Ramanujan J (2018) 45:227–251
https://doi.org/10.1007/s11139-016-9839-4

Explicit estimates of some functions over primes

Pierre Dusart[1,2]

Received: 18 March 2016 / Accepted: 10 August 2016 / Published online: 27 October 2016

Abstract New results have been found about the Riemann hypothesis. In particular, we noticed an extension of zero-free region and a more accurate location of zeros in the critical strip. The Riemann hypothesis implies results about the distribution of prime numbers. We get better effective estimates of common number theoretical functions which are closely linked to ζ zeros like $\psi(x)$, $\vartheta(x)$, $\pi(x)$, or the kth prime number p_k.

Keywords Number theory · Arithmetic functions · Chebyshev's functions · Estimates of prime numbers

Mathematics Subject Classification Primary 11N56 · Secondary 11A25, 11N05

1 Introduction

In many applications, it is useful to have explicit error bounds in the prime number theorem. Rosser [33,34] developed an analytic method which combines a numerical verification of the Riemann hypothesis with a zero-free region and derived explicit estimates for some number theoretical functions. The aim of this paper is to find sharper bounds for the Chebyshev's functions $\psi(x)$, the logarithm of the least common multiple of all integers not exceeding x, and $\vartheta(x)$, the product of all primes not exceeding x:

✉ Pierre Dusart
pierre.dusart@unilim.fr

1 XLIM - UMR CNRS 7252, Faculté des Sciences et Techniques, Université de Limoges, 87060 Limoges, France

2 Present Address: Département de Mathématiques, 123 avenue Albert Thomas, 87060 Limoges, France

$$\vartheta(x) = \sum_{p \leqslant x} \ln p, \quad \psi(x) = \sum_{\substack{p,\alpha \\ p^\alpha \leqslant x}} \ln p.$$

The prime number theorem could be written as follows:

$$\psi(x) = x + o(x), \quad x \to +\infty.$$

An equivalent formulation of the above theorem should be: for all $\varepsilon > 0$, there exists $x_0 = x_0(\varepsilon)$ such that

$$|\psi(x) - x| < \varepsilon x \quad \text{for } x \geqslant x_0$$

or

$$|\vartheta(x) - x| < \varepsilon x \quad \text{for } x \geqslant x_0.$$

This article is an updated version of some known results: the most important works on effective results have been shown by Rosser and Schoenfeld [35,36,38], Pereira [6], Robin [31], Robin and Massias [19], Dusart [8], Faber and Kadiri [12], Trudgian [40].

The proofs for estimates of $\psi(x)$ in [12,36] are based on the verification of Riemann hypothesis to a given height and an explicit zero-free region [16,20] for ζ whose form is essentially the classical one of de la Vallée Poussin. Rosser and Schoenfeld [36] have shown that the first 3 502 500 zeros of $\zeta(s)$ lie on the vertical with real part 1/2. Van de Lune et al. [41] have shown that the first 1 500 000 000 zeros are on this critical line. Wedeniwski [42] and then Gourdon [13] managed to compute zeros in a parallel way and have proved that the Riemann hypothesis is true at least for first 10^{13} nontrivial zeros. Ramaré [28] and Kadiri [17] have introduced an explicit density estimate which improves the location of the zeros in the critical strip.

This will improve bounds [10] for $\psi(x)$ and $\vartheta(x)$ for moderate values of x. Here and everywhere $f(x) = \mathcal{O}^*(g(x))$ means $|f(x)| \leqslant g(x)$. We will prove the following results (Theorems 3.3 and 4.2, respectively):

$$\psi(x) = x + \mathcal{O}^*\left(59.2x/\ln^4 x\right) \quad \text{for } x \geqslant 2,$$
$$\vartheta(x) = x + \mathcal{O}^*\left(151.3x/\ln^4 x\right) \quad \text{for } x \geqslant 2.$$

We apply the previous result on p_k, the kth prime. Denote $\ln\ln x$ by $\ln_2 x$. The asymptotic expansion of p_k is well known; Cesaro [4] then Cipolla [5] expressed it in 1902:

$$p_k = k\left\{\ln k + \ln_2 k - 1 + \frac{\ln_2 k - 2}{\ln k} - \frac{\ln_2^2 k - 6\ln_2 k + 11}{2\ln^2 k} + O\left(\left(\frac{\ln_2 k}{\ln k}\right)^3\right)\right\}.$$

A more precise work about this can be found in [32,37]. The results on p_k are (Lemma 5.14 and Proposition 5.16):

$$p_k = k\left(\ln k + \ln_2 k - 1 + \frac{\ln_2 k - 2}{\ln k} + \mathcal{O}^*\left(0.1/\ln k\right)\right) \quad \text{for } k \geqslant 178\,974.$$

We use the above results to prove (Corollary 5.5) that, for $x \geqslant 468\,991\,632$, the interval

$$\left[x, x + x/(5000\ln^2 x)\right]$$

contains at least one prime. Denote the number of primes not greater than x by $\pi(x)$. We show that (Corollary 5.2)

$$\frac{x}{\ln x}\left(1 + \frac{1}{\ln x}\right) \underset{x\geqslant 599}{\leqslant} \pi(x) \underset{x>1}{\leqslant} \frac{x}{\ln x}\left(1 + \frac{1.2762}{\ln x}\right).$$

A more precise result on $\pi(x)$ is also shown:

$$\pi(x) = \frac{x}{\ln x}\left(1 + \frac{1}{\ln x} + \frac{2}{\ln^2 x} + \mathcal{O}^*\left(0.53816/\ln^2 x\right)\right) \quad \text{for } x \geqslant 11\,813.$$

In this paper, we give also some new effective estimates for the difference between ψ and ϑ (Corollary 4.5), for $\vartheta(p_k)$ (Propositions 5.11 and 5.12), for sums over primes (Theorem 5.6 for $\sum_p \frac{1}{p}$, Theorem 5.7 for $\sum_p \frac{\ln p}{p}$), and for products over primes (Theorem 5.9).

2 Estimates of prime-related functions using the Riemann zeta theory

2.1 Relation between ψ and ζ

The Riemann zeta function $\zeta(s)$ is a function of a complex variable s and can also be defined for $\Re(s) > 1$ by the integral

$$\zeta(s) = \frac{1}{\Gamma(s)}\int_0^{+\infty} \frac{x^{s-1}}{e^x - 1}\mathrm{d}x.$$

Zeros of ζ come in (at least) two different types. The so-called "trivial zeros" occur at all negative even integers $s = -2, -4, -6, \ldots$, and "nontrivial zeros" at certain $s = \sigma + it$ for s in the critical strip $0 < \sigma < 1$.

A classic explicit formula that relates prime numbers to nontrivial zeros of ζ is given by [11, §3.8, p. 66]:

$$\psi(x) = x - \sum_\rho \frac{x^\rho}{\rho} - \ln 2\pi - \frac{1}{2}\ln(1 - x^{-2}), \tag{2.1}$$

when $x > 1$ is not a prime power. At the jumps $x = p^n$, the value of ψ is defined, as usual, to be the halfway between the new and the old values $\psi(x) = \frac{1}{2}(\psi(x-\varepsilon) + \psi(x+\varepsilon))$.

2.2 Zeros of the Riemann zeta function

2.2.1 Location of zeros

As the zeros of ζ are closely related to sums over primes by (2.1), the Riemann zeta function's zeros location is of great importance in number theory to estimate $\psi(x)$ and $\vartheta(x)$. In 1859, Riemann asserts that the nontrivial zeros of the Riemann zeta function have real part $\sigma = \Re(s) = 1/2$, a line called the critical line. This conjecture is known as the Riemann hypothesis.

The Riemann hypothesis was computationally tested and found to be true up to a height, denoted H for the rest of the paper, covering zeros $\sigma + it$ in the region $0 < t < H$. The history of Riemann hypothesis verification starts in 1903 by Gram [14], who computes the first fifteen zeros. The higher result is from Gourdon [13] in 2004 who announced to have used the Odlyzko and Schönhage's method to verify that the first ten trillion (10^{13}) nontrivial zeros of the ζ function lie on the critical line. The last computation implies that the Riemann hypothesis is true at least for $H_2 = 2\,445\,999\,556\,030$ but remains not really published. The authors of [12] mentioned the Platt's result which used another method to verify the hypothesis up to $H_1 = 30\,610\,046\,000$. We use the H_2 value in order to achieve comparable results with [12].

Classically the Riemann hypothesis testing methods do not compute exactly the zeros of ζ, but to go faster, they merely check that the number of expected zeros by interval is correct. Nevertheless if you have to compute sum over nontrivial zeros like (2.1), you must know zero ordinates with accuracy for computing at least partially this type of sum.

