MATHEMATICS OF COMPUTATION
http://dx.doi.org/10.1090/mcom/3005
Article electronically published on July 20, 2015

ESTIMATES OF ψ, θ FOR LARGE VALUES OF x WITHOUT THE RIEMANN HYPOTHESIS

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Abstract. The enlargement of known zero-free regions has enabled us to find better effective estimates for classical number-theoretic functions linked to the distribution of prime numbers. In particular we draw the quintessence of the method of Rosser and Schoenfeld on the upper bounds for the usual Chebyshev prime and prime power counting functions to find an upper bound function directly linked to a zero-free region.

1. Introduction

We recall that the first Chebyshev function $\vartheta(x)$ is given by

$$\vartheta(x) = \sum_{p \leqslant x} \ln p$$

with the sum extending over all prime numbers p that are less than or equal to x. The second Chebyshev function $\psi(x)$ is defined similarly, with the sum extending over all prime powers not exceeding x,

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

Both Chebyshev functions are asymptotic to x,

$$\vartheta(x) \sim \psi(x) \sim x \text{ as } x \to \infty,$$

a statement equivalent, by [1, Theorem 4.4], to the Prime Number Theorem proved independently by Jacques Hadamard and Charles Jean de la Vallée-Poussin in 1896.

Let $\zeta(s)$, a function of a complex s, be the continuation of the Riemann zeta function. We consider $\mathcal{R}_\zeta$ the set of non-trivial zeros of ζ which lies in the open strip $\{s \in \mathbb{C} : 0 < \mathfrak{Re}(s) < 1\}$, which is called the critical strip. A classical explicit formula, that relates the function ψ to the non-trivial zeros of ζ, is given by [3, Theorem 5.9 (p. 172)]

$$\frac{\psi(x^+) + \psi(x^-)}{2} = x + \ln(2\pi) - \frac{1}{2}\ln(1 - x^{-2}) - \lim_{T \to +\infty} \sum_{\rho \in \mathcal{R}_\zeta, |\mathfrak{Im}(\rho)| < T} \frac{x^\rho}{\rho}.$$

As the sum of the zeros is not absolutely convergent, Rosser [16, Theorem 13] uses an average of ψ on a small interval containing x to obtain bounds on ψ. This

Received by the editor March 17, 2014 and, in revised form, October 4, 2014.
2010 *Mathematics Subject Classification.* Primary 11N56; Secondary 11A25, 11N05.
Key words and phrases. Number theory, arithmetic functions.

method was improved by Rosser and Schoenfeld [17] in 1962 to give a function $\varepsilon(x)$ bounding the error term

$$E(x) = \left| \frac{\psi(x) - x}{x} \right|.$$

Their result was improved fourteen years later by Schoenfeld [19, Theorem 11], who showed that

$$\varepsilon(x) = \sqrt{\frac{8}{17\pi}} X^{1/2} e^{-X}, \tag{1}$$

where $X = \sqrt{(\ln x)/R}$ and with $R = 9.645908801$. The proof uses three key ingredients: the numerical verification of the Riemann hypothesis up to a fixed height A, an explicit zero-free region and explicit bounds for the number of zeros in the critical strip up to a fixed height.

The goal of this paper is to show that if the zero-free region has the form (called the de la Vallée Poussin form of the zero-free region)

$$\mathfrak{Re}(s) \geqslant 1 - \frac{1}{R \ln |\mathfrak{Im}(s)|} \quad \text{for } |\mathfrak{Im}(s)| \geqslant 2, \tag{2}$$

where R is a formal constant parameter, then there is no real need of the computable constant A of the Riemann hypothesis verification, to find a function $\varepsilon_R(x)$ bounding the error term $E(x)$ for large x.

Theorem 1.1. *Let $R > 0$ be a formal constant such that there exists a zero-free region of the form $\mathfrak{Re}(s) \geqslant 1 - \frac{1}{R \ln |\mathfrak{Im}(s)|}$ for $|\mathfrak{Im}(s)| \geqslant 2\pi$. Let $X = \sqrt{(\ln x)/R}$ and $\varepsilon_R(x) = \sqrt{\frac{8}{\pi}} X^{1/2} e^{-X}$. Then, for $X \geqslant \max(8.36, \frac{8}{R})$, we have*

$$\max\{|\vartheta(x) - x|, |\psi(x) - x|\} < x\varepsilon_R(x).$$

A particular value of R established in inequality (2) may thus be employed in Theorem 1.1 to obtain explicit bounds for the Chebyshev functions. In Section 3 we use a result of Kadiri [9] to conclude the following.

Corollary 1.2. *Let $R_0 = 5.69693$. Then, for $x \geqslant 3$,*

$$\max\{|\vartheta(x) - x|, |\psi(x) - x|\} < \sqrt{\frac{8}{\pi R_0^{1/2}}}\, x(\ln x)^{1/4}\, e^{-\sqrt{(\ln x)/R_0}}.$$

This function is useful for large values of x (i.e. $x \geqslant \exp(10\,000)$). As seen in Section 4, the recent advances on the check of the Riemann hypothesis have only a low impact on estimates of the Chebyshev functions for large values of x. For lower values, a direct evaluation of a bounding expression of many parameters [4, Theorem 1.1] is better. These estimates are widely used in various fields like cryptography, computer science or for explicit bounds for sums over primes [2, 6, 10, 14, 15, 20]. They can also be defined for functions with nearly the same definition. For example, in [12], Ramaré gave some estimates on $\tilde{\psi}$, a function very similar to ψ. The behavior of ψ in arithmetic progressions can also be found in [13]. In the case where the sum is over the integers congruent to 1 modulo q, Lemma 9 of [5] gave an upper bound function for ψ in this particular progression.

