Irregularities in the Distribution
of Primes and Twin Primes

By Richard P. Brent

Abstract. The maxima and minima of $\langle L(x) \rangle - \pi(x)$, $\langle R(x) \rangle - \pi(x)$, and $\langle L_2(x) \rangle - \pi_2(x)$ in various intervals up to $x = 8 \times 10^{10}$ are tabulated. Here $\pi(x)$ and $\pi_2(x)$ are respectively the number of primes and twin primes not exceeding x, $L(x)$ is the logarithmic integral, $R(x)$ is Riemann's approximation to $\pi(x)$, and $L_2(x)$ is the Hardy-Littlewood approximation to $\pi_2(x)$. The computation of the sum of inverses of twin primes less than 8×10^{10} gives a probable value $1.9021604 \pm 5 \times 10^{-7}$ for Brun's constant.

1. Approximations to $\pi(x)$. Let $P = \{2, 3, 5, \cdots\}$ be the set of primes, and let $\pi(x)$ be the number of primes not exceeding x. Two well-known approximations to $\pi(x)$ for $x > 1$ are the logarithmic integral:

(1.1)
$$L(x) = \int_0^x \frac{dt}{\log t}$$

(1.2)
$$= \gamma + \log(\log x) + \sum_{k=1}^{\infty} \frac{(\log x)^k}{k!k};$$

and Riemann's approximation:

(1.3)
$$R(x) = \sum_{k=1}^{\infty} \frac{\mu(k)}{k} L(x^{1/k})$$

(1.4)
$$= 1 + \sum_{k=1}^{\infty} \frac{(\log x)^k}{k!k\zeta(k+1)}.$$

Note that (1.1) differs by $L(2) = 1.04516378...$ from the frequently used approximation $\int_2^x dt/\log t$.

We are interested in the errors

(1.5)
$$r_1(x) = \langle L(x) \rangle - \pi(x)$$

and

(1.6)
$$r_2(x) = \langle R(x) \rangle - \pi(x),$$

where $\langle y \rangle$ denotes the integer closest to y (i.e., the integer part of $(y + \frac{1}{2})$).

Since $r_i(x)$ is usually (though not always: see below) of order $x^{1/2}/\log x$, it is useful to consider the "normalized" errors

$$(1.7) \qquad\qquad s_i(x) = r_i(x)(\log x)/x^{1/2} \qquad \text{for } i = 1, 2.$$

Littlewood showed that, for sufficiently large x, $s_i(x)/\log \log \log x$ attains arbitrarily large positive and negative values [9], [10], [13]. On the other hand, Vinogradov [22] has shown that

$$(1.8) \qquad\qquad s_i(x) = O(x^{1/2}\exp(-\alpha(\log x)^{3/5}))$$

for a positive constant α. Assuming the Riemann hypothesis, the stronger result

$$(1.9) \qquad\qquad s_i(x) = O(\log^2 x)$$

is known [10]. Explicit bounds are given by Rosser and Schoenfeld [16].

Since $\pi(x)$ has been computed, both directly and indirectly [3], [12], [14], and tabulated for various values of x up to 10^{13}, the error functions $r_i(x)$ and $s_i(x)$ are easily computed for these values of x. However, Shanks [19] observed that this gives little information about the behaviour of the error functions between the tabulated values. Let

$$(1.10) \qquad\qquad R_i(a, b) = \max_{p \in P \cap [a, b]} r_i(p)$$

and

$$(1.11) \qquad\qquad \rho_i(a, b) = \min_{p \in P \cap [a, b]} r_i(p).$$

In Section 4 we describe how $R_i(a, b)$ and $\rho_i(a, b)$ may be computed fairly efficiently for a given interval $[a, b]$. Table 1 gives the results of such computations for various intervals up to 8×10^{10}, and more detailed tables have been deposited in the UMT file of this journal. Although the maximum and minimum in (1.10) and (1.11) are taken only over primes in $[a, b]$, it is easy to see that

$$(1.12) \qquad\qquad \min_{x \in [a,b]} r_i(x) = \min(\rho_i(a, b), r_i(a))$$

and, except in the unlikely event that $r_i(x)$ does not have a jump at each prime in $[a, b]$,

$$(1.13) \qquad\qquad \max_{x \in [a,b]} r_i(x) = \max(R_i(a + 1, b) + 1, r_i(b)).$$

