A new bound for the smallest x with $\pi(x) > \mathrm{li}(x)$

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Abstract

We reduce the leading term in Lehman's theorem. This improved estimate allows us to refine the main theorem of Bays & Hudson [2]. Entering $2,000,000$ Riemann zeros, we prove that there exists x in the interval $[\exp(727.951858), \exp(727.952178)]$ for which $\pi(x) - \mathrm{li}(x) > 3.2 \times 10^{151}$. There are at least 10^{154} successive integers x in this interval for which $\pi(x) > \mathrm{li}(x)$. This interval is strictly a sub-interval of the interval in Bays & Hudson, and is narrower by a factor of about 12.

Keywords: Riemann zeros, Skewes number, primes, logarithmic integral, first crossover.

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1 Introduction

Let $\pi(x)$ denote the number of primes less than or equal to x, and let $\mathrm{li}(x)$ denote the logarithmic integral. The notation $f(x) = \Omega_{\pm} g(x)$ means that

$$\limsup_{x\to\infty} f(x)/g(x) > 0, \qquad \liminf_{x\to\infty} f(x)/g(x) < 0$$

There was, in 1914, overwhelming numerical evidence that $\pi(x) < \mathrm{li}(x)$ for all x. In spite of this, Littlewood [9] announced that

$$\pi(x) - \mathrm{li}(x) = \Omega_{\pm}(x^{1/2}(\log x)^{-1} \log\log\log x)$$

This implies that $\pi(x) - \mathrm{li}(x)$ changes sign infinitely often. Littlewood's method provided, even in principle, no definite number X before which $\pi(x) - \mathrm{li}(x)$ changes sign. For a recent proof of Littlewood's theorem, see [11, Theorem 15.11].

In the course of the 20th century, successive numerical upper bounds were found by Skewes [17], Skewes [18], Lehman [8], te Riele [15]. For Littlewood's own account of the discovery of the Skewes numbers, see [10, p. 110–112].

The smallest value of x with $\pi(x) \geq \mathrm{li}(x)$ will be denoted Ξ, as in the recent paper by Kotnik [5]. In the course of a systematic computational study, Kotnik proves that

$$10^{14} < \Xi.$$

We now explain the main idea in [8]. Lehman's theorem is an *integrated version of the Riemann explicit formula*. His method was to integrate the function $u \mapsto \pi(e^u) - \mathrm{li}(e^u)$ against a Gaussian kernel over a carefully chosen interval $[\omega - \eta, \omega + \eta]$. The definite integral so obtained is denoted $I(\omega, \eta)$. Let $\rho = 1/2 + i\gamma$ denote a Riemann zero with $\gamma > 0$ and let

$$H(T, \omega) := -2\Re \sum_{0<\gamma\leq T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha}.$$

The α in this formula is related to the kernel chosen. Lehman proved the following equality

$$I(\omega, \eta) = -1 + H(T, \omega) + R$$

together with an explicit estimate $|R| \leq \epsilon$. This creates the inequality

$$I(\omega, \eta) \geq H(T, \omega) - (1 + \epsilon).$$

The problem now is to prove that

$$H(T, \omega) > 1 + \epsilon. \tag{1}$$

If (1) holds, then $I(\omega, \eta) > 0$ and so there exists $x \in [e^{\omega-\eta}, e^{\omega+\eta}]$ for which $\pi(x) > \mathrm{li}(x)$. In order to establish (1), numerical values of the Riemann zeros with $|\gamma| < T$ are required. Each term in $H(T, \omega)$ is a complex number determined by a Riemann zero. It is necessary that the real parts of these complex numbers, which are spiralling towards 0, reinforce each other sufficiently for (1) to hold. The only known way of establishing this is by numerical computation. When T is large, this requires a computer.

In 2000, Bays & Hudson [2] made the following selection:

$$\omega = 727.95209, \quad \eta = 0.002.$$

The interval itself is $[\exp(727.95009), \exp(727.95409)]$. We note that the numerical value of $\exp(727.95409)$ is *incorrectly stated* in [2, Theorem 2].