Odlyzko [23] computes the first 2 001 052 zeros of the Riemann zeta function on the critical line, accurate to within 4×10^{-9}. Hence one can compute sums over zeros $\varrho = 1/2 + i\gamma$ based on this list of zeros. It yields,

Lemma 2.1 *Let* $T_0 = 1\,132\,490.982$. *Then* $\displaystyle\sum_{0<\gamma\le T_0} \frac{1}{\gamma} \le 11.6377324.$

2.2.2 Number of zeros

If you have to compute sum over zeros like (2.1), you need also to introduce the number of nontrivial zeros up to a fixed height. Let $T \ge 2$ and $N(T)$ be the number of nontrivial zeros $\varrho = \beta + i\gamma$ in the region $0 \le \gamma \le T$ and $0 \le \beta \le 1$. In 1941, Rosser [34, Theorem 19] proved

Theorem 2.2 (Rosser) *Let* $T \ge 2$,

$$F(T) = \frac{T}{2\pi}\ln\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8}, \quad R(T) = a_1 \ln T + a_2 \ln\ln T + a_3,$$

and $a_1 = 0.137$, $a_2 = 0.443$, $a_3 = 1.588$. *Then*

$$|N(T) - F(T)| \leq R(T).$$

The upper bound $R(T)$ and

$$q(y) = R'(y)/\ln(y/(2\pi)) = \frac{a_1 \ln y + a_2}{y \ln y \ln(y/(2\pi))} \tag{2.2}$$

are used thereafter. A recent work [39] of Trudgian updated these values, but with a low impact on our computations. In [17], Kadiri detailed the number $N(T)$ by cutting the critical strip. Let $N(\sigma_0, T)$ is the number of nontrivial zeros of zeta in the region $\sigma_0 \leq \beta \leq 1$ and $0 \leq \gamma \leq T$. She proved explicit upper bounds for $N(\sigma_0, T)$ and the result was improved by Ramaré [28, Theorem 1.1] in some cases (a factor 1/2 is required for the consistency of the two author's definitions).

Theorem 2.3 (Ramaré) *Let* $\sigma_0 \geqslant 0.52$. *Then for* $T \geq 2000$,

$$N(\sigma_0, T) \leq \tilde{F}(\sigma_0, T) = T \ln\left(1 + \frac{9.8}{2T}(3T)^{8(1-\sigma_0)/3} \ln^{5-2\sigma_0}(T)\right) + \frac{103}{2}(\ln T)^2$$

To be compliant with Kadiri's work we choose $c_2 = c_3 = 0$ and $c_1 = \tilde{F}(\sigma_0, H)/H$ to have for $\sigma_0 > 5/8$,

$$N(\sigma_0, T) \leqslant c_1 T \quad \text{for all } T \geqslant H.$$

2.2.3 Zero-free region

We make use of classical type (de la Vallée Poussin type) zero-free region. Taking over the work of Kadiri [16], the better result of this type is due to Mossinghoff and Trudgian [20, Theorem 1], with the following

Theorem 2.4 (Mossinghoff and Trudgian) *Let* $R = 5.573412$. *Then there are no zeros of* $\zeta(s)$ *in the region*

$$\Re(s) \geq 1 - \frac{1}{R \ln |\Im(s)|} \text{ and } |\Im(s)| \geq 2.$$

3 Bound for ψ

We use the Faber and Kadiri's method [12] who introduce an explicit formula for a smooth form of $\psi(x)$. Let us introduce their notations:

- $H > 0$ is such that if $\zeta(\beta + i\gamma) = 0$ and $0 < \gamma < H$, then $\beta = 1/2$,
- $T_0 > 2\pi$ is such that $\sum_{0<\gamma<T_0} \gamma^{-1}$ can be directly computed,
- T_1 is a parameter satisfying $T_0 < T_1 < H$,
- R is a constant so that $\zeta(\sigma + it)$ does not vanish in the region (3.1)
  $\sigma \geq 1 - \frac{1}{R \ln |t|}$ and $|t| \geq 2$,
- σ_0 is a parameter satisfying $5/8 \leq \sigma_0 < 1$,
- $c_1 > 0$ depend on σ_0 so that $N(\sigma_0, T) \leq c_1 T$ for all $T \geq H$.

Like Rosser and Schoenfeld, the authors used the following integral related to the modified Bessel function of second kind

$$K_\nu(z, w) = \frac{1}{2} \int_w^\infty t^{\nu-1} \exp\left(-\frac{z}{2}(t + 1/t)\right) \mathrm{d}t,$$

to explicit more easily the integrals involved in their method and introduced

$$J_m(Y) = \frac{z}{2m} K_1\left(z, \frac{2m}{z} \ln Y\right)$$

with $z = 2\sqrt{\frac{m \ln x}{R}}$. Let

$$M(a, b, m) = \frac{(2m+1)!}{m!} \int_0^1 |P_m(1-2u)| \, ((b-a)u + a)^{m+1} \, du, \tag{3.2}$$

where P_m is the m^{th} Legendre polynomial, defined by

$$P_m(x) = \sum_{k=0}^{m} \binom{m}{k}^2 \left(\frac{x+1}{2}\right)^k \left(\frac{x-1}{2}\right)^{m-k}.$$

We rewrite the main theorem of Faber and Kadiri [12]:

Theorem 3.1 *Let $m \in \mathbb{N}$, $m \geq 2$, $\delta > 0$, and the pair (a, b) takes values $(1, 1+\delta)$ or $(1-\delta, 1)$. Let $H, T_0, T_1, R, \sigma_0, c_1$ satisfy (3.1). Let b_0 be a positive constant. Then for all $x \geqslant e^{b_0}$,*

$$\begin{aligned}\frac{|\psi(x) - x|}{x} \leqslant \max_{(a,b)} \Bigg\{ & \frac{2M(a, b, m)}{\delta^m} \left(B_5 + B_3(e^{-(1-\sigma_0)} + e^{-\sigma_0 b_0}) + B_4 e^{-(1-\frac{1}{R \ln H} b_0)}\right) \\ & + 2\left(M(a, b, 0) B_1 + \frac{M(a, b, m)}{\delta^m} B_2\right) e^{-b_0/2} + \frac{\delta}{2} \\ & + \ln(2\pi) e^{-b_0} + \frac{M(a, b, 0)}{2} e^{-3b_0} \Bigg\}\end{aligned} \tag{3.3}$$

where $M(a, b, m)$ is given by (3.2), and the B_i's are defined, respectively, in (3.4), (3.5), (3.6), (3.7), and (3.8).

$$B_1(T_0, T_1) = \sum_{0<\gamma\le T_0} \frac{1}{\gamma} + \left(\frac{1}{2\pi} + q(T_0)\right)\left(\ln(T_1/T_0)\ \ln(\sqrt{T_1 T_0}/2\pi)\right) + \frac{2R(T_0)}{T_0}, \tag{3.4}$$

$$B_2(m, T_1, H) = \left(\frac{1}{2\pi} + q(T_1)\right)\left(\frac{1 + m\ln(T_1/2\pi)}{m^2 T_1^m} - \frac{1 + m\ln(H/2\pi)}{m^2 H^m}\right) + \frac{2R(T_1)}{T_1^{m+1}}, \tag{3.5}$$

$$B_3(m, H) = \left(\frac{1}{2\pi} + q(H)\right)\frac{1 + m\ln(H/2\pi)}{m^2 H^m} + \frac{2R(H)}{H^{m+1}}. \tag{3.6}$$

$$B_4(m, H, \sigma_0) = c_1\left(1 + \frac{1}{m}\right)\frac{1}{H^m}. \tag{3.7}$$

$$B_5(x, m, \sigma_0, H) = \begin{cases} c_1\left(1 + \frac{R}{2\ln x}\frac{(\ln H)^2}{\left(\frac{mR}{\ln x}\right)(\ln H)^2 - 1}\right)\frac{x^{-\frac{1}{R\ln H}}}{H^m} & \text{if } b_0 < mR(\ln H)^2 \\ c_1\frac{x^{-\frac{1}{R\ln H}}}{H^m} + c_1 J_m(H) & \text{in other case.}\end{cases} \tag{3.8}$$

Proof From [12], we use the expression (2.19) of Lemma 2.4. We delete the s_0 term which is already included in the s_1 term. Next, we respectively substitute $s_1,\ s_2,\ s_3,\ s_4$ by $B_1,\ B_2,\ B_3,\ B_4$ (2.22–2.25 of [12]). The s_5 term is bounded with (2.27) and can be bounded by (2.30) if $w > 1$ (i.e., $\ln x < mR\ln^2 H$). The modified Bessel function $K_1(z, w)$ can be computed if $0 \leqslant w \le 1$ using (2.30) and (2.35) of [36]. Next, for the two choices of the (a, b) pair, it follows by (3.3) that $\left|a - 1 + (b-a)\int_0^1 g(u)du\right| = \delta/2$. □

