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Scientific Computations Related to the Riemann Hypothesis

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1 Introduction.

The Riemann Hypothesis (RH), one of the oldest and best known unsolved problems in mathematics, continues to fascinate mathematicians. As there are a large number of equivalent formulations of the RH, many in different fields of mathematics have contributed to the general knowledge surrounding the RH. Our goal here is to survey the recent results on scientific computations and *one* such formulation of the RH.

The Riemann zeta function, defined by

(1.1) $$\zeta(z) := \sum_{n=1}^{\infty} \frac{1}{n^z} \ (z = x + iy \in \mathbb{C}),$$

is analytic in Re $z > 1$, and its representation as

(1.2) $$\zeta(z) = \prod_{p \ a \ prime} \left(1 - \frac{1}{p^z}\right)^{-1}$$

gives connections with to number theory.

Equation (1.2) can be used to show that $\zeta(z) \neq 0$ in Re $z > 1$. By means of analytic continuation, it is known that $\zeta(z)$ is analytic in the whole complex plane $\mathbb{C}$, except for a simple pole (with residue 1) at $z = 1$, and that $\zeta(z)$ satisfies the *functional equation*

(1.3) $$\zeta(z) = 2^z \pi^{z-1} \sin\left(\frac{\pi z}{2}\right) \Gamma(1-z)\zeta(1-z),$$

where $\Gamma(w)$ is the complex gamma function.

From (1.3), it can be deduced that

$$(1.4)\quad \begin{cases} \text{i)}\ \ \zeta(z) \text{ is nonzero in Re } z < 0, \text{ except for the real zeros } \{-2m\}_{m\geq 1}; \\ \text{ii)}\ \ \{-2m\}_{m\geq 1} \text{ are the only } \textit{real} \text{ zeros of } \zeta(z); \\ \text{iii)}\ \ \zeta(z) \text{ possesses infinitely many nonreal zeros in the strip } 0 \leq \text{Re} \\ \qquad z \leq 1, \text{ (so-called the) } \textit{critical strip} \text{ for } \zeta(z)). \end{cases}$$

In 1859, B. Riemann [15] formulated the following conjecture

(1.5) **The Riemann Hypothesis** : All nonreal zeros of $\zeta(z)$ lie exactly on Re $z = 1/2$.

It was later shown, (cf. Titchmarsh [16, p. 45]), independently in 1896 by Hadamard and de la Vallée-Pousin, that $\zeta(z)$ has *no* zeros on Re $z = 1$, which provided the first proof of the prime number theorem:

$$(1.6)\qquad \pi(z) \sim \frac{x}{\log x}\ (x \to +\infty),$$

where $\pi(x) := \{\text{number of primes } p \text{ for which } p \leq x\}$ (where $x > 0$). From (1.3), it also follows that $\zeta(z)$ has no zeros on Re $z = 0$; whence, (cf. (1.4iii)).

$$(1.7)\qquad \zeta(z) \text{ possesses infinitely many nonreal zeros in } 0 < \text{ Re } z < 1.$$

It is interesting to mention that

$$(1.8)\quad \begin{cases} \zeta(z) \text{ has infinitely many zeros on Re } z = 1/2 \text{ (Hardy [7])}, \\ \zeta(z) \text{ has at least } 1/3 \text{ of its zeros on Re } z = 1/2 \text{ (Levinson [9])}. \end{cases}$$

It also follows from (1.3) that if $\zeta(z) = 0$ where z is nonreal, then

$$(1.9)\qquad \{\overline{z}, 1-z, 1-\overline{z}\} \text{ are also zeros of } \zeta(z).$$

Thus, it suffices to search for the nonreal zeros of $\zeta(z)$ in the upper half-plane of the critical strip:

$$(1.10)\qquad S := \{z \in \mathbb{C} : 0 < \text{ Re } z < 1 \text{ and } Im\ z > 0\}.$$

2 Calculations.

There were numerous early ($\leq$ 1925), calculations of some zeros of $\zeta(z)$ in $0 <$ Re $z < 1$, and what was found were zeros of $\zeta(z)$ of the form $\frac{1}{2} + i\gamma_n$, where

$$\begin{aligned} &\gamma_1 = 14.13 \qquad &\gamma_4 = 30.42 \\ &\gamma_2 = 21.02 \qquad &\gamma_5 = 32.93 \\ &\gamma_3 = 25.01 \qquad &\gamma_6 = 37.58. \end{aligned} \tag{2.1}$$

