

EXPLICIT BOUNDS FOR DICKMAN'S FUNCTION

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Abstract

Dickman's function $\rho(u)$ denotes the natural density of integers n whose largest prime factor does not exceed $n^{1/u}$. We establish numerically explicit upper and lower bounds for $\rho(u)$, resulting in estimates with a relative error of less than $0.005/u^2$ for all $u \geq 5$. This allows for an approximate evaluation of $\rho(u)$ without the need to solve the delay differential equation numerically.

1. Introduction

Dickman's function $\rho(u)$ is defined as the continuous solution to the delay differential equation $u\rho'(u) + \rho(u-1) = 0$ with initial condition $\rho(u) = 1$ for $0 \leq u \leq 1$. It represents the natural density of integers n whose largest prime factor does not exceed $n^{1/u}$ [3].

For $u > 1$, let $\xi = \xi(u)$ be the unique positive solution of $e^\xi = 1 + u\xi$ and put $\xi(1) = 0$. Define

$$I(s) := \int_0^s \frac{e^z - 1}{z} dz.$$

De Bruijn [2] showed that $\rho(u) \sim \tilde{\rho}(u)$ as $u \to \infty$, where

$$\tilde{\rho}(u) := \frac{\exp\{\gamma - u\xi + I(\xi)\}}{\sqrt{2\pi I''(\xi)}}$$

and γ is Euler's constant. Alladi [1] sharpened this to $\rho(u) = \tilde{\rho}(u)(1 + O(1/u))$. Our goal is to make the estimate entirely explicit, providing a convenient way to obtain approximate values of $\rho(u)$ without the need to solve the delay differential equation numerically.

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Theorem 1. *For $u > 1$ we have*

$$\tilde{\rho}(u)\left(1-\frac{1}{12u}\right) < \rho(u) < \tilde{\rho}(u)\left(1-\frac{1}{12u(1+\frac{1}{\log u})}\right).$$

Table 1 lists numerical examples based on Theorems 1 and 2, the first four of which are consistent with the values obtained by van de Lune and Wattel [12], who iterate the trapezoidal rule to approximate $\rho(u)$ to at least five significant digits for many values of $u \le 1000$.

u	a: Thm. 1	a: Thm. 2	b
5	3.5...	3.54...	4
20	2.46...	2.461...	29
100	1.000...	1.000595...	229
1000	4.5876...	4.5876682...	3464
10000	4.8487...	4.848709620...	45867

Table 1: Values of $\rho(u) = a \cdot 10^{-b}$ from Theorems 1 and 2.

We will derive Theorem 1 from Theorem 2, which involves the expression

$$\alpha(u) := \frac{1}{8}\frac{I^{(4)}(\xi)}{(I^{(2)}(\xi))^2} - \frac{5}{24}\frac{(I^{(3)}(\xi))^2}{(I^{(2)}(\xi))^3} \sim -\frac{1}{12u},$$

where the derivatives $I^{(k)}(s)$ can easily be found from $I'(s) = (e^s - 1)/s$.

Theorem 2. *We have*

$$\rho(u) = \tilde{\rho}(u)\left(1 + \alpha(u) + \frac{\theta(u)}{u^2}\right),$$

where $|\theta(u)| < 0.005$ for $u \ge 5$, and $0 < \theta(u) < 0.005$ for $u \ge 9$.

Figure 1 shows the graph of $\rho(u)/\tilde{\rho}(u)$, the bounds from Theorem 1 and the estimate $1 + \alpha(u)$ from Theorem 2, for $1 < u \le 10$.