$s_i(x)$ oscillates so rapidly that it is difficult to plot it over any large domain of x values. However, upper and lower bounds on $s_i(p)$ for primes $p \in [a, b]$ are easily found from (1.7), (1.10) and (1.11) once $R_i(a, b)$ and $\rho_i(a, b)$ are known. These bounds are fairly sharp if b is close to a. Figure 1 shows such upper and lower bounds on $s_2(p)$, plotted against $\log_{10}((a + b)/2)$, for various intervals $[a, b]$ which cover $[10^4, 8 \times 10^{10}]$ and satisfy $1.05 \leqslant b/a \leqslant 1.10$. The graph of upper and lower bounds on $s_1(p)$ looks similar since, from (1.3),

TABLE 1

Extrema of approximation errors in $[a, b]$

| a	b	ρ_1	R_1	ρ_2	R_2	ρ_3	R_3
2	10	0	1	0	1	1	1
10	10^2	1	4	−1	0	2	4
10^2	10^3	3	10	−2	1	3	9
10^3	10^4	7	23	−6	5	3	12
10^4	10^5	13	54	−16	13	5	41
10^5	2×10^5	29	72	−19	20	13	39
2×10^5	5×10^5	35	107	−33	33	6	71
5×10^5	10^6	50	135	−36	35	37	97
10^6	2×10^6	60	174	−51	49	−88	78
2×10^6	5×10^6	79	261	−84	81	−197	−17
5×10^6	10^7	118	346	−98	95	−280	−44
10^7	2×10^7	134	435	−145	127	−281	−108
2×10^7	5×10^7	170	692	−231	260	−248	37
5×10^7	10^8	344	895	−242	260	−29	262
10^8	2×10^8	239	1149	−514	336	−143	643
2×10^8	5×10^8	585	1724	−544	565	360	1046
5×10^8	10^9	744	2668	−685	965	536	1488
10^9	2×10^9	770	3354	−1093	982	566	2669
2×10^9	5×10^9	1316	4612	−1681	1567	−336	2130
5×10^9	10^{10}	2129	7048	−2387	2657	−1930	696
10^{10}	2×10^{10}	2159	10334	−2776	3787	−5833	2143
2×10^{10}	5×10^{10}	3132	14990	−4923	4950	−7334	4443
5×10^{10}	8×10^{10}	5325	17065	−5493	6106	−2692	2846

(1.14) $s_1(x) = s_2(x) + 1 + O(1/\log x)$

as $x \rightarrow \infty$.

   The distribution of 11966 tabulated values of $s_2(n)$ for $n \in [10^3, 8.3 \times 10^{10}]$ is shown in Figure 2. The sample mean and standard deviation are 0.003 and 0.206 respectively. It is plausible to conjecture that a limiting distribution exists, with mean zero and standard deviation about 0.21.

   Some primes p for which $|s_2(p)|$ is unusually large are given in Table 2. In fact, if an "exceptional peak" is a maximal interval $[a, b]$ such that $r_2(p)$ has constant sign for all primes p in (a, b), and $|s_2(p)| \geqslant 0.6$ for at least one prime p in (a, b), then Table 2 includes a prime p (with maximal $|r_2(p)|$) from each exceptional peak in $[10^4, 8 \times 10^{10}]$. The entry $s_1(30909673) = 0.52. . .$ was found by Appel and Rosser [1]. On the basis of Mapes' computations of $\pi(1.1 \times 10^8)$ and $\pi(1.8 \times 10^8)$, Shanks [19] conjectured that lower values of

