IMPROVED RESULTS ON THE MERTENS CONJECTURE

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ABSTRACT. In this article, we study the Mertens conjecture. We revisit and improve the original constructive disproof of János Pintz. We obtain a new lower bound for the minimal counterexample and new numerical results for this conjecture.

1. INTRODUCTION AND RESULTS

The Mertens conjecture [Mer97] states that

$$|M(x)|/\sqrt{x} < 1 \text{ for } x > 1,$$

where $M(x) = \sum_{1 \leq n \leq x} \mu(n)$ and $\mu(n)$ is the Möbius function with values $\mu(1) = 1$, $\mu(n) = (-1)^k$ if n is the product of k distinct primes, and $\mu(n) = 0$ otherwise. The truth of the Mertens conjecture—but also the weaker assumption: $|M(x)|/\sqrt{x} < C$ for $x > 1$ and some $C > 1$—would imply the truth of the Riemann hypothesis. The Mertens conjecture was disproved by Odlyzko and te Riele in 1985 [OtR85] when they proved the existence of some x for which $M(x)/\sqrt{x} > 1.06$, and some other x for which $M(x)/\sqrt{x} < -1.009$. The best recent result in this direction is due to Andreas Decker [Dec10] who showed that $\limsup \pm M(x)/\sqrt{x} > 1.5$.

In 1987, Pintz [Pin87] effectively disproved the Mertens conjecture by showing that $|M(x)|/\sqrt{x} > 1$ for some $x \leq \exp(3.21 \times 10^{64})$. In this paper we revisit and improve the original effective disproof of Pintz. A new lower bound of $\exp(1.004 \times 10^{33})$ for the minimal counterexample is established and new numerical results for the Mertens conjecture are obtained.

2. THE RESULTS OF PINTZ

For a more comprehensive exposition, we will adopt the notation of Pintz's paper [Pin87]. The sequence of complex numbers $\rho_\nu = \beta_\nu + i\gamma_\nu$ will denote the sorted list of non-trivial zeros of the Riemann function ζ belonging to the upper half complex plane ($0 < \gamma_1 < \gamma_2 < ...$). Values ψ_ν are then defined such that $\pi\psi_\nu = \text{Arg}(\rho_\nu\zeta'(\rho_\nu))$. The sum $K_2(v, T, k)$, where v, T and k are positive, is defined by

$$(2.1) \qquad K_2(v, T, k) := 2 \sum_{0 < \gamma_\nu < T} e^{-k\gamma_\nu^2} \frac{\cos(\gamma_\nu v - \pi\psi_\nu)}{|\rho_\nu\zeta'(\rho_\nu)|}.$$

Note that this definition is meaningful if and only if the zeros of the Riemann function ζ are all simple, at least up to height T. The main theorem of [Pin87] is the following.

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Theorem A. *If there exists a value* $v \in [e^7, e^{5 \times 10^4}]$ *such that*

$$(2.2) \qquad |K_2(v, 1.4 \times 10^4, 1.5 \times 10^{-6})| > 1 + e^{-40},$$

then there exists x *with* $1 \le x \le e^{v + \sqrt{v}}$ *and* $|M(x)| > \sqrt{x}$.

The effective disproof of the Mertens conjecture was finally obtained by computing the left-hand side of (2.2) for a value $v \simeq 3.2097 \times 10^{64}$. This value has been determined by Odlyzko and te Riele [OtR85] and, numerically we have $K_2(v, 1.4 \times 10^4, 1.5 \times 10^{-6}) \simeq -1.00223$. Theorem 2 of [Pin87] is then:

Theorem B.

$$(2.3) \qquad \max_{x \le X} \frac{|M(x)|}{\sqrt{x}} > 1 \text{ if } X = \exp(3.21 \times 10^{64}).$$

Kotnik and te Riele [KtR06] extended these computations and were able to find lower values for X in Theorem B. During their search, they also found near miss values for X, i.e., values which were very likely to be smaller counterexamples but for which (2.2) does not hold. The main reason for this latter fact is that the value $k = 1.5 \times 10^{-6}$ was too large. Indeed, in (2.1), the terms of the summation become negligible when the index γ_ν is large. Thus these terms do not contribute sufficiently to the final sum so that these near miss values for X cannot be confirmed as counterexamples.