Dickman [3] showed that $\rho(u) = \lim_{x\to\infty} \Psi(x, x^{1/u})/x$, where $\Psi(x, y)$ denotes the number of positive integers up to x whose largest prime factor does not exceed y. Pomerance [5, Equation (1.25)] asked if $\Psi(x, y) \ge x\rho(u)$ holds for $x/2 \ge y \ge 1$, where $u = (\log x)/\log y$. Gorodetsky [4] confirmed this for x sufficiently large, assuming the Riemann hypothesis and one additional hypothesis about the error term in the prime number theorem [4, Equation (1.7)]. Together with Theorem 1 or Theorem 2, we obtain conditional lower bounds for $\Psi(x, y)$ that are easy to evaluate numerically. Hildebrand and Tenenbaum [7], Smida [10] and Xuan [14] derive asymptotic expansions for $\rho(u)$, but without being numerically explicit.

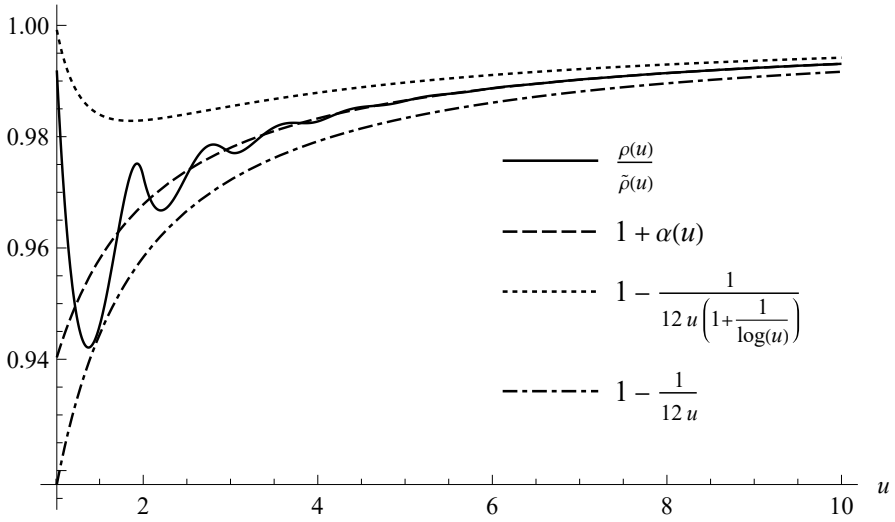

Figure 1: Theorems 1 and 2 for $1 < u \le 10$.

To compute $\tilde{\rho}(u)$ (or $\log \tilde{\rho}(u)$ when u is large) and $\alpha(u)$, note that

$$I(\xi) = \mathrm{Ei}(\xi) - \gamma - \log \xi,$$

where $\mathrm{Ei}(z)$ is the exponential integral (`ExpIntegralEi[z]` in Mathematica, and `real(-incgam(0,-z))` in PARI/GP for $z \in \mathbb{R}^+$), and

$$\xi = \xi(u) = -W_{-1}\left(-\frac{e^{-1/u}}{u}\right) - \frac{1}{u},$$

where $W_{-1}(z)$ is the lower of the two real branches, for $-1/e \le z < 0$, of the Lambert W function (`ProductLog[-1,z]` in Mathematica, and `lambertw(z,-1)` in PARI/GP).

Buchstab's function $\omega(u)$ is the unique continuous solution, for $u \ge 1$, of the delay differential equation $(u\omega(u))' = \omega(u-1)$, with initial condition $\omega(u) = 1/u$ for $1 \le u \le 2$. It arises in connection with the distribution of integers free of small prime factors [11, Chapter III.6]. Corollary 1 shows that $\tilde{\rho}(u)$ can serve as a convenient and numerically explicit upper bound for $|\omega(u) - e^{-\gamma}|$, although it is not of the smallest possible order of magnitude [6]. We obtain more accurate and numerically explicit estimates in [13].

