The Mertens conjecture revisited

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Introduction

The Möbius function $\mu(n)$ is defined as $\mu(1) = 1$, $\mu(n) = (-1)^k$ if n is the product of k different primes, and $\mu(n) = 0$ otherwise. Then

$$M(x) := \sum_{1 \le n \le x} \mu(n),$$

is the difference between the number of squarefree positive integers $n \le x$ with an *even* number of prime factors and those with an *odd* number of prime factors.

The *Mertens conjecture states that* $|M(x)|/\sqrt{x} < 1$ *for all* $x > 1$.

This – but also the weaker assumption $|M(x)|/\sqrt{x} < C$ for all $x > 1$ and some $C > 1$ – would imply the truth of the Riemann hypothesis (RH).

In fact, it is known that RH $\Longleftrightarrow \forall \epsilon > 0, \lim_{x \to \infty} M(x)/x^{\frac{1}{2}+\epsilon} = 0$.

Introduction, 2

The Mertens conjecture was shown to be false by Odlyzko and Te Riele in 1985 with help of the lattice basis reduction (L^3) algorithm of A.K. Lenstra, H.W. Lenstra, Jr., and L. Lovász (1982) for finding short vectors in lattices.
They proved the existence of some x for which $M(x)/\sqrt{x} > 1.06$, and of some other x for which $M(x)/\sqrt{x} < -1.009$.
In 1987, Pintz gave an effective disproof of the Mertens conjecture in the sense that he proved that $|M(x)|/\sqrt{x} > 1$ for some $x \le \exp(3.21 \times 10^{64})$.
Nowadays, it is generally believed that the function $M(x)/\sqrt{x}$ is unbounded, both in the positive and in the negative direction.

Kotnik and Van de Lune, e.g., have conjectured that $M(x)/\sqrt{x} =$

$\Omega_{\pm}(\sqrt{\log\log\log x})$.

Notation

The complex zeros of the Riemann zeta function are denoted by $\rho_j = \frac{1}{2} + i\gamma_j$ (we work in the range where the Riemann hypothesis is known to be true) with $\gamma_1 = 14.1347$... and $\gamma_j < \gamma_{j+1}$, $j = 1, 2, \dots$.

Furthermore, we write $\psi_j = \arg \rho_j \zeta'(\rho_j)$ and $\alpha_j = |\rho_j \zeta'(\rho_j)|^{-1}$.

We also consider the zeros ρ_j ordered according to non-increasing values of α_j, and denote them by $\rho_j^* = \frac{1}{2} + i\gamma_j^*$ with the corresponding quantities ψ_j^*, α_j^*, $j = 1, 2, \dots$.

For example, the first five ρ_j^*'s coincide with the first five ρ_j's, but $\rho_6^* = \rho_7$, $\rho_7^* = \rho_{10}$, and $\rho_8^* = \rho_6$
(with $\alpha_6^* = \alpha_7 = 0.0163\dots, \alpha_7^* = \alpha_{10} = 0.0141\dots$ and $\alpha_8^* = \alpha_6 = 0.0137\dots$).

The first ten γ_j's

j	γ_j	ψ_j	α_j	γ_j^*
1	14.1347	1.6933	0.0891	14.1347
2	21.0220	1.3264	0.0418	21.0220
3	25.0109	1.8851	0.0291	25.0109
4	30.4249	1.0169	0.0252	30.4249
5	32.9351	2.1297	0.0220	32.9351
6	37.5862	1.2636	0.0137	40.9187
7	40.9187	1.3540	0.0164	49.7738
8	43.3271	2.2052	0.0126	37.5862
9	48.0052	0.7096	0.0133	48.0052
10	49.7738	2.0372	0.0142	43.3271

Direct approach

Systematic computations of $M(x)$ for all $x \in [1, X]$ by Mertens and many others have not led to a disproof of the Mertens conjecture. For $X = 10^{14}$, Kotnik and Van de Lune found the largest positive value of $M(x)/\sqrt{x}$ to be 0.571 for $x = 7\,766\,842\,813$ and the largest negative value to be -0.525 for $x = 71\,578\,936\,427\,177$.

