A NEW BOUND FOR THE SMALLEST $x$ WITH $\pi(x) > \text{li}(x)$

CARTER BAYS AND RICHARD H. HUDSON

Abstract. Let $\pi(x)$ denote the number of primes $\leq x$ and let $\text{li}(x)$ denote the usual integral logarithm of $x$. We prove that there are at least $10^{153}$ integer values of $x$ in the vicinity of $1.39822 \times 10^{316}$ with $\pi(x) > \text{li}(x)$. This improves earlier bounds of Skewes, Lehman, and te Riele. We also plot more than 10000 values of $\pi(x) - \text{li}(x)$ in four different regions, including the regions discovered by Lehman, te Riele, and the authors of this paper, and a more distant region in the vicinity of $1.617 \times 10^{9608}$, where $\pi(x)$ appears to exceed $\text{li}(x)$ by more than $.18x^{1/2}/\log x$. The plots strongly suggest, although upper bounds derived to date for $\pi(x) - \text{li}(x)$ are not sufficient for a proof, that $\pi(x)$ exceeds $\text{li}(x)$ for at least $10^{311}$ integers in the vicinity of $1.62 \times 10^{9608}$, the density is $1 - 2.7 \times 10^{-7} = .99999973$, and that it varies from this by no more than $9 \times 10^{-8}$ over the next $10^{30000}$ integers. This should be compared to Rubinstein and Sarnak.

1. Introduction and summary

Let

$$\text{li}(x) = \lim_{\varepsilon \to 0} \left\{ \int_0^{1-\varepsilon} \frac{dt}{\log t} + \int_1^{x} \frac{dt}{1+\varepsilon(\log t)} \right\}.$$ 

In 1796, at the age of 15, Gauss (see [4, pp. 2, 305]) observed that if $\pi(x)$ denotes the number of primes $\leq x$, then

$$(1.1) \quad \pi(x) < \text{li}(x)$$

for all $x < 3000000$, and for over a century it was widely believed that (1.1) holds for all $x$. Lagarias, Miller, and Odlyzko [8] showed that (1.1) holds for selected values of $x$ as large as $4 \times 10^{16}$, and Deleglise and Rivat have recently extended these computations to $10^{20}$. For values up to $10^{18}$, see [3].

Nonetheless, in 1914, J. E. Littlewood (see [7, 11]) proved that there is a positive constant $K$ such that infinitely often

$$(1.2) \quad \pi(x) - \text{li}(x) > \frac{kx^{1/2}}{\log x} \log \log \log x.$$ 

In 1933, Skewes [16] proved that there are values of $x$ with

$$(1.3) \quad x < 10^{10^{10^{34}}}.$$ 

Received by the editor June 30, 1997 and, in revised form, April 1, 1998 and July 7, 1998.

1991 Mathematics Subject Classification. Primary 11-04, 11A15, 11M26, 11Y11, 11Y35.
such that $\pi(x) - \text{li}(x) > 0$. In 1955 Skewes [17] improved [13] by showing that the exponent 34 in [13] can be replaced by 3. The 1933 proof required the Riemann hypothesis.

The first breakthrough in lowering Skewes’ legendary bound was achieved by Lehman [3] in 1966. All subsequent work, including ours, depends on his theorem; see [2], Theorem 1.

Lehman proved that there are at least $10^{500}$ values of $x$ lying between $1.53 \times 10^{1165}$ and $1.65 \times 10^{1165}$ with $\pi(x) > \text{li}(x)$. In 1987 te Riele [13] succeeded in bringing this bound down by showing that there are at least $10^{190}$ integers in the vicinity of $6.658 \times 10^{570}$ with $\pi(x) > \text{li}(x)$. Our result depends on the accuracy of the values for the first 1,000,000 zeros of the Riemann zeta function which were generously provided to us by Andrew Odlyzko, and on the truth of the Riemann hypothesis for all complex zeros $\beta + i\gamma$ with $\gamma < 10^7$. The truth of the Riemann hypothesis for the first 3.5 million zeroes was established by Rosser, Yohe, and Schoenfeld in 1968; see [4, p. 172]. The truth for all zeroes $< 545,439,823,215$ was given by Van de Lune, te Riele, and Winter [11] in 1986.