Proposition 3.2 *Let $b_0 \ge 0$ be a fixed positive constant. Let $x \ge e^{b_0}$. Then there exists $\varepsilon_0 > 0$ such that $|\psi(x) - x| \le \varepsilon_0 x$, where ε_0 is given explicitly by (3.3) and is computed in Table 1 for $H_2 = 2\,445\,999\,556\,030$.*

Theorem 3.3 *We have*

$$|\psi(x) - x| < \eta_k \frac{x}{\ln^k x} \quad \textit{for } x \geqslant 2$$

with

k	0	1	2	3	4
η_k	0.77	0.85	1.66	8.16	59.18

Table 1 Values of $\varepsilon(x)$ for ψ

b	σ_0	m	δ	T_1	ε
20	0.86	5	1.595 $E-5$	1 132 492	1.067 $E-3$
21	0.86	5	1.468 $E-5$	1 132 492	6.498 $E-4$
22	0.86	4	1.282 $E-5$	1 132 492	3.968 $E-4$
23	0.86	4	1.160 $E-5$	1 132 492	2.431 $E-4$
24	0.85	3	9.778 $E-6$	1 132 492	1.496 $E-4$
25	0.86	3	8.629 $E-6$	1 132 492	9.250 $E-5$
30	0.86	2	2.554 $E-6$	1 882 244	9.647 $E-6$
35	0.86	2	2.458 $E-7$	19 612 863	1.078 $E-6$
40	0.87	2	2.756 $E-8$	161 338 534	1.161 $E-7$
45	0.87	3	2.721 $E-9$	2 228 096 512	1.225 $E-8$
50	0.88	5	2.572 $E-10$	37 754 757 543	1.275 $E-9$
55	0.89	15	4.374 $E-11$	568 871 547 031	1.388 $E-10$
60	0.90	23	3.812 $E-11$	973 812 914 637	2.978 $E-11$
65	0.90	23	3.751 $E-11$	989 645 080 596	2.039 $E-11$
70	0.90	22	3.697 $E-11$	963 148 272 814	1.940 $E-11$
75	0.90	22	3.658 $E-11$	973 564 683 528	1.913 $E-11$
80	0.91	22	3.621 $E-11$	987 265 077 216	1.893 $E-11$
85	0.91	22	3.573 $E-11$	996 465 239 887	1.868 $E-11$
90	0.91	22	3.533 $E-11$	1 007 775 601 523	1.847 $E-11$
95	0.91	21	3.492 $E-11$	976 821 063 390	1.830 $E-11$
100	0.91	21	3.464 $E-11$	987 265 077 216	1.815 $E-11$
200	0.94	18	2.951 $E-11$	1 003 417 649 160	1.557 $E-11$
300	0.95	16	2.642 $E-11$	1 006 421 703 556	1.404 $E-11$
400	0.96	14	2.403 $E-11$	980 285 487 059	1.288 $E-11$
500	0.96	13	2.255 $E-11$	977 429 125 922	1.215 $E-11$
600	0.97	12	2.058 $E-11$	997 132 955 137	1.115 $E-11$
700	0.97	11	1.904 $E-11$	998 061 945 822	1.039 $E-11$
800	0.97	11	1.801 $E-11$	1 019 509 030 546	9.826 $E-12$
900	0.97	10	1.688 $E-11$	1 019 509 030 546	9.281 $E-12$
1000	0.97	9	1.574 $E-11$	1 012 519 261 279	8.743 $E-12$
1500	0.98	5	8.852 $E-12$	1 019 509 030 546	5.311 $E-12$
2000	0.98	2	3.381 $E-12$	1 364 832 983 117	2.536 $E-12$
2500	0.98	2	1.193 $E-12$	2 445 999 556 029	8.941 $E-13$
3000	0.98	2	4.209 $E-13$	2 445 999 556 030	3.156 $E-13$
3500	0.98	2	1.487 $E-13$	2 445 999 556 030	1.116 $E-13$
4000	0.98	2	5.262 $E-14$	2 445 999 556 030	3.946 $E-14$
4500	0.99	2	1.699 $E-14$	2 445 999 556 030	1.274 $E-14$
5000	0.99	2	5.274 $E-15$	2 445 999 556 030	3.956 $E-15$
6000	0.99	2	6.524 $E-16$	2 445 999 556 030	4.893 $E-16$
7000	0.99	2	8.524 $E-17$	2 445 999 556 030	6.393 $E-17$

Table 1 continued

b	σ_0	m	δ	T_1	ε
8000	0.99	2	1.196 $E-17$	2 445 999 556 030	8.969 $E-18$
9000	0.99	2	3.236 $E-18$	2 445 999 556 030	2.427 $E-18$
10000	0.99	3	1.222 $E-17$	2 445 999 556 030	8.144 $E-18$
13900	0.99	2	3.144 $E-20$	2 445 999 556 030	2.358 $E-20$

Proof We compute the upper bound η_k step by step up to the end of Table 1. For example, if ε_{b_i} is the value obtained for $x = e^{b_i}$ we need to have $\eta_k \geqslant \varepsilon_{b_i} \cdot b_{i+1}^k$ for $e^{b_i} \leqslant x \leqslant e^{b_{i+1}}$ (we need to compute some intermediate values of $\varepsilon(x)$ between e^{1500} and e^{2000}). For large values outside the table, we use Theorem 1.1 of [10]. We conclude by direct inspection for small values of x. The maximum of $|\psi(x) - x|\frac{\ln^k x}{x}$ is

- for $x \geqslant 2$, $\eta_0 < (3 - \psi(3^-))/3 \approx 0.7689509398$,
- for $x \geqslant 2$, $\eta_1 < (3 - \psi(3^-))/3 \cdot \ln(3) \approx 0.8447789518618$,
- for $x \geqslant 2$, $\eta_2 < (17 - \psi(17^-))/17 \cdot \ln^2(17) \approx 1.6583011509743$,
- for $x \geqslant 2$, $\eta_3 < (223 - \psi(223^-))/223 \cdot \ln^3(223) \approx 8.15435775451$,
- for $x \geqslant 2$, $\eta_4 < (1423 - \psi(1423^-))/1423 \cdot \ln^4(1423) \approx 59.1713704$.

□

4 Bounds for ϑ

4.1 Exact computation of ϑ

Lemma 4.1 *We have*

$$\vartheta(10^{15}) = 999\,999\,965\,752\,660.939839805291048\cdots.$$

Proof From the well-known identity

$$\psi(x) = \sum_{k=1}^{\infty} \vartheta(x^{1/k}), \tag{4.1}$$

we have

$$\vartheta(x) = \psi(x) - \sum_{k=2}^{\infty} \vartheta(x^{1/k}).$$

From some exact values of $\psi(x)$ computed by [7], we obtain Table 2 (Exact values of $\vartheta(x)$) □

Table 2 Values of $\vartheta(x)$ for $10^{10} \leqslant x \leqslant 10^{15}$

x	$\vartheta(x)$	$\psi(x) - \vartheta(x)$
$1E+10$	9999939830.657757	102289.175716
$2E+10$	19999821762.768212	144339.622582
$3E+10$	29999772119.815419	176300.955450
$4E+10$	39999808348.775748	203538.541084
$5E+10$	49999728380.731899	227474.729168
$6E+10$	59999772577.550769	249003.320704
$7E+10$	69999769944.203933	268660.720820
$8E+10$	79999718357.195652	287365.266118
$9E+10$	89999644656.090911	304250.688854
$1E+11$	99999737653.107445	320803.322857
$2E+11$	199999695484.246439	453289.609568
$3E+11$	299999423179.995211	554528.646163
$4E+11$	399999101196.308601	640000.361434
$5E+11$	499999105742.583455	715211.001138
$6E+11$	599999250571.436655	783167.715577
$7E+11$	699998999499.845475	845911.916175
$8E+11$	799999133776.084743	904203.190001
$9E+11$	899998818628.952024	958602.924046
$1E+12$	999999030333.096225	1009803.669232
$2E+12$	1999998755521.470649	1427105.865316
$3E+12$	2999997819758.987859	1746299.820370
$4E+12$	3999998370195.717561	2016279.693623
$5E+12$	4999998073643.711478	2253672.042145
$6E+12$	5999997276726.877147	2467566.593710
$7E+12$	6999996936360.165729	2665065.541181
$8E+12$	7999997864671.383505	2848858.049155
$9E+12$	8999996425300.244577	3021079.319393
$1E+13$	9999996988293.034200	3183704.089025
$2E+13$	19999995126082.228688	4499685.436490
$3E+13$	29999995531389.845427	5509328.368277
$4E+13$	39999993533724.316829	6359550.652121
$5E+13$	49999992543194.263655	7109130.001413
$6E+13$	59999990297033.626198	7785491.725387
$7E+13$	69999994316409.871731	8407960.376833
$8E+13$	79999990160858.304239	8988688.375101
$9E+13$	89999989501395.073897	9531798.550749
$1E+14$	99999990573246.978538	10045400.569463
$2E+14$	199999983475767.543204	14201359.711421
$3E+14$	299999986702246.281944	17388356.540338
$4E+14$	399999982296901.085038	20074942.600622