FIGURE 1
RIEMANN'S APPROXIMATION

LOG10(P)
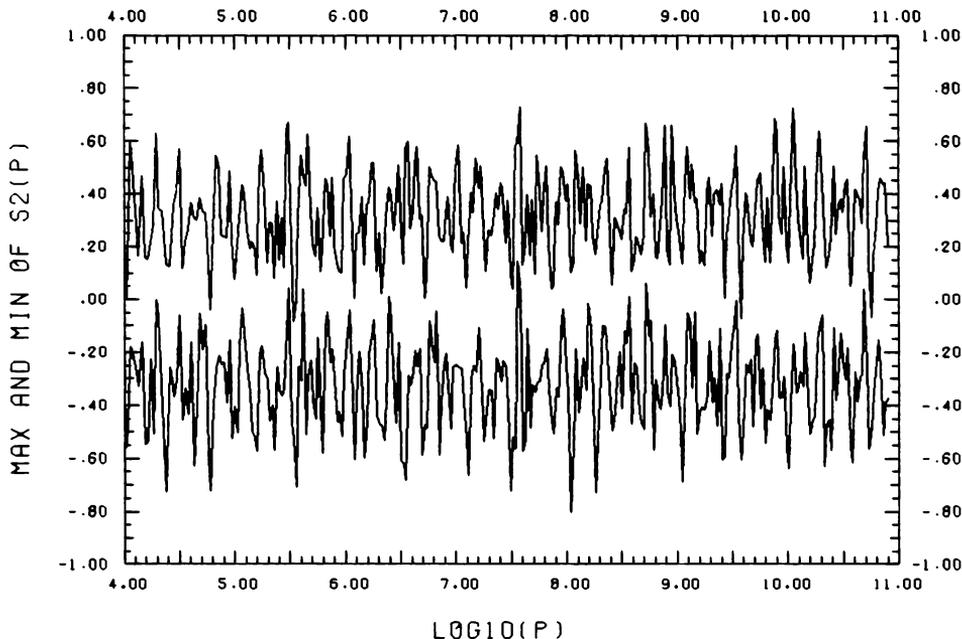
$s_1(p)$ could be found near 1.1×10^8 and 1.8×10^8, and the first and third entries in Table 2 show that this is correct.

Table 2 and an examination of the primes less than 10^4 show that

(1.15) $$s_1(p) > 0.42$$

for all prime $p \in [5, 8 \times 10^{10}]$, and hence

(1.16) $$\pi(x) < L(x)$$

for $x \leqslant 8 \times 10^{10}$. This extends the result of Rosser and Schoenfeld [16], who proved (1.16) for $x \leqslant 10^8$. Note that $|r_1(p)| < |r_2(p)|$ for several entries in Table 2. The table also shows that

(1.17) $$-0.79 < s_2(p) < 0.75$$

for all prime p in $[10^4, 8 \times 10^{10}]$, and examination of primes less than 10^4 then shows that

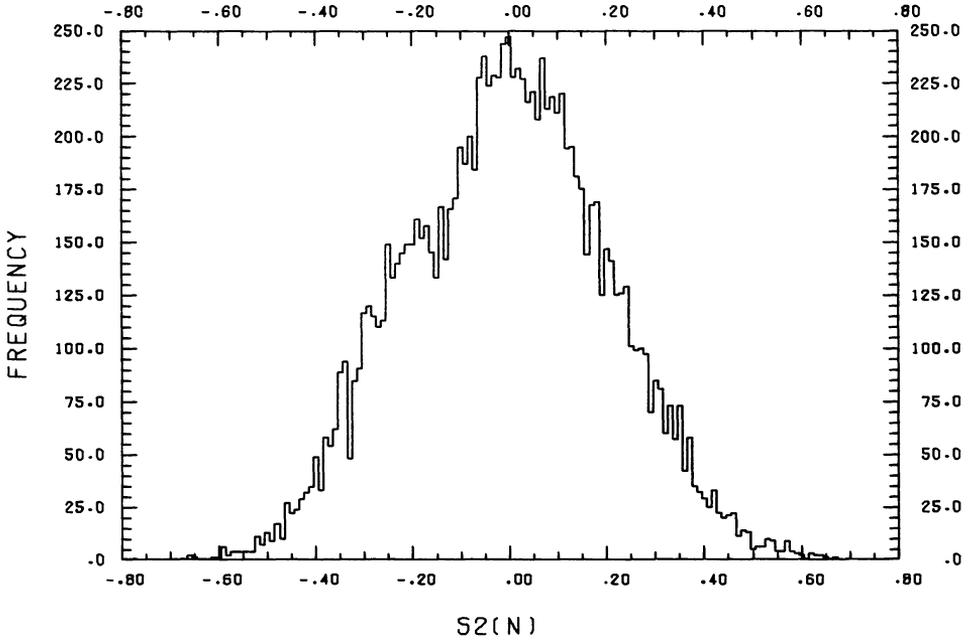(1.18) $$-0.90 < s_2(p) < 0.75$$

for all prime $p \leqslant 8 \times 10^{10}$.