We also give in this paper a plot of $\text{li}(x) - \pi(x)$ for $x < 10^{400}$. If our bound in the vicinity of $10^{316}$ is not best possible, it is highly probable that any improvement will coincide with locations (marked with small arrows) where the plot in Figures 1a and 1b appears to be close to the zero axis. If a value of $x < 10^{316}$ exists with $\pi(x) > \text{li}(x)$, substantially more than 1,000,000 zeroes of the zeta function will be required to prove its existence. We think it more likely that no such $x$ exists. However, we give in Figure 1c a high resolution plot for the best of three candidates we have found for an earlier sign change.

We also give in this paper high resolution plots of the regions found by Lehman, te Riele, and the authors of this paper. The plots strongly suggest (but do not prove) that the number of values of $x$ with $\pi(x) > \text{li}(x)$ in those three regions is a substantial proportion of the integers lying between the first and last sign changes in these regions. If so, there are more than $10^{311}$ integers $x$ with $\pi(x) > \text{li}(x)$ between $1.3981 \times 10^{316}$ and $1.3983 \times 10^{316}$ (see Figure 21). Finally, we consider the question of whether the growth rate $\log \log \log x$ in [12] is close to the truth or whether a substantially more rapid growth rate, say $\log \log x$, is more realistic. In particular, we compute $\pi(x) - \text{li}(x)$ for $x < 10^{40000}$. Ingham [7] has referred to the gap in our knowledge of the true upper and lower bounds for $\pi(x) - \text{li}(x)$ (even assuming the Riemann hypothesis) as a matter of some import. See, in this connection, Montgomery [12]. A major motivation for computing $\pi(x) - \text{li}(x)$ for such large $x$ is to corroborate the recent work of Rubinstein and Sarnak [15], who prove, under the Riemann hypothesis, that the logarithmic density of integers $x$ with $\pi(x) < \text{li}(x)$ should be (to 8 decimals) .99999973. In Section 4 (see also Table 1) we discuss a computation of the logarithmic density of $\text{li}(x) - \pi(x)$ using Lehman’s function, given in [23] of this paper, and a function introduced by Bays and Hudson in [1], and find that the logarithmic density at the end of the region in Figure 5 in both computations is .99999973, and over the range $10^{3608}$ to $10^{39969}$ the maximum difference in the computed density is bounded above by $9 \times 10^{-8}$. The reader is urged to read the Remark on Table 1 at the end of the paper, in any case to maintain proper skepticism regarding the machine computations in Table 1 until they have been independently corroborated. The problem of rigorously proving for a particular identifiable value of $x$ that $\pi(x) > \text{li}(x)$, while for all smaller $x$, $\pi(x) < \text{li}(x)$, and the related problem of rigorously proving that $\pi(x) < \text{li}(x)$...
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for a large proportion of integers in the regions found to date, is likely to remain open for a long time. Even the finest resolution plot at $10^{316}$ will plot points which are more than $10^{300}$ apart. Our knowledge of upper bounds for $\pi(x + y)$ (see the discussion of Ian Richards in [5]) is insufficient to rule out $\pi(x) - \text{li}(x)$ undergoing a sign change for a gap $y$ on the order of $10^{300}$ at $10^{316}$. Thus, while te Riele knew in his heart that there were many more than $10^{180}$ successive integers in the vicinity of $6.6578 \times 10^{370}$, and we believe that there are many more than $10^{153}$ integers in the vicinity of $1.39822 \times 10^{316}$ with $\pi(x) > \text{li}(x)$, it will not be possible, until our knowledge regarding gaps is greatly improved or machines are capable of doing more than $10^{100}$ computations, to rigorously prove what appears in Figure 2b to be true. Namely, that there are more than $10^{311}$ integers between $1.39820386 \times 10^{316}$ and $1.39821924 \times 10^{316}$ with $\pi(x) > \text{li}(x)$. Nonetheless, our experience with sign changes of $\pi_{4,3}(x) - \pi_{4,1}(x)$ certainly suggests that wildly erratic behavior of $\pi(x) - \text{li}(x)$ over short gaps is unlikely, at least for any value of $x$ accessible to a computer, so that $10^{311}$ should be much closer to the truth than $10^{153}$. Finally, we observe that totally unanticipated breakthroughs like that of R. Sherman Lehman can happen at any time, and a different approach may establish the truth of the matter far sooner than we expect.