Another approach

Another approach is based on the following theorem of Titchmarsh:

Theorem 1 *If all the zeros of the Riemann zeta-function are simple, then there is an increasing sequence* $\{T_n\}$ *such that*

$$M(x) = \lim_{n\to\infty} \sum_{|\gamma|<T_n} \frac{x^\rho}{\rho\zeta'(\rho)} - R(x) + \sum_{n=1}^{\infty} \frac{(-1)^{n-1}(2\pi/x)^{2n}}{(2n)!n\,\zeta(2n+1)} \qquad (1)$$

where $R(x) = 2 - \frac{\mu(x)}{2}$ *if* x *is an integer, and* $R(x) = 2$ *otherwise.*

On the Riemann hypothesis, we have $\rho = \frac{1}{2} + i\gamma$, giving:

$$\frac{M(x)}{\sqrt{x}} = 2 \lim_{n\to\infty} \sum_{0<\gamma<T_n} \frac{\cos(\gamma \log x - \psi_\gamma)}{|\rho\zeta'(\rho)|} + O(x^{-1/2}). \qquad (2)$$

Hence, as n increases, the sum in (2) will eventually converge to $M(x)/\sqrt{x}$, with error on the order of magnitude of $1/\sqrt{x}$. However, very little is known about the rate of this convergence, as the coefficients $|\rho_j \zeta'(\rho_j)|^{-1}$ do not form a monotonically decreasing sequence, but instead behave quite irregularly. For some values of x up to 10^{14}, this rate of convergence has been studied computationally by Kotnik and Van de Lune: several thousands of terms generally suffice to bring the error below 1%, but for much larger x this approach is not feasible.

Ingham's tric

The tric of Ingham was to consider, instead of (2), a weighted average of the function $M(x)/\sqrt{x}$. In that case the terms of the sum in (2) are multiplied by a function of bounded support, and the series in (1) is transformed into a finite sum. Two such cases will appear in what follows.

We write $x = e^y$, $-\infty < y < \infty$, and define

$$m(y) := M(x)x^{-1/2} = M(e^y)e^{-y/2},$$

$$\overline{m} := \limsup_{y\to\infty} m(y), \quad \underline{m} := \liminf_{y\to\infty} m(y).$$

Ingham's tric, 2

Then we have the following

Theorem 2 *Let*

$$h(y,T) := 2 \sum_{0<\gamma<T} \left[(1 - \frac{\gamma}{T}) \cos(\pi \frac{\gamma}{T}) + \pi^{-1} \sin(\pi \frac{\gamma}{T}) \right] \frac{\cos(\gamma y - \psi_\gamma)}{|\rho\, \zeta'(\rho)|}$$

where $\rho = \beta + i\gamma$ are the complex zeros of the Riemann zeta function which satisfy $\beta = \frac{1}{2}$ and which are simple. Then for any real y_0 we have

$$\underline{m} \le h(y_0, T) \le \overline{m}$$

and any value $h(y,T)$ is approximated arbitrarily closely, and infinitely often, by $M(x)/\sqrt{x}$.

Notice that also negative values of y_0 are allowed.

Graph of $(1 - t)\cos(\pi t) + \pi^{-1}\sin(\pi t)$

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Plot[(1 - t)*Cos[Pi*t] + Sin[Pi*t]/Pi, {t, 0, 1}]
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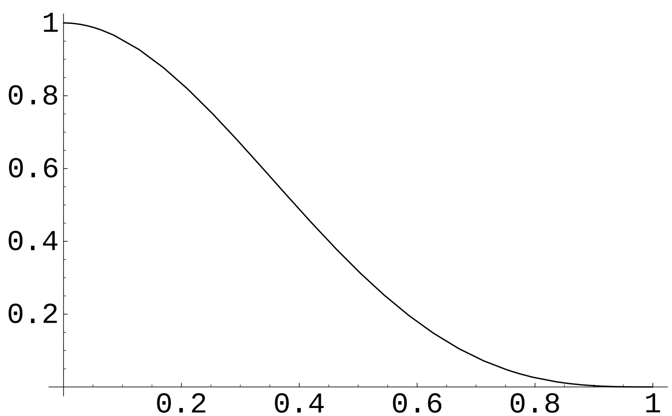