This value for k was used in the original disproof and is a consequence of the limited computational power available in 1987. Indeed, as we will see below, if we wish to confirm counterexamples, lowering k requires increasing T. A larger number of summation terms is then involved. Moreover, because of the large values for eventual candidates v, these terms have to be computed with great accuracy. This fact, in turn, requires great accuracy for the zeros ρ_ν of the Riemann function ζ, and as we will see below, the computational load of this task increases rapidly with the size of γ_ν.

Another point with (2.2) is that it has been derived using a computation of zeros of the Riemann function ζ performed by Rosser, Yohe and Schoenfeld [RYS69] in 1969. Pintz, in his derivation, used the minimal distance between consecutive zeros obtained in that paper, without information on the exact location of close zeros. As a consequence, one integral in the original work had to be bounded as if the worst case was occurring everywhere in the path of integration. As we will see below, with the knowledge of the explicit values of the zeros of the Riemann function ζ, this integral can be bounded more efficiently and the computational cost can be reduced.

3. Outline of the proof

Pintz's results are obtained by contradiction. In the first case, the Riemann hypothesis is supposed to be false. The following theorem can then be proven:

Theorem C. *Let* $\rho_0 = \beta_0 + i\gamma_0$ *be a non-trivial zero of the Riemann function* ζ *with* $\beta_0 > 1/2$ *and* $\gamma_0 > 0$. *Then*

$$(3.1) \qquad D(Y) = \frac{1}{Y} \int_0^Y |M(x)| dx > \frac{Y^{\beta_0}}{\gamma_0^5} \text{ for } Y > \gamma_0^5.$$

It is then straightforward to prove the following corollary:

Corollary D. *Let $Y > 0$ and $\varepsilon > 0$. Suppose that there exists a non-trivial zero ρ_0 of the Riemann function ζ with $\beta_0 > \frac{1}{2} + \frac{5\log|\gamma_0|+\varepsilon}{\log Y}$. Then $D(Y) > e^\varepsilon \sqrt{Y}$.*

In [Pin87], this latter result is stated in the case $\varepsilon = 0$. This new version will permit us to obtain sharper estimates for the size of the Mertens function. In the following this result will be used with $\varepsilon = 1$, which will be sufficient for our purpose.

At this point, two mean values of the Mertens function are introduced for positive u and k:

$$(3.2) \qquad M_1(u) = \frac{e^{-k/4-u/2}}{2\sqrt{\pi k}} \int_{u-2\sqrt{ku}}^{u+2\sqrt{ku}} \frac{M(x)}{x} \exp\left(-\frac{(u-\log x)^2}{4k}\right) dx,$$

$$(3.3) \qquad M_2(u) = \frac{e^{-k/4-u/2}}{2\sqrt{\pi k}} \int_1^{+\infty} \frac{M(x)}{x} \exp\left(-\frac{(u-\log x)^2}{4k}\right) dx.$$

The following lemmas are proven:

Lemma E. *If $|M(x)| \le A\sqrt{x}$ for $|\log x - u| \le 2\sqrt{ku}$, then $|M_1(u)| < A$.*

Lemma F. *$|M_2(u) - M_1(u)| < 2e^{-u/4}$ if $k < 1/4$ and $u \ge 16$.*

Lemma G. *$M_2(u) = \frac{e^{-k/4-u/2}}{2\pi i} \int_{2-i\infty}^{2+i\infty} \frac{e^{ks^2+us}}{s\zeta(s)} ds$.*

Lemma E provides by contradiction a criterion on $M_1(u)$ to prove the existence of values for $M(x)/\sqrt{x}$ larger than A. Lemma F proves that, under some conditions, values of $M_1(u)$ and $M_2(u)$ are very close. We are then left with the study of $M_2(u)$ and Lemma G gives an alternate representation of $M_2(u)$. By the use of the residue theorem, it is possible to modify the original integration path of Lemma G and we have:

Lemma H. *Let $u > 2$ and $k > 0$, $T_1 > T_0 > 0$. Suppose that the Riemann hypothesis holds up to at least height T_0. Then we have:*

$$(3.4) \qquad M_2(u) = \frac{1}{2\pi i} \int_{(L)} \frac{e^{k(s^2-1/4)+u(s-1/2)}}{s\zeta(s)} ds + K_2(u+k, T_0, k)$$

where the integration path L is formed from L_1, L_2, L_3, L_4, L_5, L_6 and their reflected image with the real axis, where we define:

$$(3.5) \quad \begin{aligned} L_1 &= \left\{ s = \frac{1}{4} + it \middle| 0 \le t \le T_0 \right\}, \\ L_2 &= \left\{ s = \sigma + iT_0 \middle| \frac{1}{4} \le \sigma \le \frac{1}{2} + \frac{1}{u} \right\}, \\ L_3 &= \left\{ s = \frac{1}{2} + \frac{1}{u} + it \middle| T_0 \le t \le T_1 \right\}, \\ L_4 &= \left\{ s = \sigma + iT_1 \middle| \frac{1}{2} + \frac{1}{u} \le \sigma \le \frac{1}{2} + \frac{5\log T_1 + 3}{u} \right\}, \\ L_5 &= \left\{ s = \sigma + it \middle| t \ge T_1, \sigma \le 2, \sigma = \frac{1}{2} + \frac{5\log t + 3}{u} \right\}, \\ L_6 &= \left\{ s = 2 + it \middle| t \ge \exp\left(\frac{3}{10}u - \frac{3}{5}\right) \right\}. \end{aligned}$$

The transformation of the integration path in Lemma H is almost the same as that of Lemma D in the original paper. There are, however, two differences. First, in paths L_4 and L_5, the numerators of the rightmost fractions are $5 \log T_1 + 2$ and $5 \log t + 2$. In our paper, the value 2 is replaced by 3 since we are going to use Corollary D with $\varepsilon = 1$. The second difference with Pintz's work is that we introduced the path L_6 which does not exist in the original paper. This point seems to be a minor error there. In fact, in [Pin87], the path L_5 is unbounded in σ while the author uses bounds on $\zeta(s)$ proven only for $0 \leq \sigma \leq 2$. Indeed, the following lemmas are used:

Lemma I. *Let $s = \sigma + it$ with $0 \leq \sigma \leq 2$ and $t \geq 4$. If $\zeta(s) \neq 0$, then we have $\log \zeta(s) = \sum_{|\gamma - t| \leq c_0} \log(s - \rho) + \theta(11 \log t + 14)$, where $\rho = \beta + i\gamma$ describes the set of non-trivial zeros of function ζ, $c_0 = \tan(1)$ and θ is a complex number depending on s with $|\theta| \leq 1$.*

Lemma J. *Let $s = \sigma + it$ with $0 \leq \sigma \leq 2$ and $t \geq 4$, and $v > 0$. If $|s - \rho| \geq 1/v$ for all zeros ρ of function ζ, then we have:*

$$(3.6) \qquad \log |1/\zeta(s)| \leq c_0 \log t \log v + 11 \log t + 14.$$

The case where $|t| \leq 4$ is treated by the following lemma:

Lemma K. $|\zeta(1/4 + it)| \geq e^{-150}$ *for* $|t| \leq 4$.

4. GENERIC BOUNDS FOR INTEGRALS

Lemmas I and J can be used to obtain upper bounds on $|1/\zeta(s)|$ provided that we have some information about the distribution of non-trivial zeros of ζ. In turn, we can obtain upper bounds for the integral part of the right-hand side of (3.4). We then expect to show that the contribution of the integral term is negligible and thus to reduce the study of $M_2(u)$ to that of $K_2(u + k, T_0, k)$.

