
 EL DIABLO DE LOS NÚMEROS

Section directed by

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A first encounter with the Riemann Hypothesis and its numerical verification

by

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1 INTRODUCTION

1.1 THE EARLY ORIGINS : FROM EUCLID TO EULER/CHEBYSHEV.

The *prime numbers* (or *primes*) 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41, 43, ... have fascinated mankind since antiquity. It seems unlikely though, that we will ever know the details surrounding *homo sapiens's* first awareness of the notion of prime number. However, we do know that Pythagoras was aware of the notion of prime number, perhaps as early as 550 B.C.E. Furthermore, Book IX of Euclid's *Elementa* (300 B.C.E.) provides us with the earliest known written record of several theorems concerning prime numbers. In particular, his proof (by contradiction) that there are infinitely many primes has become a celebrated classic and is found in the early chapters of most books on elementary number theory.¹

Also, around 240 B.C.E. Eratosthenes devised a simple but ingenious method to *generate the primes* by means of his well-known *sieve*, which is based on the following principle: $n > 1$ & $(1 < p \leq \sqrt{n} \implies p \nmid n) \implies n$ is prime.

Sometimes this procedure is described in a somewhat derogatory way as being only fit for short ranges. However, after having *precomputed* all primes $\leq n$ in a sieve block of length n , one can re-use this same sieve block repeatedly, so that the sieve-range will become n^2 . Nowadays, even on a personal computer one can easily set $n = 10\,000\,000$, so that the sieve-range will then be 10^{14} . Such an extended Eratosthenes sieve is often very useful when studying prime-related (multiplicative) arithmetic functions such as the Möbius function $\mu(n)$. For more details see [35].

¹We are also fond of Pólya's elementary combinatorial proof : $\sqrt{n} 2^{\pi(n)} \geq n$.

Throughout the known history of prime number theory, three questions have endured: (1) How to determine whether or not a given number n is prime, (2) how to find the prime factors of n when it is known that n is composite, and (3) how many primes are there, not exceeding a large positive real x .

In most of the work on primes a crucial role is played by the (non-trivial) Unique Factorization Theorem (UFT) for the positive integers: If $n = p_1^{e_1} p_2^{e_2} \cdots p_r^{e_r}$ is some prime factorization of n with $p_i < p_j$ for $i < j$, and all exponents $e_i \geq 1$, then there is no other such factorization. That this is not just a triviality may be seen from some examples: In the set of *even* integers we have $36 = 6 \times 6 = 2 \times 18$ and in the set $\{a + bi\sqrt{5}\}$ with a and b ordinary integers we have $6 = 2 \times 3 = (1 - i\sqrt{5})(1 + i\sqrt{5})$. For ages mathematicians seem to have been aware of the concept of the UFT, but it was Gauss who first succinctly stated it and provided a rigorous proof.

As an all-important consequence of the UFT we have that the logarithms of the primes are linearly independent over \mathbb{Q} (= the rationals): If $r_1 \log p_1 + r_2 \log p_2 + \cdots + r_k \log p_k = 0$, all r_i being rational, then all r_i must be = 0.

Denoting, as usual, the number of primes not exceeding x by $\pi(x)$ Euclid thus showed that $\pi(x) \uparrow \infty$ as $x \uparrow \infty$. For more details concerning the (early) development of prime number theory we strongly recommend Narkiewicz [55] and the *Einleitung* in Landau's *Handbuch* [37].

1.2 EULER'S NEW APPROACH TO PRIME NUMBER THEORY.

It was not until the 18th century, that Euler presented a new analytic proof of Euclid's theorem (see [18, Theorem 19]).

To this end Euler considered the real (harmonic) series

$$\sum_{n=1}^{\infty} \frac{1}{n^x}, \quad (\text{only convergent for } x > 1) \quad (1)$$

and showed that its sum, nowadays denoted by $\zeta(x)$, tends to ∞ as $x \downarrow 1$.

Euler's novelty consists of the observation that $\zeta(x)$ is equal to the value of the following infinite (Euler-) product (also convergent for real $x > 1$)

$$\prod_p \frac{1}{1 - \frac{1}{p^x}} \quad (\text{with } \prod_p \text{ over all primes } p), \quad (x > 1). \quad (2)$$

(Euler did not consider $\zeta(x)$ for complex x .) The basic idea behind this equality is quite simple: Write $(1 - \frac{1}{p^x})^{-1}$ as an absolutely convergent geometrical series and multiply out in (3), using the UFT mentioned above. This is why the equality of (2) and (3) is often called the analytic analogue of the UFT. Euler then argues as follows: If there were only finitely many primes, then the limit of (3), and hence that of (2), would clearly be finite for $x \downarrow 1$. This contradiction proves that there must be infinitely many primes.

After Euler it was Chebyshev [11] who took the next step. He obtained the true order of $\pi(x)$ by proving that

$$0.92129\dots \leq \liminf_{x \rightarrow \infty} \frac{\pi(x)}{x/\log x} \leq \limsup_{x \rightarrow \infty} \frac{\pi(x)}{x/\log x} \leq 1.10555\dots \quad (3)$$

He also proved that if $\lim_{x \rightarrow \infty} \frac{\pi(x)}{x/\log x}$ exists then this limit must be equal to 1.

2 RIEMANN'S APPROACH OF $\zeta(s)$ FOR COMPLEX s .

2.1 RIEMANN'S PAPER (NOVEMBER 3, 1859).

In Riemann's only published paper on number theory [68], his main contribution was to consider $\zeta(s)$ as a function of a complex variable $s = \sigma + it$, thereby also extending Euler's product to complex s with $\text{Re } s > 1$. Riemann denotes by $\zeta(s)$ the holomorphic function so defined, and shows that it extends to a meromorphic function on \mathbb{C} with a unique (simple) pole at $s = 1$ with residue 1. For this meromorphic function he then proves the functional equation

$$\text{if } f(s) = \pi^{-s/2} \Gamma(s/2) \zeta(s) \text{ then } f(s) = f(1-s) \quad (4)$$

which (using known properties of $\Gamma(s)$) may also be written as

$$\zeta(s) = \chi(s) \zeta(1-s) \quad \text{with } \chi(s) := 2^s \pi^{s-1} \sin \frac{\pi s}{2} \Gamma(1-s). \quad (5)$$

He gives two proofs of the analytic continuation and the functional equation. The second one applies the functional equation of a theta function (compare (8) below) and has become a model for the relation between more general L -functions and modular functions.