Shanks [18] suggested the plausibility of

(1.19) $$\lim_{N \to \infty} \frac{1}{N} \sum_{n=2}^{N} s_1(n) = 1$$

FIGURE 2
DISTRIBUTION OF VALUES OF S2(N)

or, equivalently in view of (1.14),

$$\text{(1.20)} \qquad \lim_{N \to \infty} \frac{1}{N} \sum_{n=2}^{N} s_2(n) = 0.$$

If true, (1.19) and (1.20) would give a sense in which Riemann's approximation (or even the simpler approximation $L(x) - \frac{1}{2}L(x^{1/2})$ obtained by taking the first two terms in (1.3)) is better than the logarithmic intergral approximation. However, Table 3 gives some evidence that the limits in (1.19) and (1.20) may not exist. If there are large intervals in which $s_2(n)$ is uniformly bounded away from zero and of constant sign, then (1.20) can hold only if the lengths of such intervals near N are $o(N)$ as $N \longrightarrow \infty$. Table 3 gives some disjoint intervals $[a, b]$ such that $10^4 \leqslant b \leqslant 8 \times 10^{10}$, $b/a \geqslant 1.08$, and $r_2(p)$ has constant sign for all prime p in $[a, b]$. The number of such intervals in each decade seems to be roughly constant. Intervals in which $|s_2(x)| \geqslant 0.01$ (say) are only slightly smaller than the intervals given in Table 3.

The limit is more likely to exist if the mean of $s_2(n)$ is taken with respect to $\log n$ rather than n. This suggests the conjecture

$$\text{(1.21)} \qquad \lim_{N \to \infty} \left(\frac{1}{\log N} \right) \sum_{n=2}^{N} s_2(n)/n = 0$$

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TABLE 2

Some primes p with $|s_2(p)| \geqslant 0.6$

p	$\pi(p)$	$r_1(p)$	$r_2(p)$	$s_1(p)$	$s_2(p)$
110102617	6308959	239	−446	0.4218	−0.7871
36917099	2256804	692	260	1.9845	0.7456
179845447	10022306	331	−514	0.4691	−0.7285
11467849447	518601767	8594	3352	1.8589	0.7250
59753	6041	19	−16	0.8548	−0.7199
30909673	1910834	170	−231	0.5274	−0.7166
24137	2688	14	−11	0.9094	−0.7145
355111	30392	35	−33	0.7506	−0.7077
7712599823	355168013	7048	2657	1.8271	0.6888
302831	26218	93	30	2.1329	0.6880
1110072773	56146451	770	−1093	0.4813	−0.6833
3445943	246651	79	−84	0.6406	−0.6811
516128797	27159319	2100	766	1.8544	0.6764
50229461677	2128963733	16289	6106	1.7908	0.6713
766449311	39507064	2489	905	1.8392	0.6687
12871811	841519	134	−145	0.6114	−0.6616
905055691	46254156	2668	965	1.8290	0.6615
18834002419	832984013	10334	3787	1.7815	0.6529
10016844407	455784972	2159	−2776	0.4967	−0.6387
19373	2192	33	9	2.3405	0.6383
463181	38685	107	33	2.0511	0.6326
1090697	85021	151	47	2.0101	0.6257
21728785387	954969014	3132	−3850	0.5057	−0.6217
3278837	235526	84	−75	0.6960	−0.6214
42863	4483	19	−12	0.9788	−0.6182
38177961203	1637252682	4075	−4923	0.5082	−0.6139
3593311	256264	242	77	1.9270	0.6131
3745619057	178440671	1504	−1681	0.5417	−0.6055
11777	1410	27	7	2.3322	0.6046
1195247	92607	60	−47	0.7680	−0.6016
10219591	678161	372	119	1.8781	0.6008

or equivalently,

(1.22)
$$\lim_{N \to \infty} \left(\frac{1}{\log N} \right) \sum_{n=2}^{N} s_1(n)/n = 1.$$

Note that (1.20) implies (1.21), but not conversely.