At this point, we make two additional assumptions on the zeros of the Riemann function ζ. First, we suppose that the Riemann hypothesis holds in fact up to at least height T_1. Second, we suppose that for any zero ρ_ν, we have $\beta_\nu \leq \frac{1}{2} + \frac{5 \log |\gamma_\nu| + 1}{\log u}$.

If this latter hypothesis is false, then Corollary D implies that $D(u) > e\sqrt{u}$. As a consequence, there exists at least one value with $1 < x < u$ and $|M(x)|/\sqrt{x} > e$. If this hypothesis is true, it can be used to provide upper bounds on integrals. Let us denote $J_i = \int_{(L_i)} \frac{e^{k(s^2 - 1/4) + u(s - 1/2)}}{s\zeta(s)} ds$ for $i \in [1 \ldots 6]$. Then we have:

$$(4.1) \qquad |M_2(u) - K_2(u + k, T_0, k)| \leq \frac{|J_1| + |J_2| + |J_3| + |J_4| + |J_5| + |J_6|}{\pi}.$$

For integral J_1, we have $s = 1/4 + it$ with $0 \leq t \leq T_0$, so that $1/|s| \leq 4$. Moreover, Lemma J holds for $v = 4$. So we have:

$$
\begin{aligned}
|J_1| &\leq 4 \int_4^{T_0} \exp\left(-\frac{3k}{16} - kt^2 - \frac{u}{4} + c_0 \log t \log 4 + 11 \log t + 14\right) dt \\
&\quad + 4 \int_0^4 \exp\left(-\frac{3k}{16} - kt^2 - \frac{u}{4} + 150\right) dt \\
&\leq 4 \exp\left(-\frac{u}{4}\right)\left(\int_4^{T_0} \exp(-kt^2 + c_0 \log T_0 \log 4 + 11 \log T_0 + 14) dt\right. \\
&\qquad\qquad \left. + \int_0^4 \exp(-kt^2 + 150) dt\right) \\
&\leq 4 \exp\left(-\frac{u}{4}\right)\left(T_0 \exp(14 \log T_0 + 14) + 4 \exp(150)\right) \\
&\leq T_0^{15} \exp\left(-\frac{u}{4} + 153\right).
\end{aligned}
$$
(4.2)

For the integral J_2, we have $s = \sigma + iT_0$ with $1/4 \leq \sigma \leq 1/2 + 1/u$, so that $1/|s| \leq 1/T_0 \leq 1$. Up to height T_1, non-trivial zeros for ζ lie on the critical line. We put $\delta = \min(T_0 - \gamma_{\nu_0}, \gamma_{\nu_0+1} - T_0)$, where ν_0 is such that $\gamma_{\nu_0} < T_0 < \gamma_{\nu_0+1}$. Then Lemma J holds for $v = K$ where $K = 1/\delta$. If we suppose that $u > 2$ and $0 < k < 1/4$, then we have:

$$
\begin{aligned}
|J_2| &\leq \int_{1/4}^{1/2+1/u} \exp(k(\sigma^2 - T_0^2 - 1/4) + u(\sigma - 1/2) \\
&\qquad\qquad + c_0 \log T_0 \log K + 11 \log T_0 + 14) d\sigma \\
&\leq \exp(-kT_0^2 - u/2 + c_0 \log T_0 \log K + 11 \log T_0 + 14) \\
&\qquad \cdot \int_{1/4}^{1/2+1/u} \exp(k\sigma^2 + u\sigma) d\sigma \\
&\leq \exp(-kT_0^2 - u/2 + c_0 \log T_0 \log K + 11 \log T_0 + 14) \exp(u/2 + 2) \\
&\leq \exp(-kT_0^2 + c_0 \log T_0 \log K + 11 \log T_0 + 16).
\end{aligned}
$$
(4.3)

Lemma J is not sufficient to bound efficiently the integral J_3. In the next section, we deal with this case with refined techniques.