In this article, we reduce the leading term in Lehman's theorem. This enables us to select the following parameters:

$$\omega = 727.952018, \quad \eta = 0.00016.$$

The interval is $[\exp(727.951858), \exp(727.952178)]$ and so an upper bound for the first crossover Ξ is

$$\Xi < \exp(727.952178) < 1.398344 \times 10^{316}$$

Our interval is strictly a sub-interval of the Bays-Hudson interval. It is narrower by a factor of about 12, and creates the smallest known upper bound.

The function $H(T, \omega)$ is an initial part of the series

$$H(\omega) := -2\Re \sum_{0<\gamma} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha}.$$

As Rademacher observed in 1956 [14], the Riemann Hypothesis plus Weyl's criterion imply that, for each $\omega > 0$, the sequence

$$\{\exp(i\gamma\omega) : \zeta(1/2 + i\gamma) = 0, \gamma > 0\}$$

is *equidistributed* in the unit circle. So we may expect a fair amount of cancellation to take place in the series $H(\omega)$. This may help to explain why it is so difficult to find a number ω for which $H(T, \omega)$ exceeds 1.

We reflect, for a moment, on the Weil explicit formula. This is an identity between two distributions [13, p.39]. It is well established that certain classical explicit formulas follow from the Weil explicit formula, by picking suitable test-functions. For example, classical formulas for Dirichlet L-series may be derived in this way, see [6, Theorem 3.2, p.340]. We are led to ask whether the Lehman formula can be obtained from the Weil explicit formula by picking a suitable test function. We hope to pursue this idea elsewhere.

We would like to thank Andrew Odlyzko for supplying us with the first 2,000,000 Riemann zeros, Jon Keating for drawing our attention to [14], Christine Lee for improvements in the exposition, Aleksandar Ivić for drawing our attention to the inequalities of Panaitopol [12], and Nick Gresham for assistance with numerical calculations. Finally, we thank the referee for his many detailed and constructive comments.

2 The Leading Term

We begin this section with Lehman's theorem.

Theorem 2.1. *(Lehman [8]) Let A be a positive number such that $\beta = \frac{1}{2}$ for all zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ for which $0 < \gamma \le A$. Let α, η and ω be positive numbers such that $\omega - \eta > 1$ and*

$$2/A \le 2A/\alpha \le \eta \le \omega/2. \tag{2}$$

Let

$$K(y) := \sqrt{\frac{\alpha}{2\pi}} e^{-\alpha y^2/2}$$

$$I(\omega, \eta) := \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) u e^{-u/2} \{\pi(e^u) - li(e^u)\} du$$

Then for $2\pi e < T \le A$

$$I(\omega, \eta) = -1 - \sum_{0<|\gamma|\le T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha} + R$$

where

$$|R| \le s_1 + s_2 + s_3 + s_4 + s_5 + s_6$$

with

$$\begin{aligned} s_1 &= \frac{3.05}{\omega - \eta} \\ s_2 &= 4(\omega+\eta) e^{-(\omega-\eta)/6} \\ s_3 &= \frac{2e^{-\alpha\eta^2/2}}{\sqrt{2\pi\alpha}\eta} \\ s_4 &= 0.08\sqrt{\alpha} e^{-\alpha\eta^2/2} \\ s_5 &= e^{-T^2/2\alpha} \{ \frac{\alpha}{\pi T^2} \log\frac{T}{2\pi} + \frac{8\log T}{T} + \frac{4\alpha}{T^3} \} \\ s_6 &= A \log A e^{-A^2/2\alpha + (\omega+\eta)/2} \{ 4\alpha^{-1/2} + 15\eta \} \end{aligned}$$

If the Riemann Hypothesis holds, then conditions (2) and the term s_6 in the estimate for R may be omitted.

For the rest of the paper $\rho = \beta + i\gamma$ will denote a zero of the Riemann zeta function $\zeta(s)$ for which $0 < \beta < 1$. We will refine a part of Lehman's proof. This allows us to reduce the term s_1 in Lehman's theorem.