Corollary 1. *For $u \ge 1$, we have*

$$|\omega(u) - e^{-\gamma}| < \rho(u) < \tilde{\rho}(u), \qquad |\omega'(u)| \le \rho(u) < \tilde{\rho}(u).$$

Proof. The inequality $\rho(u) < \tilde{\rho}(u)$ follows from Theorem 1. Tenenbaum [11, Theorem III.6.6] shows that $|\omega'(u)| \le \rho(u)$, which implies

$$|\omega(u) - e^{-\gamma}| = |\int_u^\infty \omega'(t)dt| \le \int_u^\infty \rho(t)dt < \int_u^\infty -\rho'(t)dt = \rho(u),$$

where the last inequality follows from

$$\rho(t) = \frac{1}{t}\int_{t-1}^{t} \rho(v)dv < \frac{1}{t}\rho(t-1) = -\rho'(t),$$

for $t > 1$. □

2. Proof of Theorem 2

We follow the proof of Tenenbaum [11, Theorem III.5.13], where Alladi's result [1, Equation (3.9)] with a relative error of $O(u^{-1})$ is established via the saddle point method. To obtain a relative error of $< 0.005u^{-2}$, we keep track of all constant factors, divide the range of integration into one extra interval, and use a Taylor polynomial of order seven instead of three near the saddle point. For small values of u, we verify the result by calculating $\rho(u)$ numerically as described in Section 4. We will need the following lemmas.

Lemma 1. *For real $x > 0$ and natural numbers k we have*

$$\frac{e^x - 1}{x} \ge I^{(k)}(x) \ge I^{(k+1)}(x), \qquad k \ge 1,$$
$$I^{(k)}(x) \ge \frac{e^x}{x}\left(1 - \frac{k-1}{x}\right), \qquad k \ge 2,$$
$$I^{(k)}(x) \le \frac{e^x}{x}\left(1 - \frac{k-1}{x} + \frac{(k-1)(k-2)}{x^2}\right), \qquad k \ge 3.$$

Proof. For $k \ge 1$, we have $I^{(k)}(x) = \int_0^1 h^{k-1}e^{hx}dh$, which implies the first inequality. The other two follow from applying integration by parts to this integral. □

Lemma 2. *For $u \ge 2$ we have*

$$\log(u\log u) < \xi(u) < \log(u\log u) + 1.$$

Proof. This is an easy exercise, following the same reasoning as in the proof of [11, Lemma III.5.11]. □

Lemma 3. *For real $\delta > 0$, $A > 0$, and $1 \le m < \delta^2 A + 1$, we have*

$$\int_\delta^\infty t^m e^{-At^2/2}dt \le \frac{\delta^{m+1}}{\delta^2 A - (m-1)}e^{-A\delta^2/2}.$$

Proof. This follows from a change of variables in the bound [9, Proposition 2.7]

$$\Gamma(a,x) := \int_x^\infty t^{a-1}e^{-t}dt \le \frac{x^a e^{-x}}{x-(a-1)}$$

for real x, a with $x > a-1 \ge 0$. □

Proof of Theorem 2. As in [11], we evaluate the inverse Laplace integral

$$\begin{aligned}\rho(u) &= \frac{1}{2\pi i}\int_{-\xi-i\infty}^{-\xi+i\infty} \widehat{\rho}(s)e^{us}ds = \frac{1}{2\pi i}\int_{-\xi-i\infty}^{-\xi+i\infty} e^{\gamma+I(-s)+us}ds \\ &= \frac{e^{\gamma-u\xi+I(\xi)}}{2\pi}\int_{-\infty}^{\infty} e^{I(\xi-i\tau)-I(\xi)+ui\tau}d\tau,\end{aligned} \tag{1}$$

where $s = -\xi + i\tau$. Let $\delta := \sqrt{8\log(u)/u}$ and define

$$H(\tau) := I(\xi) - \mathrm{Re}(I(\xi - i\tau)) = \int_0^1 e^{h\xi}\frac{1-\cos(h\tau)}{h}dh.$$