2. Rosser and Schoenfeld's method

The first part of the proof uses the method developed by Rosser and Schoenfeld [18] and completed by Schoenfeld [19] to estimate the sum

$$\sum_{\rho \in \mathcal{R}_\zeta} \frac{x^\rho}{\rho}. \tag{3}$$

The critical strip $\{s \in \mathbb{C} : 0 < \mathfrak{Re}(s) < 1\}$ can be split into four regions according to whether the real part is greater than half or not and if the imaginary part is smaller than a parameter T or not. Let m be a positive integer. As in [18, p. 256], we express the sum (3) according to these four regions, with $\beta = \mathfrak{Re}(\rho)$ and $\gamma = \mathfrak{Im}(\rho)$ using the new form (2) of the zero-free region. Define

$$R_m(\delta) = \left((1+\delta)^{m+1}+1\right)^m, \tag{4}$$

$$S_1(m,\delta) = 2 \sum_{\beta \leqslant 1/2; 0<\gamma\leqslant T_1} \frac{2+m\delta}{2|\rho|}, \tag{5}$$

$$S_2(m,\delta) = 2 \sum_{\beta \leqslant 1/2; T_1<\gamma} \frac{R_m(\delta)}{\delta^m |\rho(\rho+1)\cdots(\rho+m)|}, \tag{6}$$

$$S_3(m,\delta) = 2 \sum_{\beta > 1/2; 0<\gamma\leqslant T_2} \frac{2+m\delta}{2|\rho|} \exp(-X^2/\ln\gamma), \tag{7}$$

$$S_4(m,\delta) = 2 \sum_{\beta > 1/2; T_2<\gamma} \frac{R_m(\delta)\exp(-X^2/\ln\gamma)}{\delta^m |\rho(\rho+1)\cdots(\rho+m)|}. \tag{8}$$

These correspond to expressions (3.6)–(3.10) of [18] with the new form of the zero-free region. By Lemma 8 of [18], for $x > 1$ and $0 < \delta < (x-1)/(xm)$, we have

$$\begin{aligned} &\frac{1}{x}\left|\psi(x) - \{x - \ln(2\pi) - \frac{1}{2}\ln(1-x^{-2})\}\right| \\ &\leqslant \{S_1(m,\delta) + S_2(m,\delta)\}/\sqrt{x} + S_3(m,\delta) + S_4(m,\delta) + m\delta/2. \end{aligned} \tag{9}$$

We have a good idea of the repartition of non-trivial zeros. Let $T \geqslant 2$ and $N(T)$ be the number of non-trivial zeros $\rho = \beta + i\gamma$ in the region $0 \leqslant \gamma \leqslant T$ and $0 \leqslant \beta \leqslant 1$. In 1941, Rosser [16, Theorem 19, p. 223] proved for $T \geqslant 2$ that

$$|N(T) - F(T)| < R(T) \tag{10}$$

with $F(T) = \frac{T}{2\pi}\ln\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8}$ and an error term

$$R(T) = 0.137\ln T + 0.443\ln\ln T + 1.588. \tag{11}$$

The error term $R(T)$ was recently updated by Trudgian [21].

Let n be a non-negative integer, R a constant parameter for the zero-free region (2) and

$$X = \sqrt{(\ln x)/R}, \tag{12}$$

$$\phi_n(y) = y^{-(n+1)}\exp(-X^2/\ln y), \tag{13}$$

$$W_n = \exp(X/\sqrt{n+1}). \tag{14}$$

The error term (11) appears in the Corollary of Lemma 7 of [18, p. 256]. We rewrite this corollary for $W = W_n$ and $\Phi = \phi_n$:

Lemma 2.1. *Let $2\pi < U \leqslant V$. Let ϕ_n be defined by (13) and W_n by (14). Let Y be the middle number in the ordered set $\{U, V, W_n\}$. Choose $j = 0$ if $V \geqslant W_n$ and $j = 1$ in the other case. Then*

$$\sum_{U<\gamma\leqslant V} \phi_n(\gamma) \leqslant \left(\frac{1}{2\pi} + (-1)^j q(Y)\right) \int_U^V \phi_n(y) \ln \frac{y}{2\pi} dy + E_j(U, V),$$

where

$$q(y) = \frac{R'(y)}{\ln(y/(2\pi))} = \frac{0.137 \ln y + 0.443}{y \ln y \ln(y/(2\pi))} \tag{15}$$

and

$$\begin{aligned} E_0(U, V) = {} & 2R(Y)\phi_n(Y) \\ & + \ (N(V) - F(V) - R(V))\phi_n(V) - (N(U) - F(U) + R(U))\phi_n(U) \end{aligned}$$

or

$$E_1(U, V) = (N(V) - F(V) + R(V))\phi_n(V) - (N(U) - F(U) + R(U))\phi_n(U).$$

Lemma 2.2. *Let m a positive integer and ν a positive real. Let*

$$Y = X(1-\nu)^2/\nu, \tag{16}$$

$$G_0 = \nu^2\{\nu - \ln(2\pi)/X\}, \tag{17}$$

$$T_2 = \exp(\nu X). \tag{18}$$

Let T_0 be a parameter satisfying $N(T_0) = F(T_0)$ such that there are no zeros ρ satisfying $\mathfrak{Re}(\rho) \neq 1/2$ with $0 < \mathfrak{Im}(\rho) \leqslant T_0$. If $T_2 \geqslant T_0 > 2\pi$ and $\nu \leqslant 1$, then

$$\begin{aligned} S_3(m, \delta) < {} & \frac{2 + m\delta}{4\pi} T_2 \exp(-2X) \exp(-Y) X G_0 \\ & + \ (2 + m\delta) R(T_2)\phi_0(T_2). \end{aligned} \tag{19}$$