TABLE 3

Some intervals $[a, b]$ *where* $r_2(p)$ *has constant sign and* $b/a \geqslant 1.08$

a	b	b/a	$\rho_2(a, b)$	$R_2(a, b)$
9278	11046	1.191	−6	0
45894	49942	1.088	0	8
56478	62850	1.113	−16	0
164912	179748	1.090	0	20
291570	318916	1.094	0	30
324090	369790	1.141	−33	0
638372	689958	1.081	0	28
4889994	5530998	1.131	−84	0
6862134	7472358	1.089	−98	0
9867492	10673698	1.082	0	119
34225760	38856760	1.135	0	260
504454344	552984016	1.096	0	766
3219006864	3507922926	1.090	0	1567
3637747892	4013111982	1.103	−1681	0
35699734892	38858023776	1.088	−4923	0
47048490524	51040905052	1.085	0	6106
53087472258	58483092228	1.102	−5288	0

Let us return to the conjecture of a limiting distribution for $s_2(x)$. The above discussion shows that care must be taken in formalizing the conjecture, for if x and y are drawn from $[a, b]$, then $s_2(x)$ and $s_2(y)$ will certainly be dependent if b/a is too close to 1. One possibility is to conjecture that the sequence $(s_2(x_i))$ has a limiting distribution if (x_i) is a random sequence of positive numbers such that $x_i/x_{i+1} \longrightarrow 0$ (and hence $x_i \longrightarrow \infty$) as $i \longrightarrow \infty$.

If the conjecture is true, and if the limiting distribution is approximately normal, with mean 0 and standard deviation about 0.21, we would expect $s_2(x) < -1$ (or $s_1(x) < 0$) for about one in every 10^6 independent random samples. Similarly, we would expect $s_2(x) < -0.6$ for about one in 450 independent samples. Since Table 2 covers the range $4.0 \leqslant \log_{10} x \leqslant 10.9$, and includes 17 entries with $s_2(x) < -0.6$, we would expect an entry with $s_2(x) < -1$ if the table could be extended to about

$$\log_{10} x = \left(\frac{10.9 - 4.0}{17}\right)\left(\frac{10^6}{450}\right) \simeq 900.$$

Although this argument is very crude, it suggests that (1.16) probably holds for $\log_{10} x$ up to about 100 (well beyond the range of feasible computation). It is

known that (1.16) is violated long before the legendary Skewes' number [21]; specifically, Lehman proved [11] that certain integers x between 1.53×10^{1165} and 1.65×10^{1165} suffice.

2. Approximations to $\pi_2(x)$.

We say that q is a "twin prime" if both q and $q + 2$ are prime. Let $Q = \{3, 5, 11, 17, \ldots\}$ be the set of twin primes, and let $\pi_2(x)$ be the number of twin primes not exceeding x. The Hardy-Littlewood approximation to $\pi_2(x)$ is

$$(2.1) \qquad L_2(x) = 2c_2 \int_2^x \frac{dt}{\log^2 t},$$

where

$$(2.2) \qquad c_2 = \prod_{2 < p \in P} \frac{1 - 2/p}{(1 - 1/p)^2} = 0.66016181\ldots$$

is the "twin-prime" constant [24].

Properties of $\pi(x)$ may be proved using the well-known relationship between the distribution of primes and the location of the zeros of the Riemann zeta function [10, Chapter 4]. Unfortunately, no similar relationship is known for twin primes, so very little is known about $\pi_2(x)$. It is not known whether there are infinitely many twin primes, and much less whether

$$(2.3) \qquad \pi_2(x) \sim L_2(x)$$

as $x \to \infty$. However, empirical evidence suggests that (2.3) is true. In Table 4 we give $\pi_2(n)$ and

$$(2.4) \qquad r_3(n) = \langle L_2(n) \rangle - \pi_2(n)$$

for various $n \leqslant 8 \times 10^{10}$. The values of $\pi_2(n)$ were computed by enumerating the primes up to n and counting the number of twins, for no more subtle method is known. Our counts agree with those of Weintraub [23] (for $n \leqslant 2 \times 10^8$) and Bohman [4] (for $n \leqslant 2 \times 10^9$).

Let

$$(2.5) \qquad R_3(a, b) = \max_{q \in Q \cap [a,b]} r_3(q)$$

and

$$(2.6) \qquad \rho_3(a, b) = \min_{q \in Q \cap [a,b]} r_3(q).$$

The functions $R_3(a, b)$ and $\rho_3(a, b)$ were computed for various intervals $[a, b]$ up to 8×10^{10}, and some results are given in Table 1. More detailed tables have been deposited in the UMT file of this journal.

