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

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Abstract

We reduce the dominant term in Lehman's theorem. This improved estimate allows us to refine the main theorem of Bays & Hudson. Entering $2,000,000$ Riemann zeros, we prove that there exists x in the interval $[1.39792101 \times 10^{316}, 1.39847603 \times 10^{316}]$ for which $\pi(x) > \mathrm{li}(x)$. This interval is strictly a sub-interval of the interval in Bays & Hudson [1], and is narrower by a factor of about 10.

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

$$\int_0^x \frac{dx}{\log x}.$$

There was, in 1914, overwhelming numerical evidence that $\pi(x) < \mathrm{li}(x)$ for all x. In spite of this, Littlewood [8] announced that there is a positive number K such that

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

is greater than K for arbitrarily large values of x and less than $-K$ for arbitrarily large values of 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.

So began the search for an *upper bound* for the first x for which the difference $\pi(x) - \mathrm{li}(x)$ is positive. The landmarks in this subject are

- Skewes [15], 1933: the first Skewes number

$$\mathrm{Sk}_1 = 10^{10^{10^{34}}}$$

This statement is conditional on the Riemann hypothesis, see [15, p.278]. This paper develops a version of the Phragmen-Lindelóf theorem. Skewes writes the following passage:

> No further difficulties of principle arise in the calculations, and what remains to be done is the arithmetical development of the ground already covered. This is a matter of some intricacy, and it is perhaps capable of refinements. What would be more important, it is possible that the restriction of the Riemann hypothesis can be removed. I propose, therefore, to postpone the details to a later paper; in the meantime, I have obtained a value of x_0 which, though possibly capable of improvement, undoubtedly provides a solution to the original problem.

This number is Sk_1. The first Skewes number is widely quoted, see for example [5, p.17] and [14, p.421]. We repeat that *there is no published proof* that, conditional on the Riemann Hypothesis, Sk_1 is an upper bound for the first crossover. For Littlewood's own account of the Skewes number, and his notation for very large numbers, see [9, p.110].

- Skewes [16], 1955: the second Skewes number

$$\mathrm{Sk}_2 = 10^{10^{10^{1000}}}$$

This is the later paper referred to in [15]. The method of proof in [16] is as follows. Assume first a certain hypothesis (H) (not the Riemann Hypothesis) and show that (H) leads to an upper bound X_1; then assume (NH), the negation of (H), and show that (NH) leads to an upper bound X_2. Since $X_2 > X_1$, we take $Sk_2 := X_2$ as an upper bound for the first crossover. This is therefore, the first published, unconditional proof of a numerical upper bound for the first crossover. In the notation of Littlewood [9], we have $\mathrm{Sk}_2 = N_3(3)$.

- Lehman [7], 1966: an upper bound for the first crossover is

$$1.65 \times 10^{1165}$$

We attempt to explain the main idea in [7]. We think of Lehman's theorem as an *integrated version of the Riemann explicit formula.* His idea was to integrate the function $u \mapsto \pi(e^u) - \mathrm{li}(e^u)$ against a strictly positive function 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 and let

$$\Sigma_T := -\sum_{0<|\gamma|\leq T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha}.$$

Lehman proved the following equality

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

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

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

The problem now is to prove that

$$\Sigma_T > 1 + \epsilon. \tag{1}$$

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 Σ_T 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. It is interesting to note that Lehman's theorem leads to a single spiral; without this theorem, the Riemann explicit formula leads to a very large number of spirals, as in [3, p.348].

- te Riele [12], 1987: an upper bound for the first crossover is

$$6.69 \times 10^{370}$$

The article by te Riele [12] uses Lehman's theorem; see section 6 for some more details.

