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

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ABSTRACT. Let $\theta(x) = \sum_{p \le x} \log p$. We show that $\theta(x) < x$ for $2 < x < 1.39 \cdot 10^{17}$. We also show that there is an $x < \exp(727.951332668)$ for which $\theta(x) > x$.

1. Introduction

Let $\pi(x)$ denote the number of primes not exceeding x. The prime number theorem is the statement that

$$\pi(x) \sim \mathrm{li}(x) = \int_2^x \frac{dt}{\log t}. \tag{1}$$

One often deals not with $\pi(x)$ but with the less obstinate Chebyshev functions $\theta(x) = \sum_{p \le x} \log p$ and $\psi(x) = \sum_{p^m \le x} \log p$. The relation (1) is equivalent to

$$\psi(x) \sim x \quad \text{and} \quad \theta(x) \sim x.$$

Littlewood [10], showed that $\pi(x) - \mathrm{li}(x)$ and $\psi(x) - x$ change sign infinitely often. Indeed, (see, e.g., [7, Thms. 34 and 35]) he showed more than this, namely that

$$\begin{aligned} \pi(x) - \mathrm{li}(x) &= \Omega_{\pm}\left(\frac{x^{\frac{1}{2}}}{\log x} \log\log\log x\right), \\ \psi(x) - x &= \Omega_{\pm}(x^{\frac{1}{2}} \log\log\log x). \end{aligned} \tag{2}$$

By [16, (3.36)] we have

$$\psi(x) - \theta(x) \le 1.427\sqrt{x} \quad (x > 1), \tag{3}$$

which, together with the second relation in (2), shows that $\theta(x) - x$ changes sign infinitely often.

Littlewood's proof that $\pi(x) - \mathrm{li}(x)$ changes sign infinitely often was ineffective: the proof did not furnish a number x_0 such that one could guarantee that $\pi(x) - \mathrm{li}(x)$ changes sign for some $x \le x_0$. Skewes [19] made Littlewood's theorem effective; the best known result is that there must be a sign change less that $1.3972 \cdot 10^{316}$ [17]. On the other hand, Kotnik [8] showed that $\pi(x) < \mathrm{li}(x)$ for all $2 < x \le 10^{14}$.

We turn now to the question of sign changes in $\psi(x) - x$ and $\theta(x) - x$. There is nothing of much interest to be said about the first change of sign of $\psi(x) - x$: for $x \in [0, 100]$ there are 24 sign changes. The problem of determining values of C such that $\psi(x) - x$ changes sign in every interval $[x, Cx]$, for all sufficiently large x,

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is much more interesting (as examined in [11]) but it is not something we consider here. As for the first change of sign in $\theta(x) - x$, Schoenfeld [18, p. 360] showed that $\theta(x) < x$ for all $0 < x \le 10^{11}$. This range appears to have been improved by Dusart, [5, p. 4] to $0 < x \le 8 \cdot 10^{11}$. We increase this in

Theorem 1. *For* $0 < x \le 1.39 \cdot 10^{17}$, $\theta(x) < x$.

A result of Rosser [15, Lemma 4] is

Lemma 1 (Rosser)**.** *If* $\theta(x) < x$ *for* $e^{2.4} \le x \le K$ *for some* K*, then* $\pi(x) < \mathrm{li}(x)$ *for* $e^{2.4} \le x \le K$.

This enables us to extend Kotnik's result by proving

Corollary 1. $\pi(x) < \mathrm{li}(x)$ *for all* $2 < x \le 1.39 \cdot 10^{17}$.

Rosser and Schoenfeld [16, (3.38)], proved

$$\psi(x) - \theta(x) - \theta(x^{\frac{1}{2}}) < 3x^{\frac{1}{3}}, \quad (x > 0). \tag{4}$$

Table 3 in [6] gives us the bound $|\psi(x) - x| \le 7.5 \cdot 10^{-7}x$, which is valid for all $x \ge e^{35} > 1.5 \cdot 10^{15}$. This, together with (4) and Theorem 1, enables us to make the following improvement to two results of Schoenfeld [18, (5.1*) and (5.3*)].

Corollary 2. *For* $x > 0$,

$$\theta(x) < (1 + 7.5 \cdot 10^{-7})x, \quad \psi(x) - \theta(x) < (1 + 7.5 \cdot 10^{-7})\sqrt{x} + 3x^{\frac{1}{3}}.$$

We now turn to the question of sign changes in $\theta(x) - x$. In §3.1 we prove

Theorem 2. *There is some* $x \in [\exp(727.951332642), \exp(727.951332668)]$ *for which* $\theta(x) > x$.

