Adv Comput Math (2008) 29:55–70
DOI 10.1007/s10444-007-9039-2

The prime-counting function and its analytic approximations

$\pi(x)$ and its approximations

Tadej Kotnik

Received: 25 May 2006 / Accepted: 24 November 2006 /
Published online: 4 May 2007

Abstract The paper describes a systematic computational study of the prime counting function $\pi(x)$ and three of its analytic approximations: the logarithmic integral $\mathrm{li}(x) := \int_0^x \frac{dt}{\log t}$, $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$, and $R(x) := \sum_{k=1}^{\infty} \mu(k)\mathrm{li}(x^{1/k})/k$, where μ is the Möbius function. The results show that $\pi(x) < \mathrm{li}(x)$ for $2 \le x \le 10^{14}$, and also seem to support several conjectures on the maximal and average errors of the three approximations, most importantly $|\pi(x) - \mathrm{li}(x)| < x^{1/2}$ and $-\frac{2}{5}x^{3/2} < \int_2^x (\pi(u) - \mathrm{li}(u))du < 0$ for all $x > 2$. The paper concludes with a short discussion of prospects for further computational progress.

Keywords Prime-counting function · Logarithmic integral · Riemann's approximation

Mathematics Subject Classifications (2000) 11A41 · 41A60 · 11Y35 · 65G99

1 Introduction

The problem of approximating the prime-counting function $\pi(x)$ (i.e. the number of primes $\le x$) by a smooth and fairly easily computable function has been studied intensively through the last two centuries. Already in 1792 or 1793, Gauss [6] observed that the logarithmic integral, $\mathrm{li}(x) := \int_0^x \frac{dt}{\log t}$, approximates $\pi(x)$ quite accurately. His later computations showed that $\mathrm{li}(x)$ slightly, yet consistently overestimates $\pi(x)$ for

Communicated by L. Reichel

T. Kotnik (✉)
Faculty of Electrical Engineering, University of Ljubljana,
Tržaška 25, SI-1000 Ljubljana, Slovenia
e-mail: tadej.kotnik@fe.uni-lj.si

$2 \le x \le 3000000$. Although Gauss does not seem to have conjectured explicitly that $\pi(x) < \mathrm{li}(x)$ holds for all $x \ge 2$, this was widely believed to be true until 1914, when Littlewood [12] proved that

$$\pi(x) - \mathrm{li}(x) = \Omega_{\pm}\left(\sqrt{x}\,\frac{\log\log\log x}{\log x}\right), \tag{1}$$

from which it is clear that $\pi(x) - \mathrm{li}(x)$ changes sign infinitely often.

Since then, several studies have focused on the smallest value of x with $\pi(x) \ge \mathrm{li}(x)$, which will be denoted here by Ξ. The first unconditional upper bound for Ξ was obtained in 1955 by Skewes [15], who showed that $\log_{10}\log_{10}\log_{10}\log_{10}\Xi < 3$. This was strengthened in 1966 by Lehman [11] to $\Xi < 1.65 \times 10^{1165}$, in 1987 by te Riele [16] to $\Xi < 6.69 \times 10^{370}$, and in 2000 by Bays and Hudson [1] to $\Xi < 1.40 \times 10^{316}$. The first lower bound for Ξ, namely $\Xi > 3000000$, followed from the computations of Gauss described above. This was improved in 1962 by Rosser and Schoenfeld [14] to $\Xi > 10^8$, in 1975 by Brent [3] to $\Xi > 8 \times 10^{10}$, and in 1993 by Odlyzko (unpublished) to $\Xi > 1.59 \times 10^{13}$. In the present paper it is shown that $\Xi > 10^{14}$.

Another line of investigation focused on the order of magnitude of $\pi(x) - \mathrm{li}(x)$. To date, the strongest unconditional O-bound is

$$\pi(x) - \mathrm{li}(x) = O\left(x \exp\left(-0.2098\,\frac{(\log x)^{3/5}}{(\log\log x)^{1/5}}\right)\right),$$

which follows from a method developed in 1958 by Vinogradov [17] and Korobov [9], corrected in 1963 by Walfisz [20], and with the constant 0.2098 obtained in 2002 by Ford [5]. Under the Riemann hypothesis, this can be strengthened considerably, and already in 1901 von Koch [18] showed that in this case

$$\pi(x) - \mathrm{li}(x) = O(\sqrt{x}\log x), \tag{2}$$

which is still the strongest result of its kind. As (1) and (2) show, a proof of the Riemann hypothesis would bring the O- and Ω-bounds of $\pi(x) - \mathrm{li}(x)$ rather close together, but some space for improvements would remain. The results in the present paper suggest that (2) could be strengthened to at least $O(\sqrt{x})$.

Alternative approximations of $\pi(x)$ were also studied. In 1808, Legendre [10] observed that $\pi(x)$ is approximated quite well by $\frac{x}{\log x - B}$ (he originally proposed $B = 1.08366...$), but de la Vallée Poussin [4] demonstrated in 1899 that with any B, such approximations are inferior to $\mathrm{li}(x)$. Another alternative was proposed by Riemann [13], who in 1859 outlined a proof of an exact formula for $\pi(x)$

$$\pi(x) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n}\left[\mathrm{li}\left(x^{\frac{1}{n}}\right) - \sum_{\rho}\mathrm{li}\left(x^{\frac{\rho}{n}}\right) + \int_{x^{1/n}}^{\infty}\frac{du}{u(u^2-1)\log u}\right], \tag{3}$$

where μ is the Möbius function, and ρ runs through the nontrivial zeros of the Riemann zeta function. This formula, the proof of which was completed in 1895 by von Mangoldt [19], suggested to Riemann that the series

$$R(x) := \sum_{n=1}^{\infty}\frac{\mu(n)}{n}\mathrm{li}\left(x^{\frac{1}{n}}\right) = \mathrm{li}(x) - \frac{1}{2}\mathrm{li}\left(x^{\frac{1}{2}}\right) - \frac{1}{3}\mathrm{li}\left(x^{\frac{1}{3}}\right) - \frac{1}{5}\mathrm{li}\left(x^{\frac{1}{5}}\right) + \frac{1}{6}\mathrm{li}\left(x^{\frac{1}{6}}\right) - \ldots$$