We return to the interval $[e^{\omega-\eta}, e^{\omega+\eta}]$. This interval has half-length $e^{\omega} \sinh \eta$ and mid-point $e^{\omega} \cosh \eta$. Bays & Hudson make the following selection:

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

The mid-point of this interval is $1.398223656 \times 10^{316}$; the half-length of the interval is $0.002796443583 \times 10^{316}$. The interval itself is

$$[1.395427212 \times 10^{316}, 1.401020100 \times 10^{316}]$$

We note that *this interval is incorrectly stated* in Bays-Hudson [1, Theorem 2]. So we have

- Bays & Hudson [1], 2000: an upper bound for the first crossover is

$$1.401020100 \times 10^{316}.$$

We reduce the dominant term in Lehman's theorem by a factor of more than 2. This enables us to select the following parameters:

$$\omega = 727.952074, \quad \eta = 0.000198474.$$

The mid-point of this interval is $1.39819852 \times 10^{316}$; the half-length of the interval is $0.00027751 \times 10^{316}$. The interval is

$$[1.39792101 \times 10^{316}, 1.39847603 \times 10^{316}]$$

and so an upper bound for the first crossover is

- $1.39847603 \times 10^{316}$

Our interval is strictly a sub-interval of the Bays-Hudson interval. It is narrower by a factor of about 10, and creates the smallest known upper bound.

No specific X for which $\pi(X) > \mathrm{li}(X)$ is known. The 1914 article by Littlewood [8] contains the barest outline of a proof. A detailed proof of Littlewood's theorem appeared in 1918, see Hardy & Littlewood [6]. A sketch of the original argument is given in [10, Theorem 6.20].

We must mention the remarkable computer graphics of Demichel [2]. His heuristics lead to the the following upper bound for the first Littlewood violation:

$$1.39716292914 \times 10^{316}.$$

We feel bound to say that his elaborate computer graphics are dependent on the following formula:

$$\pi(x) \approx \mathrm{li}(x) - \mathrm{li}(x^{1/2})/2 - \sum_{\rho} \mathrm{li}(x^{\rho}).$$

This is not the true Riemann explicit formula, but an approximation to it. The true formula is given below, equation (4). This formula is stated in the 1859 memoir of Riemann [4, p.304]; concerning the erroneous value of $\log \xi(0)$ in this formula, see [4, p.31]. For a graphic account of the Riemann explicit formula applied to very large numbers, see Derbyshire [3, p. 348].

We thank Andrew Odlyzko for supplying us with the first $2,000,000$ Riemann zeros. We also thank Aleksandar Ivić for drawing our attention to the inequalities of Panaitopol [11].

2 Lehman's theorem

The classical function $\pi(x)$ is defined, for any real number x, as the number of primes less than or equal to x:

$$\pi(x) := \#\{p : p \leq x\}$$

where p is a prime number. Let

$$\Pi(x) = \pi(x) + \frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\pi(x^{1/3}) + ... = \sum_{k=1}^{\infty} \frac{1}{k}\pi(x^{1/k}) \qquad (2)$$

This is a finite series. We define

$$\Pi_0(x) = \lim_{\epsilon \to 0} \frac{1}{2}[\Pi(x - \epsilon) + \Pi(x + \epsilon)]$$

$$\mathrm{li}(x) = \lim_{\epsilon \to 0}\left(\int_0^{1-\epsilon} + \int_{1+\epsilon}^{x}\right)\frac{du}{\log u} \qquad (3)$$

We will describe a theorem proved by Lehman. The theorem is a powerful tool for finding where the sign of $\pi(x) - \mathrm{li}(x)$ changes.

In this section, $\rho = \beta + i\gamma$ will denote a zero of the Riemann zeta function $\zeta(s)$ for which $0 < \beta < 1$ and we denote by ϑ a number satisfying $|\vartheta| \leq 1$. This number ϑ will be different on different occasions.

Recall the Riemann explicit formula [4, p.65]

$$\Pi_0(x) = \mathrm{li}(x) - \sum_{\rho} \mathrm{li}(x^{\rho}) + \int_x^{\infty} \frac{dt}{t(t^2 - 1)\log t} - \log 2 \qquad (4)$$

where $\mathrm{li}(x^{\rho}) = \mathrm{li}(e^{\rho \log x})$ and, for $w = u + iv$, $v \neq 0$

$$\mathrm{li}(e^w) = \int_{-\infty+iv}^{u+iv} \frac{e^z}{z} dz \qquad (5)$$

If the terms in the sum are arranged according to increasing absolute values of $\gamma = \mathrm{Im}\rho$, then the series (4) converges absolutely in every finite interval $1 \leq a \leq x < b$.