2. **Proof that there are $x$ in the vicinity of $1.39822 \times 10^{316}$ with $\pi(x) > \text{li}(x)$**

Our proof, like that of te Riele, rests on the following theorem of Lehman [9].

**Theorem 1** (Lehman, 1966). Let $A$ be a positive number such that $\beta = \frac{1}{2}$ for all zeroes $\rho = \beta + i\gamma$ of $\zeta(s)$ for which $0 < \gamma \leq A$. Let $\alpha$, $\eta$, and $\omega$ be positive numbers such that $\omega - \eta > 1$ and the conditions

\begin{equation}
4A/\omega \leq \alpha \leq A^2 \quad \text{and} \quad 2A/\alpha \leq \eta < \omega/2
\end{equation}

hold. Let

\begin{equation}
K(y) = \sqrt{\frac{\alpha}{2\pi}} e^{-\alpha y^2/2}.
\end{equation}

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

\begin{equation}
\int_{\omega-\eta}^{\omega+\eta} K(u - \omega)u e^{-u/2}(\pi(e^u) - \text{li}(e^u)) du = -1 - \sum_{0 < |\gamma| \leq T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha} + R,
\end{equation}

where

\[|R| \leq S_1 + S_2 + S_3 + S_4 + S_5 + S_6\]

\[= \frac{3.05}{\omega - \eta} + 4(\omega + \eta)e^{-(\omega - \eta)/6} + \frac{2e^{-\alpha\eta^2/2}}{\sqrt{2\pi}\alpha\eta} + 0.8\sqrt{\alpha} e^{-\alpha\eta^2/2} \]

\[+ e^{-T^2/2\alpha} \left( \frac{\alpha}{\pi T^2} \log \frac{T}{2\pi} + \frac{8}{T} \log \frac{T}{T_0} + \frac{4\alpha}{T^3} \right) \]

\[+ A \log A \frac{e^{-A^2/2\alpha + (\omega + \eta)/2}}{4\alpha^{-1/2} + 15\eta}.\]

If the Riemann hypothesis holds, the conditions (2.1) and the term $S_6$ in the error bound may be omitted.
Remark. Since 1966, little has been done to improve the bounds for $S_1, \ldots, S_6$. As we will see in the following proof, it enough zeroes of $\zeta(S)$ are used so that $\alpha$ can be taken large, only the term $S_1$ contributes significantly to the error. Since

$$\frac{\pi(x^{1/2})}{2} = \frac{\mathrm{li}(x^{1/2})}{2} - \frac{x^{1/2}}{\log x} - \frac{2x^{1/2}}{\log^2 x} + o \left( \frac{x^{1/2}}{\log^2 x} \right)$$

(see [6, p. 563] or [14, p. 76]), it should be possible to reduce the 3.05 in the $S_1$ term. We will not require such an improvement, however, to prove the following theorem.

Theorem 2. There exist values of $x$ in the vicinity of $1.39822 \times 10^{316}$ (in particular, between $1.398201 \times 10^{316}$ and $1.398244 \times 10^{316}$) with $\pi(x) > \mathrm{li}(x)$.

Proof. We apply Lehman’s theorem (note that the conditions in 2.1 are satisfied) with

$$A = 10^7, \quad \alpha = 10^{10}, \quad \eta = .002, \quad T = \gamma_{1,000,000} = 600269.677 \ldots, \quad \omega = 727.95209.$$

As the Riele [13] (see also [11]) has noted, we can take $A$ as large as 545, 439, 823.215, but this is more than we need. Using the above parameters, we have

$$S_1 = \frac{3.05}{727.95009} < .00418985,$$
$$S_2 = 4(727.95409)e^{(-727.95009)/6} < 5.94 \times 10^{-50},$$
$$S_3 = (2e^{-10^{10}(0.002)^2/2})/\sqrt{2\pi}(200) < 3.64 \times 10^{-8689},$$
$$S_4 = (.08)(10^5)e^{-10^{10}(0.002)^2/2} < 1.03 \times 10^{-8682},$$
$$S_5 = e^{-(600269.677)^2/2(10^{10})} \left( \frac{10^{10}}{\pi(600269.677)^2} \log \left( \frac{600269.677}{2\pi} \right) \right)$$
$$+ \frac{8 \log(600269.677)}{600269.677} + \frac{4(10)^{10}}{(600269.677)^3} < 1.53 \times 10^{-9},$$
$$S_6 = 10^7 \log 10^7 e^{(-5000+363.977045)(.03004)} < 1.20 \times 10^{-2001}.$$

