On the first sign change of $\theta(x) - x$

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

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1 Introduction

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

$$\pi(x) \sim \operatorname{li}(x) = \int_{2}^{x} \frac{dt}{\log t}. \quad (1)$$

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

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

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

$$\pi(x) - \operatorname{li}(x) = \Omega_{\pm} \left( \frac{x^\frac{1}{2}}{\log x} \log \log \log x \right), \quad (2)$$

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

By [16, (3.36)] we have

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

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

Littlewood’s proof that $\pi(x) - \text{li}(x)$ changes sign infinitely often was ineffective: the proof did not furnish a number $x_0$ such that one could guarantee that $\pi(x) - \text{li}(x)$ changes sign for some $x \leq x_0$. Skewes [19] made Littlewood’s theorem effective; the best known result is that there must be a sign change less that $1.3971 \cdot 10^{316}$ [17]. On the other hand Kotnik [8] showed that $\pi(x) < \text{li}(x)$ for all $2 < x \leq 10^{14}$.

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 sign changes of $\psi(x)$: for $x \in [0, 100]$ there are 24 sign changes. The problem of determining an interval in which $\psi(x) - x$ changes sign is much more interesting (as examined in [11]) but it is not something we consider here. As for sign changes in $\theta(x)$: Schoenfeld, [18, p. 360] showed that $\theta(x) < x$ for all $0 < x \leq 10^{11}$. This range appears to have been improved by Dusart, [5, p. 4] to $0 < x \leq 8 \cdot 10^{11}$. We increase this in

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

A result of Rosser [15, Lemma 4] is

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

This enables us to extend Kotnik’s result by proving

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

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

$$\psi(x) - \theta(x) - \theta(x^{1/3}) < 3x^{1/3}, \quad (x > 0).$$

**(4)**

Table 3 in [6] gives us the bound $|\psi(x) - x| \leq 7.5 \cdot 10^{-7}x$, which is valid for all $x \geq e^{35} > 1.5 \cdot 10^{15}$. 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 $x > 0$

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

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 $f(x) = O^*(g(x))$ if $|f(x)| \leq g(x)$ for the range of $x$ under consideration.

**2 Outline of argument**

The explicit formula for $\psi(x)$ is [7, p. 101]

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

(5)
Since
\[ \psi(x) = \theta(x) + \theta(x^{1/2}) + \theta(x^{1/3}) + \ldots, \]
we can manufacture an explicit formula for \( \theta(x) \). Using (4) and (5) we find that
\[
\theta(x) - x > -\theta \left( x^{1/2} \right) - \sum_{\rho} \frac{x^\rho}{\rho} - \frac{\zeta'}{\zeta}(0) - 3x^{1/2}. \tag{6}
\]

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

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

Divide both sides of (6) by \( x^{1/2} \), make the substitution \( x \mapsto e^u \) and integrate against \( K(u - \omega) \). This gives
\[
\int_{\omega-\eta}^{\omega+\eta} K(u - \omega)e^{\frac{u}{2}} \{ \theta(e^u) - e^u \} du > -\int_{\omega-\eta}^{\omega+\eta} K(u - \omega)\theta \left( e^{\frac{u}{2}} \right) e^{-\frac{u}{2}} du
\]
\[
- \sum_{\rho} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u - \omega)e^{u(\rho - \frac{1}{2})} du - \frac{\zeta'(0)}{\zeta(0)} \int_{\omega-\eta}^{\omega+\eta} K(u - \omega)e^{-\frac{u}{2}} du \tag{7}
\]
\[
- 3 \int_{\omega-\eta}^{\omega+\eta} K(u - \omega)e^{-\frac{u}{2}} du = -I_1 - I_2 - I_3 - I_4,
\]
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
\[
0 < I_3 < e^{-\frac{\omega+\eta}{2}} \log 2\pi, \quad 0 < I_4 < 3e^{-\frac{\omega-\eta}{2}}.
\]

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 \( T \leq A \) 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
\[
S_1 = \sum_{|\gamma| \leq A} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u - \omega)e^{\gamma u} du, \quad S_2 = \sum_{|\gamma| > A} \frac{1}{\rho} \int_{\omega-\eta}^{\omega+\eta} K(u - \omega)e^{\rho(u - \frac{1}{2})} du.
\]

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

\[ f_\rho(s) = \rho \text{se}^{-\rho s \text{li}(e^{\rho s})e^{-\alpha(s-w)^2/2}} , \]

whence we write 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

\[ |f_\rho(s)| \leq 2 \exp(-\frac{1}{2} \alpha (s-w)^2). \]  

(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

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

provided that

\[ 4A/w \leq \alpha \leq A^2, \quad 2A/\alpha \leq \eta < w/2. \]