Proof. The proof is similar to [19] (with an update of the form of zero-free region). As there are no zeros with $\beta > 1/2$ for $|\gamma| \leqslant T_0$, the summation can begin for $\gamma > T_0$ in S_3. Using Lemma 2.1 with $n = 0$ ($\nu \leqslant 1$, hence $T_2 \leqslant W_0$),

$$S_3(m, \delta) \leqslant \frac{2 + m\delta}{2} \left(\left\{ \frac{1}{2\pi} - q(T_2) \right\} \int_{T_0}^{T_2} \phi_0(y) \ln \frac{y}{2\pi} dy + E_1 \right), \tag{20}$$

where

$$\begin{aligned} E_1 &= \{N(T_2) - F(T_2) + R(T_2)\}\phi_0(T_2) - \{N(T_0) - F(T_0) + R(T_0)\}\phi_0(T_0) \\ &< 2R(T_2)\phi_0(T_2) \qquad \text{using (10) and } R(T_0)\phi_0(T_0) > 0. \end{aligned} \tag{21}$$

For $\alpha \leqslant 1$ and $x > 0$, the upper incomplete gamma function is defined and bounded as

$$\begin{aligned} \Gamma(\alpha, x) &= \int_x^\infty t^{\alpha-1} e^{-t} dt \\ &\leqslant x^{\alpha-1} \int_x^\infty \exp(-t) dt = x^{\alpha-1} \exp(-x) \end{aligned}$$

and we also have

$$
\begin{aligned}
\int_a^b \phi_0(y) \ln \frac{y}{2\pi} dy &= \int_a^b y^{-1} \exp(-X^2/\ln y) \ln \frac{y}{2\pi} dy \\
&= X^4\{\Gamma(-2,V') - \Gamma(-2,U')\} \\
&\quad -X^2 \ln(2\pi)\{\Gamma(-1,V') - \Gamma(-1,U')\}
\end{aligned} \tag{22}
$$

with $U' = X^2/\ln a$, $V' = X^2/\ln b$ by putting $y = \exp(X^2/t)$. We apply (22) with $a = T_0$ and $b = T_2$. Observing that $T_0 > 2\pi$ and $U' = X^2/\ln T_0$ implies $X^4\Gamma(-2,U') > X^2\ln(2\pi)\Gamma(-1,U')$, we can obtain an upper bound for (22). As $q(T_2) > 0$ and $V' = X^2/\ln T_2 = X/\nu$ by (18), we find by (20) and (21) the following upper bound:

$$
\begin{aligned}
S_3(m,\delta) &< \frac{2+m\delta}{2} \cdot \frac{1}{2\pi} \exp(-V')\{X^4V'^{-3} - X^2V'^{-2}\ln(2\pi)\} + \frac{2+m\delta}{2}E_1 \\
&< \frac{2+m\delta}{4\pi} \exp(-X/\nu)\{X\nu^3 - \nu^2\ln(2\pi)\} + (2+m\delta)R(T_2)\phi_0(T_2).
\end{aligned}
$$

We have

$$
\frac{1}{\nu} = 2 - \nu + \frac{(1-\nu)^2}{\nu}.
$$

Hence, by (16),

$$
\exp(-X/\nu) = \exp(-2X)T_2\exp(-Y). \tag{23}
$$

Finally, by (17),

$$
\begin{aligned}
S_3(m,\delta) < \; &\frac{2+m\delta}{4\pi} T_2 \exp(-2X)\exp(-Y)XG_0 \\
&+ (2+m\delta)R(T_2)\phi_0(T_2).
\end{aligned}
$$

The bound for S_3 is similar to [19, (7.11), p. 342]. □

Lemma 2.3. *Let m be a positive integer and ν a positive real. Let*

$$
G_1 = \frac{m-1}{\nu^2 m - 1}\nu^2 \left(\nu + \frac{1 - m\ln(2\pi)}{mX}\right), \tag{24}
$$

$$
G_2 = \frac{R_m(\delta)}{2^m}\left(1 + 2\pi q(T_2)\right). \tag{25}
$$

If $\nu > 1/\sqrt{m}$ and $X \geqslant \frac{m\ln(2\pi)-1}{\sqrt{m}}$, then

$$
S_4(m,\delta) < \frac{G_2G_1e^{-Y}}{2\pi(m-1)}\left(\frac{2}{\delta}\right)^m Xe^{-2X}T_2^{-(m-1)} + G_2\left(\frac{2}{\delta}\right)^m E_0. \tag{26}
$$

Proof. The proof is quite similar to [19]. We just add to the proof of [19] a requirement due to the use of the new form of zero-free region

$$
1 + 2/(2X\sqrt{m}) - \sqrt{m}\ln(2\pi)/X > 0.
$$

Using Lemma 2.1 with $n = m$ for (8),

$$
S_4(m,\delta) \leqslant \frac{R_m(\delta)}{\delta^m}\left(\left\{\frac{1}{2\pi} + q(T_2)\right\}\int_{T_2}^{\infty}\phi_m(y)\ln\frac{y}{2\pi}dy + E_0\right), \tag{27}
$$

where

$$
\begin{aligned}
E_0 &\leqslant \{R(T_2) + F(T_2) - N(T_2)\}\phi_m(T_2) \\
&< 2R(T_2)\phi_m(T_2) = 2R(T_2)\phi_0(T_2)T_2^{-m} \text{ by (10) and (13).}
\end{aligned} \tag{28}
$$

The previous integral can be expressed with incomplete Bessel functions defined for $z > 0$ and $x \geqslant 0$,

$$K_\nu(z,x) = \frac{1}{2}\int_x^\infty t^{\nu-1}H^z(t)dt \tag{29}$$

with

$$H^z(t) = \exp\{-\frac{1}{2}z(t+1/t)\}.$$

We have

(30)

$$\int_{T_2}^\infty \phi_m(y)\ln\frac{y}{2\pi}dy = \frac{2X^2}{m}\left\{K_2(2X\sqrt{m},\nu\sqrt{m}) - \frac{\sqrt{m}\ln(2\pi)}{X}K_1(2X\sqrt{m},\nu\sqrt{m})\right\}.$$

Unlike Schoenfeld's proof, the coefficient before K_1 is negative and we have to minimize this term. But we know (by Lemma 4 and Lemma 5 of [18, p. 252]) that for $z > 0$ and $x > 1$:

- $K_1(z,x) < x^2H^z(x)/\{z(x^2-1)\}$,
- $K_2(z,x) < (x-1)x^2H^z(x)/\{z(x^2-1)\} + (1+2/z)K_1(z,x)$.

