

Prime Number Theorem

STEVEN FINCH

April 27, 2007

Let $\pi(x) = \sum_{p \leq x} 1$, the number of primes p not exceeding x . Gauss and Legendre conjectured an asymptotic expression for $\pi(x)$. Define the Möbius mu function

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1, \\ (-1)^r & \text{if } n \text{ is a product of } r \text{ distinct primes,} \\ 0 & \text{if } n \text{ is divisible by a square } > 1; \end{cases}$$

the von Mangoldt function

$$\Lambda(n) = \begin{cases} \ln(p) & \text{if } n = p^m \text{ for some prime } p \text{ and integer } m \geq 1, \\ 0 & \text{otherwise;} \end{cases}$$

and the Chebyshev functions

$$\theta(x) = \sum_{p \leq x} \ln(p),$$

$$\psi(x) = \sum_{\substack{p^m \leq x, \\ m \geq 1}} \ln(p) = \sum_{n \leq x} \Lambda(n) = \ln(\text{lcm}\{1, 2, \dots, \lfloor x \rfloor\}).$$

Hadamard and de la Vallée Poussin proved the Gauss-Legendre conjecture, namely,

$$\pi(x) \sim \frac{x}{\ln(x)}, \quad \theta(x) \sim x, \quad \psi(x) \sim x$$

as $x \rightarrow \infty$. These three formulas are equivalent to each other and also to

$$\sum_{n=1}^{\infty} \frac{\mu(n)}{n} = 0.$$

The Riemann zeta function clearly plays a role here since, for $\text{Re}(s) > 1$,

$$\sum_{n=1}^{\infty} \frac{1}{n^s} = \zeta(s), \quad \sum_{n=1}^{\infty} \frac{\mu(n)}{n^s} = \frac{1}{\zeta(s)}.$$

⁰Copyright © 2007 by Steven R. Finch. All rights reserved.

Of many aspects of the Prime Number Theorem, we focus on the following error estimates [1, 2, 3, 4]:

$$\begin{aligned} 1 + \int_1^{\infty} \frac{\theta(x) - x}{x^2} dx &= \lim_{N \rightarrow \infty} \left(\sum_{p \leq N} \frac{\ln(p)}{p} - \ln(N) \right) \\ &= -\gamma - \sum_p \frac{\ln(p)}{p(p-1)} = -1.3325822757\dots, \end{aligned}$$

$$1 + \int_1^{\infty} \frac{\psi(x) - x}{x^2} dx = \lim_{N \rightarrow \infty} \left(\sum_{n \leq N} \frac{\Lambda(n)}{n} - \ln(N) \right) = -\gamma = -0.5772156649\dots$$

where γ is the Euler-Mascheroni constant [5, 6]. The latter implies that

$$\sum_{n=1}^{\infty} \frac{\Lambda(n) - 1}{n} = -2\gamma.$$

What can be said about analogous expressions connected with the Prime Number Theorem for arithmetic progressions $3k + 1$ and $4k + 1$?

Nevanlinna [7, 8] gave a straightforward generalization:

$$\sum_{n \equiv 1 \pmod{3}} \frac{\mu(n)}{n} = \frac{1}{2} \frac{1}{L_{-3}(1)} = \frac{3\sqrt{3}}{2\pi},$$

$$\sum_{n \equiv 1 \pmod{4}} \frac{\mu(n)}{n} = \frac{1}{2} \frac{1}{L_{-4}(1)} = \frac{2}{\pi};$$

$$\lim_{N \rightarrow \infty} \left(\sum_{\substack{n \equiv 1 \pmod{3}, \\ n \leq N}} \frac{2\Lambda(n)}{n} - \ln(N) \right) = -\gamma - \frac{\ln(3)}{2} - \frac{L'_{-3}(1)}{L_{-3}(1)} = -\gamma - \frac{\ln(3)}{2} - \ln \left(2\pi e^{\gamma} \frac{\Gamma(\frac{2}{3})^3}{\Gamma(\frac{1}{3})^3} \right),$$

$$\lim_{N \rightarrow \infty} \left(\sum_{\substack{n \equiv 1 \pmod{4}, \\ n \leq N}} \frac{2\Lambda(n)}{n} - \ln(N) \right) = -\gamma - \ln(2) - \frac{L'_{-4}(1)}{L_{-4}(1)} = -\gamma - \ln(2) - \ln \left(2\pi e^{\gamma} \frac{\Gamma(\frac{3}{4})^2}{\Gamma(\frac{1}{4})^2} \right)$$