TABLE 4

Counts of twin primes and estimates of Brun's constant

n	$\pi_2(n)$	$r_3(n)$	$B(n)$	$B^*(n)$
10^3	35	11	1.518032463560	1.90030531
10^4	205	9	1.616893557432	1.90359819
10^5	1224	25	1.672799584828	1.90216329
10^6	8169	79	1.710776930804	1.90191335
10^7	58980	−226	1.738357043917	1.90218826
10^8	440312	56	1.758815621068	1.90216794
10^9	3424506	802	1.774735957639	1.90216024
2×10^9	6388041	984	1.778859404547	1.90215957
3×10^9	9210144	461	1.781150604842	1.90215977
4×10^9	11944438	1032	1.782724861607	1.90215950
5×10^9	14618166	291	1.783918570267	1.90215984
6×10^9	17244409	−770	1.784876490721	1.90216027
7×10^9	19830161	−119	1.785673823717	1.90216007
8×10^9	22384176	−248	1.786355995279	1.90216011
9×10^9	24911210	−1324	1.786951346213	1.90216037
10^{10}	27412679	−1262	1.787478502719	1.90216036
2×10^{10}	51509099	−4667	1.790830284135	1.90216076
3×10^{10}	74555618	−3348	1.792701319111	1.90216064
4×10^{10}	96956707	1869	1.793990899123	1.90216031
5×10^{10}	118903682	1630	1.794970693076	1.90216031
6×10^{10}	140494397	1555	1.795758170053	1.90216033
7×10^{10}	161795029	2031	1.796414982022	1.90216032
8×10^{10}	182855913	−985	1.796977508288	1.90216040

Let $s_3(x)$ be defined by (1.7) with $i = 3$. Upper and lower bounds on s_3 in various intervals were computed in the same way as for s_2, and are shown in Figure 3. Comparison of Figures 1 and 3 shows that the behaviour of s_3 is quite different from that of s_2 (or s_1). Although $s_3(q)$ changes sign, there are large intervals in which it is of constant sign. For example, $s_3(q)$ is positive for all twin primes q in $[3, 1.36 \times 10^6]$, negative in $[1.52 \times 10^6, 3.52 \times 10^7]$, positive in $[1.50 \times 10^8, 3.06 \times 10^9]$, negative in $[1.19 \times 10^{10}, 2.71 \times 10^{10}]$, etc. Hence, it seems unlikely that the limit corresponding to (1.19) exists, although it is possible that the limit corresponding to (1.22) (with s_1 replaced by s_3) exists.

Suppose that the integers $4, 5, \cdots, N$ are randomly and independently selected or rejected, with the probability of selection of n being $2c_2/\log^2 n$. If

FIGURE 3
TWIN PRIME APPROXIMATION
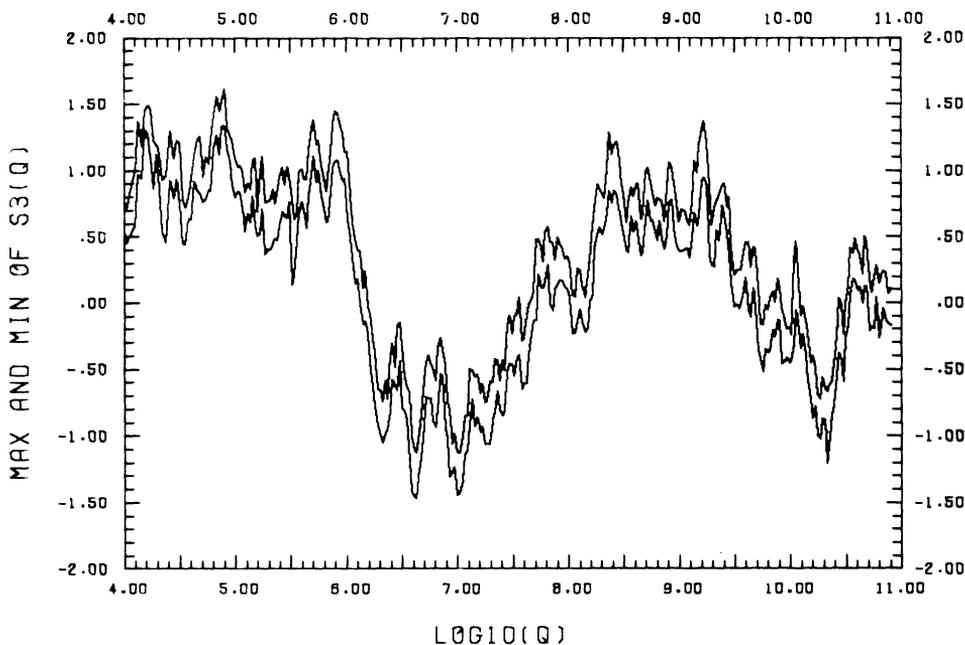
$P(N)$ is the number of integers selected, then $P(N)$ is distributed with mean $\mu(N)$ $\sim L_2(N)$ and variance $\sigma^2(N) \sim L_2(N)$, and the distribution is asymptotically normal as $N \longrightarrow \infty$. Thus $S(N) = (L_2(N) - P(N))(\log N)/N^{1/2}$ is asymptotically normal with mean zero and standard deviation $(2c_2)^{1/2} \doteq 1.15$. It is interesting to note that $\pi_2(N)$ and $s_3(N)$ appear to behave like $P(N)$ and $S(N)$ respectively. (The analogy for primes is apparently false, for it predicts that $s_1(N)$ should have mean 0 and standard deviation $O((\log N)^{1/2})$, and does not predict the frequent fluctuations in $s_1(N)$ (compare Figures 1 and 3). For some rigorous results connecting primes with random walks, see [2].)