Table 2 continued

x	$\vartheta(x)$	$\psi(x)-\vartheta(x)$
$5E+14$	499999974019856.236519	22439658.012185
$6E+14$	599999983610646.997632	24580138.242324
$7E+14$	699999971887332.157455	26545816.027402
$8E+14$	799999964680836.091645	28378339.693784
$9E+14$	899999961386694.231242	30098146.961102
$1E+15$	999999965752660.939840	31724269.567843

4.2 On the difference between ϑ and identity function

Theorem 4.2 *We have*

$$|\vartheta(x)-x| < \eta_k \frac{x}{\ln^k x} \quad \textit{for } x \geqslant x_k$$

with

k	0	1	1	2	2	2	2
η_k	1	1.2323	0.001	3.965	0.2	0.05	0.01
x_k	1	2	908 994 923	2	3 594 641	122 568 683	7 713 133 853

and

k	3	3	3	3	3	4
η_k	20.83	10	1	0.78	0.5	151.3
x_k	2	32 321	89 967 803	158 822 621	767 135 587	2

Proof We combine the estimates of $|\psi(x)-x|$ given in Proposition 3.2 with the upper bound of $|\psi(x)-\vartheta(x)| < 1.4262\sqrt{x}$ given in [35, Theorem 13]. We proceed step by step up to the end of the table. For example, if ε_{b_i} is the value obtained for $x=e^{b_i}$ we have $\eta_k \geqslant (\varepsilon_{b_i} + 1.43/\sqrt{e^{b_i}}) \cdot b_{i+1}^k$ for $e^{b_i} \leqslant x \leqslant e^{b_{i+1}}$. For large values outside the table, we use [10, Theorem 1.1] with R defined in Theorem 2.4 and we have $\eta_k \geqslant \sqrt{8/\pi}(\sqrt{\ln(x_0)/R})^{1/2} \cdot e^{-\sqrt{\ln(x_0)/R}} \cdot \ln^k(x_0)$ for $x \geqslant x_0$. The maximum of $|\vartheta(x)-x|\frac{\ln^k x}{x}$ is

- for $x \geqslant 1$, $\eta_0 < (1-\vartheta(1^-))/1 = (2-\vartheta(2^-))/2 = 1$,
- for $x \geqslant 2$, $\eta_1 < (11-\vartheta(11^-))/11 \cdot \ln(11) \approx 1.23227674$,
- for $x \geqslant 2$, $\eta_2 < (59-\vartheta(59^-))/59 \cdot \ln^2(59) \approx 3.964809$,
- for $x \geqslant 2$, $\eta_3 < (1423-\vartheta(1423^-))/1423 \cdot \ln^3(1423) \approx 20.8281933$,
- for $x \geqslant 2$, $\eta_4 < (1423-\vartheta(1423^-))/1423 \cdot \ln^4(1423) \approx 151.2235681$.

□

4.3 On the difference between ψ and ϑ

As $\vartheta(2^-) = 0$, the summation (4.1) ends:

$$\psi(x) = \sum_{k=1}^{\lfloor \frac{\ln x}{\ln 2} \rfloor} \vartheta(x^{1/k}) = \vartheta(x) + \vartheta(\sqrt{x}) + \sum_{k=3}^{\lfloor \frac{\ln x}{\ln 2} \rfloor} \vartheta(x^{1/k}).$$

4.3.1 Lower bound

Proposition 4.3 *For* $x \geqslant 121$, *we have*

$$0.9999\sqrt{x} < \psi(x) - \vartheta(x), \tag{4.2}$$

$$\left(1 - \frac{4}{\ln^3 x}\right)\sqrt{x} < \psi(x) - \vartheta(x). \tag{4.3}$$

Proof Using Theorem 4.2, we have $\psi(x) - \vartheta(x) \geqslant \vartheta(\sqrt{x}) \geqslant \sqrt{x}\left(1 - \frac{2^k \eta_k}{\ln^k x}\right)$ which can be applied with $k = 3$, $\eta_k = 0.5$ for $\sqrt{x} > 767\,135\,587$. Now by [6, p. 211],

$$\psi(x) - \vartheta(x) = \psi(\sqrt{x}) + \sum_{k \geqslant 1} \vartheta(x^{\frac{1}{2k+1}}),$$

hence

$$\psi(x) - \vartheta(x) \geqslant \psi(\sqrt{x}) + \vartheta(x^{1/3}).$$

By Theorem 19 of [35, p. 72], we have

$$\vartheta(x^{1/3}) > \sqrt[3]{x} - 2x^{1/6} \text{ for } (1423)^3 \leqslant x \leqslant (10^8)^3,$$

and by (7.2) of [38, Theorem 11], we have for $x \geqslant e^{2b}$,

$$\psi(\sqrt{x}) > \sqrt{x} - \varepsilon_b \sqrt{x}$$

where ε_b can be found in the Table in p. 358 of [38] (or in Table 1). We verify that

$$\left(\frac{4}{\ln^3 x} - \varepsilon_b\right)\sqrt{x} + \sqrt[3]{x} - 2x^{1/6} > 0$$

for $10^{16} \leqslant x \leqslant e^{46}$ by intervals (we use $b = 18.42,\ 20,\ 22$). By Theorem 24 of [35, p. 73], we conclude that (4.2) is verified for $121 \leqslant x \leqslant 10^{16}$. □

4.3.2 Upper bound

Proposition 4.4 *For $x > 0$, we have*

$$\psi(x) - \vartheta(x) - \vartheta(\sqrt{x}) < 1.777745x^{1/3}. \tag{4.4}$$

Proof For $x > 0$, we have $\vartheta(x) < 1.000081x$ by [38, p. 360]. Hence

$$\begin{aligned}\sum_{k=3}^{\lfloor \frac{\ln x}{\ln 2} \rfloor} \vartheta(x^{1/k}) &< 1.000081 \sum_{k=3}^{\lfloor \frac{\ln x}{\ln 2} \rfloor} x^{1/k} \\ &< 1.000081 \left(x^{1/3} + \left(\left\lfloor \frac{\ln x}{\ln 2} \right\rfloor - 3 \right) x^{1/4} \right) \\ &< 1.2\, x^{1/3} \text{ for } x > (10^{11})^3.\end{aligned}$$

For small values, using the result $\vartheta(x) < x$ for $x \leqslant 10^{11}$ p. 360 in [38], we proceed by intervals such as $2^n \leqslant x < 2^{n+1}$ where $\sum_{k=3}^{n} \vartheta(x^{1/k}) < \sum_{k=3}^{n} x^{1/k} < \sum_{k=3}^{n} 2^{\frac{n+1}{k}}$. We find the maximal difference of (4.4) by direct computation (maximum is reached for x=2401). With this result, we update the (3.38) part from Theorem 14 of [35]. □

Corollary 4.5 *For $x > 0$,*

$$\psi(x) - \vartheta(x) < (1 + 1.47 \cdot 10^{-7})\sqrt{x} + 1.78x^{1/3}.$$

Proof The result follows from $\vartheta(\sqrt{x}) < \sqrt{x}$ for $\sqrt{x} < 1.39 \cdot 10^{17}$ from a computational result [26] of Platt and Trudgian. Next we compute the ε value for $b = \ln(1.39 \cdot 10^{17})$ using Theorem 3.1 and Proposition 4.4 ($\sigma_0 = 0.87$, $m = 2$, $\delta = 3.048E{-8}$, $T_1 = 157\,682\,321$, $\varepsilon = 1.467E{-7}$). □

5 Estimates of prime-related functions thanks ϑ function

5.1 Estimates of π function

The prime-counting function $\pi(x)$ is the function counting the number of prime numbers less than or equal to some real number x. Let $\mathrm{li}(x)$, the logarithmic integral defined for all positive real numbers $x \neq 1$ by the definite integral:

$$\mathrm{li}(x) = \lim_{\varepsilon \to 0+} \left(\int_0^{1-\varepsilon} \frac{\mathrm{d}t}{\ln t} + \int_{1+\varepsilon}^{x} \frac{\mathrm{d}t}{\ln t} \right).$$