For the integral J_4, we have $s = \sigma + iT_1$ with $1/2 + 1/u \leq \sigma \leq 1/2 + (5 \log T_1 + 3)/u$ and $1/|s| \leq 1$. Lemma J holds for this integral with $v = u$. For this case, we suppose that $(5 \log T_1 + 3)/u < 1/2$ and $k < 1$. Then we have:

$$|J_4| \leq \int_{1/2+1/u}^{1/2+(5\log T_1+3)/u} \exp(k(\sigma^2 - T_1^2 - 1/4) + u(\sigma - 1/2)$$
$$+ c_0 \log T_1 \log u + 11 \log T_1 + 14)d\sigma$$
$$\leq \exp(-kT_1^2 - u/2 + c_0 \log T_1 \log u + 11 \log T_0 + 14)$$

(4.4)
$$\cdot \int_{1/2+1/u}^{1/2+(5\log T_1+3)/u} \exp(k\sigma^2 + u\sigma)d\sigma$$
$$\leq \exp(-kT_1^2 - u/2 + c_0 \log T_1 \log u + 11 \log T_0 + 14)$$
$$\cdot \frac{5\log T_1 + 3}{u} \exp(u/2 + 5\log T_1 + 4)$$
$$\leq (5\log T_1 + 3)\exp(-kT_1^2 + c_0 \log T_1 \log u + 16 \log T_1 + 18).$$

For the integral J_5, we have $s = \frac{1}{2} + \frac{5\log t+3}{u} + it$ for $T_1 \leq t \leq \exp(\frac{3}{10}u - \frac{3}{5})$, so that $1/|s| \leq 1$ and $|ds| \leq 2dt$. Lemma J still holds for this integral with $v = u$, for example. Then we have:

$$|J_5| \leq \int_{T_1}^{\exp(3u/10-3/5)} \exp(k(-t^2 - 1/4) + 5\log t + 3$$

(4.5)
$$+ c_0 \log t \log u + 11 \log t + 14)dt$$
$$\leq \exp(17) \int_{T_1}^{+\infty} \exp(-kt^2 + 16 \log t + c_0 \log t \log u)dt.$$

Let us put $A = c_0 \log u + 16$. Suppose that $T_1 \geq \sqrt{A/k}$ and $-\frac{k}{2}T_1^2 + A \log T_1 \leq 0$, then for $t \geq T_1$ the previous integrand is smaller than $\exp(-kt^2/2)$. Then we have:

$$|J_5| \leq \exp(17) \int_{T_1}^{+\infty} \exp(-kt^2/2)dt$$

(4.6)
$$\leq \exp(17)\frac{1}{\sqrt{k/2}}\frac{\sqrt{\pi}}{2}\mathrm{erfc}(T_1\sqrt{k/2})$$
$$\leq \frac{1}{kT_1}\exp\left(-\frac{kT_1^2}{2} + 17\right).$$

For the integral J_6, we have $s = 2 + it$ for $t \geq \exp(\frac{3}{10}u - \frac{3}{5})$. Lemma J holds for this integral with $v = 1$, so that we have:

(4.7)
$$|J_6| \leq \int_{\exp(\frac{3}{10}u-\frac{3}{5})}^{+\infty} \exp\left(-kt^2 + \frac{15k}{4} + \frac{3u}{2} + 11\log t + 14\right)dt.$$

Suppose that we have $\exp(\frac{3}{10}u - \frac{3}{5}) \geq \sqrt{11/k}$ and $-\frac{k}{2}\exp(\frac{3}{5}u - \frac{6}{5}) + \frac{33}{10}u - \frac{33}{5} \leq 0$, then we have:

(4.8)
$$|J_6| \leq \frac{1}{k\exp(\frac{3}{10}u-\frac{3}{5})}\exp\left(-\frac{k\exp(\frac{3}{5}u-\frac{6}{5})}{2} + \frac{3u}{2} + 15\right).$$

5. THE CASE OF THE PROBLEMATIC INTEGRAL

For practical candidates u, the previous upper bounds for integrals are infinitesimal or can be rendered negligible by appropriate choices for free variables. The case is a bit different for the integral J_3. Indeed, while Lemma J holds in this case

for $v = u$, the derived bound is too large to enable final conclusions to be drawn. For this particular case, we need refined techniques.