which imply that [5]

$$\sum_{n \equiv 1 \pmod{3}} \frac{2\Lambda(n) - 3}{n} = -3\gamma + \frac{\ln(3)}{2} - \frac{\sqrt{3}\pi}{6} - 4\ln(2\pi) + 6\ln(\Gamma(1/3)),$$

$$\sum_{n \equiv 1 \pmod{4}} \frac{2\Lambda(n) - 4}{n} = -3\gamma - \ln(2) - \frac{\pi}{2} - 3\ln(2\pi) + 4\ln(\Gamma(1/4)).$$

Here is a more complicated generalization. Define

$$\Lambda_{1,3}(n) = \begin{cases} \ln(p) & \text{if } n = p^m \text{ for some prime } p \equiv 1 \pmod{3} \text{ and integer } m \geq 1, \\ 0 & \text{otherwise,} \end{cases}$$

$$\Lambda_{1,4}(n) = \begin{cases} \ln(p) & \text{if } n = p^m \text{ for some prime } p \equiv 1 \pmod{4} \text{ and integer } m \geq 1, \\ 0 & \text{otherwise;} \end{cases}$$

$$\theta_{1,3}(x) = \sum_{\substack{p \leq x, \\ p \equiv 1 \pmod{3}}} \ln(p), \quad \theta_{1,4}(x) = \sum_{\substack{p \leq x, \\ p \equiv 1 \pmod{4}}} \ln(p);$$

$$\psi_{1,3}(x) = \sum_{n \leq x} \Lambda_{1,3}(n), \quad \psi_{1,4}(x) = \sum_{n \leq x} \Lambda_{1,4}(n).$$

Just as [1]

$$\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s} = -\frac{\zeta'(s)}{\zeta(s)} \sim \frac{1}{s-1} - \gamma \sim \zeta(s) - 2\gamma,$$

we have [9]

$$\begin{aligned} 2 \sum_{n=1}^{\infty} \frac{\Lambda_{1,3}(n)}{n^s} &= -\frac{\zeta'(s)}{\zeta(s)} - \frac{L'_{-3}(s)}{L_{-3}(s)} - \frac{\ln(3)}{3^s - 1} - 2 \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^{2s} - 1} \\ &\sim \zeta(s) - 2\gamma - \frac{L'_{-3}(s)}{L_{-3}(s)} - \frac{\ln(3)}{3^s - 1} - 2 \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^{2s} - 1} \end{aligned}$$

as $s \rightarrow 1$. On the one hand,

$$\sum_{n=1}^{\infty} \frac{2\Lambda_{1,3}(n) - 1}{n} = -2\gamma - \frac{L'_{-3}(1)}{L_{-3}(1)} - \frac{\ln(3)}{2} - 2 \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2 - 1}$$

but on the other hand,

$$\begin{aligned} \sum_{n \leq N} \frac{2\Lambda_{1,3}(n) - 1}{n} &\sim 2 \sum_{\substack{p \leq N, \\ p \equiv 1 \pmod{3}}} \frac{\ln(p)}{p} + 2 \sum_{\substack{p \leq N, \\ m \geq 2, \\ p \equiv 1 \pmod{3}}} \frac{\ln(p)}{p^m} - \sum_{n \leq N} \frac{1}{n} \\ &\sim \ln(N) + c_{1,3} + 2 \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p-1)} - \ln(N) - \gamma \\ &\sim -\gamma + c_{1,3} + 2 \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p-1)} \end{aligned}$$

as $N \rightarrow \infty$. It follows that

$$\begin{aligned}
1 + \int_1^{\infty} \frac{2\theta_{1,3}(x) - x}{x^2} dx &= \lim_{N \rightarrow \infty} \left(2 \sum_{\substack{p \leq N, \\ p \equiv 1 \pmod{3}}} \frac{\ln(p)}{p} - \ln(N) \right) = c_{1,3} \\
&= -\gamma - \frac{L'_{-3}(1)}{L_{-3}(1)} - \frac{\ln(3)}{2} - 2 \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2 - 1} - 2 \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p-1)} \\
&= -2.3754945198\dots
\end{aligned}$$