Riemann also introduces the entire functions $\xi(s)$ and $\Xi(t)$ by the equations²

$$\xi(s) = \frac{s(s-1)}{2} \pi^{-s/2} \Gamma(s/2) \zeta(s) \quad \text{and} \quad \Xi(t) = \xi\left(\frac{1}{2} + it\right) \quad (6)$$

and obtains the integral expression

$$\Xi(t) = 4 \int_1^\infty \frac{d(x^{\frac{3}{2}} \psi'(x))}{dx} x^{-\frac{1}{4}} \cos\left(\frac{1}{2} t \log x\right) dx \quad \text{where } \psi(x) = \sum_{n=1}^\infty e^{-\pi n^2 x} \quad (7)$$

from which it is clear that $\Xi(t)$ is real for real t .

Next he turns to the study of the zeros of $\Xi(t)$. First he proves that $\Xi(\alpha) = 0$ implies $|\text{Im}(\alpha)| \leq \frac{1}{2}$, and then states that the number of zeros α with $0 \leq \text{Re } \alpha \leq T$ is $\frac{T}{2\pi} \log \frac{T}{2\pi} - \frac{T}{2\pi}$ with an error bounded by $C \log T$. Also a very sketchy idea of the proof is given.

Riemann continues to say:

²As usual at present we do not follow the notations of Riemann.

“One finds in fact about this many real roots within these bounds and it is very likely that all of the roots are real. One would of course like to have a rigorous proof of this, but I have put aside the search for such a proof after some fleeting vain attempts because it is not necessary for the immediate objective of my investigation.” (Translation taken from Edwards [17, p. 301].)

The passage “. . . and it is very likely that all of the roots are real” has become the famous Riemann Hypothesis (RH). (In the space allocated to this paper we can only discuss a very limited part of the entire literature on the RH.)

He ends his study of the zeros of $\Xi(t)$ by giving a very sketchy idea for a proof of the product formula

$$\Xi(t) = \Xi(0) \prod_{\alpha} \left(1 - \frac{t^2}{\alpha^2}\right). \quad (8)$$

With these elements of the theory of the zeta function he turns to the main subject of the paper: To give a formula for $\pi(x)$ the number of primes $\leq x$. He considers instead the function $\pi_0(x)$ which is equal to $\pi(x)$ if x is not a prime number whereas $\pi_0(p) = \pi(p) - \frac{1}{2}$, and defines $\Pi_0(x) = \sum_n \frac{1}{n} \pi_0(x^{\frac{1}{n}})$.

Then he establishes the explicit formula

$$\Pi_0(x) = \text{Li}(x) - \sum_{\alpha} \left\{ \text{Li}(x^{\frac{1}{2}+\alpha i}) + \text{Li}(x^{\frac{1}{2}-\alpha i}) \right\} + \int_x^{\infty} \frac{1}{x^2-1} \frac{dx}{x \log x} - \log 2. \quad (9)$$

The most delicate part of the proof, the interchange of a sum and an integral is addressed by simply saying that to justify it, an additional study of the function $\Xi(t)$ is necessary.

He also mentions that $\pi_0(x)$ may be recovered by means of the relation

$$\pi_0(x) = \sum_{m=1}^{\infty} \frac{\mu(m)}{m} \Pi_0(x^{1/m}). \quad (10)$$

The paper ends with some comments on the possible influence of the “oscillatory” terms in formula (10) on the density of the prime numbers.

2.2 RIEMANN’S LETTER TO WEIERSTRASS (OCTOBER 26, 1859).

In Riemann’s Nachlass (Legacy, kept in the library of the Göttinger university) there is a draft of a letter from Riemann to Weierstrass, that explains many things about the paper. On August 11, 1859 Riemann was elected corresponding member of the Berlin Academy. Because of this event Riemann (accompanied by Dedekind) made a trip to Berlin (September 1859). In Berlin Riemann met Weierstrass, Kronecker, Kummer, Borchartd, . . . Riemann’s paper [68] is his first communication to the Academy of Berlin. It was natural then that it would be published in the “Monatsberichte der Berliner Akademie”. Weierstrass was the editor of this journal. The length of the communications in the Monatsberichte were usually two or

three pages long. On November 3, 1859 Kummer read Riemann's communication to the Berlin Academy. We present a brief summary of what Riemann wrote to Weierstrass.

First he writes that he has not yet finished his work on the frequency of primes, and that only by the insistence of Kronecker he sends a brief essay to the Academy.

If, in spite of all his efforts to be brief, the essay is considered not yet sufficiently short for a communication to the Academy, he hopes that it will be accepted anyway.

Riemann seems to be concerned about the length of the paper. Consequently, the proofs were not given in sufficient detail. In particular there are two assertions for which he does not give even a hint of proof. He details precisely those assertions of which he is speaking. The first of them, which for the sake of convenience we denote by (A), is especially interesting for us:

(A) "that between 0 and T there are approximately $\frac{T}{2\pi} \log \frac{T}{2\pi} - \frac{T}{2\pi}$ real roots of the equation $\Xi(\alpha) = 0$."

Riemann also writes (1) that these two assertions follow from an expansion of the function $\Xi(t)$ which he has not yet sufficiently simplified to communicate, (2) that in spite of this for all the rest of his assertions, for which he gives a hint of proof, he is sure Weierstrass can fill in the holes, and (3) that he wants Weierstrass to let him know whether the essay will eventually appear in the *Monatsberichte*, since otherwise he will extend it to a paper to be published by Weber in the journal of "our local (mathematical) society here".

The letter continues with a discussion of quite a different mathematical topic.

Intentionally or not, Riemann may have overestimated the capabilities of his colleagues. Apparently, neither Weierstrass, nor any other mathematician of the day, seems to have understood the hints that Riemann provided for proving his assertions.

Riemann's paper [68] was published in 1859. A generation later, in Göttingen, his successors Klein, Hilbert and Landau thought that the paper was brilliant and fruitful but that Riemann had hardly proved anything, that all was mainly heuristical reasoning. According to Landau, Riemann had only proved the functional equation and had made six additional conjectures.

This is rather surprising since the *Collected Works* had been published by Weber in 1876. The *Collected Works* contain an excerpt of Riemann's letter to Weierstrass. It seems that neither Klein, nor Hilbert or Landau have looked into the *Nachlass* in the Göttinger library, this in spite of the fact that the librarian Distel had pointed out that there was relevant material to be found.

We can only imagine how much greater our understanding of Riemann's ideas would be had he felt the freedom to use a few more pages to communicate his thoughts. (We also recommend reading Neuenschwander [56] and Quer [67]).

While acknowledging the value of Kronecker's intervention, it is obvious that the editors had ample latitude to better serve the mathematical community. As Riemann writes to Weierstrass [70], he does not consider his work on the density of primes finished. Nevertheless, he gives in to Kronecker's wishes and sends to Berlin a "brief essay" on the topic.