Calculations in 1986 by the Dutch scientists van de Lune, te Riele, and Winter [10], showed that in the set

$$\hat{S} := \{z \in \mathbb{C} : 0 < \text{ Re } z < 1 \text{ and } 0 < Im\ z < 545,439,823.215\}, \tag{2.2}$$

there are exactly 1,500,000,001 zeros of $\zeta(z)$ which satisfy

$$\text{Re } z = 1/2 \text{ and all zeros are simple .} \tag{2.3}$$

More recently, calculations by Odlyzko (1989) in [12] showed that in

$$\begin{aligned} \tilde{S} := \ &\{z \in \mathbb{C} : 0 < \text{ Re } z < 1 \text{ and } \alpha \leq Im\ z \leq \beta, \text{ where} \\ &\alpha = 15,202,440,115,916,180,028.24 \\ &\beta = 15,202,404,115,927,890,387.66\ \}, \end{aligned} \tag{2.4}$$

there are precisely 78,893,234 zeros which again satisfy (2.3).

3 Another Approach to the RH.

Riemann [15] also gave in 1859 his definition of the Riemann ξ-function:

$$\xi(iz) := \frac{1}{2}\left(z^2 - \frac{1}{4}\right)\pi^{\frac{z}{2}-\frac{1}{4}}\Gamma\left(\frac{z}{2}+\frac{1}{4}\right)\zeta\left(z+\frac{1}{2}\right). \tag{3.1}$$

It is known that $\xi(z)$ is an *entire function*, i.e., it is analytic in all of the complex plane $\mathbb{C}$. For our purposes here, it is known (cf. Titchmarsh [16, p. 255]) that

$$\frac{1}{8}\xi\left(\frac{x}{2}\right) = \frac{1}{2}\int_{-\infty}^{+\infty} \Phi(t)e^{ixt}dt = \int_{0}^{\infty} \Phi(t)\cos(xt)dt \tag{3.2}$$

for any $x \in \mathbb{C}$, where

$$\Phi(t) := \sum_{n=1}^{\infty} \left\{2\pi^2 n^4 e^{9t} - 3\pi n^2 e^{5t}\right\} \exp\left(-\pi n^2 e^{4t}\right) \tag{3.3}$$

for $t \in \mathbb{R}$. Thus, the Riemann ξ-function is a *cosine transform* having the kernel $\Phi(t)$. We remark that the critical line $\mathrm{Re}\ z = \frac{1}{2}$ for the ζ-function corresponds to the real axis for the ξ-function. Consequently,

(3.4) RH is true iff all zeros of $\xi(x)$ are real.

This certainly has a bearing on RH, in the sense that much has been developed, in the area of complex analysis, about which *changes* can be made to a kernel, whose cosine transform has only real zeros, which leaves this property invariant. Major contributions have been made here by Laguerre, Pólya, and others. We describe this is more detail.

For any real λ, place the multiplicative factor $e^{\lambda t^2}$ in the kernel of (3.2), i.e., set

$$H_\lambda(x) := \frac{1}{2}\int_{-\infty}^{+\infty} e^{\lambda t^2}\Phi(t)e^{ixt}dt = \int_{0}^{\infty} e^{\lambda t^2}\Phi(t)\cos(xt)dt, \tag{3.5}$$

for all $x \in \mathbb{C}$. From the work of Pólya (1927) in [14], it is known that

$$\text{(3.6)} \quad \begin{cases} \text{if } H_0(x) = \frac{1}{8}\xi\left(\frac{x}{2}\right) \text{ has only real zeros, then so does } H_\lambda(x), \text{ for any} \\ \lambda \geq 0. \end{cases}$$

Subsequently, de Bruijn (1950) in [1] showed that

$$\text{(3.7)} \quad \begin{cases} \text{i) } H_\lambda \text{ has only real zeros for } \lambda \geq \frac{1}{2}; \\ \text{ii) if } H_\lambda \text{ has only real zeros, then so does } H_{\lambda'} \text{ for any } \lambda' \geq \lambda. \end{cases}$$

Then, C. M. Newman (1976) in [11] showed that there is a real number Λ, with

$$-\infty < \Lambda \leq \frac{1}{2}, \tag{3.8}$$

such that

$$
(3.9) \qquad \begin{cases} H_\lambda \text{ has only real zeros when } \lambda \geq \Lambda, \text{ and} \\ H_\lambda \text{ has some nonreal zeros when } \lambda < \Lambda. \end{cases}
$$