We introduce some notation: θ and ϑ will denote real numbers for which $|\theta| < 1$ and $|\vartheta| < 1$. The values of θ and ϑ will vary according to context: but the inequalities $|\theta| < 1$ and $|\vartheta| < 1$ will always hold.

Rosser and Schoenfeld [13] have shown that, for $x > 1$, we have

$$\pi(x) = \frac{x}{\log x} + \frac{\frac{3}{2}\vartheta x}{\log^2 x}. \qquad (6)$$

Using this estimate and the more elementary estimate $\pi(x) < 2x/\log x$, we have for $x > 1$

$$\frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\pi(x^{1/3}) + ... = \frac{x^{1/2}}{\log x} + \vartheta(\frac{3x^{1/2}}{\log^2 x} + \frac{2x^{1/3}}{\log x}\left[\frac{\log x}{\log 2}\right]) \tag{7}$$

Estimating the integral in (4), we have for $x \geq e$

$$0 < \int_x^\infty \frac{dt}{(t^2-1)t\log t} < 2\int_x^\infty \frac{dt}{t^3} = \frac{1}{x^2} < \log 2$$

Since $2/\log 2 + \log 2 < 4$, we obtain, by combining (4) and (7),

$$\pi(x) = \mathrm{li}(x) - \frac{x^{1/2}}{\log x} - \sum_\rho \mathrm{li}(x^\rho) + \vartheta(\frac{3x^{1/2}}{\log^2 x} + 4x^{1/3}) \tag{8}$$

for $x \geq e$.

In this formula, it does not seem easy to determine a number x for which $\pi(x) > \mathrm{li}(x)$ by numerical computation. Because of this, Lehman derived an explicit formula for $ue^{-u/2}\{\pi(e^u) - \mathrm{li}(e^u)\}$ averaged by a Gaussian kernel and established the following theorem.

Theorem 2.1. *(Lehman [7]) 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 $\omega - \eta > 1$ and the conditions*

$$4A/\omega \leq \alpha \leq A^2 \tag{9}$$

and

$$2A/\alpha \leq \eta \leq \omega/2 \tag{10}$$

hold. Let

$$K(y) := \sqrt{\frac{\alpha}{2\pi}} e^{-\alpha y^2/2} \tag{11}$$

$$I(\omega,\eta) := \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)ue^{-u/2}\{\pi(e^u) - li(e^u)\}du \tag{12}$$

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

$$I(\omega,\eta) = -1 - \sum_{0<|\gamma|\leq T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha} + R \tag{13}$$

where

$$|R| \le \frac{3.05}{\omega-\eta} + 4(\omega+\eta)e^{-(\omega-\eta)/6} + \frac{2e^{-\alpha\eta^2/2}}{\sqrt{2\pi\alpha\eta}} + 0.08\sqrt{\alpha}e^{-\alpha\eta^2/2} \tag{14}$$

$$+e^{-T^2/2\alpha}\{\frac{\alpha}{\pi T^2}\log\frac{T}{2\pi} + \frac{8\log T}{T} + \frac{4\alpha}{T^3}\}$$

$$+A\log Ae^{-A^2/2\alpha+(\omega+\eta)/2}\{4\alpha^{-1/2}+15\eta\}$$

If the Riemann Hypothesis holds, then conditions (9) and (10) and the last term in the estimate for R may be omitted.

3 An improvement

In this section, we will improve Lehman's theorem. Quoting some results from L. Panaitopol [11], we have

$$\pi(x) > \frac{x}{\log x - 1 + (\log x)^{-0.5}} \qquad \text{for } x \ge 59 \tag{15}$$

$$\pi(x) < \frac{x}{\log x - 1 - (\log x)^{-0.5}} \qquad \text{for } x \ge 6 \tag{16}$$

Let us consider the condition $x \ge 59$. We get

$$\frac{x}{\log x - 1 + (\log x)^{-0.5}} < \pi(x) < \frac{x}{\log x - 1 - (\log x)^{-0.5}} \tag{17}$$