should be superior to $\mathrm{li}(x)$ in approximating $\pi(x)$. Since $\pi(x) - \mathrm{li}(x)$ has zeros, it is nowadays clear that this cannot be the case for all x. Moreover, as $-\frac{1}{2}\mathrm{li}(x^{1/2}) - \frac{1}{3}\mathrm{li}(x^{1/3}) - ... = O(\sqrt{x}/\log x)$, which is smaller than the Ω-bound of $\pi(x) - \mathrm{li}(x)$ in (1), it follows that $\pi(x) - R(x)$ has this same Ω-bound. This implies that $R(x)$ could at most be superior to $\mathrm{li}(x)$ on the average, in the sense that

$$\left|\int_2^x (\pi(u) - R(u))du\right| < \left|\int_2^x (\pi(u) - \mathrm{li}(u))du\right| \quad \text{for all sufficiently large } x\,, \tag{4}$$

but whether this is true remains to be resolved. It is, however, clear that even in this sense $R(x)$ is no better than its first two terms alone, i.e. $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$, since in such averaging the role of the third and the following terms is asymptotically negligible (see [8], and the results in the present paper for some numerical evidence).

Finally, if (4) is false, $\mathrm{li}(x)$ could still be inferior to $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ and $R(x)$, provided that

$$\int_2^x (\pi(u) - \mathrm{li}(u))du < 0 \quad \text{for all } x \geq 2\ , \tag{5}$$

so that on the average $\mathrm{li}(x)$ would be biased strictly toward overestimating $\pi(x)$. Assuming the Riemann hypothesis, Ingham [8] proved this inequality for all sufficiently large x, while its analogues for $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ and $R(x)$ are false, with the integrals taking both negative and positive values (see the results of this paper).

2 Methods of computation and processing

2.1 General

The program for computation and storage of the data was written in Delphi 6.0 (Borland, Scotts Valley, CA, USA) and run on a PC with a 2.4 GHz Intel Pentium 4 processor and 512 MB of RAM. All the integer variables were stored as 64-bit integers (type Int64), and all the non-integer variables as 80-bit reals (type Extended, 19-digit precision). The algorithms used for the computation of $\pi(x)$, $\mathrm{li}(x)$, and $R(x)$ are described in Sections 2.2–2.4.

As $\pi(x)$ is constant between primes, and $\mathrm{li}(x)$ is strictly increasing, all local maxima of $\pi(x) - \mathrm{li}(x)$ occur at primes. Thus, if $\pi(x) - \mathrm{li}(x)$ is negative at the start of an interval and at all primes within it, then it is negative throughout this interval. This method was used to verify the negativity of $\pi(x) - \mathrm{li}(x)$ for $2 \leq x \leq 10^{14}$.

Each decimal order of magnitude within the studied x-range was subdivided into 2400 intervals of equal length on the logarithmic scale, i.e. into intervals $\mathcal{P}_k : x_k \leq x < x_{k+1}$, with $x_{k+1} := 10^{1/2400}x_k$. For the two x-values corresponding to the largest and the smallest value of $\pi(x) - \mathrm{li}(x)$ within each $\mathcal{P}_k$, the values of $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ and $R(x)$ were computed, and the set $\{x,\ \pi(x),\ \mathrm{li}(x),\ \mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x}),\ R(x)\}$ was stored. The largest and the smallest values of $\int_2^x(\pi(u) - \mathrm{li}(u) + \frac{1}{2}\mathrm{li}(\sqrt{u}))du$ and of $\int_2^x(\pi(u) - R(u))du$ within each $\mathcal{P}_k$ were also stored, while for $\int_2^x(\pi(u) - \mathrm{li}(u))du$, which is monotonic in the investigated x-range, the value at each x_k was stored.

2.2 The function $\pi(x)$

Computation of $\pi(x)$ was based on an adaptation of the Eratosthenes sieve, with the sieving interval partitioned into blocks of $2 \times 3 \times 5 \times 7 \times 11 \times 13 \times 17 \times 19 = 9699690$ integers. Sieving of the first block with the primes ≤ 19 yielded the "small-prime variation" block that was used repeatedly as the initialization value for subsequent blocks before sieving with the primes > 19. The computed $\pi(x)$ were periodically checked with Mathematica 5.1 (Wolfram Research, Urbana, IL, USA) using the `PrimePi` routine, and no error was encountered.

2.3 The function li(x)

Computation of li(x) was based on the formula discovered by Ramanujan and proved in Berndt [2],

$$\mathrm{li}(x) = \gamma + \log\log x + \sqrt{x} \sum_{n=1}^{\infty} a_n \log^n x$$

where

$$a_n = \frac{(-1)^{n-1}}{n!\, 2^{n-1}} \sum_{m=0}^{\lfloor (n-1)/2 \rfloor} \frac{1}{2m+1}.$$

The values of li(x) were obtained by truncating the outer series at $n = 75$. Mathematica 5.1 was used to precompute the exact values of the coefficients $a_1, a_2, .., a_{75}$, which were then rounded to 20-digit precision and stored in the program as constants of type Extended. For $x > 10^{10}$ linear interpolation was used in intervals $[x, x + A]$, with $A = 2310$ up to $x = 2 \times 10^{12}$, $A = 30030$ up to $x = 2 \times 10^{13}$, and $A = 9699690$ up to $x = 10^{14}$. Section A of the Appendix shows that in the computation of li(x) using this algorithm, the absolute errors caused by truncation, interpolation, and finite precision round-off are less than 6×10^{-11}, 7×10^{-4}, and $1.54 \times 10^{-8}\sqrt{x}$, respectively, everywhere in the range $2 \leq x \leq 10^{14}$.

2.4 The function $R(x)$

Computation of $R(x)$ was based on the formula proved by Gram [7],

$$R(x) = 1 + \sum_{n=1}^{\infty} b_n \log^n x$$

where

$$b_n = \frac{1}{n!\, n\, \zeta(n+1)}$$

with ζ denoting the Riemann zeta function. The values of $R(x)$ were obtained by truncating the series at $n = 102$. Mathematica 5.1 was used to precompute the values of the coefficients $b_1, b_2, .., b_{102}$, which were then rounded to 20-digit precision and stored in the program as constants of type Extended. Section B of the Appendix shows that in the computation of $R(x)$ using this algorithm, the absolute errors caused by truncation and finite precision round-off are less than 4×10^{-11} and 1.22×10^{-3}, respectively, everywhere in the range $2 \leq x \leq 10^{14}$.