Throughout this article we make use of the following notation. For functions $f(x)$ and $g(x)$ we say that $f(x) = \mathcal{O}^*(g(x))$ if $|f(x)| \le g(x)$ for the range of x under consideration.

2. Outline of argument

The explicit formula for $\psi(x)$ is [7, Thm. 29]

$$\psi_0(x) = \frac{\psi(x+0) + \psi(x-0)}{2} = x - \sum_{\rho} \frac{x^{\rho}}{\rho} - \frac{\zeta'}{\zeta}(0) - \frac{1}{2}\log\left(1 - \frac{1}{x^2}\right). \tag{5}$$

Since

$$\psi(x) = \theta(x) + \theta(x^{\frac{1}{2}}) + \theta(x^{\frac{1}{3}}) + \dots,$$

we can manufacture an explicit formula for $\theta(x)$. Using (4) and (5) we find that

$$\theta(x) - x > -\theta\left(x^{\frac{1}{2}}\right) - \sum_{\rho} \frac{x^{\rho}}{\rho} - \frac{\zeta'}{\zeta}(0) - 3x^{\frac{1}{3}}. \tag{6}$$

One can see why $\theta(x) < x$ 'should' happen often. On the Riemann hypothesis, $\rho = \frac{1}{2} + i\gamma$; since $\gamma \ge 14$, one expects the dominant term on the right side of (6) to be $-\theta\left(x^{\frac{1}{2}}\right)$.

We proceed in a manner similar to that in Lehman [9]. Let α be a positive number. We shall make frequent use of the Gaussian kernel $K(y) = \sqrt{\frac{\alpha}{2\pi}}\exp(-\frac{1}{2}\alpha y^2)$, which has the property that $\int_{-\infty}^{\infty} K(y)\,dy = 1$.

Divide both sides of (6) by $x^{\frac{1}{2}}$, make the substitution $x \mapsto e^u$ and integrate against $K(u-\omega)$. This gives

$$\begin{aligned}\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{\frac{u}{2}}\left\{\theta(e^u)-e^u\right\} du > &-\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\theta\left(e^{\frac{u}{2}}\right)e^{-\frac{u}{2}}\, du \\ &-\sum_\rho \frac{1}{\rho}\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{u(\rho-\frac{1}{2})}\, du - \frac{\zeta'(0)}{\zeta(0)}\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{-\frac{u}{2}}\, du \\ &-3\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{-\frac{u}{6}}\, du = -I_1 - I_2 - I_3 - I_4,\end{aligned} \tag{7}$$

say. The interchange of summation and integration may be justified by noting that the sum over the zeroes of $\zeta(s)$ in (6) converges boundedly in $u \in [\omega-\eta, \omega+\eta]$. Noting that $\zeta'(0)/\zeta(0) = \log 2\pi$, we proceed to estimate I_3 and I_4 trivially to show that

$$0 < I_3 < e^{-\frac{\omega-\eta}{2}} \log 2\pi, \quad 0 < I_4 < 3e^{-\frac{\omega-\eta}{6}}.$$

It will be shown in §3 that the contributions of I_3 and I_4 to (7) are negligible — this justifies our cavalier approach to their approximation.

We now turn to I_2. Let A be the height to which the Riemann hypothesis has been verified, and let $T \le A$ be the height to which we can reasonably compute zeroes to a high degree of accuracy — we make this notion precise in §3. Write $I_2 = S_1 + S_2$, where

$$S_1 = \sum_{|\gamma| \le A} \frac{1}{\rho}\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{i\gamma u}\, du,$$

$$S_2 = \sum_{|\gamma| > A} \frac{1}{\rho}\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{(\rho-\frac{1}{2})u}\, du.$$

Our S_1 is the same as that used by Lehman in [9, pp. 402-403]. Using (4.8) and (4.9) of [9] shows that

