FIRST SIGN CHANGE OF $\theta(x) - x$

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ABSTRACT. The function $\theta(x) - x$ has been the subject of much study in analytic number theory due to its connection with the distribution of prime numbers. In this brief article, we will provide a proof that produces a region where the first sign change of $\theta(x) - x$ occurs, which is a particularly important property of this function. Specifically, we show that there is an $x < \exp(727.951332668)$ for which $\theta(x) > x$. We also provide a brief discussion on the algorithm that shows that $\theta(x) < x$ for $0 < x \leq 1.39 \times 10^{17}$.

1. INTRODUCTION

The prime number theorem states that $\pi(x)$, the number of primes less than or equal to x, is asymptotically equal to $\mathrm{li}(x)$ as $x \to \infty$ where

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

While $\pi(x)$ is the primary expression we want to study, it done so by studying the Chebyshev functions $\theta(x)$ and $\psi(x)$ due to the relation that $\pi(x) \sim \mathrm{li}(x)$ is equivalent to $\psi(x) \sim x$ and $\theta(x) \sim x$. Littlewood [Lit14] showed that $\psi(x) - x$ change signs infinitely often by showing

$$\psi(x) - x = \Omega_{\pm}(x^{\frac{1}{2}} \log\log\log x).$$

Rosser and Schoenfeld [RS62] proved that

$$\psi(x) - \theta(x) \leq 1.427\sqrt{x}, \quad \text{for } x > 1$$

which by combining with the above relation gives us that $\theta(x) - x$ change signs infinitely often. While the proof of Littlewood did not give any information as to where the sign change occurs, Skewes [Ske55] showed that there is a sign change at some point less than $\exp\exp\exp\exp(7 \times 705)$. However, Skewes's proof could not be adapted to $\theta(x) - x$. In this report, we will provide an outline of the arguments for the below two theorems regarding $\theta(x) - x$ following [PT16].

Theorem 1.1. *For $0 < x \leq 1.39 \times 10^{17}$, we have $\theta(x) < x$.*

Theorem 1.2. *There is some $x \in [\exp(727.951332642), \exp(727.951332668)]$ for which $\theta(x) > x$.*

2. SOME LEMMAS

In preparation for the theorem, we will need to prove some preliminary lemmas. Throughout this report $\rho = \beta + i\gamma$ will denote a zero of the Riemann zeta function $\zeta(s)$ for which $0 < \beta < 1$. We say that $f(x) = O^*(g(x))$ if $|f(x)| \leq g(x)$ for the range of x under consideration. Let $N(T)$ be the number of zeros for which $0 < \gamma \leq T$. Backlund [Bac16] showed that for $T \geq 2$,

$$N(T) = \frac{T}{2\pi} \log \frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8} + Q(T)$$

where $|Q(T)| \leq 0.137 \log T + 0.443 \log\log T + 4.35$. From this we can conclude that for $T \geq 2\pi e$,

$$N(T) = \frac{1}{2\pi}\int_{2\pi e}^{T} \log\frac{t}{2\pi}dt + \frac{7}{8} + O^*(2\log T). \tag{2.1}$$

Lemma 2.1. *If $\varphi(t)$ is a continuous function which is positive and monotone decreasing for $2\pi e \leq T_1 \leq t \leq T_2$, then*

$$\sum_{T_1<\gamma\leq T_2} \varphi(\gamma) = \frac{1}{2\pi}\int_{T_1}^{T_2} \varphi(t)\log\frac{t}{2\pi}dt + O^*\left(4\varphi(T_1)\log T_1 + 2\int_{T_1}^{T_2}\frac{\varphi(t)}{t}dt\right).$$

Proof. Using Stieltjes integrals, we have

$$\sum_{T_1<\gamma\leq T_2} \varphi(\gamma) = \int_{T_1}^{T_2}\varphi(t)dN(t) = \frac{1}{2\pi}\int_{T_1}^{T_2}\varphi(t)\log\frac{t}{2\pi}dt + \int_{T_1}^{T_2}\varphi(t)dQ(t).$$

