# 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

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

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

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

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

as $x \to \infty$. 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 $\operatorname{Re}(s) > 1$,

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

[0]Copyright © 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]:

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

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

where $\gamma$ 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:

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

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

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

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

which imply that [5]

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

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

Here is a more complicated generalization. Define

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

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

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

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

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]

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

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

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

but on the other hand,

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

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

$$\begin{aligned}1+\int_1^\infty \frac{2\theta_{1,3}(x)-x}{x^2}dx &= \lim_{N\to\infty}\left(2\sum_{\substack{p\le N,\\ p\equiv 1 \bmod 3}}\frac{\ln(p)}{p}-\ln(N)\right)=c_{1,3}\\ &= -\gamma-\frac{L_{-3}'(1)}{L_{-3}(1)}-\frac{\ln(3)}{2}-2\sum_{p\equiv 2 \bmod 3}\frac{\ln(p)}{p^2-1}-2\sum_{p\equiv 1 \bmod 3}\frac{\ln(p)}{p(p-1)}\\ &= -2.3754945198....\end{aligned}$$

Similarly,

$$\begin{aligned}1+\int_1^\infty \frac{2\theta_{1,4}(x)-x}{x^2}dx &= \lim_{N\to\infty}\left(2\sum_{\substack{p\le N,\\ p\equiv 1 \bmod 4}}\frac{\ln(p)}{p}-\ln(N)\right)=c_{1,4}\\ &= -\gamma-\frac{L_{-4}'(1)}{L_{-4}(1)}-\ln(2)-2\sum_{p\equiv 3 \bmod 4}\frac{\ln(p)}{p^2-1}-2\sum_{p\equiv 1 \bmod 4}\frac{\ln(p)}{p(p-1)}\\ &= -2.2248371388....\end{aligned}$$

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

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

hence

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

hence

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

Similarly,

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

More complex acceleration techniques yield [9]

$$\sum_{p\equiv 2 \bmod 3} \frac{\ln(p)}{p^2-1} = 0.3516478132..., \qquad \sum_{p\equiv 3 \bmod 4} \frac{\ln(p)}{p^2-1} = 0.2287363531...$$

which permit numerical evaluations such as

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

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

and

$$\sum_{p\equiv 1 \bmod 3} \frac{\ln(p)}{p(p-1)} = 0.0886977340..., \qquad \sum_{p\equiv 1 \bmod 4} \frac{\ln(p)}{p(p-1)} = 0.1256960010....$$

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

$$\theta_{2,3}(x) = \sum_{\substack{p\le x,\\ p\equiv 2 \bmod 3}} \ln(p), \qquad \theta_{3,4}(x) = \sum_{\substack{p\le x,\\ p\equiv 3 \bmod 4}} \ln(p)$$

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, $\theta_{2,3}(x) < 0.50933118\,x$ 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 $\theta_{1,3}(x) < 0.5040354\, x$ 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 $\psi(x) < 1.03882058\, x$ always [2]. Montgomery [14] conjectured that

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

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

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

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

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

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]

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

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

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

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

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

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

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

The fact that 0.609... > 0.581... > 0.504... 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*, $2^{\text{nd}}$ 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), 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, *Acta Arith.* 137 (2009) 51–98; arXiv:0704.0924; MR2481982.

[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 faussété 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; http://cms.math.ca/notes/v34/n5/Notesv34n5.pdf.

[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; arXiv:math/0204332; MR2034132 (2005b:11155).

[24] P. Sebah, Two modulo 8 prime sums, unpublished note (2009).

[25] S. Finch, Quartic and octic characters modulo $n$, arXiv:0907.4894.

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