From the right side of (17) and (6), we get

$$\pi(x) \quad = \frac{x}{\log x} + \frac{\frac{3}{2}\vartheta x}{\log^2 x} < \frac{x}{\log x - 1 - (\log x)^{-0.5}}$$

Denote $A = A(x) := (\log x)^{\frac{1}{2}}$, so the inequality above can be expressed in terms of A:

$$\frac{x}{A^2} + \frac{\frac{3}{2}\vartheta x}{A^4} < \frac{x}{A^2 - 1 - A^{-1}}$$

Then, we get

$$\vartheta < \frac{2}{3}\cdot\frac{A^3+A^2}{A^3-A-1} \quad \text{for all } x \ge 59.$$

In fact, the function

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

is a monotone decreasing function for $x \geq e$. Furthermore, we will choose a very large value of x well-adapted to the subject of this article. We choose $x = 10^{95}$. This leads to the following inequality for ϑ:

$$0 \leq \vartheta < 0.71523279 \quad \text{for } x \geq 10^{95}$$

From the above, we can change one coefficient in (8):

$$\frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\pi(x^{1/3}) + ... = \frac{x^{1/2}}{\log x} + \vartheta\frac{3x^{1/2}}{\log^2 x} + \theta(\frac{2x^{1/3}}{\log x}\left[\frac{\log x}{\log 2}\right])$$

and we obtain

$$\pi(x) = \text{li}(x) - \frac{x^{1/2}}{\log x} - \sum_\rho \text{li}(x^\rho) - \vartheta\frac{3x^{1/2}}{\log^2 x} + 4\theta x^{1/3} \quad \text{for } x \geq 10^{190} \tag{18}$$

Hence, by (12)and(18), we have for $u > 437.5$

$$ue^{-u/2}\{\pi(e^u) - \text{li}(e^u)\} = -1 - \sum_\rho ue^{-u/2}\text{li}(e^{\rho u}) - \vartheta\frac{3}{u} + 4\theta ue^{-u/6} \tag{19}$$

From the positivity of the kernel K, we obtain the estimate

$$\begin{aligned} |\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)(-\vartheta\frac{3}{u} + 4\theta ue^{-u/6})du| \quad &\leq \quad \frac{3\vartheta}{\omega-\eta} + 4\theta(\omega+\eta)e^{-(\omega-\eta)/6} \\ &\leq \quad \frac{2.1957}{\omega-\eta} + 4(\omega+\eta)e^{-(\omega-\eta)/6} \end{aligned}$$

For the estimates of the rest of the terms, we follow Theorem 2.1 and finally we get a new estimate of $|R|$ denoted by $|R'|$:

$$|R'| \leq \frac{2.1957}{\omega-\eta} + 4(\omega+\eta)e^{-(\omega-\eta)/6} + \frac{2e^{-\alpha\eta^2/2}}{\sqrt{2\pi\alpha}\eta} + 0.08\sqrt{\alpha}e^{-\alpha\eta^2/2} \tag{20}$$

$$+e^{-T^2/2\alpha}\{\frac{\alpha}{\pi T^2}\log\frac{T}{2\pi} + \frac{8\log T}{T} + \frac{4\alpha}{T^3}\}$$

$$+A\log Ae^{-A^2/2\alpha+(\omega+\eta)/2}\{4\alpha^{-1/2} + 15\eta\}$$

Theorem 3.1. *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 $\omega - \eta > 437.5$ and the conditions*

$$4A/\omega \le \alpha \le A^2 \tag{21}$$

and

$$2A/\alpha \le \eta \le \omega/2 \tag{22}$$

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

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

where R' is given by (20).

If the Riemann Hypothesis holds, then conditions (21) and (22) and the last term in the estimate for R' may be omitted.

Remark. When we compare Theorem 2.1 with Theorem 3.1, we see that the conditions are different: in Theorem 2.1 we have $\omega - \eta > 1$ and in Theorem 3.1 we have $\omega - \eta > 437.5$. This makes little difference because we always take a large value for ω. A comparison of R and R' shows that the dominant term in Lehman's theorem has been improved by a factor of more than 1.3. In the next section we investigate the numerical consequences of this improved estimate.