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

where

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

Lehman considers

$$f_\rho(s) = \rho s e^{-\rho s}\mathrm{li}(e^{\rho s})e^{-\alpha(s-w)^2/2},$$

whence he writes his analogous version of S_2 as a function of $f_\rho(s)$ and then estimates this using integration by parts, Cauchy's theorem, and the bound

$$|f_\rho(s)| \le 2\exp(-\tfrac{1}{2}\alpha(s-w)^2). \tag{8}$$

We consider the simpler function $f_\rho(s) = \exp(-\frac{1}{2}\alpha(s-w)^2)$, which clearly satisfies (8). We may proceed as in §5 of [9] to deduce that

$$|S_2| \le A\log A e^{-A^2/(2a)+(w+\eta)/2}\left\{4\alpha^{-\frac{1}{2}} + 15\eta\right\},$$

provided that

$$4A/w \le \alpha \le A^2, \quad 2A/\alpha \le \eta < w/2.$$

All that remains is for us to estimate

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

Table 3 in [6] and (3) give us

$$|\theta(x) - x| \le 1.5423 \cdot 10^{-9} x, \quad x \ge e^{200}, \tag{9}$$

which gives

$$I_1 < 1 + 1.5423 \cdot 10^{-9}, \quad (\omega - \eta) \ge 400.$$

Thus, we have

Theorem 3. *Let A be the height to which the Riemann hypothesis has been verified, and let T satisfy $0 < T \le A$. Let α, η and ω be positive numbers for which $\omega - \eta \ge 400$ and for which*

$$4A/\omega \le \alpha \le A^2, \quad 2A/\alpha \le \eta \le \omega/2.$$

Define $K(y) = \sqrt{\alpha/(2\pi)} \exp(-\frac{1}{2}\alpha y^2)$ and

$$I(\omega, \eta) = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-u/2} \left\{\theta(e^u) - e^u\right\} du. \tag{10}$$

Then

$$I(\omega, \eta) \ge -1 - \sum_{|\gamma| \le T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/(2\alpha)} - R_1 - R_2 - R_3 - R_4, \tag{11}$$

where

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

If one were to assume the Riemann hypothesis one could reduce the term R_4. This would give greater freedom in the choice of α; see §3.1.3.

Approximations different from (9) are available. For example, one could use Lemma 1 in [20] to obtain $|\theta(x) - x| \le 0.0045x/(\log x)^2$. One could also restrict the conditions in Theorem 3 to $\omega - \eta \ge 600$ using the slightly improved results from [6] that are applicable thereto. Neither of these improves significantly the bounds in Theorem 2.

We now need to search for values of ω, η, A, T and α for which the right side of (11) is positive.

3. Computations

3.1. **Locating a crossover.** Consider the sum $\Sigma_1 = \sum_{|\gamma| \le T} \frac{e^{i\gamma\omega}}{\rho}$. We wish to find values of T and ω for which this sum is small, that is, close to -1; for such values the sum that appears in (11) should also be small. Bays and Hudson [2], when considering the problem of the first sign change of $\pi(x) - \mathrm{li}(x)$, identified some values of ω for which Σ_1 is small. We investigated their values: $\omega = 405, 412, 437, 599, 686$ and 728.

For ω in this range, we have $R_1 = 1.5423 \cdot 10^{-9}$ so we endeavour to choose the parameters A, T, α and η to make the other error terms comparable.

3.1.1. *Choosing A.* We relied on the rigorous verification of the Riemann hypothesis for $A = 3.0610046 \cdot 10^{10}$ by the second author [13]. This computation also produced a database of the zeroes below this height computed to an absolute accuracy of $\pm 2^{-102}$ [3].

3.1.2. *Choosing T.* As already observed, we have sufficient zeroes to set $T = A \approx 3 \cdot 10^{10}$ but, since summing over roughly the 10^{11} zeroes below this height is too computationally expensive, we settled for $T = 6,970,346,000$ (about $2 \cdot 10^{10}$ zeroes). Even then, computing the sum using multiple precision interval arithmetic (see §3.1.4) takes about 40 hours on an 8 core platform.

3.1.3. *Choosing the other parameters.* To get the finest granularity on our search (i.e. to be able to detect narrow regions where $\theta(x) > x$) we aim at setting η as small as possible. This in turn means setting α (which controls the width of the Gaussian) as large as possible. However, to ensure that R_4 is manageable, we need $A^2/(2\alpha) > \omega/2$ or $\alpha < A^2/\omega$. A little experimentation led us to

$$\alpha = 1,153,308,722,614,227,968, \quad \eta = \frac{933831}{2^{44}},$$

both of which are exactly representable in IEEE double precision.