From the equation (2.1), we have

$$\begin{aligned}\left|\int_{T_1}^{T_2}\varphi(t)dQ(t)\right| &= |\varphi(T_2)Q(T_2) - \varphi(T_1)Q(T_1)| - \int_{T_1}^{T_2} Q(t)d\varphi(t)\\ &\leq 2\varphi(T_2)\log T_2 + 2\varphi(T_1)\log T_1 - 2\int_{T_1}^{T_2}\log t d\varphi(t)\\ &\leq 4\varphi(T_1)\log T_1 + 2\int_{T_1}^{T_2}\varphi(t)d(\log t).\end{aligned}$$

□

Lemma 2.2. *If $T \geq 2\pi e$, then*

$$\sum_{\gamma>T}\frac{1}{\gamma^n} < T^{1-n}\log T.$$

Proof. Applying Lemma 2.1, we have

$$\begin{aligned}\sum_{\gamma>T}\frac{1}{\gamma^n} &= \frac{1}{2\pi}\int_T^\infty t^{-n}\log\frac{t}{2\pi}dt + O^*\left(4T^{-n}\log T + \frac{2T^{-n}}{n}\right)\\ &= \frac{T^{1-n}}{2\pi}\left(\frac{\log(T/2\pi)}{n-1} + \frac{1}{(n-1)^2}\right) + O^*\left(4T^{-n}\log T + \frac{2T^{-n}}{n}\right)\\ &\leq T^{1-n}\log T\left[\frac{1}{2\pi} + \frac{1}{2\pi\log T} + \frac{4}{T} + \frac{1}{T\log T}\right]\\ &< T^{1-n}\log T.\end{aligned}$$

□

Lemma 2.3. *If $\alpha > 0$ and $\varphi(t)$ is positive and monotone decreasing for $t \geq T > 0$, then*

$$\int_T^\infty \varphi(t)e^{-\frac{t^2}{2\alpha}} < \frac{\alpha}{T}\varphi(T)e^{-\frac{T^2}{2\alpha}}.$$

Proof. Since

$$\frac{d}{dt}\left[\frac{\alpha e^{-\frac{t^2}{2\alpha}}}{t}\right] = -\frac{\alpha e^{-\frac{t^2}{2\alpha}}}{t^2} - e^{-\frac{t^2}{2\alpha}},$$

we obtain

$$\int_T^\infty \varphi(t)e^{-\frac{t^2}{2\alpha}} < -\int_T^\infty \varphi(t)\frac{d}{dt}\left(\frac{\alpha e^{-\frac{t^2}{2\alpha}}}{t}\right) \leq \frac{\alpha}{T}\varphi(T)e^{-\frac{T^2}{2\alpha}}.$$

□

Lemma 2.4. *If* $\theta(x) < x$ *for* $e^{2.4} \leq x \leq K$*, then* $\pi(x) < \mathrm{li}(x)$ *for* $e^{2.4} \leq x \leq K$.

Proof. We can write (see [Ing32, Theorem A, p.18])

$$\pi(x) = \frac{\theta(x)}{\log(x)} + \int_2^x \frac{\theta(y)}{y\log^2 y}dy. \tag{2.2}$$

We also have that

$$\int_2^{e^{2.4}} \frac{\theta(y)}{y\log^2 y}dy < \mathrm{li}(e^{2.4}) - \frac{e^{2.4}}{2.4}.$$

This is because the value of the left expression equals 1.773 while the value of the right expression is 2.008 by equation (2.2). Under the assumptions of our lemma, we can deduce that if $e^{2.4} \leq x \leq K$, then

$$\pi(x) < \frac{x}{\log x} + \mathrm{li}(e^{2.4}) - \frac{e^{2.4}}{2.4} + \int_{e^{2.4}}^x \frac{y}{y\log^2 y}dy$$

In the meantime, integration by parts gives us

$$\int_{e^{2.4}}^x \frac{y}{y\log^2 y}dy = -\frac{y}{\log y}\bigg|_{e^{2.4}}^x + \int_{e^{2.4}}^x \frac{dy}{\log y} = -\frac{x}{\log x} + \frac{e^{2.4}}{2.4} + \mathrm{li}(x) - \mathrm{li}(e^{2.4})$$

which concludes the lemma. □

The combination of Lemma 2.4 and Theorem 1.1 gives us the following important corollary.