Similarly,

$$\begin{aligned}
1 + \int_1^{\infty} \frac{2\theta_{1,4}(x) - x}{x^2} dx &= \lim_{N \rightarrow \infty} \left(2 \sum_{\substack{p \leq N, \\ p \equiv 1 \pmod{4}}} \frac{\ln(p)}{p} - \ln(N) \right) = c_{1,4} \\
&= -\gamma - \frac{L'_{-4}(1)}{L_{-4}(1)} - \ln(2) - 2 \sum_{p \equiv 3 \pmod{4}} \frac{\ln(p)}{p^2 - 1} - 2 \sum_{p \equiv 1 \pmod{4}} \frac{\ln(p)}{p(p-1)} \\
&= -2.2248371388\dots
\end{aligned}$$

A simple series acceleration technique [10] arises from the identity

$$\frac{1}{p(p-1)} - \frac{1}{p^2-1} = \frac{1}{p(p^2-1)};$$

hence

$$\begin{aligned}
\sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p-1)} &= \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p^2-1)} + \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p^2-1} \\
&= \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p^2-1)} + \left(\sum_p \frac{\ln(p)}{p^2-1} - \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2-1} - \frac{\ln(3)}{8} \right);
\end{aligned}$$

hence

$$\sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2-1} + \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p-1)} = \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p^2-1)} - \frac{\zeta'(2)}{\zeta(2)} - \frac{\ln(3)}{8};$$

hence

$$c_{1,3} = -2\gamma - 4 \log(2\pi) + \frac{9 \log(3)}{8} + 6 \log(\Gamma(1/3)) + \frac{\zeta'(2)}{\zeta(2)} - 2 \sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p^2-1)}.$$

Similarly,

$$c_{1,4} = -2\gamma - 3 \log(2\pi) + \frac{\log(2)}{3} + 4 \log(\Gamma(1/4)) + \frac{\zeta'(2)}{\zeta(2)} - 2 \sum_{p \equiv 1 \pmod{4}} \frac{\ln(p)}{p(p^2 - 1)}.$$

More complex acceleration techniques yield [9]

$$\sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2 - 1} = 0.3516478132\dots, \quad \sum_{p \equiv 3 \pmod{4}} \frac{\ln(p)}{p^2 - 1} = 0.2287363531\dots$$

which permit numerical evaluations such as

$$\begin{aligned} 1 + \int_1^{\infty} \frac{2\psi_{1,3}(x) - x}{x^2} dx &= \lim_{N \rightarrow \infty} \left(\sum_{n \leq N} \frac{2\Lambda_{1,3}(n)}{n} - \ln(N) \right) \\ &= -\gamma - \frac{L'_{-3}(1)}{L_{-3}(1)} - \frac{\ln(3)}{2} - 2 \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2 - 1} \\ &= -2(1.0990495258\dots), \end{aligned}$$

$$\begin{aligned} 1 + \int_1^{\infty} \frac{2\psi_{1,4}(x) - x}{x^2} dx &= \lim_{N \rightarrow \infty} \left(\sum_{n \leq N} \frac{2\Lambda_{1,4}(n)}{n} - \ln(N) \right) \\ &= -\gamma - \frac{L'_{-4}(1)}{L_{-4}(1)} - \ln(2) - 2 \sum_{p \equiv 3 \pmod{4}} \frac{\ln(p)}{p^2 - 1} \\ &= -2(0.9867225683\dots) \end{aligned}$$

and

$$\sum_{p \equiv 1 \pmod{3}} \frac{\ln(p)}{p(p-1)} = 0.0886977340\dots, \quad \sum_{p \equiv 1 \pmod{4}} \frac{\ln(p)}{p(p-1)} = 0.1256960010\dots$$

The estimates $-2.375\dots$ and $-2.224\dots$ for the theta function integrals are also found in [11, 12]. A parallel analysis of integrals involving

$$\theta_{2,3}(x) = \sum_{\substack{p \leq x, \\ p \equiv 2 \pmod{3}}} \ln(p), \quad \theta_{3,4}(x) = \sum_{\substack{p \leq x, \\ p \equiv 3 \pmod{4}}} \ln(p)$$

could be done as well.