An inhomogeneous Diophantine approximation problem

Since

$$(1-t)\cos(\pi t)+\pi^{-1}\sin(\pi t)>0 \text{ for } 0<t<1$$

and since it is known that $\sum_\rho |\rho\,\zeta'(\rho)|^{-1}$ diverges, the sum of the *coefficients* of $\cos(\gamma y-\psi_\gamma)$ in Theorem 2 can be made arbitrarily large by choosing T large enough. Consequently, if we could find a value of y such that all of the $\gamma y-\psi_\gamma$ are close to integer multiples of 2π, then we could make $h(y,T)$ arbitrarily large. This would contradict, by Theorem 2, the conjecture of Mertens or any weaker form given above.

An inhomogeneous ..., 2

If the γ's were linearly independent over the rationals, then by Kronecker's theorem there would indeed exist, for any $\epsilon > 0$, integer values of y satisfying

$$|\gamma y - \psi_\gamma - 2\pi m_\gamma| < \epsilon$$

for all $\gamma \in (0, T)$ and certain integers m_γ. This would show that $h(y, T)$, and hence $M(x)/\sqrt{x}$, can be made arbitrarily large. On the same assumptions, a similar argument can be given to imply that $h(y, T)$, and hence $M(x)/\sqrt{x}$, can be made arbitrarily large on the negative side.

No good reason is known why among the γ's there should exist any linear dependencies over the rationals.

The lattice basis reduction algorithm

The approach which actually led to a disproof of the Mertens conjecture was based on the now well-known lattice basis reduction (L^3–) algorithm of Lenstra (A.K.), Lenstra (H.W., Jr.) and Lovász for finding short vectors in lattices.
With this algorithm, the inhomogeneous Diophantine approximation problem could be solved for a much larger number of terms than before the time that L^3 was known.
The "prize" to pay was that any value of y that would come out was quite large. Therefore, the first 2000 γ's were computed with an accuracy of about 100 decimal digits.

The best lower and upper bounds found in 1985 for $\overline{m}$ and $\underline{m}$ were 1.06 and -1.009, respectively.

How is L^3 applied?

In order to find a y such that each of the numbers

$$(\gamma_j^* y - \psi_j^*) \bmod 2\pi,\ 1 \leq j \leq n, \tag{3}$$

is small, we transform this problem into a problem about short vectors in lattices as follows. The lattice L used is generated by the columns $\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_{n+2}$ of the following $(n+2) \times (n+2)$ matrix (here $[x]$ means the greatest integer $\leq x$):

The input matrix for L^3

$$
\begin{array}{cccccc}
-[\sqrt{\alpha_1^*}\psi_1^* 2^{\nu}] & [\sqrt{\alpha_1^*}\gamma_1^* 2^{\nu-10}] & [2\pi\sqrt{\alpha_1^*}2^{\nu}] & 0 & \ldots & 0 \\
-[\sqrt{\alpha_2^*}\psi_2^* 2^{\nu}] & [\sqrt{\alpha_2^*}\gamma_2^* 2^{\nu-10}] & 0 & [2\pi\sqrt{\alpha_2^*}2^{\nu}] & \ldots & 0 \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
-[\sqrt{\alpha_n^*}\psi_n^* 2^{\nu}] & [\sqrt{\alpha_n^*}\gamma_n^* 2^{\nu-10}] & 0 & 0 & \ldots & [2\pi\sqrt{\alpha_n^*}2^{\nu}] \\
2^{\nu}n^4 & 0 & 0 & 0 & \ldots & 0 \\
0 & 1 & 0 & 0 & \ldots & 0
\end{array}
$$

where ν is an integer satisfying $2n \leq \nu \leq 4n$.

The L^3 algorithm produces a reduced basis $\underline{v}'_1, \underline{v}'_2, \ldots, \underline{v}'_{n+2}$ for the lattice L, where each new basis vector is a linear combination of the $n+2$ given basis vectors.

Now the $(n+1)$-st coordinate of $\underline{v}_1$, which has value $2^\nu n^4$, is very large compared to all the other entries of the original basis. Since the reduced basis is a basis for the lattice L, it should contain precisely one vector $\underline{w}$ which has a nonzero coordinate in the $(n+1)$-st position and that coordinate should be $\pm 2^\nu n^4$. Without loss of generality this may be taken to be $2^\nu n^4$.