A classical result [15, Theorem 23] makes a link between these two quantities:

$$\text{if } x \to \infty, \quad \pi(x) = \mathrm{li}(x) + O\left(x e^{-C\sqrt{\ln x}}\right) \tag{5.1}$$

with some constant $C > 0$. The estimate (5.1) is better than any estimate of the form

$$\pi(x) - \mathrm{li}(x) = O\big(x/\ln^m x\big).$$

Hence the asymptotic development of $\pi(x)$ is

$$\pi(x) = \frac{x}{\ln x}\sum_{k=0}^{n}\frac{k!}{(\ln x)^k} + O\left(\frac{x}{(\ln x)^{n+1}}\right).$$

Theorem 5.1 *For $x \geqslant 4\cdot 10^9$,*

$$\pi(x) = \frac{x}{\ln x}\left(1 + \frac{1}{\ln x} + \frac{2}{\ln^2 x} + O^*\left(\frac{7.32}{\ln^3 x}\right)\right).$$

For $x > 1$,

$$\pi(x) \leqslant \frac{x}{\ln x}\left(1 + \frac{1}{\ln x} + \frac{2}{\ln^2 x} + \frac{7.59}{\ln^3 x}\right).$$

Proof We substitute an upper bound for $\vartheta(x)$ of the form $|\vartheta(x) - x| \leqslant \eta_k \frac{x}{\ln^k x}$ for $x \geqslant x_0$, in Theorem 4.3 of [1]

$$\pi(x) = \pi(x_0) - \frac{\vartheta(x_0)}{\ln x_0} + \frac{\vartheta(x)}{\ln x} + \int_{x_0}^{x}\frac{\vartheta(y)\mathrm{d}y}{y\ln^2 y}$$

to introduce

$$J(x;\eta_k) = K + \frac{x}{\ln x} + \eta_k\frac{x}{\ln^{k+1} x} + \int_{x_0}^{x}\left(\frac{1}{\ln^2 y} + \frac{\eta_k}{\ln^{k+2} y}\right)\mathrm{d}y$$

with

$$K = \pi(x_0) - \frac{\vartheta(x_0)}{\ln x_0}.$$

such that, for $x \geqslant x_0$,

$$J(x;-\eta_k) \leqslant \pi(x) \leqslant J(x;\eta_k).$$

Let $M_k(x;c) = \frac{x}{\ln x}\left(\sum_{n=0}^{k-1}\frac{n!}{\ln^n x} + \frac{c}{\ln^k x}\right)$ inspired from the beginning of the asymptotic development of $\mathrm{li}(x)$. Let us write the derivatives of $J(x;\eta_k)$ and of $M(x;c)$ with respect to x:

$$J'(x;\eta_k) = \frac{1}{\ln x} + \frac{\eta_k}{\ln^{k+1} x} - k\frac{\eta_k}{\ln^{k+2} x},$$

$$M_k'(x;c) = \frac{1}{\ln x} + \frac{c-k!}{\ln^{k+1} x} - \frac{c(k+1)}{\ln^{k+2} x}.$$

For the upper bound for $\pi(x)$, one must choose $c \geqslant (k! + \eta_k - k\eta_k/\ln x_0)/(1-(k+1)/\ln x_0)$ to have $J' < M'$ for $x \geqslant x_0$. The bound is valid if $J(x_0;\eta_k) \leqslant M_k(x_0;c)$. With $\eta_3 = 0.5$ and $x_0 = 10^{15}$, we have to choose $c \geqslant 7.303$. We verify that $J(10^{15};0.5) < M_3(10^{15};7.32)$ using Table 3 of [30] and Table 2. We use the result of [26, Corollary 1] to limit the computer verification: as $\pi(x) < \mathrm{li}(x)$ for $x < 1.39 \cdot 10^{17}$, the result is valid as $\mathrm{li}(x)$ is lower than the upper bound for $x > 1.62 \cdot 10^{10}$. The constant 7.5893, which appears in $\ln^3 x$ term, is reached for $p = 110\,102\,617$. For the lower bound, to have $J'(x;-\eta_k) > M_k'(x;c)$ we have to choose $c < (k! - \eta_k + k\eta_k/\ln x)/(1-\frac{k+1}{\ln x})$. With $k=3$, we choose $c=0$, $x_0 = 10^{11}$, and $\eta_3(1-3/\ln x) < 6$. As $M(x_0;0) < J(x_0;-1)$ and by direct computation for small values, we obtain

$$\pi(x) > \frac{x}{\ln x}\left(1 + \frac{1}{\ln x} + \frac{2}{\ln^2 x}\right) \quad \text{for } x \geqslant 88\,789.$$

□

We use the previous result to give bounds for $\pi(x)$. The lower bounds are the first terms and the upper bounds are the best bounds (best in terms of last constant) for $x > 1$ of first order of the asymptotic development of $\mathrm{li}(x)$.

Corollary 5.2

$$\underset{x \geqslant 17}{\frac{x}{\ln x} \leqslant} \pi(x) \underset{x>1}{\leqslant} 1.2551\frac{x}{\ln x}, \tag{5.2}$$

$$\frac{x}{\ln x}\left(1+\frac{1}{\ln x}\right) \underset{x \geqslant 599}{\leqslant} \pi(x) \underset{x>1}{\leqslant} \frac{x}{\ln x}\left(1+\frac{1.2762}{\ln x}\right), \tag{5.3}$$

$$\frac{x}{\ln x}\left(1+\frac{1}{\ln x}+\frac{2}{\ln^2 x}\right) \underset{x \geqslant 88\,789}{\leqslant} \pi(x) \underset{x>1}{\leqslant} \frac{x}{\ln x}\left(1+\frac{1}{\ln x}+\frac{2.53816}{\ln^2 x}\right). \tag{5.4}$$

Proof The upper bounds are reached, respectively, for $p_{30} = 113$, $p_{258} = 1\,627$, and $p_{30392} = 355\,111$. We also verify that $\pi(x) \geqslant \frac{x}{\ln x}\left(1+\frac{1}{\ln x}+\frac{2-0.53816}{\ln^2 x}\right)$ for $x \geq 11\,813$ to complete a result announced in the introduction. □

Using the asymptotic development of $1/\mathrm{li}(x)$, Panaitopol [25] showed another formula for $\pi(x)$ by proving that

$$\pi(x) = \frac{x}{\ln x - 1 - f(x)},$$

where $f(x) = k_1/\ln(x) + k_2/\ln^2(x) + \cdots + O(1/\ln^m(x))$ with k_i given by the recurrence relation

$$k_n + 1!\,k_{n-1} + 2!\,k_{n-2} + \cdots + (n-1)!\,k_1 = n \cdot n!.$$

We obtain this kind of asymptotic development

$$\pi(x) = \frac{x}{\ln x - 1 - 1/\ln(x) - 3\ln^2(x) - 13/\ln^3(x) - \cdots}$$

which is useful [2,3] for bounds for $1/\pi(x)$.

Corollary 5.3

$$\underset{x \geqslant 5\,393}{\frac{x}{\ln x - 1}} \leqslant \pi(x) \leqslant \underset{x > e^{1.112}}{\frac{x}{\ln x - 1.112}}, \tag{5.5}$$

$$\underset{x \geqslant 468\,049}{\frac{x}{\ln x - 1 - 1/\ln(x)}} \leqslant \pi(x) \leqslant \underset{x > 5.6}{\frac{x}{\ln(x) - 1 - 1.2311/\ln(x)}}. \tag{5.6}$$

Proof The upper bounds are reached, respectively, for $p_{2688} = 24\,137$ and $p_{246651} = 3\,445\,943$. □

5.2 Smallest interval containing primes

The problem of the smallest interval containing primes is linked with the problem of prime gaps (i.e., the difference between two successive prime numbers) and can be useful for the verification of the ternary Goldbach's conjecture [18] or for searching primes [40] between cubes. A result of Schoenfeld [38] showing that, for $x \geqslant 2\,010\,759.9$, the interval $]x, x + x/16597[$ contains at least one prime, was improved by [29], [40], and recently by [18].

Proposition 5.4 *For all $x \geqslant 89\,693$, there exists a prime p such that*

$$x < p \leqslant x\left(1 + \frac{1}{\ln^3 x}\right).$$

Corollary 5.5 *For all $x \geqslant 468\,991\,632$, there exists a prime p such that*

$$x < p \leqslant x\left(1 + \frac{1/5000}{\ln^2 x}\right).$$

This result is better than Trudgian's one [40]. The specific method used in [29] gives better results (if we compare with the same order of k, i.e., $k = 0$) and was updated by [18].