2.5 The integrals of $\pi(x)$, $\mathrm{li}(x)$, and $R(x)$

For $x \in \mathbb{N}$, $x \geq 3$, we have

$$\int_2^x \pi(u)du = \sum_{n=2}^{x-1} \pi(n)\,, \qquad \int_2^x \mathrm{li}(u)du = x\,\mathrm{li}(x) - \mathrm{li}(x^2) - C_1\,,$$

$$\int_2^x \mathrm{li}(u^{1/2})du = x\,\mathrm{li}(x^{1/2}) - \mathrm{li}(x^{3/2}) - C_2\,,$$

with $C_1 = -0.877257...$ and $C_2 = -2.209859...$ the values of the primitives at the lower limit of integration. The integrals of $\pi(x)$, $\mathrm{li}(x)$, and $\mathrm{li}(x^{1/2})$ were computed using these formulae and the algorithms described in Sections 2.2 and 2.3.

The series in Gram's formula (see Section 2.4) can be integrated termwise, which is justified by uniform convergence and continuity of the terms. Using

$$\int \log^n u\, du = n!u \sum_{m=0}^{n} \frac{(-1)^{n-m} \log^m u}{m!}$$

this gives

$$\int_2^x R(u)du = x\left[1 + \sum_{n=1}^{\infty} d_n \sum_{m=0}^{n} \frac{(-1)^{n-m}\log^m x}{m!}\right] - C_3\,,$$

where

$$d_n = \frac{1}{n\,\zeta(n+1)}$$

and $C_3 = 1.913594...$ is the value of the primitive at the lower limit of integration. The values at the upper limit of integration were obtained by truncating the outer series at $n = 102$. Mathematica 5.1 was used to precompute the values of the coefficients d_1, $d_2, .., d_{102}$, which were then rounded to 20-digit precision and stored in the program as constants of type Extended. Section C of the Appendix shows that in the computation of $\int_2^x R(u)du$ using this algorithm, the absolute errors caused by truncation and finite precision round-off are less than $3.27 \times 10^{-11}x$ and $1.90 \times 10^{-15}x^2$ (note that $x^{2-\varepsilon} = o(\int_2^x R(u)du)$ for every $\varepsilon > 0$), respectively, everywhere in the range $2 \leq x \leq 10^{14}$.

3 Results and discussion

The computations show that $\pi(x) < \mathrm{li}(x)$ at all primes in the range $2 \leq x \leq 10^{14}$, from which it follows (see Section 2.1) that $\Xi > 10^{14}$.

For convenience, we define

$$q_N(x) := \frac{\pi(x) - \sum_{n=1}^{N} \frac{\mu(n)}{n}\mathrm{li}(x^{1/n})}{\sqrt{x}/\log x}\,.$$

Figures 1, 2, and 3 show $q_1(x)$, $q_2(x)$, and $q_\infty(x)$, respectively, for $2 \leq x \leq 10^{14}$. In the strip at the bottom of Fig. 2, subintervals of $[10^3, 10^{14}]$ with $|q_2(x)| > |q_1(x)|$ are painted black. Similarly, in Fig. 3, subintervals of $[10^3, 10^{14}]$ with $|q_\infty(x)| > |q_1(x)|$ are marked in the upper strip, and those with $|q_\infty(x)| > |q_2(x)|$ in the lower strip.

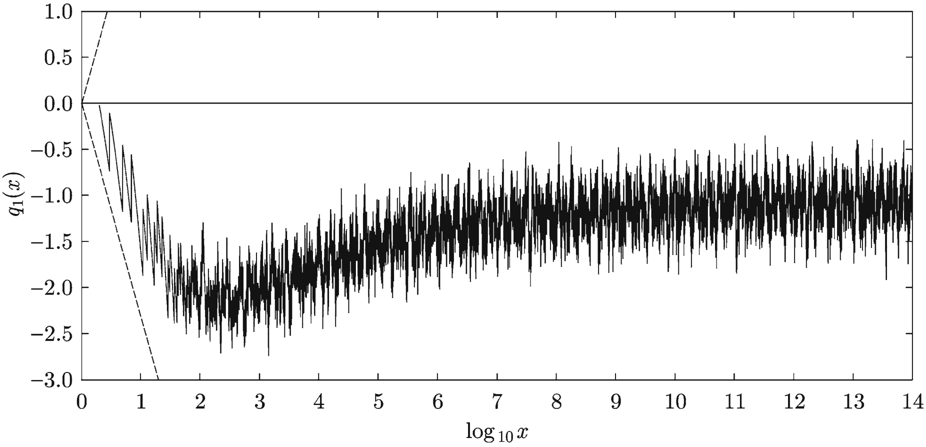

Fig. 1 $q_1(x)$ in the range $2 \leq x \leq 10^{14}$

The strips show that also in x-ranges where $\pi(x) - \mathrm{li}(x)$ is quite far from zero, $\mathrm{li}(x)$ can be superior to $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ and $R(x)$, respectively, in approximating $\pi(x)$.