The logarithmic integral is defined as follows [4, p.82]:

$$\mathrm{li}(e^z) := \int_{-\infty+iy}^{x+iy} \frac{e^t}{t} dt$$

where $z = x + iy$, $y \neq 0$. For $x > 1$, $\mathrm{li}(x)$ is then defined as follows:

$$\mathrm{li}(x) := \frac{1}{2}[\mathrm{li}(x + i0) + \mathrm{li}(x - i0)]$$

In this way, we recover the classical definition of $\mathrm{li}(x)$ as an integral principal value [4, p.82]:

$$\mathrm{li}(x) = \lim_{\epsilon \to 0} \left(\int_0^{1-\epsilon} \frac{e^t}{t} dt + \int_{1+\epsilon}^{x} \frac{e^t}{t} dt \right)$$

For a detailed account of the logarithmic integral, see [7, p.38–41].

We define

$$J(x) := \pi(x) + \frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\pi(x^{1/3}) \ldots$$

and recall the Riemann-von Mangoldt explicit formula:

$$J(x) = \mathrm{li}(x) - \sum_\rho \mathrm{li}(x^\rho) + \int_x^\infty \frac{du}{(u^2-1)u\log u} - \log 2 \tag{3}$$

valid for $x > 1$. According to [16, (3.2) and (3.6), p.69] we have, for all $x > 1$,

$$\pi(x) = \frac{x}{\log x} + \frac{3\vartheta_1(x)x/2}{(\log x)^2}$$
$$\pi(x) = \frac{\vartheta_2(x)2x}{\log x} \tag{4}$$

with $|\vartheta_1(x)| < 1$, $\vartheta_2(x) < 0.62753$. There are at most $[(\log x)/\log 2]$ terms in $J(x)$. This allows us implicitly to define $\vartheta_3(x)$ by the following equation:

$$J(x) = \pi(x) + \frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\vartheta_3(x)\pi(x^{1/3}) \left(\frac{\log x}{\log 2}\right) \tag{5}$$

Then we have $\vartheta_3(x) < 1$. Combining (4) and (6), we have

$$\pi(x) - \mathrm{li}(x) = -\sum_\rho \mathrm{li}(x^\rho) + \int_x^\infty \frac{du}{(u^2-1)u\log u} - \log 2$$
$$- \frac{1}{2}\pi(x^{1/2}) - \frac{1}{3}\vartheta_3(x)\pi(x^{1/3}) \left(\frac{\log x}{\log 2}\right).$$

Substituting the first expression in (4) for $\pi(x^{1/2})$ and the second expression for $\pi(x^{1/3})$, we get

$$\begin{aligned}\pi(x) - \mathrm{li}(x) = &-\sum_\rho \mathrm{li}(x^\rho) + \int_x^\infty \frac{du}{(u^2-1)u\log u} - \log 2 \\ &- \left(\frac{x^{1/2}}{\log x} + 3\frac{\vartheta_1(x^{1/2})x^{1/2}}{(\log x)^2}\right) - \vartheta_3(x)\left(\frac{\vartheta_2(x^{1/3})2x^{1/3}}{\log 2}\right).\end{aligned}$$

Let

$$\vartheta_4(x) := \int_x^\infty \frac{du}{(u^2-1)u\log u} - \log 2$$

For $x > 2$ we have the following bounds:

$$-\log 2 < \vartheta_4(x) < 1/2 - \log 2.$$

We now have

$$\begin{aligned}\pi(x) - \mathrm{li}(x) = &-\sum_\rho \mathrm{li}(x^\rho) - \frac{x^{1/2}}{\log x} \\ &+ 3\frac{\vartheta_1(x^{1/2})x^{1/2}}{(\log x)^2} + \vartheta_4(x) - \frac{\vartheta_3(x)\vartheta_2(x^{1/3})2x^{1/3}}{\log 2}\end{aligned}$$

Now define $\vartheta(x)$ as follows:

$$4\vartheta(x)x^{1/3} := \vartheta_4(x) - \frac{\vartheta_3(x)\vartheta_2(x^{1/3})2x^{1/3}}{\log 2}$$