2.3 THE NACHLASS (LEGACY) AND SIEGEL.

The first mathematician interested in Riemann's Legacy was Bessel-Hagen who found some new formulas. The Nachlass was far from being a polished final manuscript and Siegel was the first mathematician able to make some sense out of it.

Siegel [76] says that in Riemann's Nachlass there are two main results about the zeta function not previously published: (1) a formula found by the librarian Distel, which is an asymptotic expansion of $\zeta(s)$ in any strip $\sigma_1 \leq \operatorname{Re} s \leq \sigma_2$ (the first term of this expansion had also been given by Hardy and Littlewood (1920) in their "approximate functional equation"), (2) an expression for the zeta function by means of definite integrals found by Bessel-Hagen.

Siegel writes that he has not found, in the Nachlass, any attempt to prove either the Riemann Hypothesis, or that there are an infinite number of real zeros of $\Xi(t)$.

Siegel asserts that Riemann has arrived at assertion (A) from his asymptotic expansion (12) of $Z(t)$ by some heuristic reasoning.

The messy character of Riemann's notes, Siegel says, makes it necessary to reformulate Riemann's results. We regret that after reading Siegel's paper it is not entirely clear what was from Riemann and what was from Siegel.

Siegel then speaks about the misconceptions about Riemann of Klein's contemporaries. Siegel also makes quite explicit the fact that Riemann was in possession of very strong analytic techniques.

The asymptotic formula is written by Siegel as

$$e^{i\vartheta} \zeta\left(\frac{1}{2} + it\right) = 2 \sum_{n=1}^m \frac{\cos(\vartheta - t \log n)}{\sqrt{n}} + (-1)^{m-1} \left(\frac{t}{2\pi}\right)^{-1/4} R \quad (11)$$

$$\vartheta = -\frac{t}{2} \log \pi + \operatorname{arc} \Gamma\left(\frac{1}{4} + i\frac{t}{2}\right), \quad m = \left\lfloor \sqrt{\frac{t}{2\pi}} \right\rfloor \quad (12)$$

$$R = C_0 + C_1 t^{-1/2} + C_2 t^{-1} + C_3 t^{-3/2} + \dots \quad (13)$$

where the coefficients C_j are rather complicated expressions.

Siegel concludes that Riemann used this formula to compute some of the first few (at least 3) zeros of $\Xi(t)$.

The integral formula can be written as

$$\zeta(s) = \mathcal{R}(s) + \chi(s) \overline{\mathcal{R}(1-\bar{s})} \quad \text{where} \quad \mathcal{R}(s) = \int_{0 \searrow 1} \frac{x^{-s} e^{\pi i x^2}}{e^{\pi i x} - e^{-\pi i x}} dx. \quad (14)$$

Here the path of integration is a straight line of slope 1 through $x = 1/2$, and the function $\chi(s)$ is the same as in the functional equation. (This is not the form given by Siegel, who also deviated from Riemann's notation.)

Siegel finished his paper with a study of the function $\mathcal{R}(s)$ (a notation that we have introduced in Riemann's honor).

Siegel writes that Riemann also considered this function and tried to study its zeros, its modulus $|\mathcal{R}(\frac{1}{2} + it)|$ and its argument $\arg \mathcal{R}(\frac{1}{2} + it)$.

From his study of the zeros of $\mathcal{R}(s)$ Siegel obtains the theorem that there are at least cT real zeros of $\Xi(t)$ with $0 < t < T$, and concludes his paper by asserting that the actual means (in 1932 C.E.) does not allow for obtaining Riemann's claim (A).

2.4 AFTER THE NACHLASS.

We have no reason to doubt Riemann's sincerity in his paper [68]. Additionally, the insights he provided for a proof have not been discredited.

The only serious questions then, arose from the two assertions provided without even a sketch of proof. The second assertion, that concerning the interchange of a sum and an integral, has since been proven. So, only assertion (A), concerning the number of real zeros of $\Xi(t)$ remained unproven. Hardy [25] was the first to show that there are infinitely many real roots. Later Selberg [75] proved that there are at least $CT \log T$ such roots. Subsequently, Levinson [48] established that at least $\frac{1}{3}$ of the roots of $\Xi(t) = 0$ are real. This has been extended by Conrey [13], who has shown that a fraction of at least 40.77% of the roots are real. However, as of this writing, there is not a proof of Riemann's assertion (A).

Interestingly, Riemann definitely implies (in [68] and [70]) that he had a proof of (A). This, in stark contrast to acknowledging [68] that he had no proof of the RH.

Siegel did not find evidence that Riemann had a proof for assertion (A). However, this does not provide conclusive evidence since Siegel did not find proof of any other of Riemann's assertions either.

Here it is appropriate to acknowledge the work of Neuenschwander [57]. According to Neuenschwander, almost all the scientific correspondence of Riemann has been lost. Some of his letters can be reconstructed from scattered drafts on various pieces of paper among the 4000 or so sheets comprising the Nachlass.

Schilling, married to Riemann's only daughter Ida, writes to Weber

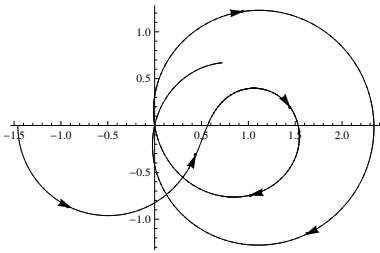
“At first mother could not come to terms with the idea that Riemann's papers should no longer remain in private hands; to her, they are something sacred, and she doesn't like to think of them being made accessible to any student, who would then also be able to read the marginal notes, some of which are purely personal.”

This and other family references suggest that many of Riemann's personal documents must have remained in the possession of Riemann's relatives, but at present, the whereabouts of these documents remains unknown.

3 THE NUMERICAL VERIFICATION OF THE RH.

3.1 THE FIRST FEW ZEROS

In order to locate the first zeros of $\zeta(s)$ in the critical strip $0 < \sigma < 1$, $t \geq 0$, we need to be able to compute $\zeta(s)$ with considerable accuracy. Nowadays such computations are much easier to perform than in the days of Gram, Backlund and Hutchinson, who, in addition to Riemann himself, were among the first to compute these zeros.



We get in this case $\text{Int} \simeq -1$, which must be due to the simple pole at $s = 1$ with residue 1. Similarly, between $t = 10$ and $t = 18$ we get $\text{Int} \simeq 1$.

Usually the zeros $\beta + i\gamma$ of $\zeta(s)$ with $\gamma > 0$ are arranged in a sequence $\rho_n = \beta_n + i\gamma_n$ so that $\gamma_{n+1} \geq \gamma_n$.

So, there is precisely one zero (on the critical line !) with $0 < t < 18$. Now we plot $|\zeta(1/2 + it)|$ for $10 \leq t \leq 18$ for finding a more precise location of $t = \gamma_1$.