Given the original lattice basis, the j-th coordinate of this vector $\underline{w}$ equals, for $1 \leq j \leq n$:

$$z\left[\sqrt{\alpha_j^*}\gamma_j^* 2^{\nu-10}\right] - \left[\sqrt{\alpha_j^*}\psi_j^* 2^{\nu}\right] - m_j\left[2\pi\sqrt{\alpha_j^*}2^{\nu}\right]$$

and the $(n+2)$-nd coordinate is z, for some integers $z, m_1, m_2, \ldots, m_n$. If the length of $\underline{w}$ is small, all of the

$$z\sqrt{\alpha_j^*}\gamma_j^* 2^{\nu-10} - \sqrt{\alpha_j^*}\psi_j^* 2^{\nu} - m_j 2\pi\sqrt{\alpha_j^*}2^{\nu}$$

will be small, i.e., all of the

$$\beta_j = \sqrt{\alpha_j^*}(y\gamma_j^* - \psi_j^* - 2\pi m_j)$$

will be very small, where $y = z/1024$.

The reason for the presence of the numbers α_j^* in the lattice basis is that we want to make the sum

$$\sum_{j=1}^{n} \alpha_j^* \cos(\gamma_j^* y - \psi_j^* - 2\pi m_j)$$

large. If the cos-arguments are all close to zero, this sum will approximately be equal to:

$$\sum_{j=1}^{n} \alpha_j^* - \frac{1}{2}\sum_{j=1}^{n}[\sqrt{\alpha_j^*}(\gamma_j^* y - \psi_j^* - 2\pi m_j)]^2,$$

and therefore we want the second sum to be small. This corresponds to minimizing the euclidean norm of the vector $(\beta_1, \beta_2, \ldots, \beta_n)$ which is what the L^3 algorithm attempts to do.

Example

$$n = 4, \nu = 8, L = \begin{bmatrix} -129 & 1 & 480 & 0 & 0 & 0 \\ -69 & 1 & 0 & 328 & 0 & 0 \\ -82 & 1 & 0 & 0 & 274 & 0 \\ -41 & 1 & 0 & 0 & 0 & 255 \\ 65536 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$L' = \begin{bmatrix} 1 & -51 & -55 & -66 & -213 & -65 \\ 1 & -51 & -55 & -262 & 61 & -5 \\ 1 & -51 & 219 & -66 & 7 & -18 \\ 1 & 204 & -55 & -66 & -12 & 23 \\ 0 & 0 & 0 & 0 & 0 & 65536 \\ 1 & -51 & -55 & -66 & -267 & 64 \end{bmatrix}$$

$z = 64, y = z/1024 = 0.0625$

Example, cont.

norms of vectors of L:

$2.236,\ 255,\ 274,\ 328,\ 480,\ 65536.227$

product=1.6×10^{15}

norms of vectors of L':

$2.236,\ 228.079,\ 245.073,\ 293.373,\ 347.235,\ 65536.070$

product=8.3×10^{14}

j	α_j^*	$\cos(\gamma_j^* y - \psi_j^*)$	$\alpha_j^* \cos(\gamma_j^* y - \psi_j^*)$
1	0.0891	0.6896	0.0614
2	0.0418	0.9999	0.0418
3	0.0291	0.9486	0.0276
4	0.0252	0.6336	0.0160
sum:	0.1852		0.1468

Application of L^3

We have applied the L^3 algorithm with the matrix (4) as input, for all the combinations (ν, n) in the range $\nu = 8, 9, \ldots, 400$, $n = [\nu/4], [\nu/4] + 1, \ldots, [\nu/2]$. To this end we used the function *qflll* from the PARI/GP package. For a given ν, the precision by which the computations were carried out was chosen to be $\log_{10}(2^{2\nu})$ decimal digits. For each combination of ν and n a number $z = z(\nu, n)$ was generated as described above and we computed the local maximum of $h(y, T)$ as defined above with y in the neighborhood of $z/1024$, and $T = \gamma_{10000}$.
The γ_j's were computed to an accuracy of about 250 decimal digits using the Mathematica package, and, as a check, using the PARI/GP package. The computing time was about 600 CPU hours on the SGI Altix 3700 Aster system of the Academic Computing Centre Amsterdam (SARA).