4 Numerical Data

As in the Introduction, let

$$\Sigma_T := - \sum_{0<|\gamma|\le T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha}. \tag{23}$$

We recall Lehman's theorem (13):

$$I(\omega, \eta) = -1 + \Sigma_T + R.$$

As a first step, Lehman looked for values of ω for which the sum

$$S_T(\omega) = - \sum_{0<|\gamma|\le T} \frac{e^{i\gamma w}}{\rho},$$

which is the sum in (23) without the factor $e^{-\gamma^2/2\alpha}$, is somewhat greater than 1. Because the zeros of the Riemann zeta function occur in complex-conjugate pairs, we can write the sum as

$$\begin{aligned} S_T(\omega) &= -\sum_{0<\gamma\leq T}\left(\frac{e^{i\gamma\omega}}{\frac{1}{2}+i\gamma}+\frac{e^{-i\gamma\omega}}{\frac{1}{2}-i\gamma}\right) \\ &= -\sum_{0<\gamma\leq T}\frac{\cos(\gamma\omega)+2\gamma\sin(\gamma\omega)}{\frac{1}{4}+\gamma^2} \end{aligned}$$

He found three values of ω,

$$727.952, \quad 853.853, \quad 2682.977$$

for which $S_{1000}(\omega)$ is approximately 0.96. In 1987, Lehman proved that there exists x with $\pi(x) > \mathrm{li}(x)$ in the vicinity of $\exp(853.853)$. In 2000, Bays & Hudson [1] improved the result in the vicinity of $\exp(727.952)$.

In the following sections, we will discuss the numerical computations based on Theorem 2.1 and its improved Theorem 3.1 and give a better result about $\pi(x) - \mathrm{li}(x) > 0$.

5 Error in computation

We introduce a notation for every term in the error R:

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

From the above discussion, between Theorem 2.1 and Theorem 3.1, s_1 is the only difference. Therefore, we denote the first term in R' as s_1', namely

$$s_1' = \frac{2.1957}{\omega-\eta}$$

We will revert to the notation in te Riele [12]:

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

and let H^* be the approximate value of H by computer and γ^* be the approximation of γ.

Before doing the computation, we need to discuss the relative error between $H(T, \alpha, \omega)$ and H^*. By the mean-value theorem, we have

$$|t(\gamma^*) - t(\gamma)| = |\gamma^* - \gamma| \cdot |t'(\overline{\gamma})| \quad \text{with} \quad |\overline{\gamma} - \gamma| < |\gamma^* - \gamma|$$

For $t'(\gamma)$, we have

$$t'(\gamma) = e^{-\gamma^2/2\alpha} \left[\frac{\cos(\omega\gamma)(2\omega\gamma - \gamma/\alpha) - \sin(\omega\gamma)(\omega + 2\gamma^2/\alpha)}{\frac{1}{4} + \gamma^2} - \frac{2\gamma\cos(\omega\gamma) + 2\gamma\sin(\omega\gamma)}{(\frac{1}{4} + \gamma^2)^2} \right]$$

and since $\gamma < \alpha$(based on the value of α we choose)

$$\begin{aligned} |t'(\gamma)| &< e^{-\gamma^2/2\alpha} \left[\frac{2\omega\gamma + \omega + 2\gamma^2/\alpha}{\frac{1}{4} + \gamma^2} + \frac{2\gamma(1 + 2\gamma)}{(\frac{1}{4} + \gamma^2)^2} \right] \\ &< e^{-\gamma^2/2\alpha} \left[\frac{2\omega}{\gamma} + \frac{\omega}{\gamma^2} + \frac{2}{\alpha} + \frac{2}{\gamma^3} + \frac{4}{\gamma^2} \right] \end{aligned}$$

In our computation, the following inequalities will hold:

$$14 < \gamma_1 \leq \gamma, \quad \omega < 854, \quad \alpha \geq 2 \times 10^8$$