When $\delta \le |\tau| \le 1$, we have $1-\cos(h\tau) \ge 0.45\tau^2h^2$ for $0 \le h \le 1$, so

$$H(\tau) \ge 0.45\tau^2\int_0^1 he^{h\xi}dh = 0.45I''(\xi)\tau^2$$

and the contribution to (1) is less than

$$\begin{aligned}\frac{1}{\pi}e^{\gamma-u\xi+I(\xi)}\int_\delta^1 \exp(-0.45I''(\xi)\tau^2)d\tau &< \frac{1}{\pi}e^{\gamma-u\xi+I(\xi)}\frac{\exp(-0.45I''(\xi)\delta^2)}{2\cdot 0.45I''(\xi)\delta} \\ &< \tilde{\rho}(u)\frac{\exp(-0.45I''(\xi)\delta^2)}{0.45\delta\sqrt{2\pi I''(\xi)}} =: \tilde{\rho}(u)E_1(u).\end{aligned}$$

Similarly, when $1 \le |\tau| \le \pi$, we have $1-\cos(h\tau) \ge 2\tau^2h^2/\pi^2$, which leads to a contribution of less than

$$\tilde{\rho}(u)\frac{\exp(-2I''(\xi)/\pi^2)}{(2/\pi^2)\sqrt{2\pi I''(\xi)}} =: \tilde{\rho}(u)E_2(u).$$

For the contribution from $\pi \le |\tau| \le 1+u\xi$, we find as in [11] that

$$H(\tau) \ge \frac{u\pi^2}{2(\pi^2+\xi^2)} - \frac{2}{\sqrt{\pi^2+\xi^2}} =: \eta(u),$$

so that these segments contribute less than

$$\frac{1}{\pi}e^{\gamma-u\xi+I(\xi)}(1+u\xi-\pi)e^{-\eta(u)} < \tilde{\rho}(u)\sqrt{2I''(\xi)/\pi}(1+u\xi-\pi)e^{-\eta(u)} =: \tilde{\rho}(u)E_3(u).$$

When $|\tau| \geq 1 + u\xi$ and $s = -\xi + i\tau$, we have $\widehat{\rho}(s) = e^{-J(s)}/s$ by [11, Equation (5.51)], where

$$|J(s)| := \left| \int_0^\infty \frac{e^{-s-t}}{s+t} dt \right| \leq \frac{e^\xi}{|\tau|} = \frac{1+u\xi}{|\tau|} \leq 1.$$

Thus,

$$|e^{-J(s)} - 1| \leq |J(s)|(e-1) \leq (e-1)\frac{1+u\xi}{|\tau|},$$

and

$$\widehat{\rho}(s) = \frac{1}{s} + \frac{\nu_{\tau,u}}{s}(e-1)\frac{1+u\xi}{|\tau|},$$

where $|\nu_{\tau,u}| \leq 1$. Substituting this into (1) and applying integration by parts to the first term, we find that the contribution from $|\tau| \geq 1 + u\xi$ to (1) is at most

$$\frac{e^{-u\xi}}{\pi}\left(\frac{2}{u(1+u\xi)} + (e-1)\right) < \frac{e^{-u\xi}}{\pi}(e+1).$$

Hence, these segments contribute less than

$$\tilde{\rho}(u)(e+1)e^{-\gamma - I(\xi)}\sqrt{2I''(\xi)/\pi} =: \tilde{\rho}(u)E_4(u).$$

For $-\delta \leq \tau \leq \delta$, we use the Taylor expansion of $I(\xi - i\tau)$ around $\tau = 0$. Since

$$|I^{(k)}(\xi - i\tau)| = |\int_0^1 h^{k-1} e^{h(\xi - i\tau)} dh| \leq I^{(k)}(\xi) \leq I'(\xi) = u,$$

for $k \geq 1$, we have

$$I(\xi - i\tau) - I(\xi) + ui\tau = \sum_{k=2}^{7} \frac{I^{(k)}(\xi)}{k!}(-i\tau)^k + \frac{I^{(8)}(\xi)\ \mu_{u,\tau}}{8!}\tau^8,$$

where $|\mu_{u,\tau}| \leq 1$. Thus,

$$\int_{-\delta}^{\delta} e^{I(\xi - i\tau) - I(\xi) + ui\tau} d\tau = \int_{-\delta}^{\delta} e^{-I''(\xi)\tau^2/2} h(u,\tau) d\tau, \tag{2}$$

where

$$h(u,\tau) := \exp\left\{ \sum_{k=3}^{7} \frac{I^{(k)}(\xi)}{k!}(-i\tau)^k + \frac{I^{(8)}(\xi)\mu_{u,\tau}}{8!}\tau^8 \right\}.$$