Proof Let $0 < f(x) < 1$ for $x \geqslant x_0$,

$$\vartheta(x(1+f(x))) - \vartheta(x) \geqslant x(1+f(x)) - \eta_k \frac{x(1+f(x))}{\ln^k(x(1+f(x)))} - \left(x + \eta_k \frac{x}{\ln^k x}\right)$$
$$> x\left(f(x) - \frac{2\eta_k}{\ln^k x} - \frac{\eta_k f(x)}{\ln^k x}\right).$$

Choose $f(x) = \frac{\beta}{\ln^k x}$ with $\beta \geqslant \frac{2\eta_k}{1+\eta_k/\ln^k x_0}$ to have

$$\vartheta\left(\left(1+\frac{\beta}{\ln^k x}\right)x\right) - \vartheta(x) > 0.$$

For $k = 3$ and $x_0 = 4 \cdot 10^{18}$, $n_3 = 0.499$ (Theorem 4.2 with a little more precision), we have $\beta \geqslant 0.998$. Using the work on maximal gaps between primes [21,22] (or resumed in [24, Table 8]), we proceed as follows. Assume that the maximal gap of all primes between x_1 and x_2 is Δ. Therefore $p_{n+1} \leqslant p_n + \Delta$ which is smaller than our bound as long as $\frac{x_1}{\ln^k x_1} \geqslant \Delta/\beta$. Hence we find easily that the result is correct between 360 653 and 4×10^{18}. We verify by computer the lower bound of the validity range. □

5.3 Estimates of sums over primes

Let γ be Euler's constant ($\gamma \approx 0.5772157$). For more accuracy, one can find more decimals and bibliography on the On-Line Encyclopedia of Integer Sequences (OEIS). The Euler's constant is referenced as sequence A001620.

Theorem 5.6 *Let M be the Meissel–Mertens constant (sequence A077761 in OEIS) given by the infinite sum*

$$M = \gamma + \sum_p (\ln(1-1/p) + 1/p) \approx 0.26149\,72128\,47643.$$

We have for $x \geqslant 2\,278\,383$,

$$\sum_{p \leqslant x} \frac{1}{p} = \ln\ln x + M + \mathcal{O}^*\left(\frac{0.2}{\ln^3 x}\right).$$

Proof The sum of prime reciprocals is related to $\vartheta(x)$ by (4.20) of [35],

$$\sum_{p \leqslant x} \frac{1}{p} = \ln_2 x + M + \frac{\vartheta(x) - x}{x \ln x} - \int_x^\infty \frac{(\vartheta(y) - y)(1 + \ln y)}{y^2 \ln^2 y} \mathrm{d}y.$$

Hence

$$\left|\sum_{p\leqslant x}\frac{1}{p}-\ln_2 x-M\right|\leqslant\frac{|\vartheta(x)-x|}{x\ln x}+\int_x^\infty\frac{|\vartheta(y)-y|(1+\ln y)}{y^2\ln^2 y}\mathrm{d}y.$$

With a form of an upper bound like $|\vartheta(x)-x|\leqslant\eta_k x/\ln^k x$ (see Theorem 4.2) and as

$$\int_x^\infty\frac{1+\ln y}{y\ln^{k+2}y}\mathrm{d}y=\frac{1}{k\ln^k x}+\frac{1}{(k+1)\ln^{k+1}x},$$

we have the result

$$\left|\sum_{p\leqslant x}\frac{1}{p}-\ln_2 x-M\right|\leqslant\frac{\eta_k/k}{\ln^k x}+\frac{\eta_k(1+\frac{1}{k+1})}{\ln^{k+1}x}. \tag{5.7}$$

For $k=3$ and $\eta_3=0.5$, the result is valid for $x\geqslant 767\,135\,587$ by Theorem 4.2. We check by computer that the result remains valid for $2\,278\,383\leqslant x\leqslant 767\,135\,587$. □

Theorem 5.7 *Let* B_3 (*sequence A083343 in OEIS*) *the constant given by the infinite sum*

$$B_3=\gamma+\sum_{n=2}^\infty\sum_p(\ln p)/p^n\approx 1.33258\,22757\,33221.$$

We have for $x\geqslant 912\,560$,

$$\sum_{p\leqslant x}\frac{\ln p}{p}=\ln x-B_3+\mathcal{O}^*\left(\frac{0.3}{\ln^2 x}\right).$$

Proof By (4.21) of [35],

$$\sum_{p\leqslant x}\frac{\ln p}{p}=\ln x-B_3+\frac{\vartheta(x)-x}{x}-\int_x^\infty\frac{\vartheta(y)-y}{y^2}\mathrm{d}y.$$

Hence

$$\left|\sum_{p\leqslant x}\frac{\ln p}{p}-\ln x+B_3\right|\leqslant\frac{|\vartheta(x)-x|}{x}+\int_x^\infty\frac{|\vartheta(y)-y|}{y^2}\mathrm{d}y.$$

As

$$\int_x^\infty \frac{dy}{y \ln^k y} = \frac{1}{(k-1)\ln^{k-1} x},$$

we obtain

$$\left| \sum_{p \leqslant x} \frac{\ln p}{p} - \ln x + B_3 \right| \leqslant \left(\frac{\eta_k}{k-1} + \frac{\eta_k}{\ln x} \right) / \ln^{k-1} x.$$

Theorem 4.2 yields the result for $x \geqslant 767\,135\,587$ with $k = 3$ and $\eta_k = 0.5$. We extended the validity range by computer. □

Remark 5.8 Considering the definition of $\tilde{\psi}(x)$ of [27], the previous theorem states bounds for $\tilde{\vartheta}(x) = \sum_{p \leqslant x} \frac{\ln p}{p}$. One may find improved constants for $\tilde{\psi}(x)$ if the bounds on $\psi(x)$ in Theorem 3.3 are used in Ramaré's proof.

5.4 Estimates of products over primes

Theorem 5.9 *We have for* $x \geqslant 2\,278\,382$,

$$\prod_{p \leqslant x} \left(1 - \frac{1}{p}\right) = \frac{e^{-\gamma}}{\ln x} \left(1 + \mathcal{O}^* \left(\frac{0.2}{\ln^3 x}\right)\right)$$

and

$$\prod_{p \leqslant x} \frac{p}{p-1} = e^{\gamma} \ln x \left(1 + \mathcal{O}^* \left(\frac{0.2}{\ln^3 x}\right)\right).$$

Proof By definition of M (see Theorem 5.6) and (5.7), we have

$$\left| -\gamma - \ln_2 x - \sum_{p > x} \frac{1}{p} - \sum_p \ln(1 - 1/p) \right| \leqslant \frac{\eta_k / k}{\ln^k x} + \frac{\eta_k (1 + \frac{1}{k+1})}{\ln^{k+1} x}.$$

Let $S = \sum_{p > x} (\ln(1 - 1/p) + 1/p) = -\sum_{n=2}^{\infty} \frac{1}{n} \sum_{p > x} \frac{1}{p^n}$. We have

$$-\gamma - \ln_2 x - \sum_{p \leqslant x} \ln(1 - 1/p) - S \geqslant -\frac{\eta_k}{k \ln^k x} - \frac{(k+2)\eta_k}{(k+1)\ln^{k+1} x}.$$

Take the exponential of both sides to obtain

$$\prod_{p \leqslant x} \left(1 - \frac{1}{p}\right) \leqslant \frac{e^{-\gamma}}{\ln x} \exp\left(-S + \frac{\eta_k}{k \ln^k x} + \frac{(k+2)\eta_k}{(k+1)\ln^{k+1} x}\right).$$

We use the lower bound for S given in [35, p. 87]:

$$-S < \frac{1.02}{(x-1)\ln x}.$$

Hence, for $k = 3$, $\eta_3 = 0.5$, and $x \geqslant 767\,135\,587$,

$$\prod_{p\leqslant x}\left(1-\frac{1}{p}\right) \leqslant \frac{e^{-\gamma}}{\ln x}\exp(0.1973/\ln^3 x) \leqslant \frac{e^{-\gamma}}{\ln x}(1+0.2/\ln^3 x).$$

We also have

$$\prod_{p\leqslant x}\frac{p-1}{p} \geqslant e^{\gamma}\ln x\exp(-0.1973/\ln^3 x).$$

In the same way, as

$$-\gamma - \ln_2 x - \sum_{p\leqslant x}\ln(1-1/p) - S \leqslant \frac{\eta_k}{k\ln^k x} + \frac{(k+2)\eta_k}{(k+1)\ln^{k+1} x},$$

we obtain the other inequalities since $S < 0$. □

5.5 Estimates involving the kth primes

5.5.1 Useful bounds

Lemma 5.10

$$p_k \leqslant k\ln p_k \quad \textit{for} \quad k \geqslant 4, \tag{5.8}$$

$$\ln p_k \leqslant \ln k + \ln\ln k + 1 \quad \textit{for} \quad k \geqslant 2. \tag{5.9}$$

Proof We deduce (5.8) from $\pi(x) > \frac{x}{\ln x}$ (Corollary 1 of [35]). By Theorem 3 of [35], we have $p_k < k(\ln k + \ln\ln k - 1/2)$ hence $p_k < ek\ln k$ for $k \geqslant 2$. □