Another type of error estimate was provided by McCurley [13]. The maximum value of $\theta_{2,3}(x)/x$ occurs at $x = 1619$ and, further, $\theta_{2,3}(x) < 0.50933118x$ for all x . This result is essentially best possible. By contrast, the maximum value of $\theta_{1,3}(x)/x$

is not known! (For $x \leq 10^8$, it occurs at $x = 52553329$.) It can be shown that $\theta_{1,3}(x) < 0.5040354x$ for all x , but improvement is likely. Sharp analyses of $\theta_{3,4}(x)$ and $\theta_{1,4}(x)$ as such seem still to be open.

The maximum value of $\psi(x)/x$ occurs at $x = 113$ and $\psi(x) < 1.03882058x$ always [2]. Montgomery [14] conjectured that

$$\liminf_{x \rightarrow \infty} \frac{\psi(x) - x}{\sqrt{x \ln(\ln(\ln(x)))^2}} = -\frac{1}{2\pi}, \quad \limsup_{x \rightarrow \infty} \frac{\psi(x) - x}{\sqrt{x \ln(\ln(\ln(x)))^2}} = \frac{1}{2\pi}.$$

Let $M(x) = \sum_{n \leq x} \mu(x)$; Odlyzko & te Riele [15] proved that

$$\liminf_{x \rightarrow \infty} \frac{M(x)}{\sqrt{x}} < -1.009, \quad \limsup_{x \rightarrow \infty} \frac{M(x)}{\sqrt{x}} > 1.06.$$

The precise growth rate of $M(x)$ has been the subject of speculation [16, 17, 18]. Most recently, Gonek and Ng [19, 20] independently conjectured that

$$\liminf_{x \rightarrow \infty} \frac{M(x)}{\sqrt{x \ln(\ln(\ln(x)))^{5/4}}} = -C, \quad \limsup_{x \rightarrow \infty} \frac{M(x)}{\sqrt{x \ln(\ln(\ln(x)))^{5/4}}} = C$$

for some positive constant C . A proof of this or of Montgomery's conjecture would be sensational!

0.1. Addendum. The second-order Landau-Ramanujan constant for counting integers of the form $a^2 + 3b^2$ is [21]

$$\frac{1}{2} \left(1 - \frac{\gamma}{2} - \frac{1}{2} \frac{L'_{-3}(1)}{L_{-3}(1)} + \frac{\ln(3)}{4} + \sum_{p \equiv 2 \pmod{3}} \frac{\ln(p)}{p^2 - 1} \right) = 0.5767761224\dots$$

and the (classical) second-order Landau-Ramanujan constant for counting integers of the form $a^2 + b^2$ is

$$\frac{1}{2} \left(1 - \frac{\gamma}{2} - \frac{1}{2} \frac{L'_{-4}(1)}{L_{-4}(1)} + \frac{\ln(2)}{2} + \sum_{p \equiv 3 \pmod{4}} \frac{\ln(p)}{p^2 - 1} \right) = 0.5819486593\dots$$

The fact that $0.576\dots < 0.581\dots$ resolves a question raised by Shanks & Schmid [22, 23]. Further, the second-order LR constant corresponding to $a^2 + 2b^2$ is [24]

$$\frac{1}{2} \left(1 - \frac{\gamma}{2} - \frac{1}{2} \frac{L'_{-8}(1)}{L_{-8}(1)} + \frac{\ln(2)}{2} + \sum_{p \equiv 5, 7 \pmod{8}} \frac{\ln(p)}{p^2 - 1} \right) = 0.6093010224\dots$$

and the second-order LR constant corresponding to $a^2 - 2b^2$ is

$$\frac{1}{2} \left(1 - \frac{\gamma}{2} - \frac{1}{2} \frac{L'_8(1)}{L_8(1)} + \frac{\ln(2)}{2} + \sum_{p \equiv 3,5 \pmod{8}} \frac{\ln(p)}{p^2 - 1} \right) = 0.5045371359\dots$$

The fact that $0.609\dots > 0.581\dots > 0.504\dots$ verifies an assertion in [22]; we used the Selberg-Delange method and formulas in [25] to deduce the preceding expressions for $a^2 \pm 2b^2$. See also [26].