Remark 1 *This constant* Λ *is now known as the* **de Bruijn-Newman constant.**

How does this all connect with RH? From (3.4) and (3.6), we see that

$$
(3.10) \qquad \text{RH is true if } H_0 \text{ has only real zeros,}
$$

so that from (3.9),

$$
(3.11) \qquad RH \text{ is true iff } \Lambda \leq 0.
$$

Note that H_0 having only real zeros implies H_Λ has only real zeros for all $\Lambda \geq 0$, but it could happen that for some $\lambda < 0$, H_λ also has only real zeros, in which case $\Lambda < 0$.

4 Lower Bounds for Λ.

We know from de Bruijn [1] that $-\infty < \Lambda \leq \frac{1}{2}$. Can these bounds in any way be *improved*? We describe below some recent results on this, in connection with *Lehmer pairs of points.*

D. H. Lehmer (1956) in [8] found a pair of close zeros of $H_0(x) = \frac{1}{8}\xi\left(\frac{x}{2}\right)$, which are

$$
(4.1) \qquad \begin{cases} x_{6709}(0) = 14,010.125\ 732\ 349\ 841, \\ x_{6710}(0) = 14,010.201\ 129\ 345\ 293. \end{cases}
$$

(Lehmer had, in his equivalent calculation of the zeros of $\zeta(z)$ on the critical line $z = \frac{1}{2} + it$, actually *missed* the above two very close zeros. His points are now called, in the literature, "*Lehmer near counterexamples*" to the RH. The following is from a paper by Csordas, Smith, and Varga [5].

Definition 1 *With* k *a positive integer, let* $x_k(0)$ *and* $x_{k+1}(0)$ *(with* $0 < x_k(0) < x_{k+1}(0)$ *be two consecutive simple positive zeros of* $H_0(x)$*, and set*

$$\Delta_k := x_{k+1}(0) - x_k(0). \tag{4.2}$$

Then, $\{x_k(0);\ x_{k+1}(0)\}$ *is a* **Lehmer pair of zeros of $\mathbf{H_0(x)}$** *if*

$$\Delta_k^2 \cdot g_k(0) < \frac{4}{5}, \tag{4.3}$$

where

$$g_k(0) := \sum_{\substack{j \neq k, k+1 \\ j \neq 0}} \left\{ \frac{1}{(x_k(0) - x_j(0))^2} + \frac{1}{(x_{k+1}(0) - x_j(0))^2} \right\}. \tag{4.4}$$

It is known (from Csordas, Norfolk and Varga [2]), that H_t is a real even entire function of order 1 and maximal type, for *each* $t \in \mathbb{R}$. As a consequence of the Hadamard Factorization Theorem, it follows that

$$H_t(x) = H_t(0) \cdot \prod_{j=1}^{\infty} \left(1 - \frac{x^2}{x_j^2(t)}\right) \quad (x \in \mathbb{C}) \tag{4.5}$$

where

$$\sum_{j=1}^{\infty} \frac{1}{|x_j(t)|^2} < \infty. \tag{4.6}$$

It is a consequence of (4.6) that the sum for $g_k(0)$ is always convergent. Note that $\{x_k(0);\ x_{k+1}(0)\}$, being a Lehmer pair of zeros of $H_0(x)$, requires *more* than just close consecutive points!

It would appear from (4.4) that *all* of $H_0(x)$ need to be known, in order to evaluate $g_k(0)$ of (4.4), which is needed in (4.3). (Of course, if all the zeros of $H_0(x)$ were known, it follows from (3.6) that all zeros of $\zeta(x/2)$ are known, and we would, from (3.4), be able to determine directly if the RH is true or false!) Fortunately, it turns out that the sum in (4.4) can be bounded above, and, in the applications below, only a *few* points $x_j(0)$ are needed, close to the pair $\{x_k(0); x_{k+1}(0)\}$, to get reasonable upper bounds for $g_k(0)$.