For the moment, we suppose that the inequality $|\log(\zeta(s))| \leq \log(u) + 11 \log t + M$ holds for s in L_3 for an appropriate value of M. Then we have, for $|u| \geq 2$ and $k \leq 1/4$:

$$(5.1) \qquad |J_3| \leq \int_{T_0}^{T_1} \exp(-kt^2 + \log(u) + 11 \log t + M + 2) dt.$$

If $T_0 \geq \sqrt{11/k}$ and $-\frac{kT_0^2}{2} + 11 \log T_0 \leq 0$, then we have:

$$(5.2) \qquad |J_3| \leq \frac{1}{kT_0} \exp\left(-\frac{kT_0^2}{2} + \log(u) + M + 2\right).$$

The inequality and the corresponding value of M required to derive this last inequality will be proven from Lemma I. First, for $s = \sigma + it$, with $0 \leq \sigma \leq 2$ and $t \geq 4$, we have:

$$
\begin{aligned}
\log|\zeta(s)| &= \mathrm{Re}(\log(\zeta(s))) \\
(5.3) \qquad &= \sum_{|\gamma - t| \leq c_0} \mathrm{Re}(\log(s - \rho)) + \mathrm{Re}(\theta(11 \log t + 14)) \\
&\geq \sum_{|\gamma - t| \leq c_0} \log|s - \rho| - 11 \log t - 14.
\end{aligned}
$$

Now if s belongs to L_3, we have $s = \frac{1}{2} + \frac{1}{u} + it$ with $T_0 \leq t \leq T_1$. Suppose that the Riemann hypothesis holds at least up to height $T_1 + c_0$. Then any zero ρ involved in the previous summation is such that $\rho = \frac{1}{2} + i\gamma$ with $T_0 - c_0 \leq \gamma \leq T_1 + c_0$. Then we have $\log|s - \rho| = \log(\sqrt{1/u^2 + (t - \gamma)^2})$. As a function of t, $|s - \rho|$ admits a global minimum equal to $-\log(u)$ for $t = \gamma$ and this function is stricly decreasing for $t \leq \gamma$ and strictly increasing for $t \geq \gamma$. Moreover, if $t \neq \gamma$, we have $\log|s - \rho| \geq \log|t - \gamma|$.

We define now $\theta_\nu = \frac{\gamma_\nu + \gamma_{\nu+1}}{2}$ and we suppose that $t \in [\theta_{\nu-1}, \theta_\nu]$. Then any zero $\rho = 1/2 + i\gamma$ of ζ, such that $|\gamma - t| \leq c_0$ is such that $\theta_{\nu-1} - c_0 \leq \gamma \leq \theta_\nu + c_0$.

First, if $\rho = 1/2 + i\gamma_\nu$, we have $\log|s - \rho| \geq -\log(u)$. Suppose now that $\rho = 1/2 + i\gamma_{\nu'}$ with $\theta_{\nu-1} - c_0 \leq \gamma_{\nu'} \leq \theta_\nu + c_0$ and $\nu \neq \nu'$. Then we have $\log|s - \rho| > \log|t - \gamma_{\nu'}|$. If $\gamma_{\nu'} < \gamma_\nu$, this gives $\log|s - \rho| > \log|\theta_{\nu-1} - \gamma_{\nu'}|$, while if $\gamma_{\nu'} > \gamma_\nu$, we have $\log|s - \rho| > \log|\theta_\nu - \gamma_{\nu'}|$.

For a given $\rho = 1/2 + i\gamma_{\nu'}$, the two previous lower bounds are effective for the summation of (5.3), for any $s = \frac{1}{2} + \frac{1}{u} + it$ with $t \in [\theta_{\nu-1}, \theta_\nu]$ only if $\gamma_{\nu'} - c_0 \leq \theta_{\nu-1}$ and $\theta_\nu \leq \gamma_{\nu'} + c_0$.