Scatter plot of the large positive values of h

Figure 1 gives for each $\nu = 8, 9, \ldots, 400$ and for each value of $z(\nu, n)$ which was found by the L^3 algorithm, a scatter plot of the positive values of

$$h(z(\nu, n)/1024, \gamma_{2000}).$$

For increasing values of ν, the corresponding h-values are increasing on average, but at a rate that seems to decrease. For the negative values of h the pattern is very similar. Reaching 1.3 and -1.3 would likely require a value of ν in the neighborhood of 800.

Large positive values of h, hence of $M(x)/\sqrt{x}$

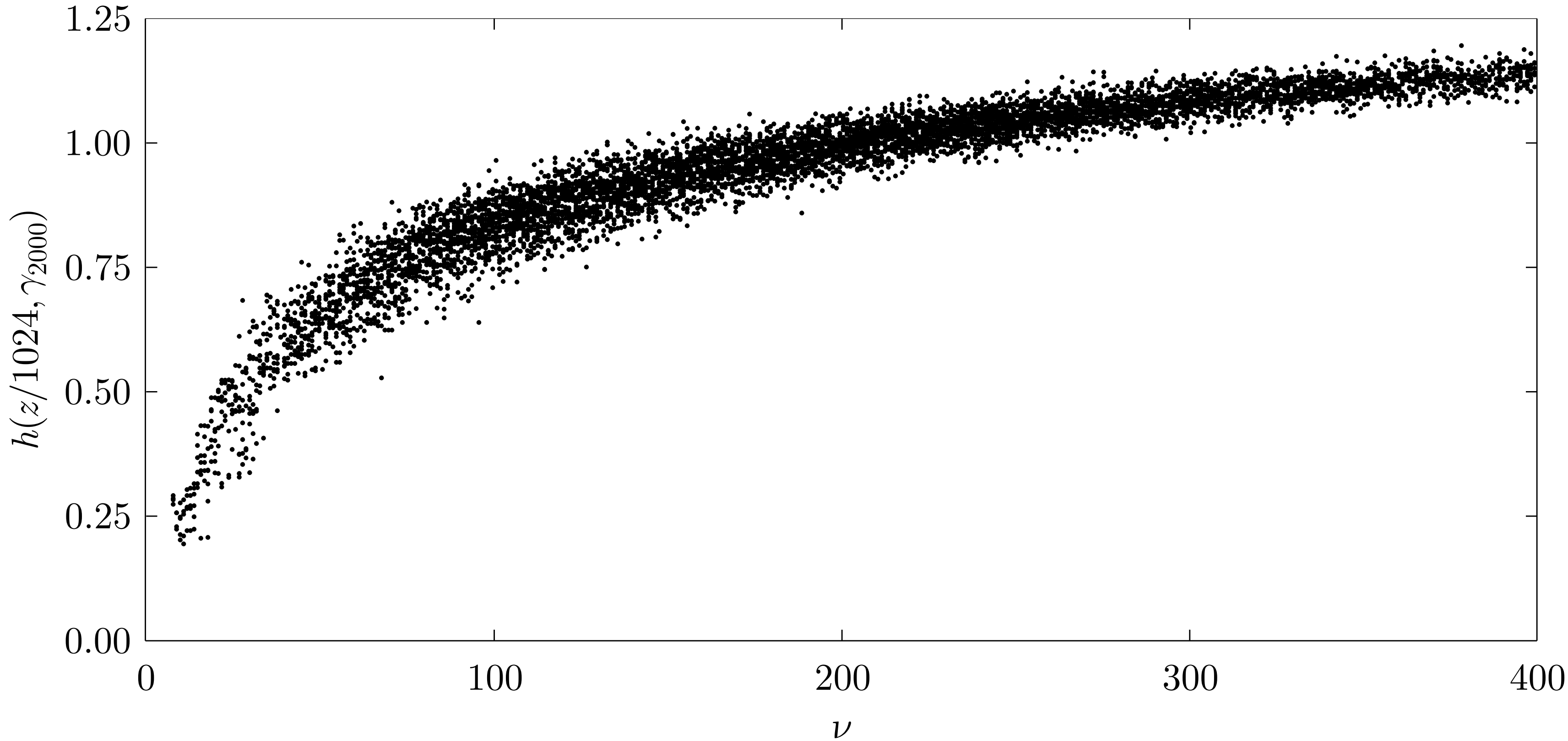

FIGURE 1

Champions

For the most promising values of h obtained, we computed the local maximum resp. minimum of $h(y, \gamma_{10000})$ in the neighborhood of $y = z/1024$. On the positive side, our champion (found with $\nu = 379, n = 98$) is