Integrating by parts, we get

$$\mathrm{li}(\sqrt{x}) = \frac{2\sqrt{x}}{\log x}\left(1 + O\left(\frac{1}{\log x}\right)\right),$$

so that

$$q_1(x) - q_2(x) = -\frac{\mathrm{li}(\sqrt{x})/2}{\sqrt{x}/\log x} = -1 - O\left(\frac{1}{\log x}\right)$$

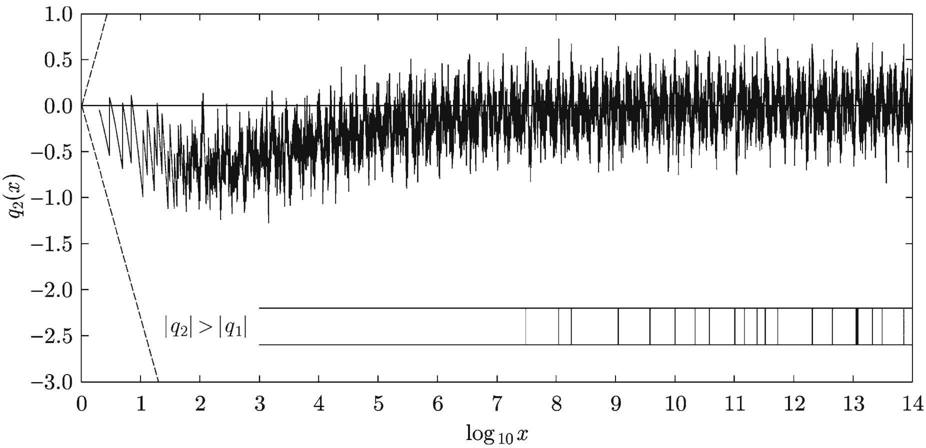

Fig. 2 $q_2(x)$ in the range $2 \leq x \leq 10^{14}$

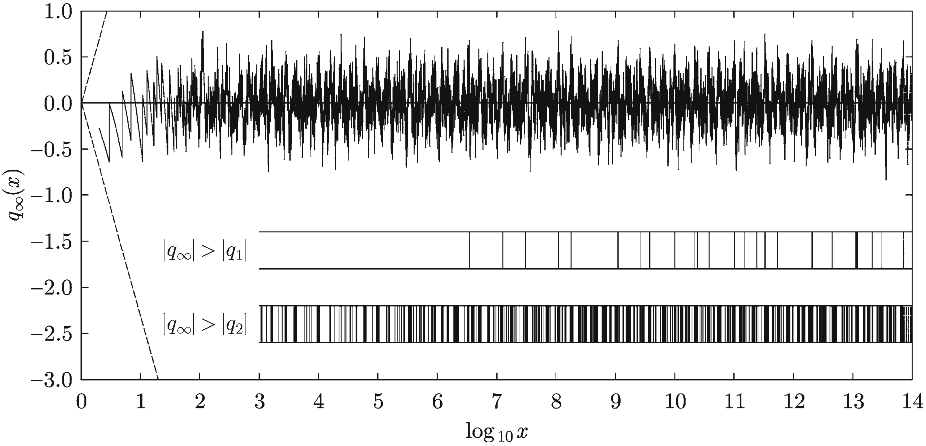

Fig. 3 $q_\infty(x)$ in the range $2 \le x \le 10^{14}$

and

$$q_1(x) - q_\infty(x) = -\frac{\mathrm{li}(\sqrt{x})/2 + O(x^{1/3}/\log x)}{\sqrt{x}/\log x} = -1 - O\left(\frac{1}{\log x}\right).$$

From the figures it appears that the nonoscillating component of $q_1(x)$ asymptotically approaches -1, and those of $q_2(x)$ and $q_\infty(x)$ asymptotically approach 0. The behavior of $q_1(x)$, $q_2(x)$, and $q_\infty(x)$ also seems to suggest the following

Conjecture 1 For all $x \ge 2$

$$|\pi(x) - \mathrm{li}(x)| < \sqrt{x},$$

$$\left|\pi(x) - \mathrm{li}(x) + \frac{1}{2}\mathrm{li}(\sqrt{x})\right| < \sqrt{x},$$

$$|\pi(x) - R(x)| < \sqrt{x}.$$

As x increases, the confinement of these three functions with respect to $\pm\sqrt{x}$ (corresponding to the dashed lines in Figs. 1, 2 and 3) rapidly grows stronger, which seems to suggest that their order is actually $o(\sqrt{x})$, and perhaps even considerably closer to Littlewood's Ω-bound than to von Koch's conditional O-bound, not to mention the Vinogradov–Korobov–Walfisz–Ford unconditional O-bound.

We now turn to the average errors of the three considered approximations. In analogy to the "normalization" used in $q_N(x)$, we define here

$$e_N(x) := \frac{\frac{1}{x-2}\int_2^x \left(\pi(u) - \sum_{n=1}^N \frac{\mu(n)}{n}\mathrm{li}(u^{1/n})\right) du}{\sqrt{x}/\log x}.$$

Figures 4, 5, and 6 show the plots of $e_1(x)$, $e_2(x)$, and $e_\infty(x)$, respectively, in the range $2 \le x \le 10^{14}$ (note that the vertical scale of Fig. 4 differs from those of Figs. 5 and 6). In the strip at the bottom of Fig. 6, subintervals of $[10^3, 10^{14}]$ with $|e_\infty(x)| > |e_2(x)|$ are painted black, showing that for x beyond billions, the average superiority of $R(x)$

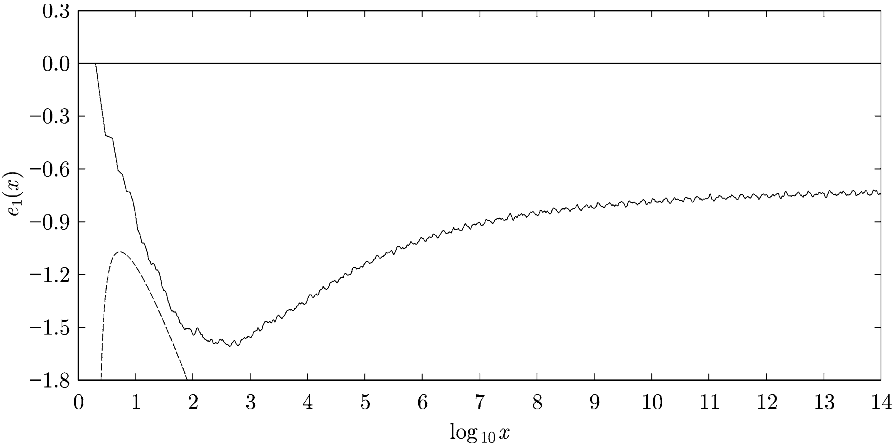

Fig. 4 $e_1(x)$ in the range $2 \le x \le 10^{14}$

over $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ ceases to be the case. The two, however, appear to retain their superiority over li(x), suggesting