We thus find that $\gamma_1 \simeq 14.1$ (higher accuracy is easily obtained). In similar plots of $|\zeta(1 + it)|$ we may already recognize the zeros $\gamma_2 \simeq 21$, $\gamma_3 \simeq 25$, $\gamma_4 \simeq 30$ and $\gamma_5 \simeq 33$.

We will come back to this in Section 3.7 and make things more precise by other (more economical) means. The first five γ_n are :

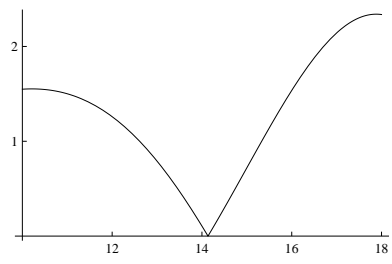


Figure 3: $|\zeta(\frac{1}{2} + it)|$ for $10 \leq t \leq 18$

- $\gamma_1 = 14.1347251417\ 3469379045\ 7251983562\ 4702707842\ 5711569924$ (early)
- $\gamma_2 = 21.0220396387\ 7155499262\ 8479593896\ 9027773343\ 4052490278$ (late)
- $\gamma_3 = 25.0108575801\ 4568876321\ 3790992562\ 8218186595\ 4967255799$ (early)
- $\gamma_4 = 30.4248761258\ 5951321031\ 1897530584\ 0913201815\ 6002371544$ (late)
- $\gamma_5 = 32.9350615877\ 3918969066\ 2368964074\ 9034888127\ 1560351703$ (early)

Riemann indicated that all zeros are on the critical line. So, one has concentrated on zeros of $\zeta(1/2 + it)$. But, also possible zeros off the critical line have to be excluded !

That $t = 14.134\dots$ is the first zero of $\zeta(1/2 + it)$ may also be shown (as Riemann actually did) by using the formula (for more details see Edwards [17, p. 159–160])

$$\sum_{n=1}^{\infty} \frac{1}{\gamma_n^2 + \frac{1}{4}} = 1 + \frac{1}{2} \gamma - \frac{1}{2} \log \pi - \log 2 = 0.02309\ 57089\ 66121\ 03381\dots \quad (16)$$

We also observe that for $\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}$, where $0 < a \leq 1$, there exists an Euler-Maclaurin formula similar to (16).

There are alternative ways to guess the first few zeros. For example, note the position of the up-zeros of $\arg \zeta(1 + it)$. See Fig. 4.

Continuing as indicated above one easily finds the first 100 (simple) zeros of $\zeta(s)$ (all on the critical line). (See [59] for a list of the first 2001052 zeros accurate to within 3×10^{-9} .)

According to Siegel, Riemann applied his asymptotic formula in an extensive computation to locate the first few zeros (Siegel is not very precise, but it seems that

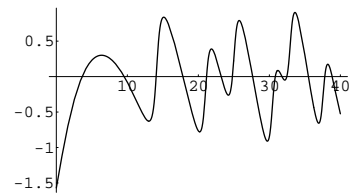


Figure 4: $\arg \zeta(1 + it)$ for $0 \leq t \leq 40$

Riemann computed at least three zeros).

We have the following time table for the numerical verification of the RH:

Time Table		
Year	Investigator	Number of zeros
(1859)	Riemann (using (12)–(14))	≥ 3
	↓ using Euler-Maclaurin	
(1903)	Gram [22]	15
(1916)	Backlund [1]	79
(1925)	Hutchinson [29]	138
	↓ using Riemann-Siegel	
(1936)	Titchmarsh & Comrie [80]	1 041
(1953)	Turing [83]	1 104
(1956)	Lehmer [41]	25 000
(1958)	Meller [53]	35 337
(1966)	Lehman [39]	250 000
(1969)	Rosser, Yohe, Schoenfeld [72]	3 502 500
(1979)	Brent [7]	81 000 001
(1982)	Brent, van de Lune, te Riele & Winter [9]	200 000 001
(1983)	van de Lune & te Riele [43]	300 000 001
(1986)	van de Lune, te Riele & Winter [46]	1 500 000 001
(2001)	van de Lune (unpublished)	10 000 000 000
(2003)	Wedeniowski (Zeta-grid) [87]	250 000 000 000
(2004)	By a new method of Odlyzko and Schönhage [62] Gourdon [20]	10 000 000 000 000

3.2 THE RIEMANN-SIEGEL FORMULA.

By means of the functional equation it is possible to define two *real continuous* functions $\vartheta(t)$ and $Z(t)$, $t \geq 0$, satisfying $\zeta(\frac{1}{2} + it) = Z(t)e^{-i\vartheta(t)}$ and $\vartheta(0) = 0$. See Edwards [17, p. 119]. From the functional equation it follows that $\vartheta(t)$ depends only on the Gamma-function:

$$\vartheta(t) := \operatorname{Im} \log \Gamma\left(\frac{1}{4} + i\frac{t}{2}\right) - \frac{t}{2} \log \pi. \quad (17)$$

The function $\vartheta(t)$ is rather easy to compute ([20]) whereas the computation of $Z(t)$ is quite complicated, especially in view of the inherent error terms.

The Riemann-Siegel formula for $\zeta(\frac{1}{2} + it)$ reads (for $t > 0$):

$$Z(t) = \sum_{n=1}^m \frac{\cos(\vartheta(t) - t \log n)}{\sqrt{n}} + R_m(t) \quad (18)$$

where $m = \lfloor \sqrt{t/2\pi} \rfloor$ and $R_m(t)$ is a rather complicated sum of linear combinations of derivatives of $\Psi(p) = \frac{\cos 2\pi(p^2 - p - \frac{1}{16})}{\cos 2\pi p}$. For the rather delicate error $R_m(t)$, see

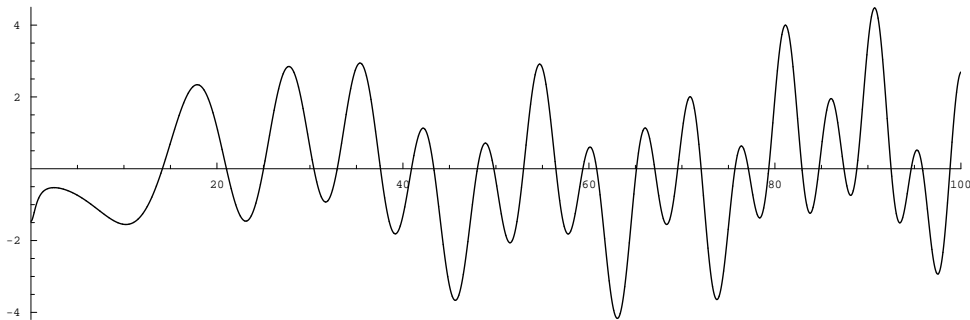


Figure 5: A plot of $Z(t)$ for $0 \leq t \leq 100$

Edwards [17], Gabcke [19] or Crary & Rosser [14]. Once the error $R_m(t)$ has been mastered this (Riemann-Siegel) formula is quite effective (provided t is not too small). Indeed, this method requires the computation of some $\sqrt{t/2\pi}$ terms, whereas the Euler-Maclaurin formula requires the computation of $O(t)$ terms.