Then we have

$$|\vartheta(x)| < 4^{-1}x^{-1/3}(1/2 - \log 2) + 1/2 < 1 - \log 2 < 1$$

for all $x > 2$. Here is where our method differs from Lehman's approach: we keep the estimate $\vartheta_1(x)$ separate from $\vartheta(x)$. We have

$$\pi(x) - \mathrm{li}(x) = -\sum_\rho \mathrm{li}(x^\rho) - \frac{x^{1/2}}{\log x} + \frac{3\vartheta_1(x^{1/2})x^{1/2}}{(\log x)^2} + \vartheta(x)4x^{1/3} \quad (6)$$

Now we improve the bound for $\vartheta_1(x)$. We quote a result of Panaitopol [12, Theorem 1]:

$$\pi(x) < \frac{x}{\log x - 1 - (\log x)^{-0.5}} \quad \text{for all} \quad x \geq 6 \quad (7)$$

From (4) and (7), we get

$$\frac{x}{\log x} + \frac{\frac{3}{2}x\vartheta_1(x)}{\log^2 x} < \frac{x}{\log x - 1 - (\log x)^{-0.5}} \tag{8}$$

Denote $y = y(x) := (\log x)^{\frac{1}{2}}$. The inequality (8) will lead to an upper bound for $\vartheta_1(x)$:

$$0 < \vartheta_1(x) < \frac{2}{3} \cdot \frac{y^3 + y^2}{y^3 - y - 1} \quad \text{for all } x \geq 6. \tag{9}$$

We define

$$F(y) := \frac{y^3 + y^2}{y^3 - y - 1}.$$

We have $F(y) > 1,\ F(y) \to 1$ as $y \to \infty$, and

$$F'(y) = (-4y^3 - 3y^2 - 1)/(y^3 - y - 1)^2 < 0$$

so that F is a monotone decreasing function. By (9) we have

$$\vartheta_1(e^v) < \frac{2}{3} \cdot F(\sqrt{v})$$

and so

$$3\vartheta_1(e^{u/2}) < 2F(\sqrt{\tfrac{727}{2}}) < 2.1111$$

if $u \geq 727$.

From (6) we have immediately:

$$ue^{-u/2}\{\pi(e^u) - \mathrm{li}(e^u)\} = -1 - \sum_\rho ue^{-u/2}\mathrm{li}(e^{\rho u}) + \vartheta_1(e^{u/2})\frac{3}{u} + 4\vartheta(e^u)ue^{-u/6}$$

Now K is a standard Gaussian distribution, and so

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)du = \int_{-\eta}^{\eta} K(v)dv < 1.$$

If $\omega - \eta > 727$ then we have the estimate

$$\left| \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)(\vartheta_1(e^{u/2})\frac{3}{u} + 4\vartheta ue^{-u/6})du \right| \leq \frac{2.1111}{\omega-\eta} + 4(\omega+\eta)e^{-(\omega-\eta)/6}$$

We have replaced the term s_1 by s_1':

$$s_1' = \frac{2.1111}{\omega - \eta}$$

Following the steps in Lehman's proof [8], we are led to a new estimate $|R'|$:

$$|R'| \leq s_1' + s_2 + s_3 + s_4 + s_5 + s_6 \tag{10}$$

Theorem 2.2. *Let A be a positive number such that $\beta = \frac{1}{2}$ for all zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ for which $0 < \gamma \leq A$. Let α, η and ω be positive numbers such that $\omega - \eta > 727$ and*

$$2/A \leq 2A/\alpha \leq \eta \leq \omega/2. \tag{11}$$

Let $K(y)$ and $I(\omega, \eta)$ be defined as in Theorem 2.1. Then for $2\pi e < T \leq A$ we have

$$I(\omega, \eta) = -1 - \sum_{0<|\gamma|<T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha} + R'$$

where an upper bound for R' is given by (10).

If the Riemann Hypothesis holds, then conditions (11) and the term s_6 in the estimate for R' may be omitted.