$y = -233029271\,5134531215\,0140181996\,7723401020\,4456785091\backslash$
$6681557518\,6743434036\,9240230890\,8933261706\,9029233958\backslash$
2730162362.807965 $(\log_{10}|y| = 108.3\ldots)$

with $h(y, \gamma_{10000}) = 1.218429$

and on the negative side, our champion (found with $\nu = 396, n = 102$) is

$$y = -1608\,7349754400\,0919817483\,9640165505\,4685212472\backslash$$
$2284778177\,5539303027\,5350690810\,7957194829\,6433602695\backslash$
$1442102295\,3212754000.679958$ $(\log_{10}|y| = 113.2\ldots)$

with $h(y, \gamma_{10000}) = -1.229385$.

Behaviour of $M(e^y)/e^{y/2}$ near the champions

Figure 2 compares the typical behaviour of $M(e^y)/e^{y/2}$ (top) with the behaviour of $h(y, \gamma_{10000})$ around the 1.218–spike (middle) and around the -1.229–spike (bottom).

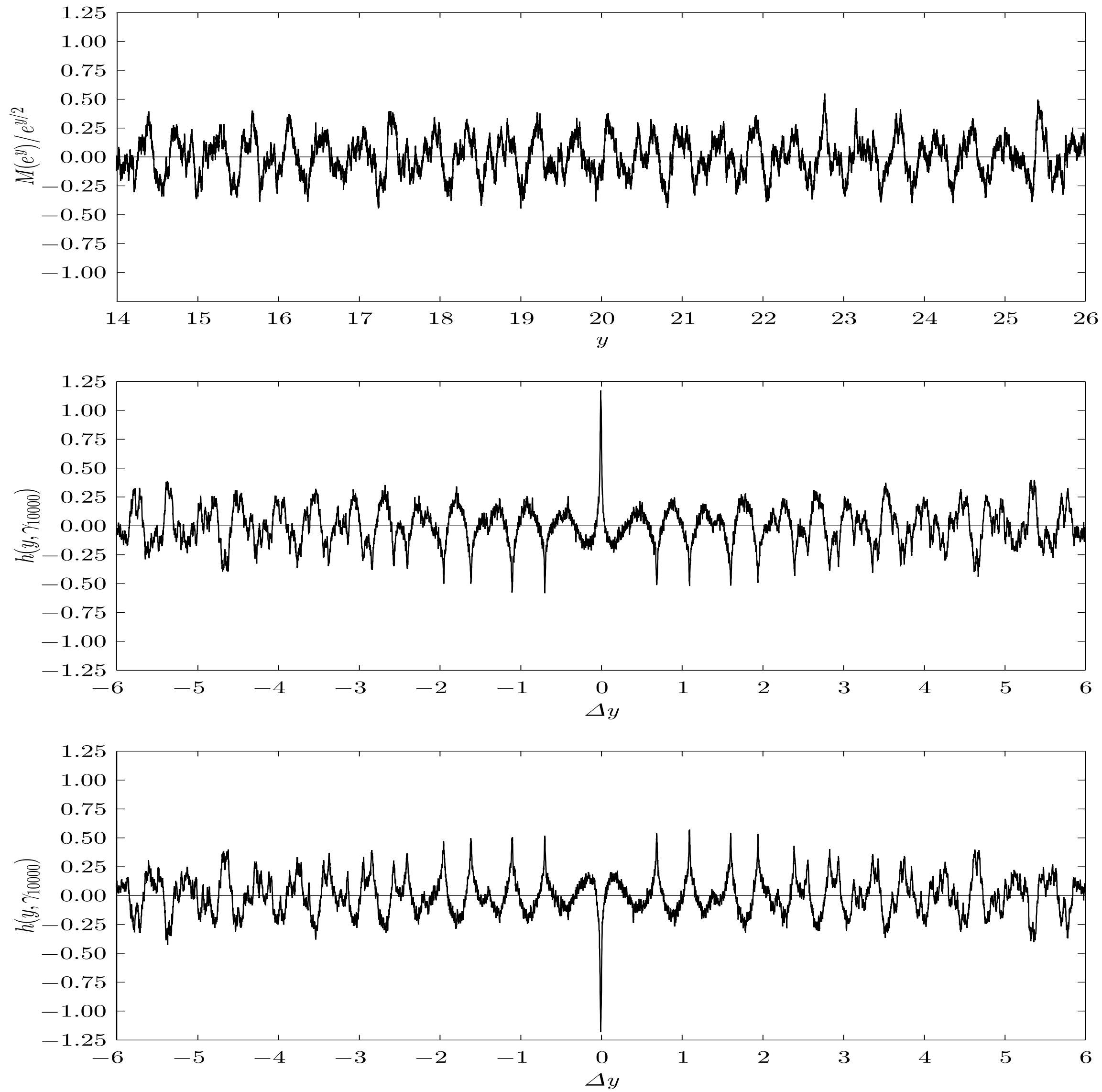
1.25
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
$M(e^y)/e^{y/2}$
14 15 16 17 18 19 20 21 22 23 24 25 26
y
$h(y, \gamma_{10000})$
−1.25
−6 −5 −4 −3 −2 −1 0 1 2 3 4 5 6
Δy
$h(y, \gamma_{10000})$
−6 −5 −4 −3 −2 −1 0 1 2 3 4 5 6
Δy