Corollary 2.5. $\pi(x) < \mathrm{li}(x)$ *for all* $2 < x \leq 1.39 \times 10^{17}$.

3. Outline of the argument

Recall the two formulas discussed in class. The explicit formula for $\psi(x)$ is given by

$$\psi_0(x) = \frac{\psi(x+0^+) + \psi(x-0^+)}{2} = x - \sum_\rho \frac{x^\rho}{\rho} - \frac{\zeta'}{\zeta}(0) - \frac{1}{2}\log\left(1 - \frac{1}{x^2}\right) \tag{3.1}$$

where ρ are the non-trivial zeros of the Riemann-zeta function $\zeta(s)$. Second one is the identity relating the two Chebyshev functions

$$\psi(x) = \theta(x) + \theta(x^{\frac{1}{2}}) + \theta(x^{\frac{1}{3}}) + \cdots. \tag{3.2}$$

From the above two identities, we can actually manufacture the explicit formula for $\theta(x)$. A direct substitution of the explicit formula (3.1) into (3.2) gives

$$\begin{aligned}\theta(x) - x &= -\sum_{\rho} \frac{x^{\rho}}{\rho} - \frac{\zeta'}{\zeta}(0) - \frac{1}{2}\log\left(1 - \frac{1}{x^2}\right) - \sum_{n=2}^{\infty} \theta(x^{\frac{1}{n}}) \\ &\leq -\theta(x^{\frac{1}{2}}) - x^{\frac{1}{2}} \sum_{\gamma>0} \left(\frac{x^{i\gamma}}{\frac{1}{2}+i\gamma} + \frac{x^{-i\gamma}}{\frac{1}{2}-i\gamma}\right) - \frac{1}{2}\log\left(1 - \frac{1}{x^2}\right) \quad \text{(assuming RH)}. \quad (3.3)\end{aligned}$$

If Riemann hypothesis is true, we can write $\rho = \frac{1}{2} + i\gamma$ and from our knowledge on the first zero of $\zeta(s)$, we have $\gamma \geq 14$. Hence, we expect the dominant term on RHS of (3.3) is $-\theta(x^{\frac{1}{2}})$, which explains our expectation on why $\theta(x) < x$ should happen often. We have the following result by Rosser and Schoenfeld [RS62, Theorem 14]

$$\psi(x) - \theta(x) < \theta(x^{\frac{1}{2}}) - 3x^{\frac{1}{3}}. \quad (3.4)$$

Substituting (3.1) into (3.4) gives

$$\theta(x) - x > -\theta(x^{\frac{1}{2}}) - \sum_{\rho} \frac{x^{\rho}}{\rho} - \frac{\zeta'}{\zeta}(0) - 3x^{\frac{1}{3}}. \quad (3.5)$$

Let α, ω and η be positive numbers such that $\omega - \eta > 1$. Define the Gaussian Kernel $K(y) = \sqrt{\frac{\alpha}{2\pi}} \exp(\frac{-1}{2}\alpha y^2)$. For any real number γ,

$$\int_{-\infty}^{\infty} K(y) e^{i\gamma y} dy = e^{-\frac{\gamma^2}{2\alpha}} \sqrt{\frac{\alpha}{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha}{2}(y - \frac{\gamma}{\alpha} i)^2} dy = e^{-\frac{\gamma^2}{2\alpha}}. \quad (3.6)$$

In particular, $\int_{-\infty}^{\infty} K(y)dy = 1$. We divide both sides of (3.5) by $x^{\frac{1}{2}}$, make the substitution $x \mapsto e^u$ and integrate against $K(u - w)$, which gives

$$\begin{aligned}\int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-\frac{u}{2}} (\theta(e^u) - e^u) du &> -\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\theta(e^{\frac{u}{2}}) e^{-\frac{u}{2}} \\ &- \sum_{\rho} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{u(\rho - \frac{1}{2})} du - \frac{\zeta'(0)}{\zeta(0)} \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-\frac{u}{2}} du \\ &- 3\int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-\frac{u}{6}} du = -I_1 - I_2 - I_3 - I_4.\end{aligned}$$

The interchange of summation and integration is valid by noting that the sum over the zeros of $\zeta(s)$ in (3.5) converges boundedly in $u \in [\omega - \eta, \omega + \eta]$. Noting that $\frac{\zeta'(0)}{\zeta(0)} = \log 2\pi$, we estimate I_3 trivially as follows

$$0 < I_3 < (\log 2\pi) \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-\frac{\omega-\eta}{2}} du < e^{-\frac{\omega-\eta}{2}} \log 2\pi.$$

We proceed similarly to estimate I_4 trivially to obtain

$$0 < I_4 < 3e^{-\frac{\omega-\eta}{6}}.$$

The contributions of I_3 and I_4 are actually negligible as shown in latter part of calculations.

