<table>
<thead>
<tr>
<th>Title</th>
<th>Scientific Computations Related to the Riemann Hypothesis (Numerical Solution of Partial Differential Equations and Related Topics)</th>
</tr>
</thead>
<tbody>
<tr>
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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

\begin{equation}
\xi(z) := \sum_{n=1}^{\infty} \frac{1}{n^z} \quad (z = x + iy \in \mathbb{C}),
\end{equation}

is analytic in Re \( z > 1 \), and its representation as

\begin{equation}
\xi(z) = \prod_{p \text{ prime}} \left( 1 - \frac{1}{p^z} \right)^{-1}
\end{equation}

gives connections with to number theory.

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

\begin{equation}
\xi(z) = 2^z \pi^{z-1} \sin \left( \frac{\pi z}{2} \right) \Gamma(1-z) \xi(1-z),
\end{equation}

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

From (1.3), it can be deduced that
\[ \begin{align*}
\text{i) } & \zeta(z) \text{ is nonzero in } \text{Re} \ z < 0, \text{ except for the real zeros } \{-2m\}_{m \geq 1}; \\
\text{ii) } & \{-2m\}_{m \geq 1} \text{ are the only real zeros of } \zeta(z); \\
\text{iii) } & \zeta(z) \text{ possesses infinitely many nonreal zeros in the strip } 0 \leq \text{Re} \ z \leq 1, \text{ (so-called the critical strip for } \zeta(z)).
\end{align*} \]

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

\textbf{(1.5) The Riemann Hypothesis}: All nonreal zeros of \( \zeta(z) \) lie exactly on \( \text{Re} \ z = 1/2 \).

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

\textbf{(1.6)} \[ \pi(x) \sim \frac{x}{\log x} \quad (x \to +\infty), \]

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 \( \text{Re} \ z = 0 \); whence, (cf. (1.4iii)).

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

It is interesting to mention that

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

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

\textbf{(1.9)} \[ \{ \overline{z}, 1 - z, 1 - \overline{z} \} \text{ are also zeros of } \zeta(z). \]

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

\textbf{(1.10)} \[ S := \{ z \in \mathbb{C} : 0 < \text{Re} \ z < 1 \text{ and } \text{Im} \ z > 0 \}. \]
2 Calculations.

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

$$
\begin{align*}
\gamma_1 &= 14.13 & \gamma_4 &= 30.42 \\
\gamma_2 &= 21.02 & \gamma_5 &= 32.93 \\
\gamma_3 &= 25.01 & \gamma_6 &= 37.58.
\end{align*}
$$  
(2.1)

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

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

there are exactly 1,500,000,001 zeros of ζ(z) which satisfy

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

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

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

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

It is known that ξ(z) is an entire function, i.e., it is analytic in all of the complex plane C. For our purposes here, it is known (cf. Titchmarsh [16, p. 255]) that
\[(3.2)\quad \frac{1}{8} \xi \left( \frac{x}{2} \right) = \frac{1}{2} \int_{-\infty}^{+\infty} \Phi(t) e^{ixt} dt = \int_{0}^{\infty} \Phi(t) \cos(xt) dt\]

for any \(x \in \mathbb{C}\), where

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

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

\[(3.4)\quad \text{RH is true iff all zeros of } \xi(x) \text{ are real.}\]

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

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

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

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

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

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

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

\[(3.8)\quad -\infty < \Lambda \leq \frac{1}{2},\]
such that

\begin{equation}
\begin{cases}
H_\lambda \text{ has only real zeros when } \lambda \geq \Lambda, \\
H_\lambda \text{ has some nonreal zeros when } \lambda < \Lambda.
\end{cases}
\end{equation}

Remark 1 This constant \( \Lambda \) 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

\begin{equation}
\text{RH is true if } H_0 \text{ has only real zeros,}
\end{equation}

so that from (3.9),

\begin{equation}
\text{RH is true iff } \Lambda \leq 0.
\end{equation}

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

4 Lower Bounds for \( \Lambda \).

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

\begin{equation}
\begin{aligned}
x_{6709}(0) &= 14,010.125732349841, \\
x_{6710}(0) &= 14,010.201129345293.
\end{aligned}
\end{equation}

(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
\[(4.2)\quad \Delta_k := x_{k+1}(0) - x_k(0).\]

Then, \(\{x_k(0); x_{k+1}(0)\}\) is a Lehmer pair of zeros of \(H_0(x)\) if
\[(4.3)\quad \Delta_k^2 \cdot g_k(0) < \frac{4}{5},\]
where
\[(4.4)\quad g_k(0) := \sum_{j \neq 0, j \neq k, k+1} \left\{ \frac{1}{(x_k(0) - x_j(0))^2} + \frac{1}{(x_{k+1}(0) - x_j(0))^2} \right\}.\]

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
\[(4.5)\quad H_t(x) = H_t(0) \cdot \prod_{j=1}^{\infty} \left( 1 - \frac{x^2}{x_j^2(t)} \right) \quad (x \in \mathbb{C})\]
where
\[(4.6)\quad \sum_{j=1}^{\infty} \frac{1}{|x_j(t)|^2} < \infty.\]

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

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

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

\[
\lambda_k < \Lambda.
\]

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,

\[
x'(t) = \frac{H''_t(x(t))}{H'_t(x(t))} \quad (t \in I).
\]

Proof. Implicit function theorem! \( \square \)

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).
$x'_k(t) < 0$ 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

$$H_{t_0}(x_0) = H'_{t_0}(x_0) = H''_{t_0}(x_0) = 0.$$  \hspace{1cm} (4.10)

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

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

so that

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

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

$$H_t \in L - P \text{ iff } t \geq \Lambda,$$  \hspace{1cm} (4.11)

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

$$L_1(f(x)) \geq 0 \text{ for all } x \in \mathbb{R}.$$  \hspace{1cm} (4.12)

(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

$$t_0 - \delta < \Lambda$$

for all $\delta > 0$ 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

(4.13) \hspace{1cm} -7.113 \cdot 10^{-4} < \Lambda

was obtained.

But since we are interested in that best lower bound for $\Lambda$, 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

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

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

(4.15) \hspace{1cm} -5.895 \cdot 10^{-9} < \Lambda.
We list below the accumulated research, consisting of analysis and computation, in finding lower bounds for $\Lambda$:

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

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

\[
\text{(4.17) RH is true iff } \Lambda \leq 0,
\]

and (4.16) suggests strongly that

\[
\text{(4.18) } \Lambda \gtrsim 0,
\]


5 Open Problems.

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

2. Obtain a new upper bound for $\Lambda$. 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 $H_\lambda$ 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.

References