3.1.4. *Summing over the zeroes.* Since

$$\frac{\exp(i\gamma\omega)}{\frac{1}{2} + i\gamma} + \frac{\exp(-i\gamma\omega)}{\frac{1}{2} - i\gamma} = \frac{\cos(\gamma\omega) + 2\gamma\sin(\gamma\omega)}{\frac{1}{4} + \gamma^2},$$

the dominant term in Σ_1 is roughly $2\sin(\gamma\omega)/\gamma$. Though one might expect a relative accuracy of 2^{-53} when computing this in double precision, the effect of reducing $\gamma\omega \bmod 2\pi$ degrades this to something like 2^{-17} when $\gamma = 10^9$ and $\omega = 400$. We are therefore forced into using multiple precision, even though that entails a performance penalty perhaps as high as a factor of 100. To avoid the need to consider rounding and truncation errors at all, we use the MPFI [14] multiple precision interval arithmetic package for all floating point computations. Making the change from scalar to interval arithmetic probably costs us another factor of 4 in terms of performance.

3.1.5. *Results.* We initially searched the regions around $\omega = 405, 412, 437, 599, 686$ and 728 using only those zeroes $\frac{1}{2} + i\gamma$ with $0 < \gamma < T = 5,000$. Although these results were not rigorous, it was hoped that a sum approaching -1 would indicate a potential crossover worth investigating with full rigour. As an example, Figure 1 shows the results for a region near $\omega = 437.7825$. This is some way from dipping below the -1 level and indeed a rigorous computation using the full set of zeroes and with $\omega = 437.78249$ fails to get over the line. The same pattern repeats for ω near $405, 412, 599$ and 686.

In contrast, we expected the region near 728 to yield a point where $\theta(x) > x$. The lowest published interval containing an x such that $\pi(x) > \mathrm{li}(x)$ is

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

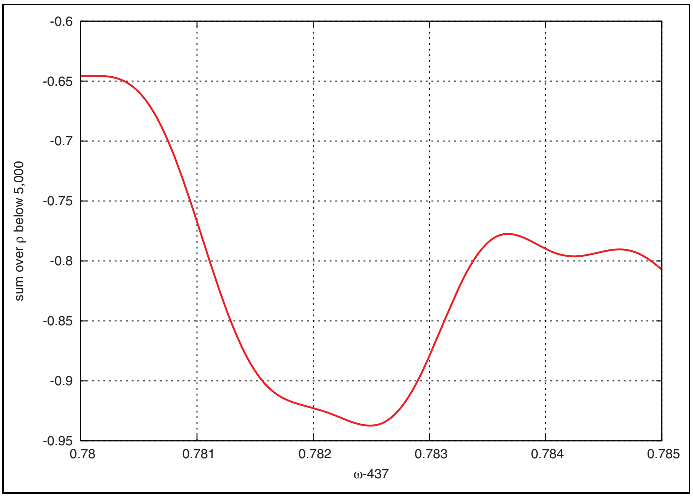

FIGURE 1. Plot of $\sum_{|\gamma|\le 5000} \frac{e^{i\omega\gamma}}{\rho}$ for $\omega \in [437.78, 437.785]$.

in [17]. 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, we can do better. Using $\omega = 727.951332655$ we get

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

We also have $R_1 + R_2 + R_3 + R_4 < 1.7 \cdot 10^{-9}$, so that

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega) e^{-u/2} \{\theta(e^u) - e^u\}\, du > 0.0013360261. \tag{12}$$

3.1.6. *Sharpening the region.* Using the same argument as [17, §9], we can analyse the tails of the integral (10) and sharpen the region considerably. Consider, for $\eta_0 \in (0, \eta]$,

$$T_1 = \int_{\omega+\eta_0}^{\omega+\eta} K(u-\omega) e^{-\frac{u}{2}} \{\theta(e^u) - e^u\}\, du$$

and

$$T_2 = \int_{\omega-\eta}^{\omega-\eta_0} K(u-\omega) e^{-\frac{u}{2}} \{\theta(e^u) - e^u\}\, du.$$

Another appeal to Table 3 in [6], and (3), gives us

$$|\theta(x) - x| \le 1.3082 \cdot 10^{-9} x, \quad x \ge e^{700}.$$

Thus for $\omega - \eta > 700$ we have

$$|T_1| + |T_2| \le 1.3082 \cdot 10^{-9} (\eta - \eta_0) K(\eta_0) \left[e^{\frac{\omega+\eta}{2}} + e^{\frac{\omega-\eta_0}{2}} \right]. \tag{13}$$