Note. We are setting out to narrow the interval $[\omega - \eta, \omega + \eta]$. However, the inequalities (11) include a *lower bound* on η. We explain briefly how this lower bound arises. Without the Riemann Hypothesis, Lehman proves, by means of several intricate estimates [8, p.404–406], that the inequalities (11) are a sufficient condition for the following crucial estimate:

$$\left| \sum_{|\gamma|>A} \int_{\omega-\eta}^{\omega+\eta} K(u - \omega) u e^{-u/2} \mathrm{li}(e^{\rho u}) du \right| \leq s_6.$$

3 Numerical Results

In this section we exploit the reduced term s_1' to obtain improved numerical results. We commence with some remarks concerning the accuracy of computing by machine. Adopting notation similar to te Riele [15] we set

$$H(T, \alpha, \omega) = - \sum_{0<|\gamma|\leq T} e^{-\gamma^2/2\alpha} \cdot \frac{e^{i\omega\gamma}}{\rho} = - \sum_{0<\gamma\leq T} t(\gamma, \alpha, \omega)$$

where

$$t(\gamma, \alpha, \omega) = e^{-\gamma^2/2\alpha} \cdot \frac{\cos(\omega\gamma) + 2\gamma \sin(\omega\gamma)}{\frac{1}{4} + \gamma^2}$$

Fixing $N = 2,000,000$, we denote by γ_i^* the approximations to the true values of γ_i, correct to nine decimal places, computed by Odlyzko for $1 \leq i \leq N$, and set $T = 1131944.47182487 > \gamma_N$. Let $H^*(T, \alpha, \omega)$ be the value obtained by taking the sum up to T using $t(\gamma^*, \alpha, \omega)$ and let $H^*_M(T, \alpha, \omega)$ be the result of computing the same sum by machine. The function H^*_M therefore depends on many machine-specific details, including the implementation of standard library functions `sin`, `cos` and `exp`; similar considerations apply to the evaluation of $s'_1, \ldots, s_6$. In the case of H the quantity we wish to control is

$$|H - H^*_M| \leq |H - H^*| + |H^* - H^*_M|$$

The terms on the right represent errors arising from the conditioning of H upon the γ_i and numerical instability in computing by machine respectively.

Following [15] we have for $\gamma < \alpha$

$$|H(T, \alpha, \omega) - H^*(T, \alpha, \omega)| < \sum_{0<\gamma\leq T} |\gamma - \gamma^*| \cdot M(\gamma, \alpha, \omega)$$

with

$$M(\gamma, \alpha, \omega) = e^{-\gamma^2/2\alpha} \left(\frac{2\omega}{\gamma} + \frac{\omega}{\gamma^2} + \frac{2}{\alpha} + \frac{2}{\gamma^3} + \frac{4}{\gamma^2} \right) < \frac{3\omega + 8}{\gamma}$$

Now $14 < \gamma < 1131945 < \alpha$, and in the region of interest, we have $\omega < 728$, so we may use the estimate

$$|H(T, \alpha, \omega) - H^*(T, \alpha, \omega)| < 10^{-9} \cdot 2192 \cdot \sum_{i=1}^{N} \frac{1}{\gamma_i}$$

and we find numerically that $\sum_{i=1}^{N} \frac{1}{\gamma_i} < 12$, so that $|H - H^*|$ is bounded above by 3×10^{-5}.

It remains to address the extent of the additional error arising from machine computation of H^* and the quantities $s'_1, \ldots, s_6$. Let us denote by R'_M the machine-evaluated sum $s'_1 + \cdots + s_6$. Our initial experiments were conducted using MATLAB, but to speed sampling of the space of parameters $(\omega, \alpha, \eta, A)$ we re-implemented matters in `C` on an `x86_64 GNU/Linux` system using native double precision and routines from the `GNU` standard mathematics library `libm`. The results for specific valid choices of $(\omega, \alpha, \eta, A)$ with $H^*_M - (1 + R'_M) > 1 \times 10^{-4}$ were then re-computed using the arbitrary-precision libraries ARPREC[1] and MPFR[3], running at up to 100 digits and 1024 bits of precision respectively. Upon rounding to 7 decimal places all values obtained were in agreement; we are therefore confident that the cumulative effects of adverse numerical phenomena lie well below the threshold of 1×10^{-6}.