Writing M for the exponent, we have

$$h(u,\tau) = e^M = \sum_{j=0}^{5} \frac{M^j}{j!} + \frac{1.1 M^6 \nu_M}{6!},$$

for $\mathrm{Re}(M) \le \log 1.1$, where $|\nu_M| \le 1$. Since $|\tau| \le \delta$ and $I^{(k+1)}(\xi) \le I^{(k)}(\xi)$, we have

$$\mathrm{Re}(M) \le \frac{I^{(4)}(\xi)}{4!}\tau^4 + \frac{I^{(8)}(\xi)}{8!}\tau^8 \le \frac{I^{(4)}(\xi)\delta^4}{4!}\left(1 + \frac{\delta^4}{1680}\right),$$

which implies that $\mathrm{Re}(M) < \log 1.1$ for $u \ge 980$.

Let h_k be M^k without all the terms that contribute zero to the integral in (2) and write

$$I_k := I^{(k)}(\xi) \quad \text{and} \quad a_k := \frac{I^{(k)}(\xi)}{k!} = \frac{I_k}{k!}.$$

We have

$$\begin{aligned}
h_0 &= 1,\\
h_1 &= a_4\tau^4 - a_6\tau^6 + \theta_1\tau^8 R_1(\tau),\\
h_2 &= -a_3^2\tau^6 + 2a_3a_5\tau^8 + a_4^2\tau^8 - \tau^{10}S_2 + \theta_2\tau^{10}R_2(\tau),\\
h_3 &= -3a_3^2a_4\tau^{10} + \tau^{12}S_3 + \theta_3\tau^{12}R_3(\tau),\\
h_4 &= a_3^4\tau^{12} - \tau^{14}S_4 + \theta_4\tau^{14}R_4(\tau),\\
h_5 &= \tau^{16}S_5 + \theta_5\tau^{16}R_5(\tau),
\end{aligned}$$

where $|\theta_i| \le 1$ and $S_1 = 0$, $R_1(\tau) := I_8/8!$,

$$S_2 := \sum_{\substack{3\le i,j\le 8\\ i+j=10}} \frac{I_iI_j}{i!j!}, \qquad R_2(\tau) := \sum_{\substack{3\le i,j\le 8,\ i+j\ge 11\\ i+j\equiv 0 \bmod 2 \text{ or } \max(i,j)=8}} \frac{\tau^{i+j-10}}{i!j!}I_iI_j,$$

$$S_3 := \sum_{\substack{3\le i,j,k\le 8,\\ i+j+k=12}} \frac{I_iI_jI_k}{i!j!k!}, \qquad R_3(\tau) := \sum_{\substack{3\le i,j,k\le 8,\ i+j+k\ge 13\\ i+j+k\equiv 0 \bmod 2 \text{ or } \max(i,j,k)=8}} \frac{\tau^{i+j+k-12}}{i!j!k!}I_iI_jI_k,$$

et cetera.

With the help of Lemma 1, we verify that $I_8 < I_2^4u^{-3}$ for $u \ge 14 =: u_1$; each product I_iI_j appearing in S_2 or R_2 satisfies $I_iI_j < I_2^5u^{-3}$ for $u \ge 5 =: u_2$; each product $I_iI_jI_k$ appearing in S_3 or R_3 satisfies $I_iI_jI_k < I_2^6u^{-3}$ for $u \ge 3 =: u_3$, et cetera, with $u_4 = u_5 = 1$. Since $|\tau| \le \delta \le 1/4$, which holds for $u \ge 870$, we have $|R_j(\tau)| \le R_j(1/4)$. Let α_j, β_j denote the values of the sums S_j and $R_j(1/4)$, respectively, but without the products of the I's. Then

$$0 \le S_j \le \alpha_j I_2^{j+3}u^{-3}, \quad |R_j(\tau)| \le \beta_j I_2^{j+3}u^{-3}.$$