FIGURE 2

Effective result of Pintz

Theorem 3 (Pintz, 1987) *Let*

$$h_P(y,T) := 2 \sum_{0<\gamma<T} e^{-1.5\times 10^{-6}\gamma^2} \frac{\cos(\gamma y - \psi_\gamma)}{|\rho\zeta'(\rho)|}. \quad (4)$$

If there exists a $y \in [e^7, e^{5\times 10^4}]$ *with* $|h_P(y,T)| > 1 + e^{-40}$ *for* $T = 1.4 \times 10^4$*, then* $|M(x)|/\sqrt{x} > 1$ *for some* $x < e^{y+\sqrt{y}}$*.*

For the number $y = y_0 \approx 3.2097 \times 10^{64}$ as given by Odlyzko and Te Riele, on request of Pintz, Te Riele computed $h_P(y_0, T)$ and found the value -1.00223, which implies, by Pintz's Theorem, that the Mertens conjecture is false for some $x < \exp(3.21 \times 10^{64})$.

Improvement of Pintz's result

We have computed $h_P(y,T)$ for many *smaller* values of y, resulting from our application of the L^3 algorithm above, in order to attempt to reduce the upper bound for the smallest x for which the Mertens conjecture is false. The smallest y for which we found a value of $|h_P(y,T)| > 1 + e^{-40}$ is:

$$y = 1\,5853191167\,3595000428\,9014722171\,6268116204.984802$$

with $h_P(y,T) = -1.00819$. This shows that there exists an

$$x < \exp(1.59 \times 10^{40})$$

for which the Mertens conjecture is false.

$\Omega_{\pm}$-behaviour of $M(x)/\sqrt{x}$

In Figure 3, we extend the study of Kotnik and van de Lune with our results obtained here. The hollow squares and circles give the increasingly large values of $M(e^y)/\sqrt{e^y}$ and $h_1(y, \gamma_{10^6})$, respectively, found by Kotnik and Van de Lune and the solid circles give the values of $h_1(y, \gamma_{10^4})$ found by the L^3 algorithm.