First, as we assume that $\nu > 1/\sqrt{m}$, we can apply these bounds for K_2 with $z = 2X\sqrt{m} > 0$ and $x = \nu\sqrt{m} > 1$. Then the upper bound for K_2 involves a K_1 part. As we assume that $X \geqslant \frac{m\ln(2\pi)-1}{\sqrt{m}}$, the total coefficient before K_1 becomes positive. Hence we can apply the previous upper bounds (for K_2 and K_1) and get

$$\begin{aligned} &K_2(2X\sqrt{m},\nu\sqrt{m}) + \frac{-\sqrt{m}\ln(2\pi)}{X}K_1(2X\sqrt{m},\nu\sqrt{m}) \\ &< \left(\nu + \frac{1-m\ln(2\pi)}{mX}\right)\frac{\nu^2 m}{2X(\nu^2m-1)}\exp\left\{-X\sqrt{m}\left(\nu\sqrt{m}+\frac{1}{\nu\sqrt{m}}\right)\right\}.\end{aligned}$$

Now, by (16) and (24), we have

$$X\sqrt{m}\left(\nu\sqrt{m}+\frac{1}{\nu\sqrt{m}}\right) = m\nu X + (2X - \nu X + Y)$$

and

$$\begin{aligned} &K_2(2X\sqrt{m},\nu\sqrt{m}) + \frac{-\sqrt{m}\ln(2\pi)}{X}K_1(2X\sqrt{m},\nu\sqrt{m}) \\ &< \frac{m}{2(m-1)}G_1X^{-1}e^{-Y}e^{-2X}(T_2)^{-m+1}.\end{aligned}$$

Hence by (30),

$$\int_{T_2}^\infty \phi_m(y)\ln\frac{y}{2\pi}dy = \frac{G_1}{m-1}e^{-Y}T_2^{-(m-1)}Xe^{-2X}.$$

We have by (27) and (25),

$$S_4(m,\delta) < \frac{G_2G_1e^{-Y}}{2\pi(m-1)}\left(\frac{2}{\delta}\right)^m Xe^{-2X}T_2^{-(m-1)} + G_2\left(\frac{2}{\delta}\right)^m E_0.$$

The bound for S_4 is similar to the expression to that of [19, (7.20), p. 344]. □

Some parameters will be set for optimizing the sum of the S_3 and S_4 bounds.

Lemma 2.4. *Let G_0, G_1, G_2, T_0, T_2 be defined as above and a function k defined by*

$$k(\nu) = \frac{X}{2\pi}\left(\frac{G_0^3}{G_1}\right)^{1/2} e^{-2X(1-\nu)} e^{-X(1-\nu)^2/\nu}. \tag{31}$$

If there exists a real $\nu \in]1/\sqrt{2}, 1]$ such that $k(\nu) = 1$ and if $X > \sqrt{2}\ln(2\pi)$, then

$$T_2 \;=\; (G_1/G_0)^{1/4}\{2\pi e^Y/G_0\}^{1/2} X^{-1/2} e^X, \tag{32}$$

$$\delta \;=\; \sqrt{\frac{2}{\pi}}(G_0G_1)^{1/4} e^{-Y/2} X^{1/2} e^{-X}, \tag{33}$$

and, moreover, if $T_2 \geqslant T_0 > 2\pi$, then

$$\begin{aligned} S_3(2,\delta) + S_4(2,\delta) + \delta < G_2\left\{G_0G_1\right\}^{1/4} e^{-Y/2}\sqrt{\frac{8}{\pi}} X^{1/2} e^{-X} \\ +\; 2G_2\left\{1 + G_0/G_1\right\} R(T_2)\phi_0(T_2). \end{aligned} \tag{34}$$

Proof. By (4) and (25), we have $2 + m\delta < 2R_m(\delta)/2^m < 2G_2$. We gather the estimates (19) and (26) of S_3 and S_4:

$$\begin{aligned} S_3(m,\delta) + S_4(m,\delta) \;<\; & \frac{G_2 e^{-Y}}{2\pi} X e^{-2X}\left\{G_0T_2 + \frac{G_1}{m-1}\left(\frac{2}{\delta}\right)^m T_2^{-(m-1)}\right\} \\ & + 2G_2R(T_2)\phi_0(T_2)\left\{1 + \left(\frac{2}{\delta T_2}\right)^m\right\}. \end{aligned}$$

We choose

$$T_2 = (G_1/G_0)^{1/m}\cdot 2/\delta \tag{35}$$

to minimize the first expression between braces. We obtain

$$\begin{aligned} S_3(m,\delta) + S_4(m,\delta) + \frac{1}{2}m\delta \;<\; & \frac{1}{2}mG_2\left\{G_0^{1-1/m}G_1^{1/m}\frac{2e^{-Y}}{(m-1)\pi} X e^{-2X}\delta^{-1} + \delta\right\} \\ & + 2G_2R(T_2)\phi_0(T_2)\left\{1 + G_0/G_1\right\}. \end{aligned}$$

The expression inside braces is minimized by choosing

$$\delta = \left\{G_0^{1-1/m}G_1^{1/m}\frac{2e^{-Y}}{(m-1)\pi}\right\}^{1/2} X^{1/2}e^{-X}. \tag{36}$$

