

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

D. J. PLATT AND T. S. TRUDGIAN

ABSTRACT. Let  $\theta(x) = \sum_{p \leq x} \log p$ . 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

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

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

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

By [16, (3.36)] we have

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

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 than  $1.3972 \cdot 10^{316}$  [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 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  $0 < x \leq 10^{11}$ . 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

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

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  $x > 0$ ,*

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

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  $|f(x)| \leq g(x)$  for the range of  $x$  under consideration.

## 2. OUTLINE OF ARGUMENT

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

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

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

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

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  $-\theta \left( x^{\frac{1}{2}} \right)$ .

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

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

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  $T \leq A$  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

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

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

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

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

$$(8) \quad |f_{\rho}(s)| \leq 2 \exp(-\frac{1}{2}\alpha(s-w)^2).$$

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

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

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

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

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

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

Then

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

where

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

If one were to assume the Riemann hypothesis one could reduce the term  $R_4$ . This would give greater freedom in the choice of  $\alpha$ ; 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  $\Sigma_1 = \sum_{|\gamma| \leq T} \frac{e^{i\gamma\omega}}{\rho}$ . 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 be 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 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  $\eta$  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 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  $\Sigma_1$  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  $\gamma\omega \bmod 2\pi$  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  $\omega$  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

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

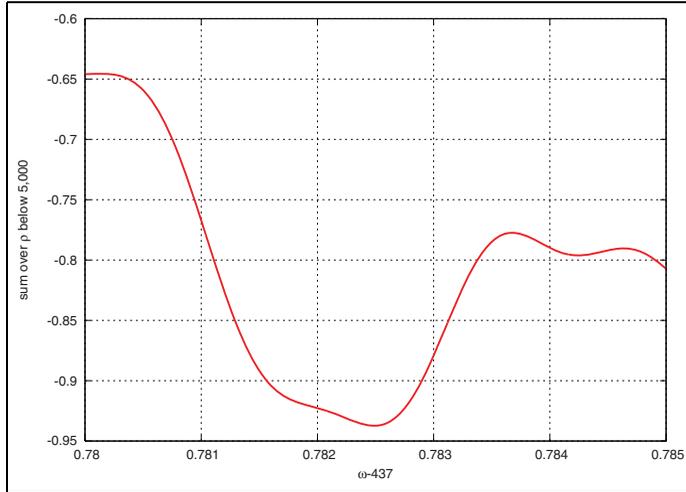


FIGURE 1. Plot of  $\sum_{|\gamma| \leq 5000} \frac{e^{i\omega\gamma}}{\rho}$  for  $\omega \in [437.78, 437.785]$ .

in [17]. Since the error terms for  $\theta(x) - x$  are tighter than those for  $\pi(x) - \text{li}(x)$  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

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

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

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

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

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

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 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.

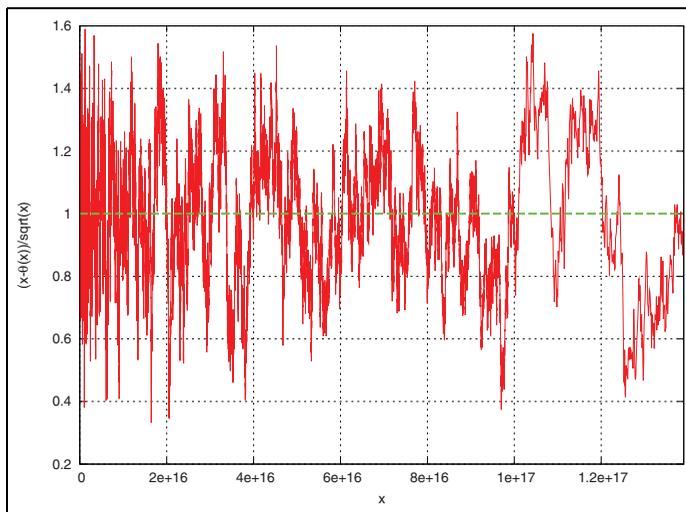


FIGURE 2. Plot of  $\frac{x-\theta(x)}{\sqrt{x}}$ .

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HEILBRONN INSTITUTE FOR MATHEMATICAL RESEARCH UNIVERSITY OF BRISTOL, BRISTOL,  
UNITED KINGDOM

*E-mail address:* `dave.platt@bris.ac.uk`

MATHEMATICAL SCIENCES INSTITUTE, THE AUSTRALIAN NATIONAL UNIVERSITY, ACT 0200,  
AUSTRALIA

*E-mail address:* `timothy.trudgian@anu.edu.au`