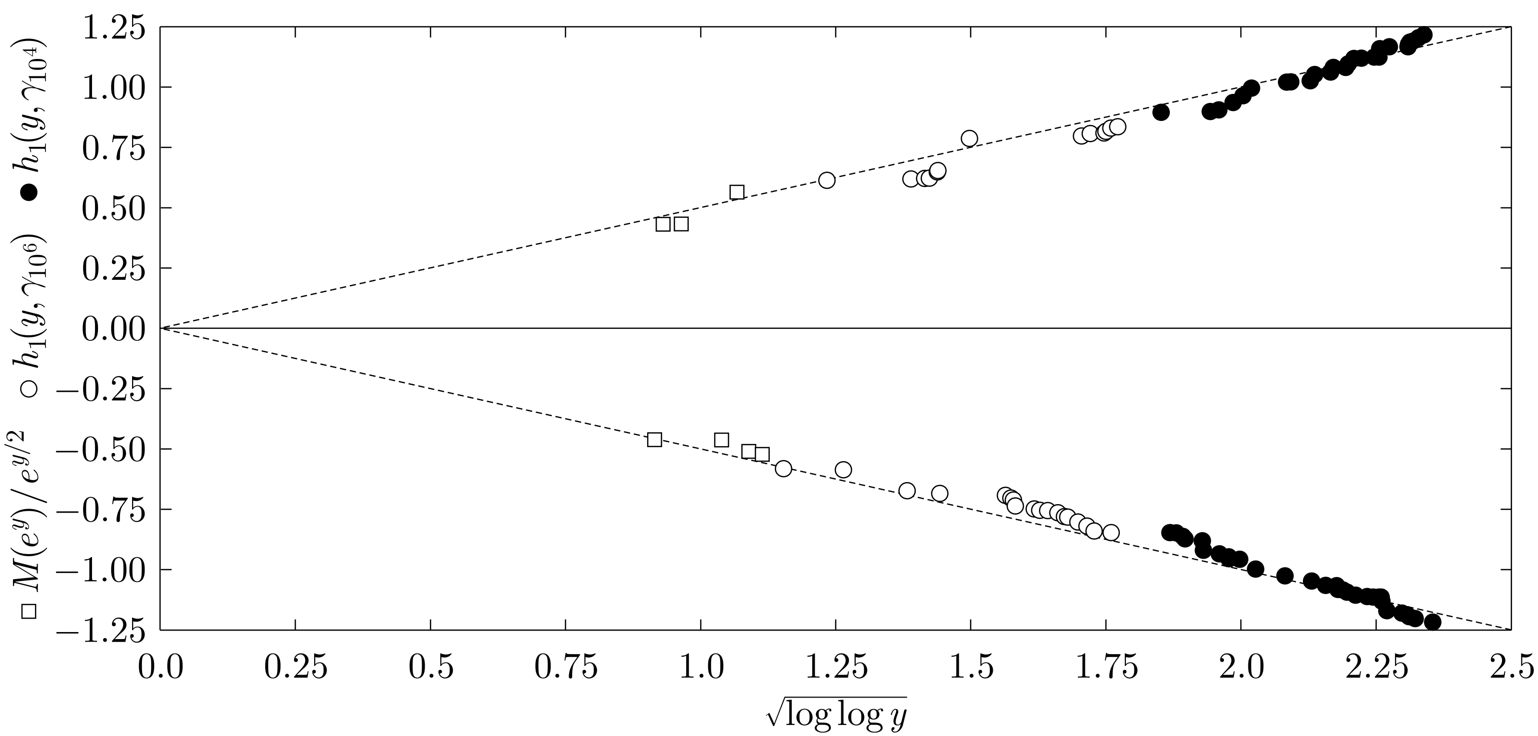

FIGURE 3

We observe that the estimates of the largest positive and negative values of $M(x)/\sqrt{x}$ are quite close to $\frac{1}{2}\sqrt{\log\log\log x}$ and $-\frac{1}{2}\sqrt{\log\log\log x}$, respectively.

Nevertheless, at the very largest y-values the positive and negative estimates appear to be systematically somewhat above the first and somewhat below the second of these two functions, respectively.

Conclusions

- known lower bound 1.06 for $\limsup M(x)/\sqrt{x}$ raised to 1.218
  known upper bound -1.009 for $\liminf M(x)/\sqrt{x}$ lowered to -1.229
- explicit upper bound $\exp(3.21 \times 10^{64})$ of Pintz on the smallest number for which the Mertens conjecture is false, reduced to $\exp(1.59 \times 10^{40})$
- numerical evidence for $M(x)/\sqrt{x} = \Omega_{\pm}(\sqrt{\log\log\log x})$