3.3 THE FUNCTION $\vartheta(t)$.

Equation (18) shows that $\vartheta(t)$ does not depend on $\zeta(\frac{1}{2} + it)$, although, it has been shown (van de Lune, 1996) that we also have

$$\vartheta(t) = - \int_0^t \operatorname{Re} \frac{\zeta'(\frac{1}{2} + iu)}{\zeta(\frac{1}{2} + iu)} du. \tag{19}$$

Usually $\vartheta(t)$ is computed by means of the asymptotic expansion

$$\vartheta(t) = \frac{t}{2} \log \frac{t}{2\pi} - \frac{t}{2} - \frac{\pi}{8} + \sum_{n=1}^{\infty} \frac{(2^{2n-1} - 1) |B_{2n}|}{2^{2n} (2n - 1) 2n} \frac{1}{t^{2n-1}}, \quad t \rightarrow \infty. \tag{20}$$

(For more details and its practical use see Edwards [17] or Gabcke [19]). However, this formula is not suitable for small values of t . From the functional equation (5) and the Weierstrass product for $\Gamma(s)$ it may be shown that for all $t \geq 0$:

$$\vartheta(t) = -(\gamma + \log \pi + 3 \log 2 + \frac{\pi}{2}) \frac{t}{2} + \sum_{k=0}^{\infty} \left(\frac{2t}{4k+1} - \arctan \frac{2t}{4k+1} \right) \tag{21}$$

(van de Lune, 1996) which is useful only for small values of t . From (22) it is clear that $\vartheta(t)$ is analytic on \mathbb{R} , and differentiating (22) twice we see that $\vartheta(t)$ is convex and from this it easily follows that $\vartheta(t)$ is eventually *strictly increasing* (for $t > 2.28984$). (When using Mathematica one may directly use $\vartheta(t) := \text{RiemannSiegelTheta}[t]$.)

3.4 GRAM POINTS.

In all modern computations concerning the RH, some special points play a very important role: the Gram points g_k (or $g(k)$). For integral $k \geq -1$ the Gram point $t = g_k (> 7)$ is defined as the unique solution of $\vartheta(t) = k\pi$ (Note that the minimum of $\vartheta(t)$ is $\simeq -3.53097$ at $t \simeq 6.28984$). This equation may easily be solved by Newton iteration. Gram's "law" (to which there are many exceptions) says that (quite often) $(-1)^k Z(g(k)) > 0$. In case $(-1)^k Z(g(k)) > 0$ the Gram point $g(k)$ is called good, otherwise bad. The first bad Gram point is g_{126} with $Z(g_{126}) \simeq -0.02763$. In all numerical work on $Z(t)$ one observes that $Z(g_k) \neq 0$ for all k . So, the Gram points are the points (different from the zeros) where the orbit of $\zeta(\frac{1}{2} + it)$ intersects the real axis.

Often it is useful to generalize the notion of Gram point. In order to do so we recall that $\vartheta(t)$ is strictly increasing for $t > 6.28984\dots$ with $\vartheta(6.28984\dots) = -3.53097\dots$. So, also $\frac{1}{\pi}\vartheta(t)$ is strictly increasing (and continuous) and therefore has an inverse function $g(x)$ for $x > -\frac{1}{\pi}3.53097\dots$. Hence $\{\frac{1}{\pi}\vartheta\}^{-1} = g$. So, for appropriate x and t , we have $\frac{1}{\pi}\vartheta(g(x)) = x$ (or $\vartheta(g(x)) = \pi x$) and $g(\frac{1}{\pi}\vartheta(t)) = t$. We now define the Gram index of $t (> 6.28984\dots)$ as the unique solution $x = x(t)$ of $g(x) = t$. From this it is clear that this solution equals $x = x(t) = \frac{1}{\pi}\vartheta(t)$. (Note that the Gram index of the Gram point $g_k = g(k)$ is k .)

We note here that Titchmarsh has shown that :

$$\frac{1}{N} \sum_{n=1}^N Z(g(2n)) \rightarrow 2 \quad \text{and} \quad \frac{1}{N} \sum_{n=1}^N Z(g(2n-1)) \rightarrow -2 \quad \text{as } N \rightarrow \infty. \quad (22)$$

From this it is clear that $Z(t)$ must have infinitely many (real) zeros. It occurs to us that, in addition to this, it should not be too difficult to prove the following generalization:

$$-1 < x \leq 1 \quad \implies \quad \frac{1}{N} \sum_{n=1}^N Z(g(2n+x)) \rightarrow 2 \cos \pi x \quad \text{as } N \rightarrow \infty. \quad (23)$$

First Gram points					
g_{-1}	=	9.6669080561 3019214126	g_5	=	38.9992099640 2607481744
g_0	=	17.8455995404 1086081682	g_6	=	42.3635503920 5733796940
g_1	=	23.1702827012 4630927899	g_7	=	45.5930289815 0352227397
g_2	=	27.6701822178 1633796093	g_8	=	48.7107766217 9333294037
g_3	=	31.7179799547 6405317955	g_9	=	51.7338428133 4610437069
g_4	=	35.4671842971 0021611605	g_{10}	=	54.6752374468 5325626632

It can be shown that $g_k \sim 2\pi \frac{k}{\log k}$ asymptotically as $k \rightarrow \infty$. The bad Gram points with index ≤ 500 are $g_{126}, g_{134}, g_{195}, g_{211}, g_{232}, g_{254}, g_{288}, g_{367}, g_{377}, g_{379}, g_{397}, g_{400}, g_{461}$.

According to Gram's law we should have $g(k-2) < \gamma_k < g(k-1)$. So, we might say that the "ideal location of γ_k " is $g(k - \frac{3}{2})$. The distribution of the γ_k around

the points $g(k - \frac{3}{2})$ seems to be Gaussian. In relation to this we define: *Early/late* zeros: a zero $\frac{1}{2} + i\gamma_k$ will be called “early” if $\gamma_k < g(k - \frac{3}{2})$ and “late” otherwise. We have never observed that a zero is “right on time”. Of the first five zeros given on page 9 the first, third and fifth are early, whereas the second and fourth are late.