We get

$$\begin{aligned} S_3(m,\delta) + S_4(m,\delta) + \frac{1}{2}m\delta \;<\; & G_2\left\{G_0^{1-1/m}G_1^{1/m}\frac{2e^{-Y}}{\pi}\right\}^{1/2}\frac{m}{\sqrt{m-1}} X^{1/2}e^{-X} \\ & + 2G_2\left\{1 + G_0/G_1\right\} R(T_2)\phi_0(T_2). \end{aligned}$$

The coefficient $m/\sqrt{m-1}$ is minimized by choosing $m = 2$. For this value, we obtain (32) by (35) and (36)

$$T_2 = (G_1/G_0)^{1/4}\{2\pi e^Y/G_0\}^{1/2} X^{-1/2} e^X$$

and by (24) with $m = 2$,

$$G_1 = \frac{\nu^2}{2\nu^2 - 1}\left(\nu + \frac{1 - 2\ln(2\pi)}{2X}\right). \tag{37}$$

We have two definitions (18) and (32) of T_2. They are consistent if

$$\exp(\nu X) = \sqrt{2\pi}\left(\frac{G_1}{G_0^3}\right)^{1/4} e^{Y/2} X^{-1/2} e^X.$$

By taking squares (assume $\nu > 1/\sqrt{2}$ and $X > \sqrt{2}\ln(2\pi)$), the definitions are consistent if there exists ν such that $k(\nu) = 1$ where

$$k(\nu) = \frac{X}{2\pi}\left(\frac{G_0^3}{G_1}\right)^{1/2} e^{-2X(1-\nu)} e^{-X(1-\nu)^2/\nu}.$$

It is the same definition as in [19, (7.27), p. 345]. □

3. Upper bound function

Lemma 3.1. *Let $k(\nu)$ defined by* (31). *For $X \geq 8.36$, the solution ν of $k(\nu) = 1$ is unique and belongs to the interval*

$$0.97 < 1 - \frac{1}{2X}\ln\left(\frac{X}{2\pi}\right) < \nu < 1. \tag{38}$$

Proof. For $\nu \in]1/\sqrt{2}, 1]$, G_0, defined by (17), is a positive and increasing function of ν if $X > \frac{2}{3}\sqrt{2}\ln(2\pi)$ and G_1, defined by (37), decreases assuming that $X > 2\ln(2\pi) - 1$. Hence, for $X > 2\ln(2\pi) - 1$, k increases for $\nu \in]1/\sqrt{2}, 1]$. Now, as $\lim_{\nu \to 1^+/\sqrt{2}} k(\nu) = 0$ and

$$\begin{aligned} k(1) &= \frac{X}{2\pi}\left(\frac{(1 - \frac{\ln(2\pi)}{X})^3}{1 + \frac{1 - 2\ln(2\pi)}{2X}}\right)^{1/2}, \\ k(1) &> 1 \text{ for } X \geqslant 8.36, \end{aligned}$$

we have a unique $\nu \in]1/\sqrt{2}, 1[$ such that $k(\nu) = 1$. The validity bound (8.36 value) can be exactly computed: $\frac{\sqrt{3}}{3}(4\pi\cos(\frac{1}{3}\arctan(\sqrt{\frac{(8\pi)^2}{27} - 1})) + \sqrt{3}\ln(2\pi))$. Let

$$\nu_0 = 1 - \frac{1}{2X}\ln\left(\frac{X}{2\pi}\right). \tag{39}$$

For $X \geqslant 8.36$, the function $X \mapsto 1 - \frac{1}{2X}\ln\left(\frac{X}{2\pi}\right)$ reaches its minimum for $X = 2\pi e$ with the value 0.97 and has an asymptotic maximum equal to 1. We now show that $k(\nu_0) < 1$. We have by (39) and (31)

$$k(\nu_0) = \left(\frac{G_0^3}{G_1}\right)^{1/2} \exp\left(-\frac{1}{4\nu_0 X}\ln^2(X/(2\pi))\right)$$

with, by (17) and (24),

$$\frac{G_0^3}{G_1} = \nu_0^4(2\nu_0^2 - 1)\left(\nu_0 - \frac{\ln(2\pi)}{X}\right)^2\left(1 - \frac{1}{2X\nu_0 - 2\ln(2\pi) + 1}\right).$$

With $\nu_0 \in]1/\sqrt{2}, 1]$, we have for $X > \ln(2\pi)$,

$$0 < \frac{G_0^3}{G_1} < 1. \tag{40}$$

□

Lemma 3.2. *Let G_0, G_1, G_2 defined as above, with $m = 2$. For $X \geqslant 8.36$ and $0.97 < 1 - \frac{1}{2X}\ln\left(\frac{X}{2\pi}\right) < \nu < 1$, we have the following bounds:*

$$0.61 < G_0G_1 < 1,$$

$$G_0/G_1 < 1,$$

$$1 \leqslant e^Y < 1.0223,$$

$$G_2 > 1.$$

Proof. With $m = 2$, by (17) and (24), we have

$$G_0G_1 = \frac{\nu^6}{2\nu^2 - 1}\left(1 + \frac{1 - 2\ln(2\pi)}{2X\nu}\right)\left(1 - \frac{\ln(2\pi)}{X\nu}\right).$$

For $0.97 < \nu \leqslant 1$, the function $\nu \mapsto \frac{\nu^6}{2\nu^2-1}$ is increasing. Then we have for $X > 0$ and $\nu < 1$, $G_0G_1 < \frac{\nu^6}{2\nu^2-1} < 1$ and for $X \geqslant 8.36$ and $\nu > 0.97$, $G_0G_1 > 0.61$. We have by (17) and (24), for $m = 2$, $G_0/G_1 < 2\nu^2 - 1 < 1$. As $1 - \frac{1}{2X}\ln\left(\frac{X}{2\pi}\right) < \nu < 1$ and the function $(1-\nu)^2/\nu$ decreases for $\nu \in]0, 1]$, we have by (16), $0 \leqslant Y \leqslant \frac{\ln\frac{X}{2\pi}}{4X - 2\ln\frac{X}{2\pi}}$ which is bounded by $0.022\cdots$ for $X > 2\pi$ (maximum reached for $X \approx 45.43$). By (4) and (25), we have $1 < 1 + m\delta/2 < R_m(\delta)/2^m < G_2$. □