Thus,

$$|R| = S_1 + \cdots + S_6 < .00419.$$

Now let

$$H = \sum e^{\gamma \omega} \rho e^{-\gamma^2/2\alpha}.$$

Defining $H^*$ to be the finite sum obtained when (2.4) is summed over all $\gamma$ with $0 < |\gamma| < 600269.677$, $\alpha$ is taken to be $10^{10}$, and $\omega$ is taken to be 727.95209, we obtain

$$H^* = 1.012762 \ldots,$$

where $H^*$ is our machine computation approximation of $H$ defined in [13].

It follows that

$$\int^{\omega+\eta}_{\omega-\eta} K(u-\omega)ue^{-u/2}(\pi(e^u) - \mathrm{li}(e^u))du > 0,$$
unless there is an error in our computation of $H^*$ greater than .0078. We have ruled this out in a large number of ways, some of which are described in the following section. Suffice to say here that for the parameters chosen by te Riele in discovering the sign change in the vicinity of $e^{853.852286}$, our computed value $H^*$ differs from te Riele’s by at most .0000012. This alone makes the likelihood of a machine error as large as .0078 appear remote.  

Finally, assuming for the moment that such a machine error does not take place, the positivity of the kernel $K$ implies that there is a value of $u$ between $\omega - \eta$ and $\omega + \eta$ where $\pi(e^u) - \text{li}(e^u) > 0$. This completes the proof of Theorem 2.  

3. Machine computations

We ruled out the likelihood of a machine error serious enough to affect the result in this paper in several ways.

First, we carried out the computation on two different computers and performed the computation several times. Second, we chose a value of $\alpha$ considerably less than the largest possible value which maximizes (2.5). For example, if we chose $\alpha = 2.5 \times 10^{11}$, then $H^* = 1.016145$, but the error in $\delta$ increases markedly. A choice of $\alpha = 2.5 \times 10^{11}$ allows one to show that there are more than $(1.016145 - .0042)e^{\alpha/2}/u > 10^{153}$ successive integers between $1.39821924 \times 10^{316}$ and $1.39821925 \times 10^{316}$ with $\pi(x) > \text{li}(x)$. However, we achieve effectively the same result with $H^* = 1.012762$.

Since we believe there are probably more than $10^{311}$ integers in the region in Figure 2a with $\pi(x) > \text{li}(x)$, we chose to guard against machine error rather than trying to maximize $H$. Observe that for $\alpha = 10^{10}$ at a height of $T = 300,000$ we have $e^{-\gamma^2/2\alpha} < .01111$, so that a reduction of $\alpha$ significantly reduces the effect (and so the error) in using zeroes to a greater height than te Riele (for $\alpha = 2.5 \times 10^{11}$, $e^{-\gamma^2/2\alpha} > .1652$).

Third, we computed $\pi(x) - \text{li}(x)$ using the theorem established by Hudson in [1], which assumes the Riemann hypothesis, employing constants which agree closely with machine computations to date. The regions plotted in Figures 1-5 are indistinguishable from one another if we use this theorem or if we use (2.3).

Finally, we utilized te Riele’s analysis [13, p. 327]. In this worst case scenario, where effectively all million zeroes of the zeta function conspire simultaneously to make the computed value $H^*$ larger than its true value $H$, we can, nonetheless, rule out a machine error nearly as large as $|H - H^*| = .0078$ as follows.