Applying (13) to (12), we find we can take $\eta_0 = \eta/4.2867$ so that

$$\int_{\omega-\eta_0}^{\omega+\eta_0} K(u-\omega)e^{-u/2}\left\{\theta(e^u) - e^u\right\} du > 2.75 \cdot 10^{-6},$$

which proves Theorem 2. Therefore, there is at least one $u \in (\omega - \eta_0, \omega + \eta_0)$ with $\theta(e^u) - e^u > 0$. Owing to the positivity of the kernel $K(u - \omega)$ we deduce that there is at least one such u with

$$\theta(e^u) - e^u > 2.75 \cdot 10^{-6} e^{u/2} > 10^{152}.$$

Since $\theta(x)$ is nondecreasing this proves

Corollary 3. *There are more than* 10^{152} *successive integers* x *satisfying*

$$x \in [\exp(727.951332642), \exp(727.951332668)],$$

for which $\theta(x) > x$.

3.2. **A lower bound.** Having established an upper bound for the first x for which $\theta(x)$ exceeds x, we now turn to a lower bound. A simple method would be to sieve all the primes p less than some bound B, sum $\log p$ starting at $p = 2$, and compare the running total each time to p. We set $B = 1.39 \cdot 10^{17}$ since this was required by the second author for another result in [4]. By the prime number theorem we would expect to find about $3.5 \cdot 10^{15}$ primes below this bound. Since this is far too many for a single thread computation we must look for some way of computing in parallel.

3.2.1. *A parallel algorithm.* We divide the range $[0, B]$ into contiguous segments. For each segment $S_j = [x_j, y_j]$ we set $T = \Delta = \Delta_{\min} = 0$. We look at each prime p_i in this segment, compute $l_i = \log p_i$, and add it to T. We set $\Delta = \Delta + l_i - p_i + p_{i-1}$ and $\Delta_{\min} = \min(\Delta_{\min}, \Delta)$. Thus, at any p, $\Delta_{\min}$ is the maximum amount by which $\theta(p)$ has caught up with or gone further ahead of p within this segment. After processing all the primes within a segment, we output T and $\Delta_{\min}$.

Now, for each segment $S_j = [x, y]$ the value of $\theta(x)$ is simply the sum of T_k with $k < j$ and $\theta(y) = \theta(x) + T_j$. Furthermore, if $\theta(x) < x$ and $\theta(x) + \Delta_{\min} > 0$, then $\theta(w) < w$ for all $w \in [x, y]$.

3.2.2. *Results.* We implemented this algorithm in C++ using Kim Walisch's "primesieve" [21] to enumerate the primes efficiently, and the second author's double precision interval arithmetic package to manage rounding errors.

We split B into $10,000$ segments of width 10^{13} followed by 390 segments of width 10^{14}. This pattern was chosen so that we could use Oliveira e Silva's tables of $\pi(x)$ [12] as an independent check of the sieving process.

We used the 16 core nodes of the University of Bristol Bluecrystal Phase III cluster [1] and we were able to utilise each core fully. In total we used about $78,000$ node hours. This established Theorem 1.

We plot $(x - \theta(x))/\sqrt{x}$ measured at the end of each segment in Figure 2. As one would expect, this appears to be a random walk around the line 1.

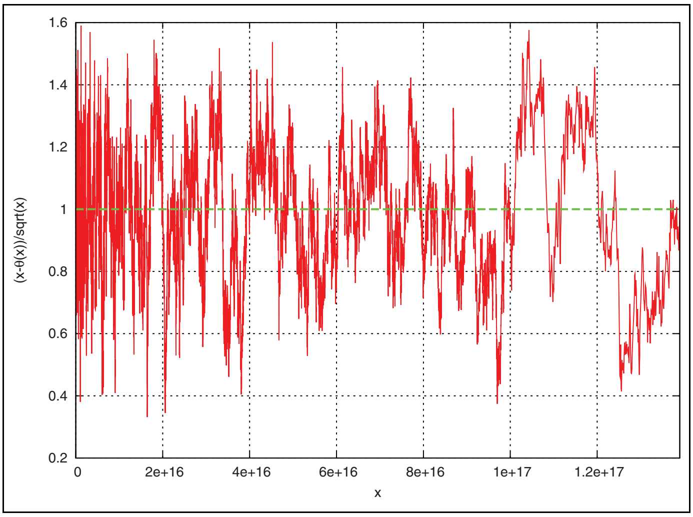

FIGURE 2. Plot of $\frac{x-\theta(x)}{\sqrt{x}}$.

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