5.5.2 Estimates of $\vartheta(p_k)$

We have an asymptotic development of $\vartheta(p_k)$ whose the first terms by [5] are

$$\vartheta(p_k) = k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2}{\ln k} - \frac{\ln\ln^2 k - 6\ln\ln k + 11}{2\ln^2 k} + O\left(\frac{\ln\ln^3 k}{\ln^3 k}\right)\right).$$

Massias and Robin [19, Th. B(v)] obtained an upper bound which corresponds to the first terms of the asymptotic development

$$\vartheta(p_k) \leqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2}{\ln k}\right) \quad \text{for } k \geqslant 198. \tag{5.10}$$

Here, we obtain the following lower bounds:

Proposition 5.11

$$\vartheta(p_k) \geqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2.050735}{\ln k}\right) \quad \textit{for } p_k \geqslant 10^{11},$$
$$\vartheta(p_k) \geqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2.04}{\ln k}\right) \quad \textit{for } p_k \geqslant 10^{15}.$$

Proof We proceed in the same manner as [19]. Let f_β defined by

$$n \mapsto n\left(\ln n + \ln\ln n - 1 + \frac{\ln\ln n - \beta}{\ln n}\right).$$

We want to prove that $\vartheta(p_n) \geqslant f_\beta(n)$. Define the function h_a by

$$h_a(n) = n\left(\ln n + \ln\ln n - a\right).$$

Suppose there exists a such that $p_k \geqslant h_a(k)$ for $k \geqslant k_0$. Hence

$$\vartheta(p_k) - \vartheta(p_{k_0}) = \sum_{n=k_0+1}^{k} \ln p_n \geqslant \sum_{n=k_0+1}^{k} \ln h_a(n).$$

We have $f'_\beta \leqslant \ln h_a$ if

$$\frac{\ln\ln n - \beta + 1}{\ln n} - \frac{\ln\ln n - \beta - 1}{\ln^2 n} \leqslant \ln\left(1 + \frac{\ln\ln n - a}{\ln n}\right). \tag{5.11}$$

We can rewrite (5.11) as

$$\beta(1 - 1/\ln n) \geqslant 1 + \ln\ln n - \ln\left(1 + \frac{\ln\ln n - a}{\ln n}\right)\ln n - \frac{\ln\ln n - 1}{\ln n}. \tag{5.12}$$

For $a \in [0.95, 1]$ and $t \geqslant 22$, the function $t \mapsto (\ln t + 1 - t\ln\left(1 + \frac{\ln t - a}{t}\right) - \frac{\ln t - 1}{t})/(1 - 1/t)$ is decreasing. By [9], we can choose $a = a_0 = 1$. For $k \geqslant e^{100}$, the value $\beta = 2.048$ satisfies (5.12). For $\pi(10^{11}) \leqslant k \leqslant e^{100}$, the value $\beta_0 = 2.094$ satisfies (5.12). Hence

$$\vartheta(p_k) \geqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - \beta_0}{\ln k}\right).$$

Then $p_k \geqslant \vartheta(p_k) - \eta_2 \frac{k}{\ln k}$ by (4.2) and (5.8), hence $p_k \geqslant h_{a_1}(k)$ with $a_1 = 1 - \frac{\ln\ln k - (\beta_0 + \eta_2)}{\ln k}$. Splitting the interval of k, we use different values of a with adapted values of η_2. By iterating the process, we obtain $\beta = 2.050735$ for $k \geqslant k_0 = \pi(10^{11})$. This value of β verifies $\vartheta(p_{k_0}) \geqslant f_\beta(k_0)$.

By same way, we obtain $\beta = 2.038$ for $k \geqslant \pi(10^{15})$ thanks to Lemma 4.1. □

Proposition 5.12 *For* $k \geqslant 781$,

$$\vartheta(p_k) \leqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2}{\ln k} - \frac{0.782}{\ln^2 k}\right)$$

Proof Use Lemmas 5.14 and 5.13. □

Lemma 5.13 *Let two integers* k_0, k *and a real* $\gamma > 0$. *Suppose that for* $k_0 \leqslant n \leqslant k$,

$$p_n \leqslant n\left(\ln n + \ln\ln n - 1 + \frac{\ln\ln n - 1.95}{\ln n}\right).$$

Let $s(k) = k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2}{\ln k} - \frac{\gamma}{\ln^2 k}\right)$. *Let* $f(k) = s(k) - (\ln k + \ln\ln k + 1)$. *If* $\vartheta(p_{k_0 - 1}) \leqslant f(k_0)$ *then* $\vartheta(p_k) \leqslant s(k)$ *for all* $k \geqslant k_0$.

Proof Let $S_a(n)$ be an upper bound for p_n for $k_0 \leqslant n \leqslant k$ where

$$S_a(n) = n\left(\ln n + \ln\ln n - 1 + \frac{\ln\ln n - a}{\ln n}\right).$$

Now, for $2 \leqslant k_0 \leqslant k$, we write

$$\vartheta(p_{k-1}) - \vartheta(p_{k_0} - 1) = \sum_{n=k_0}^{k-1} \ln p_n \leqslant \sum_{n=k_0}^{k-1} \ln S_a(n) \leqslant \int_{k_0}^{k} \ln S_a(n) dn.$$

Next we shall prove that $\ln S_a(n) \leqslant f'(n)$. We have

$$\ln S_a(n) = \ln n + \ln\ln n + \ln(1 + u(n))$$

with $u(n) = \frac{\ln\ln n - 1}{\ln n} + \frac{\ln\ln n - a}{\ln^2 n}$ and

$$f'(n) = \ln n + \ln\ln n + \frac{\ln\ln n - 1}{\ln n} - \frac{\ln\ln n + \gamma - 3}{\ln^2 n} + \frac{2\gamma}{\ln^3 n} - \frac{1}{n}(1 + 1/\ln n).$$

Let $\beta < 1/2$ such that $\ln(1 + u(n)) \leqslant u(n) - \beta u^2(n)$ for $n \geqslant k_0$. Then $\ln S_a(n) \leqslant f'(n)$ if

$$\beta\left(\frac{\ln\ln n - 1}{\ln n} + \frac{\ln\ln n - a}{\ln^2 n}\right)^2 - \frac{2\ln\ln n + \gamma - 3 - a}{\ln^2 n} + 2\gamma/\ln^3 n - 1/n - 1/(n\ln n) \geqslant 0,$$

that we can simplify in

$$\frac{A}{\ln^2 n} + 2\frac{B}{\ln^3 n} + \beta\frac{(\ln\ln n - a)^2}{\ln^4 n} - 1/n - 1/(n\ln n) \geqslant 0$$

where

$$A = \beta\ln\ln^2 n - 2(\beta+1)\ln\ln n + 3 + a + \beta - \gamma$$
$$B = \beta\ln\ln^2 n - \beta(a+1)\ln\ln n + a\beta + \gamma$$

We have $1/n + 1/(n\ln n) \leqslant 0.02/\ln^3 n$ for $n \geqslant 10^5$.

We study each parts, denoting $\ln\ln n$ by X:

- $\beta X^2 - 2(\beta+1)X + 3 + a + \beta - \gamma \geqslant 0$ for all X if $\gamma - a - 1 + 1/\beta \leqslant 0$,
- $X^2 - (a+1)X + (a + \gamma/\beta + 0.01/\beta) \geqslant 0$ for all X if $a^2 - 2a + 1 - 4(\gamma/\beta + 0.01/\beta) \leqslant 0$,
- $X^2 - 2aX + a^2 = (X-a)^2 \geqslant 0$.

We choose γ such that $\gamma - a - 1 + 1/\beta = 0$. We choose $\beta = \frac{u(k_0) - \ln(1+u(k_0))}{u^2(k_0)}$. With $a = 1.95$ and $k_0 = 178974$, we have $\beta = 0.461291475\cdots$ and $\gamma = 0.78217325\cdots$.