Conjecture 2

$$\left|\int_2^x (\pi(u) - \mathrm{li}(u) + \frac{1}{2}\mathrm{li}(\sqrt{u}))du\right| < \left|\int_2^x (\pi(u) - \mathrm{li}(u))du\right| \quad \text{for all } x > 2.222\,,$$

$$\left|\int_2^x (\pi(u) - R(u))du\right| < \left|\int_2^x (\pi(u) - \mathrm{li}(u))du\right| \quad \text{for all } x > 4.003\,.$$

From the data it is also clear that $\int_2^x (\pi(u) - \mathrm{li}(u))du$ remains negative for $2 \le x \le 10^{14}$, while $\int_2^x (\pi(u) - \mathrm{li}(u) + \frac{1}{2}\mathrm{li}(\sqrt{u}))du$ and $\int_2^x (\pi(u) - R(u))du$ both take negative

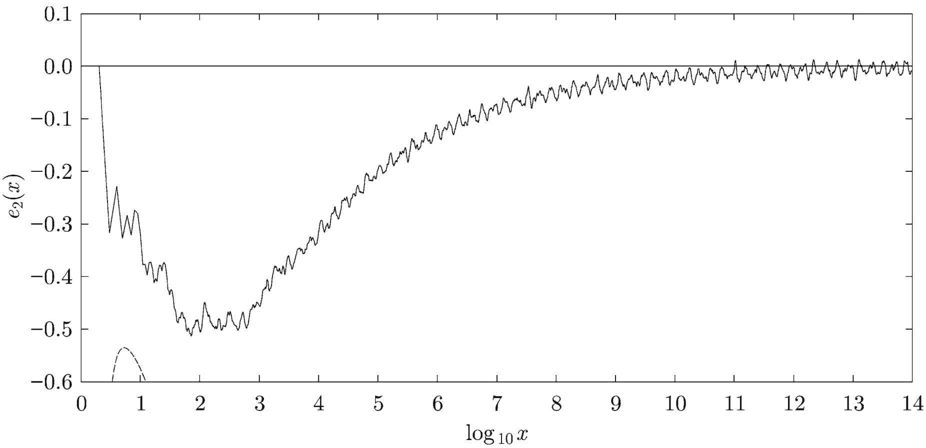

Fig. 5 $e_2(x)$ in the range $2 \le x \le 10^{14}$

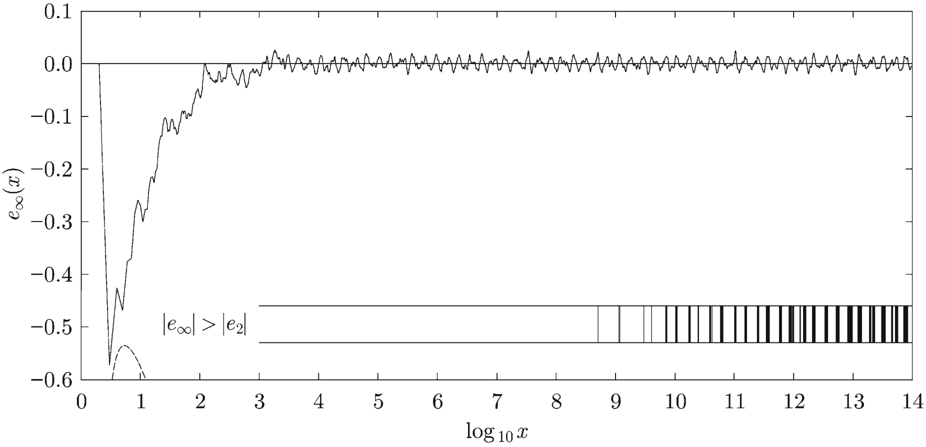

Fig. 6 $e_\infty(x)$ in the range $2 \le x \le 10^{14}$

and positive values; the former integral first becomes positive at $x = 1.020... \times 10^{11}$, and the latter at $x = 1.201... \times 10^2$.

Assuming the Riemann hypothesis, it can be shown [8] that the unbounded oscillations which contribute the factor $\Omega_\pm(\log\log\log x)$ in the integrands are smoothed out by the averaging, so that the oscillations in $e_1(x)$, $e_2(x)$, and $e_\infty(x)$ are bounded. This is a key step in Ingham's conditional proof that $\int_2^x(\pi(u) - \mathrm{li}(u))du < 0$ for sufficiently large x (see Section 1), and from the data shown in Fig. 4 it appears that this might well be the case for all $x \ge 2$. Together with the general behavior of $e_1(x)$, $e_2(x)$, and $e_\infty(x)$, this suggests

Conjecture 3 For all $x \ge 2$

$$-\frac{2}{5}x^{3/2} < \int_2^x (\pi(u) - \mathrm{li}(u))du < 0\,,$$

$$-\frac{1}{5}x^{3/2} < \int_2^x (\pi(u) - \mathrm{li}(u) + \frac{1}{2}\mathrm{li}(\sqrt{u}))du < \frac{1}{5}x^{3/2}\,,$$

$$-\frac{1}{5}x^{3/2} < \int_2^x (\pi(u) - R(u))du < \frac{1}{5}x^{3/2}\,.$$

As x increases, the confinement of the integrals with respect to the conjectured bounds ($-\frac{2}{5}x^{3/2}$ corresponds to the dashed curve in Fig. 4, and the negative branch of $\pm\frac{1}{5}x^{3/2}$ to the dashed curves in Figs. 5 and 6) rapidly grows stronger.

If the nonoscillating component of $q_1(x)$ asymptotically approaches -1 , it would seem reasonable to assume that the nonoscillating component of $e_1(x)$ asymptotically approaches $-\frac{2}{3}$. This also appears to be in agreement with the behavior of $e_1(x)$ displayed in Fig. 4.

4 Prospects for further progress

The computations presented in this paper took approximately six months to complete. The x-range covered turned out to be broad enough to provide specific examples of several theoretically established properties of the three considered approximations of $\pi(x)$, such as the values of x for which $\mathrm{li}(x)$ is closer to $\pi(x)$ than either $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ or $R(x)$, and the values of x for which the average errors of $\mathrm{li}(x) - \frac{1}{2}\mathrm{li}(\sqrt{x})$ and $R(x)$ are positive. In principle, an extension to larger x could shed additional light on the accuracy of certain tentative observations, such as the oscillations of $e_1(x)$ being asymptotically "centered" at $-\frac{2}{3}$, but for substantial improvements this extension would probably have to span far beyond the computationally accessible x-range.