Lemma 3.3. *Let $R(T), \phi_0(T)$ defined respectively by* (11) *and* (13), *$T_2 > 2\pi$ defined by* (18) *with $\nu \leqslant 1$. Then, with Y defined by* (16) *and $X \geqslant 8.36$, we have*

$$R(T_2)\phi_0(T_2) < 1.15Xe^{-2X}.$$

Proof. We have $R(T_2)\phi_0(T_2) = \frac{R(T_2)}{\ln T_2}\ln(T_2)e^{-Y}e^{-2X}$ by (16). By Lemma 3.2, $e^{-Y} < 1$. As $\nu \leqslant 1$, $\ln T_2 \leqslant X$. We study the function $\frac{R(y)}{\ln y}$, which decreases for $y \geqslant 1.1$. For $y \geqslant 2\pi$, $\frac{R(y)}{\ln y} \leqslant \frac{R(2\pi)}{\ln 2\pi} \approx 1.1477\cdots$. □

Lemma 3.4. *Let X and R be defined respectively by* (12) *and* (2). *We assume $X > 8/R$. Then, with the choice* (33) *of δ, we have for $X \geqslant 8.36$,*

(41)
$$\frac{1}{\sqrt{x}}\{S_1(2,\delta) + S_2(2,\delta)\} + 1.43/\sqrt{x} + \ln(2\pi)/x \leqslant 0.0033\sqrt{\frac{8}{\pi}}G_2(G_0G_1)^{1/4}Xe^{-2X}.$$

Proof. Taking $T_1 = 0$, we obtain by (5) and (6),

$$\begin{aligned}
\frac{1}{\sqrt{x}}\{S_1(2,\delta) + S_2(2,\delta)\} &\leqslant \frac{1}{\sqrt{x}}\frac{R_2(\delta)}{\delta^2}\sum_\gamma \frac{1}{|\gamma|^3} \\
&< \frac{1}{\sqrt{x}}G_2\left(\frac{2}{\delta}\right)^2\sum_\gamma \frac{1}{|\gamma|^3} \\
&< \frac{4}{\delta^2\sqrt{x}}G_2 \cdot 0.00167 \text{ by Lemma 17 of [16]} \\
&< C_0\sqrt{\frac{8}{\pi}}G_2(G_0G_1)^{1/4}Xe^{-2X} \text{ by (33)}
\end{aligned}$$

with $C_0 = \frac{0.00167\pi\sqrt{\pi/2}e^Y}{(G_0G_1)^{3/4}}e^{4X}/\sqrt{x}$. As $X \geqslant 8/R$, $e^{4X}/\sqrt{x} \leqslant 1$ by (12). For $X \geqslant 8.36$ by Lemma 3.2, $C_0 < 0.003277$. In the same manner,

$$\frac{1.43}{\sqrt{x}} + \frac{\ln(2\pi)}{x} < C_1\sqrt{\frac{8}{\pi}}G_2(G_0G_1)^{1/4}Xe^{-2X}$$

with $C_1 = \sqrt{\frac{\pi}{8}}\frac{1.43e^{-2X}+e^{-6X}\ln(2\pi)}{G_2(G_0G_1)^{1/4}X} < 10^{-8}$ by Lemma 3.2. $\square$

Lemma 3.5. *Let G_2 be defined by* (25) *with $\nu > 1/\sqrt{2}$. With the choices $m = 2$ and δ set by* (33)*, assuming $k(\nu) = 1$ exists, we have for $X \geqslant 2\pi$,*

$$G_2 < \exp\left(2.64X^{1/2}e^{-X}\right). \tag{42}$$

Proof. By Lemma 3.2, $(G_0G_1)^{1/4} < 1$ and $e^{-Y/2} < 1$, hence $\delta < \sqrt{\frac{2}{\pi}}X^{1/2}e^{-X}$ by (33) and for $X \geqslant 2\pi$, $\delta < \sqrt{\frac{2}{\pi}}\sqrt{2\pi}e^{-2\pi}$ and $3 + 3\delta + \delta^2 < 3.01122$.

$$\begin{aligned}
\frac{R_2(\delta)}{2^2} &= \left\{\frac{(1+\delta)^3+1}{2}\right\}^2 = \left\{1 + \frac{1}{2}\delta(3+3\delta+\delta^2)\right\}^2 \\
&< \left(1 + \frac{3.01122}{2}\delta\right)^2 \\
&< \exp\left(\frac{3.01122}{2}\delta\right)^2 = \exp(3.01122\delta) \\
&< \exp(2.41 \cdot X^{1/2}e^{-X}) \text{ by (33).}
\end{aligned}$$

As $X > 2\pi$, $\nu > 1/\sqrt{2}$ and $T_2 = \exp(\nu X)$ by (18), we have $T_2 > \exp(2\pi/\sqrt{2})$. Then

$$\begin{aligned}
\{1 + 2\pi q(T_2)\} &= 1 + \frac{0.137 + 0.443/\ln T_2}{\ln(T_2/(2\pi))} \cdot \frac{2\pi}{T_2} \quad \text{by (15)} \\
&= 1 + \frac{0.137 + \frac{0.443}{\ln T_2}}{\ln(T_2/(2\pi))} \cdot \sqrt{2\pi}\left(\frac{G_0^3}{G_1}\right)^{1/4} e^{-Y/2}X^{1/2}e^{-X} \text{ by (32)} \\
&< 1 + 0.23X^{1/2}e^{-X} \text{ by (40)} \\
&< \exp(0.23 \cdot X^{1/2}e^{-X}).
\end{aligned}$$