A simple strategy for selecting suitable $(\omega, \alpha, \eta, A)$ is to make order of magnitude estimates of the exponential factors in the terms $s_2, \ldots, s_6$. To start note that with two million zeros and ω near 728 the exponential factor in s_5 will be of the same order of magnitude as the leading term s_1' when α is near 10^{11}. A larger α means that η may be taken smaller, resulting in a narrower interval $(\omega - \eta, \omega + \eta)$, but pushing α to 1.35×10^{11} seems to be as far as one may safely travel in this direction. By repeated subdivision and scanning over subintervals of $(727, 728)$ with this α we find $H_M^* - 1$ can be made to exceed the leading term $s_1' > 2 \times 10^{-3}$ near $\omega = 727.95202$. To control the contribution from s_6 we need to take an A the same order of magnitude as $(\alpha\omega)^{1/2}$, whereupon the constraint $\alpha \leq A^2$ forces A near 1×10^7. We cannot take η an order of magnitude smaller than 10^{-5} without losing control of s_4, and the constraint $\alpha\eta \geq 2A$ forces η close to 2×10^{-4}. To keep $H_M^* - 1 - R_M'$ safely above 1×10^{-4} we chose the following values:

$$\omega = 727.952018 \qquad \eta = 0.00016$$
$$\alpha = 1.34 \times 10^{11} \qquad A = 1.022 \times 10^7$$

Then we obtain $H_M^* > 1.006569$ and the estimates

$$s_1' < 0.002901 \qquad s_2 < 10^{-49}$$
$$s_3 < 10^{-746} \qquad s_4 < 10^{-740}$$
$$s_5 < 0.003380 \qquad s_6 < 10^{-5}$$

so that

$$\begin{aligned} I(\omega, \eta) &\geq H - (1 + |R'|) \\ &\geq H_M^* - (1 + R_M') - 3 \times 10^{-5} - 1 \times 10^{-6} \\ &\geq 2 \times 10^{-4} > 0 \end{aligned}$$

Thus there is a value of u in the interval

$$(\omega - \eta, \omega + \eta) = (727.951858, 727.952178)$$

for which $\pi(e^u) > \mathrm{li}(e^u)$. Let

$$F(u) = ue^{-u/2} \cdot (\pi - \mathrm{li})(e^u)$$

then we have shown that

$$I(\omega, \eta) = \int_{\omega-\eta}^{\omega+\eta} K(u - \omega) \cdot F(u) du \geqslant \delta$$

with $\delta = 2 \times 10^{-4}$, therefore since $K(u)du$ is a probability measure,

$$0 < \delta \leq \int_{\omega-\eta}^{\omega+\eta} K(u - \omega) \cdot \sup F(u) du < \sup F(u)$$

Now $F(u)$ is continuous except where u happens to be the logarithm of a prime, so it follows that for u in some subinterval of $(\omega - \eta, \omega + \eta)$ we have $F(u) > \delta$, that is to say

$$\pi(e^u) - \mathrm{li}(e^u) > u^{-1}e^{u/2} \cdot \delta > 3.2 \times 10^{151}$$

We have

$$\mathrm{li}(N + r) - \mathrm{li}(N) - \frac{r}{\log N} = \int_N^{N+r} \frac{du}{\log u} - \frac{r}{\log N} \le 0 \le \pi(N + r) - \pi(N)$$

and so we obtain

$$\pi(N + r) - \mathrm{li}(N + r) \ge \pi(N) - \mathrm{li}(N) - \frac{r}{\log N}$$

This shows that if $\pi(e^u) - \mathrm{li}(e^u) > M > 0$ then $\pi(e^u) - \mathrm{li}(e^u)$ will remain positive for another $[Mu]$ consecutive integers. Here, $Mu > 10^{154}$.

Theorem 3.1. *There is a value of u in the interval*

$$(727.951858, 727.952178)$$

for which $\pi(e^u) - li(e^u) > 3.2 \times 10^{151}$. There are at least 10^{154} successive integers x between $\exp(727.951858)$ *and* $\exp(727.952178)$ *for which $\pi(x) > li(x)$.*

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