The frequency of bad Gram points apparently increases with increasing t . Experimentally, we found these frequencies to be: 6.25% for $k \sim 10^3$, 9.90% for $k \sim 10^4$, 12.62% for $k \sim 10^5$, 13.99% for $k \sim 10^6$, 15.37% for $k \sim 10^7$, 16.06% for $k \sim 10^8$, 17.52% for $k \sim 10^9$, and 19.25% for $k \sim 10^{10}$. Selberg has shown [75] that there is (at least) a positive proportion of failures of Gram’s law.

3.5 A (PARTLY HEURISTIC) NOTE ON THE EXACT LOCATION OF THE γ_n .

When plotting the orbit of $\zeta(\frac{1}{2} + it)$ we observe, for example, that for $t > 3$, this orbit is *convex to the right*. We have not seen any exception to this “rule”. (It can be shown that this behavior follows from the RH.) Moreover, all computations so far indicate that $\zeta'(\frac{1}{2} + it) \neq 0$ for all real t . (On the critical line $\zeta'(s)$ can be zero only at a zero of $\zeta(s)$. See Titchmarsh [81, p. 381].) So, it seems that all zeros of $\zeta(s)$ are simple.

Based on these two ingredients we can compute $\lim_{t \uparrow \gamma_1} \arg \zeta(\frac{1}{2} + it)$ in two different ways resulting in (note that the tangent to the orbit of $\zeta(\frac{1}{2} + it)$ and the vector $\zeta'(\frac{1}{2} + it)$ are always perpendicular)

$$\pi - \vartheta(\gamma_1) = \lim_{t \uparrow \gamma_1} \arg \zeta(\frac{1}{2} + it) = \arg \zeta'(\frac{1}{2} + it) + \frac{\pi}{2} + \pi \tag{24}$$

so that

$$\frac{1}{2} - \frac{1}{\pi}(\vartheta(\gamma_1) + \arg \zeta'(\frac{1}{2} + i\gamma_1)) = 1. \tag{25}$$

A similar reasoning reveals that for all $n \in \mathbb{N}$

$$\frac{1}{2} - \frac{1}{\pi}(\vartheta(\gamma_n) + \arg \zeta'(\frac{1}{2} + i\gamma_n)) = n. \tag{26}$$

This observation draws our attention to the function (van de Lune, 1997):

$$\kappa(t) := \frac{1}{2} - \frac{1}{\pi}(\vartheta(t) + \arg \zeta'(\frac{1}{2} + it)) \tag{27}$$

where $\vartheta(t)$ and $\arg \zeta(\frac{1}{2} + it)$ are continuous with $\vartheta(0) = 0$ and $\arg \zeta'(1/2) = \pi$.

This way we thus find that (assuming RH) $t = \gamma_n$ is the (unique) solution of the equation $\kappa(t) = n$.

We observe that $\arg \zeta'(\frac{1}{2} + it)$ is decreasing for $t > 2.75648\ 83863\ 8962\dots$, which is equivalent to the convexity to the right of the orbit of $\zeta(\frac{1}{2} + it)$. We also observe that the rate of decrease consistently overpowers the rate of increase of $\vartheta(t)$ to such an extent that $\kappa(t)$ is strictly increasing for $t > 0.78$, say, with $\kappa'(t) > 0$. One may verify that $\kappa(t = 6.28983\ 5988\dots) = 0$.

Since $\kappa(t)$ is strictly increasing it has an inverse function $\gamma(u)$: $\kappa(\gamma(u)) = u$ for $u > -0.67025\ 97987\dots$. We might say that in this way we get a *linearization of the*

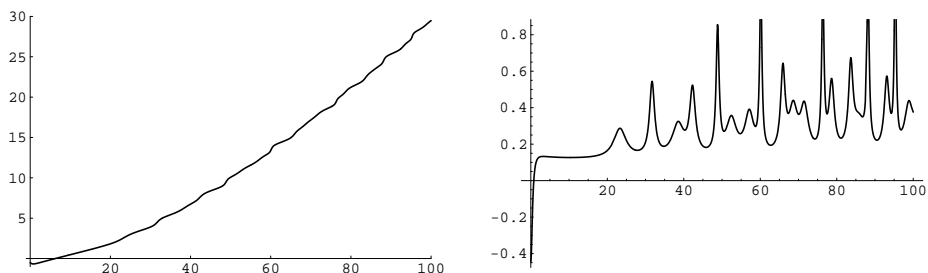


Figure 6: Plot of $\kappa(t)$ for $0 \leq t \leq 100$. Plot of $\kappa'(t)$ for $0 \leq t \leq 100$

γ_n . That is $\gamma(n) = \gamma_n$. It may be shown that $Z'(t) = 0 \Leftrightarrow t = \gamma(n - \frac{1}{2})$, so that also the local maxima and minima of $Z(t)$ are *linearized*. If a local minimum (maximum) of $Z(t)$ would be > 0 (< 0) then the RH would be violated.

Differentiating (28) and then integrating again we find that we also have the remarkable formula (it can be shown that the integrand is continuous)

$$\kappa(t) = -\frac{1}{2} + \frac{1}{\pi} \int_0^t \operatorname{Re} \left(\frac{\zeta'(\frac{1}{2} + iu)}{\zeta(\frac{1}{2} + iu)} - \frac{\zeta''(\frac{1}{2} + iu)}{\zeta'(\frac{1}{2} + iu)} \right) du. \quad (28)$$

The derivative

$$\kappa'(t) = \frac{1}{\pi} \operatorname{Re} \left(\frac{\zeta'(\frac{1}{2} + it)}{\zeta(\frac{1}{2} + it)} - \frac{\zeta''(\frac{1}{2} + it)}{\zeta'(\frac{1}{2} + it)} \right) \quad (29)$$

appears to be positive for $t > 0.7798535753\dots$ and shows a “tendency of being increasing”. See Figure 6.

It goes without saying that $\kappa'(t)$ must be quite large in the vicinity of close zeros! For example: $\kappa'(17143.804216267293) \simeq 519.27$ and

$$\kappa'(1239587702.547487092560555) \simeq \frac{1}{\pi} 154818579.027278937671 > 49 \times 10^6.$$

It can be shown that $\kappa'(\gamma_n) = \frac{1}{\pi} \vartheta'(\gamma_n) \simeq \frac{1}{2} \log \frac{\gamma_n}{2\pi}$ which is of “very moderate size”.

3.6 ROSSER BLOCKS.

In every modern systematic check of the RH a very prominent role is also played by *Rosser blocks*³. A Rosser block (of length L) is an interval $[g_k, g_{k+1}, \dots, g_{k+L}]$ where the end points g_k and g_{k+L} are good Gram points and the inner points $g_{k+1}, \dots, g_{k+L-1}$ are bad Gram points. This block is denoted by B_k (or rather by $B_{k,L}$). Note that a Rosser block of length $L = 1$ is just a good Gram interval.