It follows that

$$|t'(\gamma)| < \frac{1770}{\gamma} \tag{24}$$

From above and the Riemann zeros given by Odlyzko, we have $|\gamma_i - \gamma_i^*| < 10^{-9}$

for $1 \leq i \leq 2 \times 10^6$ and can deduce

$$\begin{aligned} |H - H^*| &< \sum_{i=1}^{N} |t(\gamma_i) - t(\gamma_i^*)| \\ &= \sum_{i=1}^{N} |\gamma_i - \gamma_i^*| \cdot |t'(\overline{\gamma_i})| \\ &< 10^{-9} \sum_{i=1}^{N} \frac{1770}{\overline{\gamma_i}} \\ &< 10^{-9} \sum_{i=1}^{N} \frac{1770}{\gamma_i - 10^{-9}} \end{aligned}$$

where N is the number of zeros we use. Hence,we get

$$I(\omega, \eta) > -1 + H^* - |H - H^*| - |R|.$$

6 Computation

We will use Theorem 3.1 to find where the sign of $\pi(x) - \mathrm{li}(x)$ changes; we will also make some comparisons between Theorems 2.1 and 3.1.

In all the computations in this section, we use MATLAB. In fact, we do the computations with $2,000,000$ zeros. This is a very large number to store in a computer programme. So, we group the zeros together in blocks of $50,000$ and input two $50,000 \times 20$ matrices by MS-Excel. Then, we transfer these two matrices to our computer programme by some commands in MATLAB.

First, we compare Theorems 2.1 and 3.1 via numerical examples.

Computation 1. We take the same parameters as in Bays & Hudson [1, p.1288], using Theorem 2.1 and Theorem 3.1:

$$A = 10^7, \quad \alpha = 10^{10}, \quad \eta = 0.002,$$
$$T = \gamma_{1000000} = 600269.677..., \quad \omega = 727.95209$$

This leads to

$$H^* \approx 1.0128206$$

and the inequalities

$$\begin{aligned} |s_1| &< 0.00418985, & |s_1'| &< 0.00301627 \\ |s_2| &< 10^{-51}, & |s_3| &< 10^{-8688} \\ |s_4| &< 10^{-8681}, & |s_5| &< 10^{-8} \\ |s_6| &< 10^{-2000}, & |H - H^*| &< 1.606959 \times 10^{-5} \end{aligned}$$

This example shows that s_1(or s_1') is the most important term to change the value of $I(\omega,\eta)$. Reducing the term s_1 is an effective method to get a more accurate result. With Theorem 2.1, we need 432379 zeros; with Theorem 3.1, we need 426139 zeros.

COMPUTATION 2. In this computation, we decrease the parameters ω, η. We change the values used in Bays & Hudson [1]. After several experiments, we choose these values:

$$\begin{aligned} A = 7.8\times 10^6, \quad \alpha = 7.86\times 10^{10}, \quad \eta = 0.000198474, \\ T = \gamma_{2000000} = 1131944.4718..., \quad \omega = 727.952074 \end{aligned}$$

and apply Theorem 3.1 with $2,000,000$ Riemann zeros. Our results are as follows:

$$\begin{aligned}
s_1' &= \frac{2.1957}{727.951875526} < 0.003016271 \\
s_2 &= 4(727.952272474)e^{-(727.951875526)/6} < 5.933\times 10^{-50} \\
s_3 &= \frac{2e^{-7.86\times 10^{10}(0.000198474)^2/2}}{\sqrt{2\pi(7.86\times 10^{10})}(0.000198474)} < 10^{-1000} \\
s_4 &= 0.08\sqrt{7.86\times 10^{10}}e^{-7.86\times 10^{10}(0.000198474)^2/2} < 10^{-1000} \\
s_5 &= e^{(-1131944.4718)^2/2(7.86\times 10^{10})}\{\frac{7.86\times 10^{10}}{\pi(1131944.4718)^2}\log(\frac{1131944.4718}{2\pi})\} \\
&+ \frac{8\log(1131944.4718)}{1131944.4718} + \frac{4(7.86\times 10^{10})}{1131944.4718^3} < 0.00006820541 \\
s_6 &= (7.8\times 10^6)\log(7.8\times 10^6)e^{-(7.8\times 10^6)^2/2(7.86\times 10^{10})+(727.952272474)/2} \\
&\{ \; 4(7.86\times 10^{10})^{-1/2} + 15(0.000198474)\} \\
&< \; 0.000036261861
\end{aligned}$$