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

\[ |\theta(x) - x| \leq 1.5423 \cdot 10^{-9} x, \quad x \geq e^{200} , \]  

(9)

which gives

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

Thus, we have

**Theorem 3.** Let \( A \) be the height to which the Riemann hypothesis has been verified, and let \( T \) satisfy \( 0 < T \leq A \). Let \( \alpha, \eta \) and \( \omega \) be positive numbers for which \( \omega - \eta \geq 400 \) and for which

\[ 4A/\omega \leq \alpha \leq A^2, \quad 2A/\alpha \leq \eta \leq \omega/2. \]

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

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

(10)

Then

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

(11)

where

\[ R_1 = 1.5423 \cdot 10^{-9} \]

\[ R_2 = 0.08 \sqrt{\alpha} e^{-\alpha \eta^2/2} + e^{-T^2/2\alpha} \left\{ \frac{\alpha}{\pi T^2} \log \frac{T}{2\pi} + 8 \log \frac{T}{T} + \frac{4\alpha}{T^3} \right\} \]

\[ R_3 = e^{-(\omega-\eta)/2} \log 2\pi + 3 e^{-(\omega-\eta)/6} \]

\[ R_4 = A(\log A) e^{-A^2/(2\alpha) + (w+\eta)/2} \left\{ 4\alpha^{\frac{1}{2}} + 15\eta \right\}. \]
We note that if one were to assume the Riemann Hypothesis for $\zeta$, then the $R_4$ term could be reduced. This would give us greater freedom in our choice of $\alpha$—see §3.1.3.

Approximations different from (9) are available. For example, one could use Lemma 1 in [20] to obtain $|\theta(x) - x| \leq 0.0045x/(\log x)^2$. One could also restrict the conditions in Theorem 3 to $\omega - \eta \geq 600$ 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 $\omega$, $\eta$, $A$, $T$ and $\alpha$ for which the right-side of (11) is positive.

3 Computations

3.1 Locating a crossover

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

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

3.1.1 Choosing $A$

We chose to rely on the rigorous verification of RH for $A = 3.0610046 \cdot 10^{10}$ by the second author [13]. This computation also produced a database of the zeros below this height computed to an absolute accuracy of $\pm 2^{-102}$ [3].

3.1.2 Choosing $T$

As already observed, we have sufficient zeros to set $T = A \approx 3 \cdot 10^{10}$ but, since summing over the roughly $10^{11}$ zeros below this height is too computationally expensive, we settled for $T = 6,970,346,000$ (about $2 \cdot 10^{10}$ zeros). 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 $\eta$ as small as possible. This in turn means setting $\alpha$ (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

$$\alpha = 1, 153, 308, 722, 614, 227, 968, \quad \eta = \frac{933831}{244},$$

both of which are exactly representable in IEEE double precision.
3.1.4 Summing over the zeros

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 \(\Sigma_1\) 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 \(\gamma \omega \mod 2\pi\) 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 zeros \(\frac{1}{2} + i\gamma\) 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 zeros and with \(\omega = 437.78249\) fails to get over the line. The same pattern repeats for \(\omega\) 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 \(\pi(x) > \text{li}(x)\) is

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

in [17]. Since the error terms for \(\theta(x) - x\) are tighter than those for \(\pi(x) - \text{li}(x)\) this necessarily means that the same \(x\) will satisfy \(\theta(x) > x\). In fact, we can do better. Using \(\omega = 727.951332655\) we get

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

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

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

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 \(\eta_0 \in (0, \eta]\),

\[
T_1 = \int_{\omega + \eta_0}^{\omega + \eta} K(u - \omega)e^{-u/2} \{\theta(e^u) - e^u\} \, du,
\]
Figure 1: Plot of $\sum_{|\gamma|\leq 5000} \frac{e^{i\omega \gamma}}{\rho}$ for $\omega \in [437.78, 437.785]$. 
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

\[ |\theta(x) - x| \leq 1.3082 \cdot 10^{-9} x, \quad x \geq e^{700}. \]

Thus for \( \omega - \eta > 700 \) we have

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

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

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

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 non-decreasing 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 time that \( \theta(x) \) exceeds \( x \), we now turn to a lower bound. A simple method would be to sieve all the primes \( p < B \), 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 \( T = \Delta = \Delta_{\text{min}} = 0 \). We look at the 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 \( \Delta_{\text{min}} = \min(\Delta_{\text{min}}, \Delta) \). Thus at any \( p \), \( \Delta_{\text{min}} \) 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 \( \Delta_{\text{min}} \).

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 \( \theta(x) + \Delta_{\text{min}} > 0 \) 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.

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