³Sometimes called Gram blocks. They were introduced by Rosser et al [72].

A Rosser block of length L is called good if it contains *at least* L zeros of $Z(t)$. Otherwise it is called bad.

Rosser's rule (to which there are infinitely many exceptions) reads: All Rosser blocks are good.

We present some examples of first occurrences of Rosser blocks:

$L = 2$ starts at	$n =$	125	$L = 6$ starts at	$n =$	1 181 229
$L = 3$ starts at	$n =$	2 144	$L = 7$ starts at	$n =$	13 869 654
$L = 4$ starts at	$n =$	18 243	$L = 8$ starts at	$n =$	112 154 948
$L = 5$ starts at	$n =$	68 084	$L = 9$ starts at	$n =$	542 964 969

The largest Rosser block found so far has $L = 13$ (see Gourdon [20] and [21]). The zero pattern of a Rosser block is the finite sequence of integers counting the number of zeros of $Z(t)$ in each Gram interval of the block and its relevant neighbors. The first violation of Rosser's rule occurs at $n = 13\,999\,525$ (with $L = 2$ and zero pattern (00)3).

3.7 SYSTEMATIC SEPARATION OF THE ZEROS IN THE CRITICAL STRIP.

In practice, the numerical verification of the RH in a given range of the critical strip consists of *separating* the zeros of $Z(t)$, or, equivalently, of finding sufficiently many sign changes of $Z(t)$. So, its goal is *not* to compute the zeros of $Z(t)$ to any high degree of accuracy! We note in advance that it has never been observed that for any $n \geq -1$ we have $Z(g(n)) = 0$.

The main steps of the strategy in the separation-process are (briefly):

- (0) observe that the first Gram point $g(-1)$ is good
- (1) evaluate $Z(t)$ at the next Grampoint
- (2) as long as this (next) Grampoint is good, one has actually detected (at least) one zero (= sign change), and one goes to the next Gram point
- (3) as soon as one detects a bad Gram point $g(n+1)$ a Rosser block $B_{n,L} := [g(n), g(n+1), \dots, g(n+L-1), g(n+L)]$ of length $L \geq 2$ is set up
- (4) in such a block one has implicitly already detected $L-2$ zeros (in the interval $[g(n+1), \dots, g(n+L-1)]$)
- (5) so there are "two zeros missing"
- (6) now search for the "missing two":
 - (6a) first search inside the Rosser block for an (= one) "extra" sign change
 - (6b) if found then the Rosser block is good and one goes to the next Gram point $g(n+L+1)$
 - (6c) if not successful in finding the "missing two" one searches in one or more neighboring Rosser blocks
 - (6d) if still not successful: print an appropriate message and carry on, just pretending(!) that the "missing two" were found (such a "naughty" Rosser block will later be scrutinized "by hand".)

- (7) continue with evaluating $Z(g(n+L+1))$ and repeat the separation-procedure as sketched above.

An essential ingredient of the above strategy is a procedure to guarantee the sign of $Z(t)$. This requires a rigorous analysis of the Riemann-Siegel and Euler-Maclaurin formulas. A fully detailed FORTRAN-program of the procedure briefly sketched above may be found in van de Lune, te Riele & Winter [42] or [45].

So far, this strategy has never failed. The first example of a bad Rosser block was found by Brent: at $n = 13\,999\,525$ with length 2 (with zero-pattern (00)3).

A separation-run is usually finished by applying the following

THEOREM (Brent [7, Theorem 3.2]). *Let the interval $[g(n), g(p)]$ be the union of K consecutive good Rosser blocks where*

$$K \geq 0.0061 \log^2 g(p) + 0.08 \log g(p). \quad (30)$$

Then $N(g(n)) \leq n + 1$ and $N(g(p)) \geq p + 1$.

The systematic computation as sketched above is aiming at establishing $N(g(n)) \geq n + 1$. So, if Brent's theorem applies, then the conclusion will be that $N(g(n)) = n + 1$ and *no* violation of the RH has been detected.

So, at the time of writing we know that the first 10^{13} non-trivial zeros are on the critical line and are simple. See the time table.

All computations so far have shown that the "naughty" Rosser blocks of item (6d) occur quite rarely. Brent reports only 15 such blocks in the interval $0 < t < 32\,585\,736$. There seems to be no general rule predicting where the "missing two" are located.

We present a few interesting examples. In Figure 7 we consider for $n = 1\,048\,449\,112$ the Rosser block $B_{n,2} = [g(n), g(n+2))$. In this case the "missing two" are (as two very close zeros) located in the (bad) Gram interval $[g(n), g(n+1))$. Indeed, one may verify that $Z(g(n+0.88896415)) \simeq -0.000\,000\,221\,8$. So, this Rosser block turns out to be good with zero-pattern (20).

In Figure 8 we consider for $n = 30\,930\,927$ the Rosser block $B_{n,2} = [g(n), g(n+2))$. In this case the "missing two" are (as two extra zeros) located in the (good) Gram interval $[g(n-1), g(n))$. So, this $B_{n,2}$ turns out to be a bad Rosser block with zero-pattern 3(00).

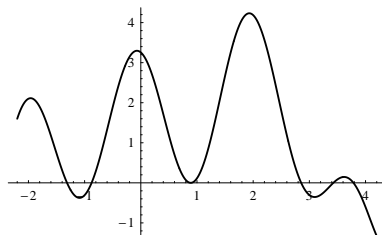


Figure 7: $Z(g(n+t))$ for $-2 \leq t \leq 4$

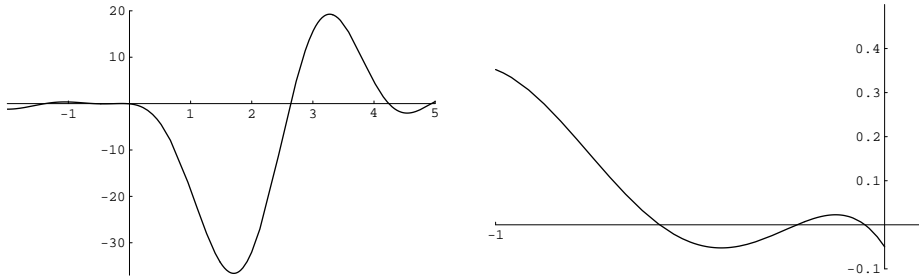


Figure 8: $Z(g(n+t))$ for $-2 \leq t \leq 5$ $Z(g(n+t))$ for $-1 \leq t \leq 0$

In Figure 9 we take $n = 61\,331\,766$ and consider the interval $[g(n), g(n+4))$. This interval consists of two adjacent Rosser blocks $B_{n,2} = [g(n), g(n+2))$ and $B_{n+2,2} = [g(n+2), g(n+4))$. From Figure 9 we infer that the “missing two” for $B_{n,2}$ as well as for $B_{n+2,2}$ are simultaneously located in the (bad) Gram interval $[g(n+2), g(n+3))$, which contains 4 zeros! So, $B_{n,2}$ is bad, whereas $B_{n+2,2}$ is a good Rosser block. The zero-patterns are (00)4 and (40), respectively.