To exploit the alternating $\pm$ pattern in front of the S_j's, we define $\gamma_1^+ = \gamma_1^- = \beta_1 = 1/8!$; for $1 \le j \le 2$, let $\gamma_{2j}^+ := \beta_{2j}$, $\gamma_{2j}^- := \alpha_{2j} + \beta_{2j}$, $\gamma_{2j+1}^+ := \alpha_{2j+1} + \beta_{2j+1}$, $\gamma_{2j+1}^- := \beta_{2j+1}$.

Since $I_{k+1} \le I_k$, we have

$$|M| \le \sum_{k=3}^{8} \frac{I_k}{k!}|\tau|^k \le \frac{I_3|\tau|^3}{3!}1.065761,$$

for $|\tau| \le \delta \le 1/4$, and therefore,

$$|1.1M^6| \le \frac{I_3^6\tau^{18}}{(3!)^6}1.612 < \frac{u^{-3}I_2^9\tau^{18}}{(3!)^6}1.612 =: u^{-3}I_2^9\tau^{18}\gamma_6,$$

as $I_3^6 < u^{-3}I_2^9$ for $u \ge 1$. With $\gamma_6^+ = \gamma_6^- = \gamma_6$, the contribution of the S_j's, the R_j's, and $|1.1M^6|$ to (2) is less than

$$\sum_{k=1}^{6}\frac{\gamma_k^+ I_2^{3+k}}{u^3 k!}\int_{-\infty}^{\infty} e^{-I''(\xi)\tau^2/2}\tau^{6+2k}d\tau = \sqrt{\frac{2\pi}{I''(\xi)}}\sum_{k=1}^{6}\frac{\gamma_k^+ I_2^{3+k}}{u^3 k!}\frac{(5+2k)!!}{I_2^{3+k}}$$
$$< \sqrt{\frac{2\pi}{I''(\xi)}}\frac{1}{u^3}\sum_{k=1}^{6}\frac{\gamma_k^+(5+2k)!!}{k!} < \sqrt{\frac{2\pi}{I''(\xi)}}\frac{5.39}{u^3},$$

and, similarly, it is greater than

$$-\sqrt{\frac{2\pi}{I''(\xi)}}\frac{1}{u^3}\sum_{k=1}^{6}\frac{\gamma_k^-(5+2k)!!}{k!} > -\sqrt{\frac{2\pi}{I''(\xi)}}\frac{4.37}{u^3},$$

where $n!!$ is the product of all the positive integers up to n that have the same parity as n.

Writing the main terms as $g(\tau) := 1 + \sum_{j=2}^{6} c_j(u)\tau^{2j}$, Lemma 3 yields

$$\int_{\delta}^{\infty} e^{-I''(\xi)\tau^2/2}|g(\tau)|d\tau \le \frac{e^{-I''(\xi)\delta^2/2}}{I''(\xi)\delta}\left(1 + \frac{3}{2}\sum_{j=2}^{6}|c_j(u)|\delta^{2j}\right),$$

provided $I''(\xi)\delta^2 \ge 33$, which is the case if $u \ge 127$. We find that

$$1 + \frac{3}{2}\sum_{j=2}^{6}|c_j(u)|\delta^{2j} \le 7$$

for $u \ge 380$, which implies

$$2\int_{\delta}^{\infty} e^{-I''(\xi)\tau^2/2}|g(\tau)|d\tau < \frac{14e^{-I''(\xi)\delta^2/2}}{\delta\sqrt{2\pi I''(\xi)}}\sqrt{\frac{2\pi}{I''(\xi)}} =: E_5(u)\sqrt{\frac{2\pi}{I''(\xi)}}.$$