We are now going to estimate I_2. Let A be the height to which the Riemann hypothesis has been verified, and let $T \leq A$ be the height to which we can reasonably compute zeros to a high degree of accuracy. We write

$$\begin{aligned} I_2 &= \sum_{|\gamma|\leq A} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{(\rho-\frac{1}{2})u} du + \sum_{|\gamma|>A} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{(\rho-\frac{1}{2})u} du \\ &= \sum_{|\gamma|\leq A} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{i\gamma u} du + \sum_{|\gamma|>A} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{(\rho-\frac{1}{2})u} du = S_1 + S_2 \end{aligned}$$

which is valid since we know Riemann hypothesis is true up to height A. By (3.6) and the change of variable $y = u - \omega$,

$$\begin{aligned} S_1 &= \sum_{|\gamma|\leq A} \frac{e^{i\gamma\omega}}{\rho} \int_{-\eta}^{\eta} K(y) e^{i\gamma y} dy \\ &= \sum_{|\gamma|\leq A} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}} + O^*\left(\frac{4}{\gamma}\left|\int_{\eta}^{\infty} K(y) e^{i\gamma y}\right|\right) \end{aligned}$$

We want to give an estimate the the term $\int_\eta^\infty K(y)e^{i\gamma y}$. Integration by parts yields

$$\int_{\eta}^{\infty} K(y) e^{i\gamma y} = \int_{\eta}^{\infty} K'(y) \frac{e^{i\gamma\eta} - e^{i\gamma y}}{i\gamma} dy.$$

Hence, from the monotonic decreasing of $K(y)$ for $y > 0$,

$$\left|\int_{\eta}^{\infty} K(y) e^{i\gamma y}\right| \leq \int_{\eta}^{\infty} \left|K'(y) \frac{e^{i\gamma\eta} - e^{i\gamma y}}{i\gamma}\right| dy \leq \frac{2}{\gamma} \int_{\eta}^{\infty} |K'(y)| dy = \frac{2}{\gamma} K(\eta) = \frac{2}{\gamma} \sqrt{\frac{\alpha}{2\pi}} e^{-\frac{\alpha\eta^2}{2}}. \tag{3.7}$$

Now, we apply the following numerical estimate

$$\sum_{0<\gamma<\infty} \frac{1}{\gamma^2} < 0.025,$$

the inequality $(2\pi)^{-\frac{1}{2}} < 0.4$ and (3.7) to obtain

$$S_1 = \sum_{|\gamma|\leq A} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}} + O^*\left(8\sqrt{\frac{\alpha}{2\pi}} \sum_{0<\gamma\leq A} \frac{1}{\gamma^2}\right) = \sum_{|\gamma|\leq A} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}} + O^*\left(0.08\sqrt{\alpha} e^{-\frac{\alpha\eta^2}{2}}\right).$$

Instead of taking the sum over zeros for which $|\gamma| \leq A$, we would like to take the sum over zeros for which $|\gamma| \leq T$. Indeed, for $T \geq 2\pi e$,

$$\left|\sum_{T<|\gamma|\leq A} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}}\right| \leq 2 \sum_{T<|\gamma|\leq A} e^{-\frac{\gamma^2}{2\alpha}} \leq \int_T^\infty \frac{e^{-\frac{t^2}{2\alpha}}}{\pi t} \log\frac{t}{2\pi} dt + \frac{8e^{-\frac{T^2}{2\alpha}} \log T}{T} + 4\int_T^\infty \frac{e^{-\frac{t^2}{2\alpha}}}{t^2} dt. \tag{3.8}$$