$\square$

Proof of Theorem 1.1. By (9) or Lemma 8 of [18] with $m = 2$, we have $\frac{1}{x}|\psi(x) - x| < (S_1(2,\delta) + S_2(2,\delta))/\sqrt{x} + S_3(2,\delta) + S_4(2,\delta) + \delta + \frac{\ln(2\pi)}{x}$, with δ defined by (33). The choice for δ satisfies the conditions (9) set by Lemma 8 of [18] for $X \geqslant \max(8.36, 8/R)$ with Lemma 3.2. Now Theorem 13 of [17] gives

$$\frac{1}{x}|\vartheta(x) - x| < \frac{1}{x}|\psi(x) - x| + 1.43/\sqrt{x}.$$

We choose $T_0 = 17.8478\cdots$ such that $F(T_0) = N(T_0)$. We have $T_0 > 2\pi$ and T_0 satisfies the condition on zeros with the verification [8] of the Riemann hypothesis up to T_0. By Lemmas 3.1, 2.4 and 3.2,

$$\begin{aligned}
&S_3(2,\delta)+S_4(2,\delta)+\delta \\
&\quad < \quad G_2(G_0G_1)^{1/4}\sqrt{\frac{8}{\pi}}X^{1/2}e^{-X} + 4G_2R(T_2)\phi_0(T_2) \\
&\quad < \quad G_2(G_0G_1)^{1/4}\sqrt{\frac{8}{\pi}}X^{1/2}e^{-X}(1+3.2618X^{1/2}e^{-X}) \text{ by Lemmas 3.3 and 3.2.}
\end{aligned}$$

By Lemma 3.4,

$$\begin{aligned}
&(S_1(2,\delta)+S_2(2,\delta))/\sqrt{x}+S_3(2,\delta)+S_4(2,\delta)+\delta+\frac{\ln(2\pi)}{x}+\frac{1.43}{\sqrt{x}} \\
&\quad < \quad G_2(G_0G_1)^{1/4}\sqrt{\frac{8}{\pi}}X^{1/2}e^{-X}(1+3.27X^{1/2}e^{-X}) \\
&\quad < \quad G_2(G_0G_1)^{1/4}\sqrt{\frac{8}{\pi}}X^{1/2}e^{-X}\exp(3.27X^{1/2}e^{-X}) \\
&\quad < \quad (G_0G_1)^{1/4}\sqrt{\frac{8}{\pi}}X^{1/2}e^{-X}\exp(5.91X^{1/2}e^{-X}) \text{ by Lemma 3.5.}
\end{aligned}$$

Let $G_3 = (G_0G_1)^{1/4}\exp(5.91X^{1/2}e^{-X}) = \left[(\nu^2G_1)\left(\frac{G_0}{\nu^2}\exp(23.64X^{1/2}e^{-X})\right)\right]^{1/4}$. By (24), we have $\nu^2G_1 = \frac{\nu^5}{2\nu^2-1}\left(1+\frac{1-2\ln(2\pi)}{2X\nu}\right)$. The derivative of the function $\nu \mapsto \nu^2G_1$ has the same sign as the expression $6X\nu^3+(2-4\ln(2\pi))\nu^2-5X\nu+4\ln(2\pi)-2$. For $X>0$ and $\nu\in[0.97,1]$, this expression is positive. Then $\nu^2G_1 < 1+\frac{1-2\ln(2\pi)}{2X}$. By (17) and $\nu<1$, $\frac{G_0}{\nu^2}\exp(\alpha X^{1/2}e^{-X}) = (\nu-\ln(2\pi)/X)\exp(\alpha X^{1/2}e^{-X}) < (1-\ln(2\pi)/X)\exp(\alpha X^{1/2}e^{-X})$. By studying the derivative, if $\frac{\ln(2\pi)}{X^2} > \alpha\sqrt{X}e^{-X}$, the function increases and is bounded by 1. For $\alpha = 23.64$, the condition is valid for $X \geqslant 7.64$. Then an upper bound function for $|\psi(x)-x|/x$ or $|\vartheta(x)-x|/x$ is

$$\varepsilon_R(x) = \sqrt{\frac{8}{\pi}}\left(1-\frac{\ln(2\pi)-1/2}{X}\right)^{1/4}X^{1/2}e^{-X}. \qquad \square$$

Proof of Corollary 1.2 . We apply the Theorem 1.1 with the value $R = 5.69693$ found by Kadiri [9]. Our result is sharper than Schoenfeld's (1) only for $x > \exp(300)$. We show that the result holds between $\exp(300)$ and $\exp(400)$ using [19] (entry $b = 300$ of Table p. 358). We have checked numerically the bounds for $3 \leqslant x \leqslant 101$. $\square$

4. Estimates for moderate values of x

For moderate values of x, direct computations are significantly better than the global upper bound and can be computed to extend the area where the global upper bound holds.

Lemma 4.1. *Let $T_1 \geqslant 12\,030.00896$ and $b > 1/2$. Let T_2 be such that $A \leqslant T_2 \leqslant \exp\sqrt{b/R}$. Let m be a positive integer, $z = 2X\sqrt{m} = 2\sqrt{mb/R}$, $Y =$*