Now, $f(u) := u^3\sum_{k=1}^{5}E_k(u) = u^{3-(0.45)8+o(1)} = u^{-0.6+o(1)}$ has a limit of zero and is decreasing for $u \ge 70$, while $f(922) < 0.05$. Combining everything, we obtain

$$\rho(u) = \tilde{\rho}(u)\left(1 + \alpha(u) + \beta(u) + \lambda(u)u^{-3}\right), \tag{3}$$

where $|\lambda(u)| < 5.39 + 0.05 = 5.44$ for $u \ge 980$,

$$\alpha(u) := \frac{a_4 3!!}{I''(\xi)^2} - \frac{a_3^2 5!!}{2!I''(\xi)^3} = \frac{I^{(4)}(\xi)}{8I''(\xi)^2} - \frac{5I^{(3)}(\xi)^2}{24I''(\xi)^3} \sim -\frac{1}{12u},$$

$$\begin{aligned}\beta(u) &:= -\frac{a_6 5!!}{I''(\xi)^3} + \frac{(2a_3a_5 + a_4^2)7!!}{2!I''(\xi)^4} - \frac{3a_3^2a_4 9!!}{3!I''(\xi)^5} + \frac{a_3^4 11!!}{4!I''(\xi)^6} \\ &= -\frac{I^{(6)}(\xi)}{48I''(\xi)^3} + \frac{7I^{(3)}(\xi)I^{(5)}(\xi)}{48I''(\xi)^4} + \frac{35I^{(4)}(\xi)^2}{384I''(\xi)^4} - \frac{35I^{(3)}(\xi)^2I^{(4)}(\xi)}{64I''(\xi)^5} + \frac{385I^{(3)}(\xi)^4}{1152I''(\xi)^6} \\ &\sim \frac{1}{288u^2}.\end{aligned}$$

Lemma 1 shows that $u^2\beta(u) = \frac{1}{288}(1 - 2/\xi + O(1/\xi^2))$, so that $\lim_{u\to\infty} u^2\beta(u) = \frac{1}{288}$. Moreover, $u^2\beta(u)$ is increasing and positive for $u \geq 7$, so $|u^2\beta(u)| < \frac{1}{288}$ for $u \geq 7$. From (3) we obtain

$$|\theta(u)| := |u^2(\beta(u) + \lambda(u)u^{-3})| < \frac{1}{288} + \frac{5.5}{u}.$$

Thus, $|\theta(u)| < 0.005$ for $u \geq 3600$. For $5 \leq u \leq 3600$, we calculate $\rho(u)$ (resp. $\rho(u)/\tilde{\rho}(u)$) numerically as described in Section 4 and graph $\theta(u) := (\rho(u)/\tilde{\rho}(u) - 1 - \alpha(u))u^2$, to find that $|\theta(u)| \leq 0.0036$ in this range.

We have $\theta(u) = u^2\beta(u) + \lambda(u)/u > u^2\beta(u) - 5.5/u$ for $u \geq 980$, which implies $\theta(u) > 0$ for $u \geq 2250$. For $9 \leq u \leq 2250$, we verify that $\theta(u) > 0$ by computing $\rho(u)$ as described in Section 4 and graphing $\theta(u)$. □

In proving Theorem 2, we also proved Theorem 3, where the range $1 \leq u \leq 980$ is again established by calculating $\rho(u)$ as in Section 4. The upper bound 5.44 is likely far from best possible.

Theorem 3. *Equation (3) holds with $|\lambda(u)| < 5.44$ for $u \geq 1$.*

3. Proof of Theorem 1

Lemma 4. *For $u \geq 2$ we have*

$$-\frac{\xi}{12e^\xi}\left(1 - \frac{1}{\xi} + \frac{1.75}{\xi^2}\right) < \alpha(u) < -\frac{\xi}{12e^\xi}\left(1 - \frac{1}{\xi} + \frac{0.5}{\xi^2}\right).$$