We shall briefly mention some other approximations to $\pi_2(x)$. The simplest is $2c_2 x/\log^2 x$, which differs from $L_2(x)$ by terms of order $x/\log^3 x$. The empirical results discussed above show that

(2.7) $|s_3(q)| < 2.3$

for all twin primes $q \leqslant 8 \times 10^{10}$, so $|L_2(x) - \pi_2(x)|$ is of order $x^{1/2}/\log x$ for $x \leqslant 8 \times 10^{10}$. Hence, $L_2(x)$ is a more accurate approximation, at least in the range considered.

Other approximations are obtained by replacing $1/\log^2 t$ in (2.1) by $(R'(t))^2$ or by $(2R'(t)/\log t - 1/\log^2 t)$, as suggested by Fröberg [8] and Shanks and Wrench [20], respectively. Since these approximations differ from $L_2(x)$ by terms of order

$x^{1/2}/\log^2 x$ they are not appreciably better or worse than $L_2(x)$ over most of the range $x \leqslant 8 \times 10^{10}$. The advantage of $L_2(x)$ is that it is easy to compute, e.g., from

$$(2.8) \qquad L_2(x) = 2c_2(L(x) + K - x/\log x),$$

where $K = 2/\log 2 - L(2) = 1.84022630\cdots$.

3. Brun's Constant. Let

$$(3.1) \qquad B(x) = \sum_{x \geqslant q \in Q} \left(\frac{1}{q} + \frac{1}{q+2} \right).$$

Brun [7] showed that "Brun's constant" $B(\infty) = \lim_{x \to \infty} B(x)$ is finite (although the sum of reciprocals of primes has been known to be infinite since Euler's time). We have followed the definition of Shanks and Wrench [20], although Brun [7] and Selmer [17] consider $B(\infty) - (1/3 + 1/5)$, and Bohman [4] considers $B(\infty) - 1/5$.

Assuming that twin primes are distributed randomly with density $L_2'(x) = 2c_2/\log^2 x$ (see Section 2), we can estimate

$$(3.2) \qquad B(\infty) - B(x) \simeq 4c_2 \int_x^\infty \frac{dt}{t \log^2 t} = 4c_2/\log x,$$

which suggests the definition

$$(3.3) \qquad B^*(x) = B(x) + 4c_2/\log x.$$

Although $\lim_{x \to \infty} B^*(x) = \lim_{x \to \infty} B(x) = B(\infty)$, it is probable that the rate of convergence of $B^*(x)$ is much faster than that of $B(x)$. In fact, in contrast to (3.2), we expect that $B^*(x) - B(\infty)$ is asymptotically normally distributed with mean $o(1/(x^{1/2}\log x))$ and standard deviation $\sim (8c_2)^{1/2}/(x^{1/2}\log x)$.

