | δ | M | Probability | Reference |
|-------------------------|------------------------|--------------------|-------------|------------|
| -5.90×10^{-9} | 1.09×10^{-4} | 1.5×10^9 | 0.049 | [COSV93] |
| -2.63×10^{-9} | 1.45×10^{-4} | 5×10^9 | 0.994 | [Odl00] |
| -1.15×10^{-11} | 2.084×10^{-5} | 1×10^{14} | 0.629 | This paper |

6. FINAL REMARKS

The result we obtained was enabled by the discovery of a close pair of zeros for the Riemann ζ function by Gourdon and Demichel [GD04]. In the conclusion of [Odl00], Odlyzko expresses the idea that systematic computations of zeros should produce still better and better lower bounds for Λ . A question then comes to mind: is the current Lehmer pair we used exceptional or not? The exact distribution law of zeros of the Riemann ζ function is unknown, but it is conjectured to be the same as that of eigenvalues of matrices of the Gaussian unitary ensemble. This conjecture comes from practical observations, but it agrees with Hilbert and Pólya's conjecture that the zeros of the Riemann ζ function correspond to eigenvalues of some positive linear operator.

The Gaussian unitary ensemble has been widely studied in physics. Odlyzko compared the results from this model to the numerical data of zeros of the Riemann ζ function [Odl87]. For instance, the GUE conjecture implies that if you define $\delta_n = (t_{n+1} - t_n) \frac{\log \frac{t_n}{2\pi}}{2\pi}$, then the probability that the minimal value, amongst M consecutive values, for δ_n is less than $\alpha M^{-1/3}$, is approximately equal to $1 - \exp(-\pi^2 \alpha^3/9)$, provided that α^3/M is small. From this relation, and taking into account the number of zeros which have been computed, it is possible to give a quantitative appreciation of close Lehmer pairs that have been used in this and earlier work. These values are recorded in Table 3. Thus, we can observe that, while in [COSV93] the Lehmer pair that has been used was rather exceptional, the one used in [Odl00] was almost totally predictable. The probability of the pair used in this paper lies between these two: neither exceptional, nor certain. The strategies to obtain these pairs differ. In [COSV93], the pair was obtained by a complete enumeration of the first 1.5×10^9 zeros of the Riemann ζ function. In [Odl00], the pair considered was obtained by computing 5×10^9 zeros around the 10^{20} -th zero. Finally, the computation in this paper is based on a complete enumeration of the first 10^{14} zeros, performed by Gourdon and Demichel [GD04]. If 10^{14} zeros around the 10^{20} -th zero had been computed, then, with the same probability as in this paper, we could have expected to obtain a close pair with $\delta \simeq 2 \times 10^{-5}$ and thus a lower bound of approximately -1.1×10^{-12} for Λ . However, it has to be noted that complete enumerations of first zeros of ζ have widespread applications in computational number theory. For instance, this kind of result can be used to refine knowledge of the prime number distribution [Dus98]. This is not the case for isolated computations.

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INSTITUT TELECOM BREST, BRETAGNE, FRANCE
E-mail address: Yannick.Sauter@telecom-bretagne.eu

DASSAULT SYSTEMES, VELIZY-VILLACOUBLAY, FRANCE
E-mail address: xgourdon@gmail.com

HEWLETT-PACKARD FRANCE, LES ULIS, FRANCE
E-mail address: patrick.demichel@hp.com