One of the rigorous results obtained in this paper, and from a certain perspective also its main finding, is the bound $\Xi > 10^{14}$. It is easy to envisage that using more powerful computers and/or distributing the computations among a number of machines, this aspect of the study could be extended by several orders of magnitude. Finding an x with $\pi(x) > \mathrm{li}(x)$ in this manner, however, does not appear very likely. Namely, the method used by Lehman [11], te Riele [16], and finally Bays and Hudson [1] in imposing upper bounds for Ξ (see Section 1) can be used for generating rough sketches of $\pi(x) - \mathrm{li}(x)$ for ranges far broader than those amenable to exact computation of $\pi(x)$. Such sketches (see [1], p. 1291) suggest that Ξ could perhaps be in the vicinity of 10^{176}, 10^{179}, 10^{190}, 10^{260}, or 10^{298}, but a smaller value seems quite unlikely. A continuation of systematic computation of $\pi(x)$ and $\mathrm{li}(x)$ at all primes can thus lead to improved lower bounds for Ξ, but probably not to Ξ itself. In view of the idle time on so many computers, this may still be a goal worth pursuing.

Acknowledgements I would like to thank Dr Jan van de Lune (Hallum, The Netherlands), Prof Richard P. Brent (Oxford University), and Prof Robert C. Vaughan FRS (Pennsylvania State University) for many instructive discussions and suggestions.

Appendix A: Error analysis for li(x)

A.1 The truncation error

Truncation of the exact formula

$$\mathrm{li}(x) = \gamma + \log\log x + \sqrt{x}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}\log^n x}{n!\,2^{n-1}}\sum_{m=0}^{\lfloor (n-1)/2\rfloor}\frac{1}{2m+1}$$

at $n = N$ results in an error $E_1(N, x)$ with

$$|E_1(N,x)| < \sqrt{x}\sum_{n=N+1}^{\infty}\frac{\log^n x}{n!\,2^{n-1}}\sum_{m=0}^{\lfloor (n-1)/2\rfloor}\frac{1}{2m+1}$$

$$\overset{(1)}{\leq} \sqrt{x}\sum_{n=N+1}^{\infty}\frac{\log^n x}{(n-1)!\,2^{n-1}} \overset{(2)}{=} 2t\sqrt{x}\sum_{n=N+1}^{\infty}\frac{t^{n-1}}{(n-1)!}$$

$$
\begin{aligned}
&= 2t\sqrt{x}\sum_{n=N}^{\infty}\frac{t^n}{n!} = 2\sqrt{x}\frac{t^{N+1}}{N!}\sum_{n=0}^{\infty}\frac{t^n N!}{(N+n)!} \\
&< 2\sqrt{x}\frac{t^{N+1}}{N!}\sum_{n=0}^{\infty}\frac{t^n}{(N+1)^n} \overset{(3)}{=} 2\sqrt{x}\frac{t^{N+1}}{N!}\frac{1}{1-\frac{t}{N+1}} \\
&= \frac{\sqrt{x}\log^{N+1} x}{2^N N!}\frac{1}{1-\frac{\log x}{2(N+1)}}
\end{aligned}
$$

where in step (1) we used the fact that $\sum_{m=0}^{\lfloor (n-1)/2 \rfloor} \frac{1}{2m+1} \le n$, in step (2) we wrote $t := \frac{\log x}{2}$, and in step (3) we assumed that $\frac{t}{N+1} < 1$. With $x \le 10^{14}$ and $N = 75$, this is the case, and we get $|E_1(75, x)| < 5.84 \times 10^{-11}$.

A.2 The interpolation error

Linear interpolation of the value of $\mathrm{li}(x)$ in the interval $[x_0, x_0 + A]$ results in an error

$$
U(x_0, A, x) = \mathrm{li}(x_0) + \frac{\mathrm{li}(x_0 + A) - \mathrm{li}(x_0)}{A}(x - x_0) - \mathrm{li}(x)\,.
$$

As $\mathrm{li}(x)$ is concave, $U(x_0, A, x)$ is convex everywhere and negative for $x_0 < x < x_0 + A$, and it clearly equals 0 at the endpoints of this interval. Thus the maximum of $|U(x_0, A, x)|$ in the interval $[x, x_2]$ is located at the only zero of the first derivative of $U(x_1, x_2, x)$, which is at

$$
x = \exp\frac{A}{\mathrm{li}(x_0 + A) - \mathrm{li}(x_0)}
$$

and hence

$$
|U(x_0, A, x)| \le -U\left(x_0, A, \exp\frac{A}{\mathrm{li}(x_0 + A) - \mathrm{li}(x_0)}\right)\,.
$$

As x increases, the second derivative of $\mathrm{li}(x)$ approaches 0 monotonically, so that for a fixed A, the maximal error in the linear interpolation of $\mathrm{li}(x)$ decreases. Since in this paper we used $A_1 = 2310$ for $x > 10^{10}$, $A_2 = 30030$ for $x > 2 \times 10^{12}$, and $A_3 = 9699690$ for $x > 2 \times 10^{13}$, we obtain

$$
\begin{aligned}
|U(x_0, A_1, x)| &\le -U\left(10^{10}, A_1, \exp\frac{A_1}{\mathrm{li}(10^{10} + A_1) - \mathrm{li}(10^{10})}\right) \\
&< 1.3 \times 10^{-7} \qquad \text{for } 10^{10} < x \le 2 \times 10^{12}, \\
|U(x_0, A_2, x)| &\le -U\left(2 \times 10^{12}, A_2, \exp\frac{A_2}{\mathrm{li}(2 \times 10^{12} + A_2) - \mathrm{li}(2 \times 10^{12})}\right) \\
&< 7.1 \times 10^{-8} \qquad \text{for } 2 \times 10^{12} < x \le 2 \times 10^{13}, \\
|U(x_0, A_3, x)| &\le -U\left(2 \times 10^{13}, A_3, \exp\frac{A_3}{\mathrm{li}(2 \times 10^{13} + A_3) - \mathrm{li}(2 \times 10^{13})}\right) \\
&< 6.3 \times 10^{-4} \qquad \text{for } 2 \times 10^{13} < x \le 10^{14}.
\end{aligned}
$$