Hence $\vartheta(p_{k-1}) - f(k) \leqslant \vartheta(p_{k_0} - 1) - f(k_0)$. As $\vartheta(p_{k_0} - 1) \leqslant f(k_0)$, we have $\vartheta(p_{k-1}) - f(k) \leqslant 0$. We obtain the upper bound $\vartheta(p_k) = \vartheta(p_{k-1}) + \ln p_k \leqslant f(k) + \ln p_k < s(k)$ by (5.9). □

5.5.3 Estimates of p_k

Lemma 5.14 *For $k \geqslant 178\,974$,*

$$p_k \leqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 1.95}{\ln k}\right).$$

Proof Substituting x by p_k in $|\vartheta(x) - x| \leqslant \eta_2\frac{x}{\ln^2 x}$, we obtain

$$|p_k - \vartheta(p_k)| \leqslant \eta_2\frac{p_k}{\ln^2 p_k}.$$

By (5.8), we have $\frac{p_k}{\ln^2 p_k} \leqslant \frac{k}{\ln k}$ and

$$|p_k - \vartheta(p_k)| \leqslant \eta_2\frac{k}{\ln k}. \tag{5.13}$$

Using the upper bound (5.10) of $\vartheta(p_k)$, we have

$$p_k \leqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2 + \eta_2}{\ln k}\right).$$

We use $\eta_2 = 0.05$ for $p_k \geqslant 122\,568\,683$ by Theorem 4.2. □

Proposition 5.15 *For* $k \geqslant 688\,383$,

$$p_k \leqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2}{\ln k}\right).$$

Proof Use Proposition 5.12 with $\eta_3 = 0.78$ of Theorem 4.2 for $\ln p_k > 27$. A computer verification concludes the proof. □

Proposition 5.16 *For* $k \geqslant 3$,

$$p_k \geqslant k\left(\ln k + \ln\ln k - 1 + \frac{\ln\ln k - 2.1}{\ln k}\right).$$

Proof Using (5.13), we have

$$p_k \geqslant \vartheta(p_k) - \eta_2 \frac{k}{\ln k}.$$

By Proposition 5.11 and $\eta_2 = 0.04913$, we conclude the proof. □

Acknowledgements The author wishes to thank the anonymous reviewers for their helpful comments.

References

1. Apostol, T.M.: Introduction to Analytic Number Theory. Springer, New York (1976)
2. Axler, C.: New bounds for the prime counting function $\pi(x)$. arXiv: 1409.1780 (2014)
3. Berkane, D., Dusart, P.: On a constant related to the prime counting function. Mediterr. J. Math. **13**(3), 929–938 (2016). doi:10.1007/s00009-015-0564-9
4. Cesaro, E.: Sur une formule empirique de M. Pervouchine. Comptes Rendus hebdo. des Séances de l'Académie des Sciences *CXIX* **119**, 848–849 (1894)
5. Cipolla, M.: La determinazione assintotica dell'n^{imo} numero primo. Rend. Acad. Sci. Fis. Mat. Napoli **8**, 132–166 (1902)
6. Costa P.N.: Estimates for the Chebyshev function $\psi(x) - \vartheta(x)$. Math. Comput. **44**(169), 211–221 (1985). See corrigendum [Math. Comput. **48**(177), 447 (1987)]
7. Deléglise, M., Rivat, J.: Computing $\psi(x)$. Math. Comput. **67**(224), 1691–1696 (1998)
8. Dusart, P.: Inégalités explicites pour $\psi(X)$, $\vartheta(X)$, $\pi(X)$ et les nombres premiers. C. R. Math. Acad. Sci. Soc. R. Can. **21**(2), 53–59 (1999)
9. Dusart, P.: The kth prime is greater than k(ln k + ln ln k - 1) for k ≥ 2. Math. Comput. **68**(225), 411–415 (1999)
10. Dusart, P.: Estimates of ψ, ϑ for large values of x without the Riemann hypothesis. Math. Comput. **85**(298), 875–888 (2016)
11. Edwards, H.M.: Riemann's Zeta Function. Academic Press, New York–London, 1974. Pure and Applied Mathematics, Vol. 58. Reprinted by Dover Publications Inc., Mineola (2001)
12. Faber, L., Kadiri, H.: New bounds for $\psi(x)$. Math. Comput. **84**(293), 1339–1357 (2015)
13. Gourdon, X.: The 10^{13} first zeros of the Riemann zeta function, and zeros computation at very large height. http://numbers.computation.free.fr/Constants/Miscellaneous/zetazeros1e13-1e24.pdf (2004). Accessed 24 Oct 2004
14. Gram, J.P.: Note sur les zéros de la fonction $\zeta(s)$ de Riemann. Acta Math. **27**(1), 289–304 (1903)
15. Ingham, A.: The Distribution of Prime Numbers. Cambridge Mathematical Library, Cambridge University Press, Cambridge (1932)
16. Kadiri, H.: Une région explicite sans zéros pour la fonction ζ de Riemann. Acta Arith. **117**(4), 303–339 (2005)

17. Kadiri, H.: A zero density result for the Riemann zeta function. Acta Arith. **160**(2), 185–200 (2013)
18. Kadiri, H., Lumley, A.: Short effective intervals containing primes. Integers 14, Paper No. A61 (2014)
19. Massias, J.-P., Robin, G.: Bornes effectives pour certaines fonctions concernant les nombres premiers. J. Théor. Nombres Bordeaux **8**(1), 215–242 (1996)
20. Mossinghoff, M.J., Trudgian, T.S.: Nonnegative trigonometric polynomials and a zero-free region for the Riemann zeta-function. J. Number Theory **157**, 329–349 (2015)
21. Nicely, T.R.: New maximal prime gaps and first occurrences. Math. Comput. **68**(227), 1311–1315 (1999)
22. Nyman, B., Nicely, T.R.: New prime gaps between 10^{15} and 5×10^{16}. J. Integer Seq. **6**, 3 (2003). Article 03.3.1, 6
23. Odlyzko, A.M.: The 10^{22}-nd zero of the Riemann zeta function. In: van Frankenhuysen, M., Lapidus, M.L. (eds.) Dynamical, Spectral, and Arithmetic Zeta Functions. American Mathematical Society, Contemporary Mathematics, vol. 290, pp. 139–144 (2001)
24. Oliveira e Silva, T., Herzog, S., Pardi, S.: Empirical verification of the even Goldbach conjecture and computation of prime gaps up to $4{\cdot}10^{18}$. Math. Comput. **83**, 288 (2014)
25. Panaitopol, L.: A formula for $\pi(x)$ applied to a result of Koninck-Ivić. Nieuw Arch. Wiskd. (5) **1**, 55–56 (2000)
26. Platt, D.J., Trudgian, T.S.: On the first sign change of $\vartheta(x) - x$. Math. Comput. **85**, 1539–1547 (2016)
27. Ramaré, O.: Explicit estimates for the summatory function of $\Lambda(n)/n$ from the one of $\Lambda(n)$. Acta Arith. **159**(2), 113–122 (2013)
28. Ramaré, O.: An explicit density estimate for Dirichlet L-series. Math. Comput. **85**(297), 325–356 (2016)
29. Ramaré, O., Saouter, Y.: Short effective intervals containing primes. J. Number Theory **98**(1), 10–33 (2003)
30. Riesel, H.: Prime Numbers and Computer Methods for Factorization. Birkhauser Boston, Cambridge, MA (1985)
31. Robin, G.: Estimation de la fonction de Tchebychef ϑ sur le k-ième nombre premier et grandes valeurs de la fonction $\omega(n)$ nombre de diviseurs premiers de n. Acta Arith. **42**(4), 367–389 (1983)
32. Robin, G.: Permanence de relations de récurrence dans certains développements asymptotiques. Publ. l'Inst. Math. **43**(57), 17–25 (1988)
33. Rosser, J.B.: The n-th prime is greater than $n \ln n$. Proc. Lond. Math. Soc. **45**, 21–44 (1939)
34. Rosser, B.: Explicit bounds for some functions of prime numbers. Am. J. Math. **63**, 211–232 (1941)
35. Rosser, J.B., Schoenfeld, L.: Approximate formulas for some functions of prime numbers. Ill. J. Math. **6**, 64–94 (1962)
36. Rosser, J.B., Schoenfeld, L.: Sharper bounds for the Chebyshev functions $\vartheta(x)$ and $\psi(x)$. Math. Comput. **29**(129), 243–269 (1975)
37. Salvy, B.: Fast computation of some asymptotic functional inverses. J. Symb. Comput. **17**(3), 227–236 (1994)
38. Schoenfeld, L.: Sharper bounds for the Chebyshev functions $\vartheta(x)$ and $\psi(x)$. II. Math. Comput. **30**(134), 337–360 (1976)
39. Trudgian, T.: An improved upper bound for the error in the zero-counting formulae for Dirichlet L-functions and Dedekind zeta-functions. Math. Comput. **84**(293), 1439–1450 (2015)
40. Trudgian, T.: Updating the error term in the prime number theorem. Ramanujan J. **39**(2), 225–234 (2016). doi:10.1007/s11139-014-9656-6
41. van de Lune, J., te Riele, H.J.J., Winter, D.T.: On the zeros of the Riemann zeta function in the critical strip. IV. Math. Comput. **46**(174), 667–681 (1986)
42. Wedeniwski, S.: Zetagrid. In: Schoder, D., Fischbach, K., Teichmann, R. (eds.) Peer-to-Peer: Ökonomische, Technische und Juristische Perspektiven, pp. 173–188. Springer, Berlin, Heidelberg (2002)