Assume that the computed value $\gamma_i^*$ differs from the true value $\gamma_i$ by less than $10^{-9}$. Probably the first 2,000 zeroes provided to us by Odlyzko are even more accurate, but we do not need such an assumption. Referring to (3.5) and (3.7) in [9] and noting that for Odlyzko’s zeroes we do have $|\gamma_i - \gamma_i^*| < 10^{-9}$ for $1 \leq i \leq 10^6$, we must have (since $e^{-\gamma^2/2\alpha} < 1$ for all $\gamma$ if $\alpha = 10^{10}$) that, for $\omega = 728$, and

$14 < \gamma_1 \leq \gamma \leq \gamma_{50000} < 40434 < \gamma_{1,000,000} < 600270$, using te Riele’s notations,

\begin{equation}
|t'(\gamma)| < \frac{1}{\gamma} \left(2\omega + \frac{\omega}{\gamma} + \frac{2}{\alpha} + \frac{2}{\gamma^2} + \frac{4}{\gamma}\right) < \frac{1509}{\gamma}.
\end{equation}

\footnote{We are most grateful to the referee of this paper for computing $H^*$ using 1,000,000 zeroes computed independently. He obtained $H^*(\gamma_{1,000,000}, 10^{10}, 728.952088813) = 1.0127617\ldots$.}
But then, by te Riele’s analysis,

\[ |H - H^*| < 10^{-9} \sum_{i=1}^{10^6} \left( \frac{1509}{\gamma_i} \right) < 10^{-9} \left( \frac{15000}{14} + \frac{35000}{14040} + \frac{950000}{40434} \right) < .00166. \]

In fact, a machine computation gives

\[ P_{10^6}(1509) = 14255.702 \ldots \]

so that the actual machine error is probably bounded above by 1.5 \times 10^{-5}, but this computation uses Odlyzko’s zeroes and (3.2) does not.

Remark. As te Riele noted, it is not possible to obtain Theorem 2 using 50,000 zeroes of the Riemann-zeta function. The 1,000,000 zeroes provided to us by Andrew Odlyzko are required for the proof of this result (see the acknowledgment at the end of this paper).

4. Logarithmic density of the set of \( x \) with \( \text{li}(x) > \pi(x) \)

Let \( P \) be the set of positive real \( x \) with \( \text{li}(x) > \pi(x) \). Using \( \text{li}(x) = \int_0^x (\log^{-1} t) dt \), which differs from the Cauchy principal value of \( \int_0^x (\log^{-1} t) dt \) by about 1.045 [4, p. 46], Rubinstein and Sarnak proved, using the Riemann hypothesis, that the logarithmic density of the set \( P \), denoted by \( \delta(P) \), is \(.99999973 \ldots \), where

\[ \delta(P) = \overline{\delta}(P) = \underline{\delta}(P) \]

and

\[ \overline{\delta}(P) = \limsup_{x \to \infty} \frac{1}{\log x} \int_{t \in P \cap [2, x]} \frac{dt}{t} \]

\[ \underline{\delta}(P) = \liminf_{x \to \infty} \frac{1}{\log x} \int_{t \in P \cap [2, x]} \frac{dt}{t} \]

This motivated us to compute the logarithmic density of \( \text{li}(x) - \pi(x) \) using (2.4) and also using a theorem established by Hudson in [1], which has been shown to give highly accurate results for the related difference \( \pi_{4.3}(x) - \pi_{4.1}(x) \). Using both methods (with \( x \) chosen somewhat larger in (2.4)), we find the logarithmic density at 1.62 \times 10^{9608} (which appears to be the sixteenth region with \( \pi(x) > \text{li}(x) \)) is \(.99999973 \ldots \). Over the next 10^{30000} integers, the logarithmic density differs from this figure by at most 9 \times 10^{-8}.

5. Description of figures

Figures 1a and 1b. These plots show \( \text{li}(x) - \pi(x) \) on a logarithmic scale for values of \( x \) from \( 10^6 \) to \( 10^{400} \). The numbers give values of \( x \) (as powers of ten). The small vertical bars cross the zero axis (the plot dips below this horizontal line when \( \text{li}(x) - \pi(x) \) exhibits a sign change). The top horizontal line represents \( \pi(x^{1/2}) \); the middle line, about which the plot hovers, depicts \( \pi(x^{1/2})/2 \). The large arrows indicate the crossings in the vicinity of \( 10^{316} \) and \( 10^{370} \). The small arrows show “near crossings”; if a crossing earlier than \( 10^{316} \) exists, it is likely to be at one of these spots.

Figures 2 through 5. Detailed plots of the regions in the vicinity of \( 10^{316}, 10^{370}, 10^{1165}, \) and \( 10^{9608} \) are given in Figures 2 through 5, which are all drawn to the same scale. The top line represents \( \pi(x^{1/2}) \); the bottom line is the zero axis. The reference line between is at \( \pi(x^{1/2})/4 \). Compare the relatively miniscule expanse of the region
Figure 1a.