A.3 The round-off error

In this section, we use an underscore to indicate that the finite-precision value obtained and/or stored by the computer is being considered. The absence of an underscore will thus always mean that we are referring to the exact value. Thus if a real number x is stored in a variable $\underline{x}$ with the precision of K digits, we have

$$(1-10^{-K+1})x < \underline{x} < (1+10^{-K+1})x\,,$$

as well as

$$(1-10^{-K+1})\underline{x} < x < (1+10^{-K+1})\underline{x}\,.$$

Since 80-bit reals have a precision of 19 digits, we may take $K = 19$ for all the non-integer variables used in the computations presented here. As described in Section 2.3, the coefficients a_n in the sum

$$\sqrt{x}\sum_{n=1}^{75} a_n \log^n x$$

were precomputed and stored with 19-digit precision. Thus

$$\left(1-10^{-18}\right)|a_n| < \underline{|a_n|} < \left(1+10^{-18}\right)|a_n|\ .$$

For a term $\log^n x$, we have

$$\left(1-10^{-18}\right)^{2n}\left(\log\left(1-10^{-18}\right)x\right)^n < \underline{\left(\underline{\log \underline{x}}\right)^n}$$
$$< \left(1+10^{-18}\right)^{2n}\left(\log\left(1+10^{-18}\right)x\right)^n\ .$$

For the left-hand side of this inequality we have

$$\begin{aligned}
&\left(1-10^{-18}\right)^{2n}\left(\log\left(1-10^{-18}\right)x\right)^n \\
&\quad > \left(1-2n\times 10^{-18}\right)(\log x - 2\times 10^{-18})^n \\
&\quad > \left(1-2n\times 10^{-18}\right)(1-3\times 10^{-18})^n \log^n x \\
&\quad > \left(1-2n\times 10^{-18}\right)(1-3n\times 10^{-18})\log^n x \\
&\quad > \left(1-5n\times 10^{-18}\right)\log^n x \ge \left(1-3.75\times 10^{-16}\right)\log^n x\,.
\end{aligned}$$

A similar result, with subtractions replaced by additions, follows for the right-hand side of the same inequality. Therefore

$$\left|\underline{\underline{a_n}\,\underline{\left(\underline{\log\underline{x}}\right)^n}} - a_n\log^n x\right| < 3.77\times 10^{-16}\,|a_n|\log^n x\,,$$

$$\left|\underline{\sum_{n=1}^{75}\underline{\underline{a_n}\,\underline{\left(\underline{\log\underline{x}}\right)^n}}} - \sum_{n=1}^{75} a_n\log^n x\right| < 3.77\times 10^{-16}\sum_{n=1}^{75}|a_n|\log^n x\,.$$

Also

$$\left|\underline{\sqrt{\underline{x}}} - \sqrt{x}\right| < 2 \times 10^{-18}\sqrt{x}$$

so that

$$\left| \underline{\underline{\sqrt{\underline{x}}} \sum_{n=1}^{75} \underline{\underline{a_n} \, \underline{\underline{\left(\underline{\log \underline{x}}\right)^n}}}} - \sqrt{x}\sum_{n=1}^{75} a_n \log^n x \right|$$

$$< 3.8 \times 10^{-16}\sqrt{x}\sum_{n=1}^{75} |a_n| \log^n x$$

$$\leq 3.8 \times 10^{-16}\sqrt{x}\sum_{n=1}^{75} |a_n| \log^n 10^{14} < 1.54 \times 10^{-8}\sqrt{x}\,.$$

Appendix B: Error analysis for $R(x)$

B.1 The truncation error

Truncation of the exact formula

$$R(x) = 1 + \sum_{n=1}^{\infty} \frac{\log^n x}{n!\, n\, \zeta(n+1)}$$

at $n = N$ results in an error $E_2(N, x) > 0$ with

$$\begin{aligned} E_2(N, x) &= \sum_{n=N+1}^{\infty} \frac{\log^n x}{n!\, n\, \zeta(n+1)} \overset{(1)}{<} \sum_{n=N+1}^{\infty} \frac{\log^n x}{n!\, n} \\ &= \sum_{n=N+1}^{\infty} \frac{\log^n x}{n^2 (n-1)!} < \frac{1}{(N+1)^2} \sum_{n=N+1}^{\infty} \frac{\log^n x}{(n-1)!} \\ &= \frac{1}{(N+1)^2} \sum_{n=N}^{\infty} \frac{\log^{n+1} x}{n!} = \frac{\log^{N+1} x}{N!\,(N+1)^2} \sum_{n=0}^{\infty} \frac{\log^n x\, N!}{(N+n)!} \\ &< \frac{\log^{N+1} x}{N!\,(N+1)^2} \sum_{n=0}^{\infty} \frac{\log^n x}{(N+1)^n} \overset{(2)}{=} \frac{\log^{N+1} x}{N!\,(N+1)^2} \frac{1}{1 - \frac{\log x}{N+1}} \end{aligned}$$

where in step (1) we used the fact that $\zeta(n+1) > 1$, and in step (2) we assumed that $\frac{\log x}{N+1} < 1$. With $x \leq 10^{14}$ and $N = 102$, this is the case, and we get $E_2(102, x) < 3.27 \times 10^{-11}$.