$\max(T_2, W_m)$, $T_2' = (2m/z)\ln T_2$. *Let*

$$\begin{aligned}
(43)\qquad \Omega_1 &= \frac{2+m\delta}{4\pi}\left\{\left(\ln\frac{T_1}{2\pi}+\frac{1}{m}\right)^2+\frac{1}{m^2}+G(T_1)\right\}\\
&\qquad \textit{with } G(T_1) = -0.212544 - \frac{2.31m}{(m+1)T_1},\\
(44)\qquad \Omega_2^* &= \frac{(0.159155)zR_m(\delta)}{2m^2}\left\{zK_2(z,T_2') - 2m\ln(2\pi)K_1(z,T_2')\right\}\\
&\quad + R_m(\delta)\{2R(Y)\phi_m(Y)\},\\
(45)\qquad \Omega_3 &= \frac{2+m\delta}{4\pi}\left[X^4\left\{\Gamma(-2,\frac{b}{R\ln T_2}) - \Gamma(-2,\frac{b}{R\ln A})\right\}\right.\\
&\qquad\left. -X^2\ln(2\pi)\left\{\Gamma(-1,\frac{b}{R\ln T_2}) - \Gamma(-1,\frac{b}{R\ln A})\right\}\right]\\
&\quad + \frac{2+m\delta}{2}\left[2R(T_2)\phi_0(T_2) - R(A)\phi_0(A)\right] + \Omega_2^*\delta^{-m}.
\end{aligned}$$

If $0 < \delta < (1-e^{-b})/m$ *then, for all* $x \geqslant e^b$,

$$|\psi(x) - x| < \varepsilon x$$

where

$$\varepsilon = \Omega_1 e^{-b/2} + \Omega_3 + m\delta/2 + e^{-b}\ln(2\pi).$$

Proof. It is a rewriting of Theorem 5 of [18, p. 264] for the new zero-free region, combined with Lemma 9* of [19, p. 352]. □

Theorem 4.2. *If* $x \geqslant e^b$, *then*

$$|\psi(x) - x| < \varepsilon_b x,$$

where ε_b *can be chosen in the tabulated values of* ε *against* b *in Tables* 1 *or* 2 .

Proof. The last work on numerical verification of the Riemann Hypothesis is from Platt [11] in 2011. His method does not reach great heights but his approach is different from previous ones. In particular, Wedeniwski [22] in 2003 and Gourdon [7] in 2004 had announced higher values of A.

We use two values for A: the first, $A_0 = 30\ 610\ 046\ 000$ is deduced from the work of [11, p. 12], and the second $A_1 = 2\ 445\ 999\ 556\ 030.34$ from the work of [7]. We use Lemma 4.1 to compute the values ε. These values have been computed by Pari/GP software, using approximations of $K_1(z, x)$ and $K_2(z, x)$ given in pp. 251–252 of [18]. The dichotomy method was used to find the best T_2 value between A and $\exp(X)$. The values have been also checked with Maple software. Note that the influence of the height A fades for large values of x. Note also that, for $b \leqslant 5\,000$, the method and the values obtained by [4] are better. □

TABLE 1. $|\psi(x) - x| \leqslant \varepsilon x$ for $x \geqslant \exp(b)$ with $A = A_0$

b	m	δ	T_2	ε
4 000	2	$1.1890 \cdot 10^{-11}$	176 299 633 876	$2.2732 \cdot 10^{-11}$
4 500	2	$2.4925 \cdot 10^{-12}$	818 607 249 859	$4.8205 \cdot 10^{-12}$
5 000	2	$5.5813 \cdot 10^{-13}$	3 689 208 595 186	$1.0887 \cdot 10^{-12}$
6 000	2	$3.4159 \cdot 10^{-14}$	62 122 177 420 055	$6.7839 \cdot 10^{-14}$
7 000	2	$2.6079 \cdot 10^{-15}$	836 413 627 936 444	$5.2649 \cdot 10^{-15}$
8 000	2	$2.3743 \cdot 10^{-16}$	9 408 404 902 762 368	$4.8646 \cdot 10^{-16}$
9 000	2	$2.4968 \cdot 10^{-17}$	91 354 948 828 713 929	$5.1847 \cdot 10^{-17}$
9 963	2	$3.2000 \cdot 10^{-18}$	725 724 755 308 452 870	$6.7240 \cdot 10^{-18}$
10 000	2	$2.9627 \cdot 10^{-18}$	784 268 545 258 411 610	$6.2288 \cdot 10^{-18}$
13 900	2	$1.7387 \cdot 10^{-21}$	1 416 256 696 499 307 770 372	$3.8041 \cdot 10^{-21}$
20 000	2	$9.7193 \cdot 10^{-26}$	26 995 134 915 435 610 800 632 362	$2.2294 \cdot 10^{-25}$

TABLE 2. $|\psi(x) - x| \leqslant \varepsilon x$ for $x \geqslant \exp(b)$ with $A = A_1$

b	m	δ	T_2	ε
4 700	2	$1.1561 \cdot 10^{-12}$	2 445 999 556 030	$1.7342 \cdot 10^{-12}$
5 000	2	$5.5901 \cdot 10^{-13}$	3 671 451 453 116	$9.3307 \cdot 10^{-13}$
6 000	2	$3.3945 \cdot 10^{-14}$	63 329 872 175 071	$6.7604 \cdot 10^{-14}$
7 000	2	$2.6067 \cdot 10^{-15}$	837 621 322 691 459	$5.2647 \cdot 10^{-15}$
8 000	2	$2.3741 \cdot 10^{-16}$	9 409 612 597 517 383	$4.8646 \cdot 10^{-16}$
9 000	2	$2.4968 \cdot 10^{-17}$	91 356 156 523 468 944	$5.1847 \cdot 10^{-17}$
9 963	2	$3.2000 \cdot 10^{-18}$	725 725 963 003 207 885	$6.7240 \cdot 10^{-18}$
10 000	2	$2.9627 \cdot 10^{-18}$	784 269 752 953 166 625	$6.2288 \cdot 10^{-18}$
13 900	2	$1.7387 \cdot 10^{-21}$	1 416 256 697 707 002 525 387	$3.8041 \cdot 10^{-21}$
20 000	2	$9.7193 \cdot 10^{-26}$	26 995 134 915 436 818 495 387 377	$2.2294 \cdot 10^{-25}$

ACKNOWLEDGEMENT

The author would like to thank the anonymous reviewers for their valuable comments and suggestions to improve the quality of this paper.

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