This leads to the following estimate of R'

$$|R'| = s_1' + s_2 + s_3 + s_4 + s_5 + s_6 < 0.003120738272$$

and H is summed over all γ with $0 < |\gamma| < 1131944.4718$. We obtain the approximation

$$H^* = 1.00319601829755$$

and the inequality

$$|H - H^*| < 2.05971416\times 10^{-5}$$

It follows that

$$I(\omega,\eta) > -1 + H^* - |H - H^*| - |R'| > 5.468288 \times 10^{-5} > 0 \tag{25}$$

The positivity of the kernel K implies that there is a value of u between $\omega-\eta$ and $\omega+\eta$ where $\pi(e^u) - \text{li}(e^u) > 0$. That means we have proved that there exists x in the vicinity of $\exp(727.952074)$ with $\pi(x) > \text{li}(x)$ by computer. Moreover, since

$$\int_{-\infty}^{\infty} K(u)du = 1 \tag{26}$$

it follows that

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)ue^{-u/2}\{e^{u/2}/u\}du < 1. \tag{27}$$

By (26) and (27), it follows that for some values of u between $\omega-\eta$ and $\omega+\eta$ we have

$$\pi(e^u) - \text{li}(e^u) > 5.468288 \times 10^{-5} e^{u/2}/u > 10^{150}$$

This implies that there are more than 10^{150} successive integers x between $1.39792101 \times 10^{316}$ and $1.39847603 \times 10^{316}$ for which $\pi(x) > \text{li}(x)$.

Theorem 6.1. *There exist values of x in the vicinity of $1.39819852 \times 10^{316}$, in particular, between $1.39792101 \times 10^{316}$ and $1.39847603 \times 10^{316}$, with $\pi(x) > li(x)$.*

Proof. See above. □

We feel bound to say that the interval in Bays & Hudson is incorrectly stated [1, Theorem 2]: the correct statement is

> *There exists values of x in the vicinity of 1.39822×10^{316} (in particular, between 1.395427×10^{316} and 1.401201×10^{316}) with $\pi(x) > li(x)$.*

We have succeeded in decreasing ω and η. Maybe there exists x with $\pi(x) > \text{li}(x)$ in another interval. In Bays & Hudson [1], they gave some possible candidates. We will use some rough computation to check their possibilities. Firstly, we point out what the candidates are:

$$10^{176}, \quad 10^{179}, \quad 10^{190}, \quad 10^{260}, \quad 10^{298}.$$

We find that the most likely candidate is in the vicinity of 10^{190} and Table 3 below records the values of S_{1000}, S_{50000} and H^*.

ω	S_{1000}	S_{50000}	H^*
437.763500	0.88258736	0.88666106	0.87987776
437.782672	0.88873669	0.88987227	0.87703253

Table 3. Estimated values in the vicinity of 10^{190}

From the table above, we can see S_{1000}, S_{50000} and H^* are less than 0.9. In fact, S_{1000} and S_{50000} are the sums H without the factor $e^{-\gamma^2/2\alpha}$. When doing the computation, we need to take this factor into account. On the other hand, when $\gamma \geq \gamma_{2000000} = 1131944.4718$, the value of $e^{-\gamma^2/2\alpha}$ is less than $10^{-1271038775}$. It is very small and this is why H^* is less than S_T when T is sufficiently large. Furthermore, let us consider every term in H,

$$-e^{-\gamma^2/2\alpha}\frac{\cos(\gamma\omega) + 2\gamma\cos(\gamma\omega)}{0.25 + \gamma^2} < e^{-\gamma^2/2\alpha}\frac{2\gamma}{\gamma^2} = \frac{2e^{-\gamma^2/2\alpha}}{\gamma}$$

From this inequality and the estimate of $e^{-\gamma^2/2\alpha}$, we see that the value of every term is extremely small when γ is sufficiently large. We know that if there exists x satisfying $\pi(x) - \mathrm{li}(x) > 0$, then H must be greater than 1. It seems that in the vicinity of 10^{190} it is almost impossible to make $\pi(x) > \mathrm{li}(x)$. Hence, the vicinity of 10^{316} is likely to be the first location for which $\pi(x) - \mathrm{li}(x) > 0$.

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