The first inequality comes from $|\frac{e^{i\gamma\omega}}{\rho}| = \frac{1}{|\beta+i\gamma|} \leq \frac{1}{\gamma}$ and the second inequality is just a direct application of Lemma 2.1. Each integral in RHS of (3.8) can be estimated by using Lemma 2.3, which gives

$$\left|\sum_{T<|\gamma|\le A} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}}\right| \le e^{-\frac{T^2}{2\alpha}} \left(\frac{\alpha}{\pi T^2}\log\frac{T}{2\pi} + \frac{8}{T}\log T + \frac{4\alpha}{T^3}\right).$$

Combining our results of the estimation for S_1 yields

$$S_1 = \sum_{|\gamma|\le T} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}} + E_1,$$

where

$$|E_1| < 0.08\sqrt{\alpha} e^{-\frac{\alpha\eta^2}{2}} + e^{-\frac{T^2}{2\alpha}} \left(\frac{\alpha}{\pi T^2}\log\frac{T}{2\pi} + \frac{8}{T}\log T + \frac{4\alpha}{T^3}\right).$$

Define

$$f_\rho(s) = \exp(-\frac{1}{2}\alpha(s-w)^2).$$

By using integration by parts, residue theorem and Lemma 2.2, we can deduce that (following the same idea as Lehman in [Leh65, Section 5])

$$|S_2| \le A\log\left[Ae^{-\frac{A^2}{2a}+\frac{\omega+\eta}{2}}\left(4\alpha^{-\frac{1}{2}} + 15\eta\right)\right]$$

provided that

$$\frac{4A}{w} \le \alpha \le A^2, \quad \frac{2A}{\alpha} \le \eta < \frac{w}{2}.$$

It remains to estimate

$$I_1 = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\theta(e^{\frac{u}{2}})e^{-\frac{u}{2}}.$$

The result from Rosser and Schoenfeld [RS62, Theorem 13] says

$$\psi(x) - \theta(x) \le 1.4263\sqrt{x}, \quad \text{for all } x > 0.$$

Meanwhile, Faber and Kadiri [FK15, Table 3] had explicitly computed

$$|\psi(x) - x| \le (1.5423 \times 10^{-9})x, \quad \text{for } x \ge e^{200}.$$

Using these two results and the positivity of I_1, for $\omega - \eta \ge 400$, hence $e^{\frac{\omega-\eta}{2}} \ge e^{200}$ and

$$\begin{aligned} I_1 &\le \int_{\omega-\eta}^{\omega+\eta} [e^{\frac{u}{2}} + (1.5423\times 10^{-9})e^{\frac{u}{2}}]e^{-\frac{u}{2}} K(u-\omega)du \\ &\le (1 + 1.5423\times 10^{-9}) \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)du \\ &< 1 + 1.5423\times 10^{-9}. \end{aligned}$$

We combine all our estimates into the following theorem.

Theorem 3.1. *Let A be the height to which the Riemann hypothesis has been verified, and let T satisfy $0 < T < A$. Let α, η and ω be positive numbers for which $\omega - \eta \geq 400$ and for which*

$$\frac{4A}{w} \leq \alpha \leq A^2, \quad \frac{2A}{\alpha} \leq \eta < \frac{w}{2}.$$

Let $K(y) = \sqrt{\frac{\alpha}{2\pi}} \exp -\frac{1}{2}\alpha y^2$ be the Gaussian kernel and

$$I(\omega, \eta) = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-\frac{u}{2}} (\theta(e^u) - e^u) du.$$

Then,

$$I(\omega, \eta) \geq -1 - \sum_{|\gamma| \leq T} \frac{e^{i\gamma\omega}}{\rho} e^{-\frac{\gamma^2}{2\alpha}} - R_1 - R_2 - R_3 - R_4, \tag{3.9}$$

where

$$\begin{aligned}
R_1 &= 1.5423 \times 10^{-9} \\
R_2 &= 0.08\sqrt{\alpha} e^{-\frac{\alpha\eta^2}{2}} + e^{-\frac{T^2}{2\alpha}} \left(\frac{\alpha}{\pi T^2} \log \frac{T}{2\pi} + \frac{8}{T} \log T + \frac{4\alpha}{T^3} \right) \\
R_3 &= e^{-\frac{\omega-\eta}{2}} \log 2\pi + 3e^{-\frac{\omega-\eta}{6}} \\
R_4 &= A \log \left[A e^{-\frac{A^2}{2\alpha} + \frac{\omega+\eta}{2}} \left(4\alpha^{-\frac{1}{2}} + 15\eta \right) \right].
\end{aligned}$$

Remark 3.2. This is an unconditional result since we do not assume RH. However, the proof of the theorem does rely on rigorous verification of RH.