The basic result of Csordas, Smith, and Varga [5] is

Theorem 1 *Let* $\{x_k(0);\ x_{k+1}(0)\}$ *be a Lehmer pair of zeros of* $H_0(x)$. *If* $g_k(0) \leq 0$, *then* $\Lambda > 0$. *If* $g_k(0) > 0$, *set*

$$\lambda_k := \frac{\left(1 - \frac{5}{4}\Delta_k^2 \cdot g_k(0)\right) - 1}{8g_k(0)}, \tag{4.7}$$

so that $-\dfrac{1}{8g_k(0)} < \lambda_k < 0$. *Then,*

$$\lambda_k < \Lambda. \tag{4.8}$$

The proof of this theorem depends upon

Lemma 1 *Suppose* x_0 *is a simple zero of* H_{t_0}, t_0 *real. Then, in some open interval* I *containing* x_0, *there is a real differentiable function* $x(t)$, *defined on* I, *satisfying* $x(t_0) = x_0$, *such that* $x(t)$ *is a simple zero of* H_t *and* $H_t(x(t)) \equiv 0$ *for* $t \in I$. *Moreover,*

$$x'(t) = \frac{H_t''(x(t))}{H_t'(x(t))} \quad (t \in I). \tag{4.9}$$

Proof. Implicit function theorem! □

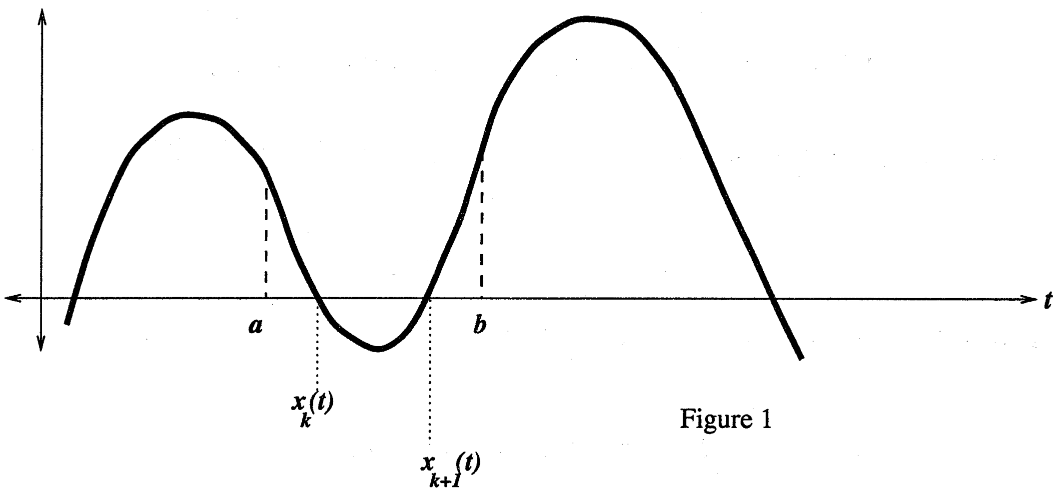

Figure 1

Suppose, as in Figure 1, that $H_t''(z) > 0$ in (a,b), where $x_k(t)$ and $x_{k+1}(t)$ are two consecutive simple zeros of $H_t(x)$ in (a,b). In the above Figure 1, $H_t'(x_k(t)) < 0$ and $H_t'(x_{k+1}(t)) > 0$, so that from (4.9).

$$x'_k(t) < 0 \text{ and } x'_{k+1}(t) > 0.$$

This means that, on increasing t, these two zeros of $H_t(x)$ are moving *away* from one another. So, on *reversing directions* and *decreasing* t, makes these zeros *approach one another*! It is the *coalescence* of these zeros which interests us!

Lemma 2 *Suppose, for some real t_0 and real x_0, that*

(4.10) $$H_{t_0}(x_0) = H'_{t_0}(x_0) = H'_{t_0}(x_0) = 0.$$

Then, $t_0 \leq \Lambda$.

Proof. Assume that $H''_{t_0}(x_0) \neq 0$; the case of a higher order zero at x_0 is similar. If

$$L_1(g(x)) := (g'(x))^2 - g(x) \cdot g''(x) \quad (x \in \mathbb{R})$$

for a real entire function $g(x)$, then for small $\delta > 0$, the hypothesis of (4.10) gives that

$$L_1\left(H_{t_0-\delta}(x_0)\right) = -\delta\left(H''_{t_0}(x_0)\right)^2 + O\left(\delta^2\right), \quad \delta \downarrow 0,$$

so that

$$L_1\left(H_{t_0-\delta}(x_0)\right) < 0 \quad \text{for all } \delta > 0 \text{ sufficiently small.}$$