Figure 1b.
at $10^{316}$ with the deep crossing at $10^{9608}$. The region at $10^{316}$ has been enlarged in Figure 2b. Here, the top horizontal line is the $\pi(x^{1/2})/4$ line. Note the large arrow in Figure 2b: the authors have been unable to ascertain if this “touching” point crosses the axis. Further calculations (involving more zeroes of the Riemann zeta function) must be made in order to determine whether this is the first actual crossing region in the vicinity of $1.398 \times 10^{316}$.

**Remark.** For additional information on how the plots in Figures 1-5 were obtained, see [1].
Remark on Table 1. The expectation that \( \pi(x) \) will exceed \( \text{li}(x) \) when \( g(x) < 0 \), at least if the Riemann hypothesis is true, has long been known, and is noted by Lehman on p. 398 of \([9]\). The function \( f(x) \) is referred to implicitly in the work of Rubinstein and Sarnak \([15]\), and is used by Bays and Hudson \([1]\) to successfully duplicate the distribution of \( \pi_{4,3}(x) - \pi_{4,1}(x) \) with the Riemann-zeta function replaced by \( L(s, \chi) \), \( \chi \) the nonprincipal character modulo 4. The difference between the bias computations using \( f(x) \) and \( g(x) \) shows up only in the eleventh decimal place over the entire range presented. Nonetheless, Table 1 is not intended to convince the reader that the logarithmic density at \( \infty \) is .99999973. This has already been proven, using the Riemann hypothesis, by Rubinstein and Sarnak \([15]\). What is remarkable is that Table 1 suggests that as early as the sixteenth region of integers \( x \), this convergent is close to the logarithmic density computed using \( f(x) \) or \( g(x) \). This suggests that giant fluctuations of \( \pi(x) - \text{li}(x) \), which must occur because of \([1.2]\), occur very infrequently on a logarithmic scale.
Table 1.
The first 20 regions where \( f(x) = \sum_{i=1}^{10^6} \left( \frac{1}{2} + \frac{\sin \gamma_i \log x}{\gamma_i} + \frac{1}{\log x} \right) < 0 \)

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<th>Region</th>
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<th>Bias out</th>
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<td>.999999999...</td>
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*The “bias in” approximates the logarithmic density of \( \text{li}(x) - \pi(x) \) at the beginning of each region, and “bias out” approximates the logarithmic density at the end of each region. Results are very similar for the beginning point and the bias if \( f(x) \) is replaced by values of \( x \) with

\[
g(x) = 1 - \sum_{i=1}^{10^6} e^{-\gamma_i^2/2a} \left( \cos \gamma_i \log x + 2\gamma_i \sin \gamma_i \log x \right) < 0,
\]

choosing \( \alpha = 4 \times 10^{10} \).
We are grateful to Carl Pomerance for pointing out that the density calculations in Table 1 are suspect if the numerical calculations do not accurately find the beginning and end of regions with $\pi(x) > \text{li}(x)$. Our optimism that this is not the case is based on the astonishing accuracy of our duplication of the logarithmic density calculations were very close to actual computed values, and the logarithmic density of .99592... computed for $x$ in the vicinity of $10^{30}$ agrees with the value .9959... obtained by Rubinstein and Sarnak in [15] under the generalized Riemann hypothesis. In [2] we obtain similarly accurate results for the moduli 3, 5, 7, 11 and 13. On numerical grounds, we would expect the values obtained in Table 1 to be more accurate than results in [1] and [2], if for no other reason, because of the use of 1,000,000 zeroes of the Riemann zeta function.

We concede that our program could have missed shallow regions or included ones that do not exist. Nonetheless, Table 1 represents the first serious attempt to analyze the distribution of $\text{li}(x)$ over the first $10^{30}$ integers. That this effort will be improved upon, we have no doubt.

Acknowledgments

We would like to thank Michael Rubinstein, Peter Sarnak, Robert Rumely, Carl Pomerance, and Andrew Odlyzko for their support and encouragement. Indeed, as noted above, the proof of the main result of this paper would have been impossible without the 1,000,000 zeroes of the Riemann-zeta function provided to us by Andrew Odlyzko.

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