4. Computations

4.1. **Upper Bound.** Using the above theorem, we need to substitute appropriate values for ω, η, A, T and α such that the right side of the inequality (3.9) is positive. We refer the reader to [PT16] for a detailed analysis on the reasoning for choosing these specific values of the parameters given below.

Consider the sum $\sum_1 = \sum_{|\gamma| \leq T} \frac{e^{i\gamma\omega}}{\rho}$. We need to substitute appropriate values of T and ω such that this value is close to -1. Bays and Hudson [BH00] has provided a list of values for ω for which $\sum_1$ is small, namely $\omega = 405, 412, 437, 599, 686$ and 728. We aim to choose the remaining parameters to make the other error terms R_2, R_3 and R_4 comparable to $R_1 = 1.5423 \times 10^{-9}$. The rigorous verification of Riemann hypothesis has been made in [PT21] for $A = 3.0610046 \times 10^{10}$. We can pick $T = A \approx 3 \times 10^{10}$. A trade-off between good error bounds and computation power has been made for choosing $T = 6970346000$.

Our goal is to detect a narrow region $[\exp(\omega - \eta), \exp(\omega + \eta)]$ for which $\theta(x) > x$ for some $x \in [\exp(\omega - \eta), \exp(\omega + \eta)]$. We have to pick η as small as possible. Next, we choose α as large as possible because the smaller the width (variance) of the Gaussian distribution, the narrower the region we obtain. However, to make the error term R_4 manageable, we need $\frac{A^2}{2\alpha} > \frac{\omega}{2}$. A little experimentation has led to picking

$$\alpha = 1153308722614227968 \text{ and } \eta = \frac{933831}{2^{44}}.$$

The authors in [PT16] searched the regions around $\omega = 405, 412, 437, 599$ and 686. The computation shows $\sum_1$ is far away from dipping below the -1 level for these values of ω. It is believed that $\theta(x) < x$ around all these values of ω.

It is natural to expect that the region near $\omega = 728$ yields a point where $\theta(x) > x$. This is because the lowest published interval containing an x such that $\pi(x) > \mathrm{li}(x)$ is

$$x \in [\exp(727.951335231), \exp(727.951335621)]$$

in [STD15]. Since the error terms for $\theta(x) - x$ are tighter than those for $\pi(x) - \mathrm{li}(x)$, this necessarily means that the same x will satisfy $\theta(x) > x$. In fact choosing $\omega = 727.951332655$ gives

$$\sum_{|\gamma| \le T} \frac{\exp(i\gamma\omega)}{\rho} \exp\left(-\frac{\gamma^2}{2\alpha}\right) \in [-1.0013360278, -1.0013360277].$$

Our choice of parameters gives $R_1 + R_2 + R_3 + R_4 < 1.7 \times 10^{-9}$. Subsequent calculations show

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-u/2} (\theta(e^u) - e^u) du > 0.0013360261$$

which proves Theorem 1.2.

4.2. **Lower bound.** Having established an upper bound for the first time that $\theta(x)$ exceeds x, we now turn to a lower bound. A simple method would be to run through all the primes p less than some bound B. Compute the sum $\log p$ starting from $p = 2$ and compare the running sum total each time to p. To obtain the desired error we would need to set $B = 1.39 \times 10^{17}$. By the prime number theorem we would expect to find about 3.5×10^{15} primes below this bound. Since this is far too many for a single thread computation, we opt for parallel computing.

We refer the reader to [PT16, Section 3.2.1] for a discussion on the following algorithm[1]. Divide the range $(0, B]$ into contiguous intervals. For each interval $S_j = (x_j, y_j]$, set $T_j = \Delta_j = \Delta_{j,\max} = 0$. Let $P_j = [p_{j,1}, p_{j,2}, \ldots, p_{j,n}]$ be the ordered list of primes in the interval S_j with usual number ordering "$<$". In particular, $x_j < p_{j,1} < p_{j,2} < \cdots < p_{j,n} \le y_j$. We run the following algorithm over all primes $p_{j,i}$ in P_j starting with the smallest one $p_{j,1}$.