On the other hand, it is known, from (Csordas, Ruttan and Varga (1991) in [4], that

(4.11) $$H_t \in L - P \text{ iff } t \geq \Lambda,$$

while it is also known, for any $f(x) \in \mathcal{L} - P$, that

(4.12) $$L_1(f(x)) \geq 0 \text{ for all } x \in \mathbb{R}.$$

(Here, $\mathcal{L} - P$ denotes the *Laguerre-Pólya class*, i.e., the set of all real entire functions of the form

$$f(z) = Ce^{-\lambda z^2+\beta z} z^n \prod_{j=1}^{\omega} \left(1 - \frac{z}{x_j}\right) e^{z/x_j} \quad (z \in \mathbb{C}),$$

where $\lambda \geq 0$, $\beta \in \mathbb{R}$, and x_j are real and nonzero with $\sum_{j=1}^{\omega} \frac{1}{x_j^2} < \infty$.)

Hence, putting together these facts gives us that

$$t_0 - \delta < \Lambda \text{ for all } \delta > 0 \text{ sufficiently small,}$$

so that

$$t_0 \leq \Lambda.$$

□

Applying the above Theorem to the original pair of zeros of (4.1) discovered by Lehmer, it can be shown that this pair of zeros is indeed a "Lehmer pair of zeros," in the sense of Definition 1 in this section, and that, on suitably bounding above $g_k(0)$ of (4.4), the result of

$$-7.113 \cdot 10^{-4} < \Lambda \tag{4.13}$$

was obtained.

But since we are interested in that *best* lower bound for Λ, we use a *spectacularly* close pair of zeros of H_0, bound by te Riele, et al., in 1986 in [10]. With

$$K := 1,048,449,114,$$

these zeros are

$$\begin{cases} x_K(0) = 777,717,772.0045\ 702\ 406, \\ x_{K+1}(0) = 777,717,772.0047\ 873\ 798, \end{cases} \tag{4.14}$$

Applying Theorem 1, it was shown in Csordas, Odlyzko, Smith, and Varga [3] that

$$-5.895 \cdot 10^{-9} < \Lambda. \tag{4.15}$$

We list below the accumulated research, consisting of analysis and computation, in finding lower bounds for Λ:

$$
(4.16)\quad \begin{cases}
-50 < \Lambda & \text{(Csordas, Norfolk, Varga, 1988)} \\
-5 < \Lambda & \text{(te Riele, 1991)} \\
-0.385 < \Lambda & \text{(Norfolk, Ruttan, Varga, 1992)} \\
-0.0991 < \Lambda & \text{(Csordas, Ruttan, Varga, 1991)} \\
-4.379 \cdot 10^{-6} < \Lambda & \text{(Csordas, Smith, Varga, 1994)} \\
-5.895 \cdot 10^{-9} < \Lambda & \text{(Csordas, Odlyzko, Smith, Varga, 1993)} \\
-2.7 \cdot 10^{-9} < \Lambda & \text{(Odlyzko (2000))}
\end{cases}
$$

The lower bounds were found in chronological order; their appearance in print is not! The first five lower bounds of (4.16) were each based on a different mathematical analysis. The analysis of the last and best lower bound of Odlyzko [13] is also based on the theory developed in [5].

We remind the readers that

$$(4.17)\qquad \text{RH is true iff } \Lambda \leq 0,$$

and (4.16) suggests strongly that

$$(4.18)\qquad \Lambda \overset{?}{\geq} 0,$$

which was already conjectured by C. M. Newman in [11] in 1976.

5 Open Problems.

1. Show that $0 \overset{?}{\leq} \Lambda$. Note that this would not prove or disprove the RH!

2. Obtain a new *upper* bound for Λ. Recall that de Bruijn in 1950 in [1] showed that

$$-\infty < \Lambda \leq \frac{1}{2},$$

but, in the intervening 50 years, there has been *no* improvement of the upper bound, $\frac{1}{2}$. Note that showing $\Lambda \leq \lambda$ would require showing that *all* zeros of H_λ are real, which is formidable.

3. It was shown in Csordas, Smith, and Varga [6] in 1994, that if H_0 has infinitely many Lehmer pairs of zeros, in the sense of the Definition, then $0 \leq \Lambda$. Thus, show that H_0 has **infinitely many Lehmer pairs of zeros.**

Remark 2 *This was already suggested by D. H. Lehmer.*

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