Proof. Let

$$A(x) := \frac{1}{8}\frac{I^{(4)}(x)}{(I^{(2)}(x))^2} - \frac{5}{24}\frac{(I^{(3)}(x))^2}{(I^{(2)}(x))^3},$$

so that $\alpha(u) = A(\xi(u))$, and define $\kappa(x)$ by

$$A(x) = -\frac{x}{12e^x}\left(1 - \frac{1}{x} + \frac{\kappa(x)}{x^2}\right).$$

Lemma 1 shows that $\kappa(x)$ is bounded. A calculus exercise, aided by a computer, reveals that $\kappa(x)$ is increasing on the interval $(0, 2.749...)$, where it reaches its maximum of 1.746... at $x = 2.749...$, and decreasing on $(2.749..., \infty)$ with $\lim_{x\to\infty} \kappa(x) = 1/2$. We have $\kappa(1/3) = 0.511... > 0.5$. The result now follows since $\xi > 1/3$ for $u \geq 2$. □

Lemma 5. *For $u \geq 1$ we have*

$$-\frac{1}{12u} < \alpha(u) - \frac{0.02}{u^2} < \alpha(u) + \frac{0.02}{u^2} < -\frac{1}{12u(1+1/\log u)}.$$

Proof. For $u \geq 4$, we have $u^2(1-1.75/\xi) > (0.02)12(u\xi+1) = (0.02)12e^{\xi}$, by Lemma 2. Lemma 4 implies

$$\alpha(u) - \frac{0.02}{u^2} > -\frac{\xi}{12e^{\xi}}\left(1 - \frac{1}{\xi} + \frac{1.75}{\xi^2}\right) - \frac{0.02}{u^2} > \frac{-\xi}{12e^{\xi}} = \frac{-\xi}{12(u\xi+1)} > \frac{-1}{12u}.$$

For $u \geq 1$, we have $u^2 \geq (0.02)24\xi e^{\xi} = (0.02)24\xi(u\xi+1)$. Lemma 4 yields

$$\alpha(u) + \frac{0.02}{u^2} < -\frac{\xi}{12e^{\xi}}\left(1 - \frac{1}{\xi} + \frac{0.5}{\xi^2}\right) + \frac{0.02}{u^2} < \frac{-\xi}{12e^{\xi}}\left(1 - \frac{1}{\xi}\right) = \frac{-(\xi-1)}{12(u\xi+1)}.$$

We claim that

$$-\frac{\xi-1}{12(u\xi+1)} < -\frac{1}{12u(1+1/\log u)}.$$

Indeed, this is equivalent to $\xi > 1 + (1+1/u)\log u$, which follows from Lemma 2 for $u \geq 23$. This demonstrates the result for $u \geq 23$. For $1 \leq u \leq 23$ we confirm the result by graphing the four quantities in question multiplied by u. □

Proof of Theorem 1. For $u \geq 5$ the result follows from Theorem 2 and Lemma 5. For $1 \leq u \leq 5$, we calculate $\rho(u)$ as described in Section 4 and graph the three expressions as in Figure 1. □

4. Numerical Calculation of $\rho(u)$

In the range $1 \leq u \leq 50$, we calculate $\rho(u)$ with the algorithm of Marsaglia, Zaman, and Marsaglia [8]. To approximate $\rho(u)$ in the interval $[n, n+1]$, where n is an integer, we find the coefficients of the Taylor polynomial of order 250 centered at $n+1/2$, recursively from the coefficients of the polynomial centered at $n-1/2$.

For larger u, we evaluate the inverse Laplace integral numerically. After the change of variables $t = \tau\sqrt{I''(\xi)}$, Equation (1) implies

$$\frac{\rho(u)}{\tilde{\rho}(u)} = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left\{I(\xi - it/\sqrt{I''(\xi)}) - I(\xi) + uit/\sqrt{I''(\xi)}\right\} dt.$$

The proof of Theorem 2 shows that the real part of the integrand approaches the standard normal density function as u grows. Numerical integration in Mathematica converges well for $u \geq 15$.

With this way of calculating $\rho(u)$, our values match those in [12] to the accuracy they claim, namely at least five significant digits.

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