1. Compute $l_{j,i} = \log p_{j,i}$.
2. Set $T_j = T_j + l_{j,i}$ and $\Delta_j = \Delta_j + l_{j,i} - p_{j,i} + p_{j,i-1}$, where $p_{j,0} = 0$.
3. Set $\Delta_{j,\max} = \max\{\Delta_{j,\max}, \Delta_j\}$.

After running the algorithm, output T_j and $\Delta_{j,\max}$. Mathematically, we can express T_j and $\Delta_{j,\max}$ as

$$T_j = \sum_{i=1}^{n} \log p_{j,i} = \theta(y_j) - \theta(x_j)$$

and

$$\Delta_{j,\max} = \max_{1 \le k \le n} \left[\sum_{i=1}^{k} \log p_{j,i} - p_{j,k} \right] = \max_{1 \le k \le n} [\theta(p_{j,k}) - p_{j,k}] - \theta(x_j)$$

[1] There are possibly some typos in [PT16, Section 3.2.1]. We make some appropriate amendments in our exposition.

respectively. After obtaining the output T_j and Δ_j for each S_j, we can easily compute

$$\theta(y_j) = \sum_{k=1}^{j} T_k.$$

Note that

$$\max_{1\le k\le n} [\theta(p_{j,k}) - p_{j,k}] = \max_{x\in S_j} [\theta(x) - x]$$

for all j, and hence,

$$\theta(x_j) + \Delta_{j,\max} = \max_{1\le k\le n} [\theta(p_{j,k}) - p_{j,k}] = \max_{x\in S_j} [\theta(x) - x].$$

If $\theta(x_j) + \Delta_{j,\max} < 0$, then we can conclude $\theta(x) < x$ for all $x \in (x_j, y_j]$.

By splitting B into $10,000$ segments of width 10^{13} followed by 390 segments of width 10^{14}, the authors in [PT16] were able to prove Theorem 1.1 with computer aids.

References

[Bac16] R. J. Backlund. Über die Nullstellen der Riemannschen Zetafunktion. *Acta Mathematica*, 41:345 – 375, 1916.

[BH00] C. Bays and R. H. Hudson. A new bound for the smallest x with $\pi(x) > \mathrm{li}(x)$. *Mathematics of computation*, 69(231):1285–1297, 2000.

[FK15] L. Faber and H. Kadiri. New bounds for $\psi(x)$. *Mathematics of computation*, 84(293):1339–1357, 2015.

[Ing32] A. E. Ingham. *The distribution of prime numbers*. Cambridge mathematical library. Cambridge University Press, Cambridge, 1990 - 1932.

[Leh65] R. S. Lehman. On the difference $\pi(x) - \mathrm{li}(x)$. *Acta arithmetica*, 11(4):397–410, 1965.

[Lit14] J. E. Littlewood. Sur la distribution des nombres premiers. *CR Acad. Sci. Paris*, 158(1869):1872, 1914.

[PT16] D. J. Platt and T. S. Trudgian. On the first sign change of $\theta(x) - x$. *Mathematics of computation*, 85(299):1539–1547, 2016.

[PT21] D. Platt and T. Trudgian. The Riemann hypothesis is true up to $3 \cdot 10^{12}$. *Bull. Lond. Math. Soc.*, 53(3):792–797, 2021.

[RS62] J. B. Rosser and L. Schoenfeld. Approximate formulas for some functions of prime numbers. *Illinois Journal of Mathematics*, 6(1):64 – 94, 1962.

[Ske55] S. Skewes. On the difference $\pi(x) - \mathrm{li}(x)$ (II). *Proceedings of the London Mathematical Society*, s3-5(1):48–70, 1955.

[STD15] Y. Saouter, T. Trudgian, and P. Demichel. A still sharper region where $\pi(x) - \mathrm{li}(x)$ is positive. *Math. Comp.*, 84(295):2433–2446, 2015.