REFERENCES

- [1] E. Landau, *Handbuch der Lehre von der Verteilung der Primzahlen*, 2nd ed., Chelsea, 1953, pp. 197–203; MR0068565 (16,904d).
- [2] J. B. Rosser and L. Schoenfeld, Approximate formulas for some functions of prime numbers, *Illinois J. Math.* 6 (1962) 64–94; MR0137689 (25 #1139).
- [3] W. Ellison and F. Ellison, *Prime Numbers*, Wiley, 1985, p. 111; MR0814687 (87a:11082).
- [4] N. J. A. Sloane, On-Line Encyclopedia of Integer Sequences, A003418, A014963, A034386.
- [5] S. R. Finch, Euler-Mascheroni constant, *Mathematical Constants*, Cambridge Univ. Press, 2003, pp. 28–40.
- [6] S. R. Finch, Meissel-Mertens constants, *Mathematical Constants*, Cambridge Univ. Press, 2003, pp. 94–98.
- [7] V. Nevanlinna, On constants connected with the prime number theorem for arithmetic progressions, *Annales Academiae Scientiarum Fennicae Ser. A I* (1973) n. 539, 1–11; MR0342473 (49 #7219).
- [8] S. R. Finch, Quadratic Dirichlet L-series, unpublished note (2005).
- [9] P. Moree, Chebyshev’s bias for composite numbers with restricted prime divisors, *Math. Comp.* 73 (2004) 425–449; MR2034131 (2005b:11154).
- [10] X. Gourdon and P. Sebah, Some constants from number theory (Numbers, Constants and Computation), available online at <http://numbers.computation.free.fr/Constants/constants.html>.
- [11] M. P. Young, Lower-order terms of the 1-level density of families of elliptic curves, *Int. Math. Res. Notices* (2005) 587–633; math.NT/0408359; MR2147004 (2006c:11076).

- [12] S. J. Miller, Lower order terms in the 1-level density for families of holomorphic cuspidal newforms, arXiv:0704.0924.
- [13] K. S. McCurley, Explicit estimates for $\theta(x; 3, l)$ and $\psi(x; 3, l)$, *Math. Comp.* 42 (1984) 287–296; MR0726005 (85g:11085).
- [14] H. L. Montgomery, The zeta function and prime numbers, *Queen's Papers in Pure and Applied Mathematics*, n. 54, Proc. 1979 Queen's Number Theory Conf., ed. P. Ribenboim, 1980, pp. 1–31; MR0634679 (82k:10047).
- [15] A. M. Odlyzko and H. J. J. te Riele, Disproof of the Mertens conjecture, *J. Reine Angew. Math.* 357 (1985) 138–160; MR0783538 (86m:11070).
- [16] I. J. Good and R. F. Churchhouse, The Riemann hypothesis and pseudorandom features of the Möbius sequence, *Math. Comp.* 22 (1968) 857–861; MR0240062 (39 #1416).
- [17] B. Saffari, Sur la fausseté de la conjecture de Mertens, *C. R. Acad. Sci. Paris Sér. A-B* 271 (1970) A1097–A1101; MR0280447 (43 #6167).
- [18] T. Kotnik and J. van de Lune, On the order of the Mertens function, *Experiment. Math.* 13 (2004) 473–481; MR2118272 (2005i:11139).
- [19] N. Ng, The distribution factor of values of the summatory function of the Möbius function, *CMS Notes*, v. 34 (2002) n. 5, 5–8; available online at <http://www.journals.cms.math.ca/Notes/>.
- [20] N. Ng, The distribution of the summatory function of the Möbius function, *Proc. London Math. Soc.* 89 (2004) 361–389; MR2078705 (2005f:11215).
- [21] S. R. Finch, Landau-Ramanujan constant, *Mathematical Constants*, Cambridge Univ. Press, 2003, pp. 98–104.
- [22] D. Shanks and L. P. Schmid, Variations on a theorem of Landau. I, *Math. Comp.* 20 (1966) 551–569; MR0210678 (35 #1564).
- [23] P. Moree and H. J. J. te Riele, The hexagonal versus the square lattice, *Math. Comp.* 73 (2004) 451–473; available online at <http://arxiv.org/abs/math.NT/0204332>; MR2034132 (2005b:11155).
- [24] P. Sebah, Two modulo 8 prime sums, unpublished note (2009).
- [25] S. Finch, Quartic and octic characters modulo n , <http://arxiv.org/abs/0907.4894>.

- [26] S. R. Finch, Mertens' formula, unpublished note (2007).