B.2 The round-off error

As described in Section 2.4, the coefficients b_n in the sum

$$\sum_{n=1}^{102} b_n \log^n x, \qquad \text{where } b_n = \frac{1}{n!\, n\, \zeta(n+1)}$$

were precomputed and stored with 19-digit precision. Proceeding similarly as in Section A.3 , we obtain

$$\left| \underline{\underline{\sum_{n=1}^{102} \underline{b_n} \left(\underline{\log \underline{x}}\right)^n}} - \sum_{n=1}^{102} b_n \log^n x \right| < 3.77 \times 10^{-16} \sum_{n=1}^{102} b_n \log^n x$$
$$< 3.77 \times 10^{-16} \sum_{n=1}^{102} b_n \log^n 10^{14} < 1.21 \times 10^{-3} .$$

Appendix C: Error analysis for $\int_2^x R(u)du$

C.1 The truncation error

Denote

$$R_N(x) := 1 + \sum_{n=1}^{N} \frac{\log^n x}{n!\, n\, \zeta(n+1)} \quad .$$

Then

$$\int_2^x R(u)du = \int_2^x R_N(u)du + \int_2^x (R(u) - R_N(u))du = \int_2^x R_N(u)du + E_3(N, x)\,,$$

where $E_3(N, x) > 0$ and

$$E_3(N, x) \le \int_2^x |R(u) - R_N(u)|\, du \le (x-2) \max_{2\le u\le x} |R(u) - R_N(u)|$$
$$= (x-2)\, E_2(N, x) < x\, E_2(N, x)\,.$$

From $E_2(102, x) < 3.27 \times 10^{-11}$ it then follows that $E_3(102, x) < 3.27 \times 10^{-11} x$.

C.2 The round-off error.

As described in Section 2.5, the coefficients d_n in the sum

$$\sum_{n=1}^{127} d_n \sum_{m=0}^{n} \frac{(-1)^{n-m} \log^m x}{m!}, \qquad \text{where } d_n = \frac{1}{n\, \zeta(n+1)}$$

were precomputed and stored with 19-digit precision, and the coefficients $g_{m,n} = (-1)^{n-m}/m!$ were computed to the same precision. Proceeding similarly as in Section A.3, we obtain

$$\left| \underline{\underline{\underline{g_{m,n}} \left(\underline{\underline{\log \underline{x}}}\right)^m}} - g_{m,n} \log^m x \right| < 3.77 \times 10^{-16} \frac{\log^m x}{m!} \,,$$

$$\left| \underline{\underline{\sum_{m=0}^{n} \underline{g_{m,n}} \left(\underline{\underline{\log \underline{x}}}\right)^m}} - \sum_{m=0}^{n} g_{m,n} \log^m x \right| < 3.77 \times 10^{-16} \sum_{m=0}^{n} \frac{\log^m x}{m!}$$

$$< 3.77 \times 10^{-16} \sum_{m=0}^{\infty} \frac{\log^m x}{m!} = 3.77 \times 10^{-16} x \,,$$

$$\left| \underline{\underline{\underline{d_n} \sum_{m=0}^{n} \underline{g_{m,n}} \left(\underline{\underline{\log \underline{x}}}\right)^m}} - d_n \sum_{m=0}^{n} g_{m,n} \log^m x \right| < 3.8 \times 10^{-16} d_n x \,,$$

$$\left| \underline{\underline{\underline{x} \sum_{n=1}^{127} \underline{d_n} \sum_{m=0}^{n} \underline{g_{m,n}} \left(\underline{\underline{\log \underline{x}}}\right)^m}} - x \sum_{n=1}^{127} d_n \sum_{m=0}^{n} g_{m,n} \log^m x \right| < 3.8 \times 10^{-16} x^2 \sum_{n=1}^{127} d_n$$

$$< 1.9 \times 10^{-15} x^2 \,.$$

References

1. Bays, C., Hudson, R.: A new bound for the smallest x with $\pi(x) > \mathrm{li}(x)$. Math. Comp. **69**, 1285-1296 (2000)
2. Berndt, B.C.: Ramanujan's Notebooks, Part IV. pp. 126–131. Springer, New York (1994)
3. Brent, R.P.: Irregularities in the distribution of primes and twin primes. Math. Comp. **29**, 43–56 (1975)
4. de la Vallée Poussin, C.J.: Sur la fonction $\zeta(s)$ de Riemann et le nombre des nombres premiers inférieurs à une limite donnée. Mem. Cour. Acad. Roy. Belg. **59**, 1 (1899)
5. Ford, K.: Vinogradov's integral and bounds for the Riemann zeta function. Proc. London Math. Soc. **85**, 565–633 (2002)
6. Gauss, C.F.: Werke, Vol. II. Königliche Gesellschaft der Wissenschaften zu Göttingen, pp. 444–447 (1863)
7. Gram, J.P.: Undersøgelser angående Mængden af Primtal under en given Grænse. Kong. Dansk. Videnskab. Selsk. Skr. (VI) **2**, 183–308 (1884)
8. Ingham, A.E.: The distribution of prime numbers, pp. 105–106. Cambridge University Press, New York (1932)
9. Korobov, N.M.: Estimates of trigonometric sums and their applications. Usp. Mat. Nauk. **13**, 185–192 (1958) (in Russian)
10. Legendre, A.M.: Essai sur la théorie des nombres, 2ème dition, p.394. Courcier, Paris (1808)
11. Lehman, R.S.: On the difference $\pi(x) - \mathrm{li}(x)$. Acta Arith. **11**, 397–410 (1966)
12. Littlewood, J.E.: Sur la distribution des nombres premiers. C. R. Acad. Sci. Paris **158**, 1869–1872 (1914)
13. Riemann, B.: Ueber die Anzahl der Primzahlen unter einer gegebenen Grösse. Monatsber. Preuss. Akad. Wiss. **1859** 671–680 (1859)
14. Rosser, J.B., Schoenfeld, L.: Approximate formulas for some functions of prime numbers. Illinois J. Math. **6**, 64–94 (1962)
15. Skewes, S.: On the difference $\pi(x) - \mathrm{li}(x)$. II. Proc. London Math. Soc. (3) **5**, 48–70 (1955)

16. te Riele, H.J.J.: On the sign of the difference $\pi(x) - \mathrm{li}(x)$. Math. Comp. **48**, 323–328 (1987)
17. Vinogradov, I.M.: A new estimate for $\zeta(1 + it)$ [in Russian]. Izv. Akad. Nauk SSSR, Ser. Mat. **22**, 161–164 (1958)
18. von Koch, H.: Sur la distribution des nombres premiers. Acta Math. **24**, 159–182 (1901)
19. von Mangoldt, H.: Zu Riemann's Abhandlung 'Ueber die Anzahl der Primzahlen unter einer gegebenen Grösse'. J. Reine Angew. Math. **114**, 255–305 (1895)
20. Walfisz, A.: Weylsche Exponentialsummen in der neueren Zahlentheorie, pp. 175-188. VEB Deutscher Verlag, Berlin (1963)