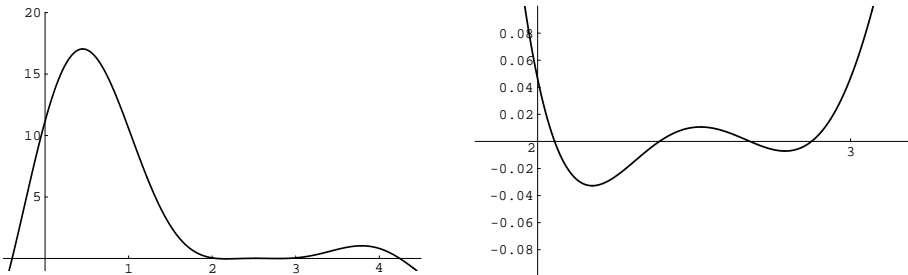


Figure 9: $Z(g(n+t))$ for $0 \leq t \leq 4$ $Z(g(n+t))$ for $2 \leq t \leq 3$

In Gourdon [20, p. 37] the reader may find a similar example in which there are 5 roots in one and the same (good) Gram interval.

4 “EQUIVALENCES” OF THE RH

In Titchmarsh [81, Chapter XIV] we find some necessary and sufficient conditions for the RH: the conditions of Riesz and Hardy & Littlewood. Later these were generalized by Brent [8]. The sufficient condition of Turán reads: If for all $N \in \mathbb{N}$ the sums $\zeta_N(s) = \sum_{n=1}^N n^{-s}$ have no zeros with $\sigma > 1$ then the RH is true. Unfortunately this condition is not true. We only mention the counter example $\zeta_{23}(1.00849693 \dots + i 8645.52442332 \dots) = 0$. For further information we refer to Spira [77] [78], van de Lune & te Riele [44], and Montgomery [54].

There is also a necessary and sufficient condition related to Farey series. For details see Landau's Vorlesungen [37, II, 167 – 177].

Mertens's sufficient condition reads: $M(x) \leq \sqrt{x}$ for all $x \geq 1$. Here $M(x) := \sum_{n \leq x} \mu(n)$, where $\mu(n)$ is the Möbius function. However, in 1985 it was shown by Odlyzko & te Riele [61] that "Mertens's conjecture" is not true. After te Riele and Odlyzko disproved the Mertens hypothesis, Pintz [65] was the first to show that actually the first violation occurs below $x = \exp(3.22 \times 10^{64})$. This bound was sharpened by Kotnik and te Riele [36] to $x = \exp(1.59 \times 10^{40})$. Some numerical computations by Kotnik & van de Lune [33] indicate that the first x with $M(x) > \sqrt{x}$ may very well be $> 10^{2 \times 10^{23}}$.

The Lindelöf hypothesis: $\zeta(\frac{1}{2} + it) = O(t^\varepsilon)$ for every $\varepsilon > 0$, follows from the RH; however, the converse does not hold.

More recently several other necessary and sufficient conditions for the RH have been presented (also see Bruinier [10]):

(1984) Robin's condition [71]: $\sigma(n) < e^\gamma n \log \log n$ for all $n \geq 5041$, where $\sigma(n) := \sum_{d|n} d$, and γ is Euler's constant.

(2000) Lagarias's condition [47]: $\sigma(n) \leq h(n) + e^{h(n)} \log h(n)$ for all $n \in \mathbb{N}$, where $h(n) := \sum_{j=1}^n \frac{1}{j}$.

No counter examples to these conditions have been found.

(1983) Nicolas's condition [58]: $\frac{N_k}{\varphi(N_k)} > e^\gamma \log \log N_k$, where $\phi(\cdot)$ is Euler's totient, and N_k the product of the first k primes.

This condition may also be written as

$$\Delta(k) := - \sum_{j=1}^k \log \left(1 - \frac{1}{p_j} \right) - \gamma - \log \log \sum_{j=1}^k \log p_j > 0. \quad (31)$$

Numerical computations by Kotnik & van de Lune [34] have shown that for all $2 \leq k \leq 10^{13}$ we actually have the sharper $\Delta(k) > \frac{1}{k}$. They also observe that for $k \geq 5$ one even has $\Delta(k) > \frac{1}{\sqrt{k(\log k)^2}}$.

Hence, so far the Nicolas criterion is amply satisfied.

(1992) Keiper [32] proved that if the RH is true then

$$\lambda_n := \frac{1}{n} \sum_{\varrho} (1 - (1 - \varrho^{-1})^n) > 0 \quad \text{for all } n \in \mathbb{N}. \quad (32)$$

It seems to us that Keiper was definitely a forerunner of Li.

(1997) Li's condition [49]: For all $n \geq 1$ the numbers $\lambda_n := \sum_{\varrho} (1 - (1 - \varrho^{-1})^n)$, where ϱ runs over the complex zeros of the zeta-function, are positive for all $n \geq 1$.

As for Li's criterion we restrict ourselves by referring to Li [49], Biane, Pitman & Yor [4] and Oesterlé [63]. We note that Bombieri & Lagarias [6] have shown that Li's criterion is a special case of a much more general theorem. Also, it is now known that if the first N zeros of $\zeta(s)$ are on the critical line then Li's criterion is satisfied for all $n \leq N^2$. See [63].

We mention the following sufficient condition: (J van de Lune, 2003) If, for every $\varepsilon > 0$, $\sum_{n \leq N} |\mu(n)| - 6N/\pi^2 = O(N^{1/4+\varepsilon})$ then the RH is true. (In this context

we mention that $\sum_{n \leq N} |\mu(n)|$ can be computed very fast by means of a sieve as mentioned in Section 1.1. Numerical computations (by Kotnik and van de Lune) for $N \leq 225 \times 10^{12}$ indicate that $\sum_{n \leq N} \{|\mu(n)| - 6/\pi^2\} = O(N^{1/4} \log N)$. More precisely, for all $N \leq 225 \times 10^{12}$ they found that $\left| \sum_{n \leq N} (|\mu(n)| - 6/\pi^2) \right| < 1.126 \times N^{1/4}$. We also note that this sufficient condition can be generalized considerably.

Finally there still is the condition by Baez-Duarte [3], and the condition that RH \Leftrightarrow the de Bruijn-Newman constant is ≤ 0 . See Wolf [88]. For the de Bruijn-Newman constant see Odlyzko [62].

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