Selmer [17] estimated $B(\infty) = 1.901 \pm 0.014$ by extrapolation from $B(200000)$. Fröberg [8] computed $B(n)$ for several $n \leqslant 2^{20}$ and estimated $B(\infty) = 1.90195 \pm 3 \times 10^{-5}$. Shanks and Wrench [20] found $B(32452843)$ and estimated $B(\infty) = 1.90218 \pm 2 \times 10^{-5}$. Finally, Bohman [4] computed $B(2 \times 10^9)$ and estimated $B(\infty) = 1.90216 \pm 5 \times 10^{-6}$. During the computation of $\pi_2(n)$ as described above, we computed $B(n)$ and $B^*(n)$ for various $n \leqslant 8 \times 10^{10}$. Some values are given in Table 4, and more are given in a table deposited in the UMT file of this journal. From our computation of $B^*(8 \times 10^{10})$ we estimate that $B(\infty)$ probably lies in the range

$$(3.4) \qquad B(\infty) = 1.9021604 \pm 5 \times 10^{-7}.$$

In the computation of $B(n)$ we used floating-point arithmetic with a 60-bit fraction, and accumulated the sum using Moller's "quasi double-precision" device [15]. Hence, rounding errors should not affect the entries in Table 4. (Our values of $B(n)$

differ from Bohman's (corrected) values in the 9th decimal place, possibly because of the effect of rounding errors in his calculations.)

Although we do not know how to bound the error in our estimate (3.4), the discussion above suggests that $x^{1/2}\log x(B^*(x) - B(\infty))$ is asymptotically normally distributed, and we certainly have

(3.5) $$|x^{1/2}\log x(B^*(x) - 1.9021604)| < 3.5$$

for all tabulated values in the range $[10^4, 8 \times 10^{10}]$. (The maximum value of 3.4927 is at $x = 860000$, in the region of the sharp drop in Figure 3.) Hence, it is probable that

(3.6) $$|B^*(8 \times 10^{10}) - B(\infty)| < \frac{3.5}{(8 \times 10^{10})^{1/2}\log(8 \times 10^{10})} < 5 \times 10^{-7},$$

which explains the error estimate in (3.4). If the constant $(8c_2)^{1/2}$ above is correct, the probability that $B(\infty)$ is in the range given by (3.4) is about 0.88.

Different methods of extrapolating $B(x)$ to the limit have been suggested by Fröberg [8] and Shanks and Wrench [20], but their extrapolations differ from $B^*(x)$ by $O(1/x^{1/2}\log^2 x)$, so are probably not much better or worse than $B^*(x)$. It seems difficult to obtain an appreciably better extrapolation than $B^*(x)$ without being able to predict the large-scale oscillations of $s_3(x)$ (see Figure 3).

4. Computation of $R_i(a, b)$ and $\rho_i(a, b)$. If R_i and ρ_i are defined by (1.10) and (1.11), the most time-consuming part of their computation is not the generation of the primes in $[a, b]$, which may be done efficiently by a sieve method (as in [5], [6]), but the frequent evaluation of $L(x)$ and $R(x)$ to a precision sufficient to determine $\langle L(x)\rangle$ and $\langle R(x)\rangle$. (Similarly for R_3 and ρ_3 defined by (2.5) and (2.6), although the situation is not so clear here, because it takes longer, on the average, to generate a twin prime than a prime.)

To avoid evaluating $\langle L(p)\rangle$ and $\langle R(p)\rangle$ for every prime p in $[a, b]$, we can use simple upper and lower bounds for $L(p)$ and $R(p)$, and only evaluate $\langle L(p)\rangle$ and $\langle R(p)\rangle$ if the upper and lower bounds fail to show that $r_i(p)$ lies within the maxima and minima already found. The following lemmas indicate how suitable upper and lower bounds may be found.

LEMMA 1. *Suppose $f''(x) < 0$ on $[a, b]$, and $a < a' < x < x' < b' < b$. Then*

$$\frac{f(a') - f(a)}{a' - a} > \frac{f(x') - f(x)}{x' - x} > \frac{f(b') - f(b)}{b' - b}.$$

The proof is immediate from a mean value theorem.

LEMMA 2. *$L''(x), R''(x)$ and $L_2''(x)$ are negative for $x > 1$.*

Proof. From (1.1), (2.1) and (1.4) we have $L''(x) = -1/(x\log^2 x) < 0$, $L_2''(x) = -4c_2/(x\log^3 x) < 0$, and

$$(4.1) \qquad R''(x) = -x^{-2} \sum_{k=1}^{\infty} \left(\frac{k+1}{\zeta(k+1)} - \frac{k}{\zeta(k+2)} \right) \frac{(\log x)^{k-1}}{(k+1)!}.$$

Now $\zeta(k+1) < 1 + 1/k$ for $k \geqslant 1$, so $(k+1)/\zeta(k+1) > k/\zeta(k+2)$, and the result follows from (4.1).

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