If one of these two conditions is not met, it means that the eventual lower bound is not valid for the whole interval. In this case, the corresponding $\log|\theta - \gamma_{\nu'}|$ value is kept in the summation if it is negative. If it turns out to be positive, this value is discarded from the summation. Since we are looking for a global lower bound, this strategy gives a correct result for the entire interval.

Thus we have performed numerical computations in order to determine lower bounds of the expression $\sum_{|\gamma - t| \leq c_0} \log|s - \rho|$ of (5.3). The first 22 million intervals $[\theta_{\nu-1}, \theta_\nu]$ have been considered. The results are summarized in Table 1. In this table, column N records successive extremal values for valid lower bounds of the summation. Thus the last value $N = -9.05$ is valid for the whole interval of computation, i.e., for $4 \leq t \leq 10379424.827854489$. The column M then gives

TABLE 1. Constants for lower bounds for $\log(\zeta(\frac{1}{2} + \frac{1}{u} + it))$ with $4 \leq t \leq 10379424.827854489$

$[\theta_{\nu-1}, \theta_\nu]$	N	M
[197268.960264916,197268.976758059]	-6.33	20.33
[218899.718347201,218900.221843291]	-6.43	20.43
[234016.329120325,234016.894982296]	-6.66	20.66
[273192.971337030,273193.663137712]	-7.21	21.21
[511464.060978107,511464.895650786]	-7.24	21.24
[663317.570720223,663318.508310486]	-7.67	21.67
[1961773.274790168,1961773.993356110]	-7.98	21.98
[2159847.653552496,2159847.660178352]	-8.01	22.01
[2218149.038583455,2218149.333203491]	-8.21	22.21
[2650983.947015138,2650984.610665275]	-8.77	22.77
[4316831.857820662,4316832.467101349]	-9.05	23.05

the value to be used in (5.2). Values of Table 1 can then be used provided that $T_1 \leq 10379424.827854489$.

Our computations enabled us to prove that $\log|1/\zeta(s)| \leq \log(u) + 11\log t + 23.05$ for $s = \frac{1}{2} + \frac{1}{u} + it$ and $4 \leq t \leq 10^7$. As a comparison, the corresponding inequality derived by Pintz is found in [Pin87, Lemma 6] and asserts that $\log|1/\zeta(s)| \leq \log(u) + 23.01\log t + 14$ for $4 \leq t \leq 1.1 \times 10^6$.

6. Finding new counterexamples

Eventual counterexamples to the Mertens conjecture can be found with the L^3 algorithm [LLL82] applied to an $(n+2) \times (n+2)$ matrix, the details of which are given in [OtR85, (3.3)] and in [KtR06, (7)]. This results in an integer value z with the property that many values of $(\gamma_j z/1024 - \pi\psi_j) \bmod 2\pi$ for $1 \leq j \leq n$ in (2.1) are close to zero or to 2π, so that the corresponding $\cos(\gamma_j z/1024 - \pi\psi_j)$-values are close to 1 and the corresponding value of K_2 is relatively large. This matrix also depends on an integer parameter ν and in [KtR06] we have run the L^3 algorithm for all combinations (ν, n) in the range $\nu = 8, 9, \ldots, 400$, $n = [\nu/4], [\nu/4]+1, \ldots, [\nu/2]$. For $\nu = 133$, $n = 57$ we found the 38D-integer

$$z = 36351141\ 6925600240\ 0926330274\ 8479207105$$

with $K_2^*(z) = K_2(z/1024, 1.4 \times 10^4, 1.5 \times 10^{-6}) = 0.98856$ giving a near counterexample. This result was one of the motivations for the work in the present paper. In the meantime, we found a second, smaller, candidate counterexample, namely, for $\nu = 130$, $n = 45$, the 37D-integer

$$(6.1) \qquad z = 1027817\ 3478789657\ 9893810100\ 6330785076$$

with $K_2^*(z) = -0.97553$.

Table 2 lists values of z, ν, and n which we have found for $|z| < 10^{38}$ and $|K_2^*(z)| > 0.95$.

TABLE 2. Possible counterexamples to the Mertens conjecture.

z	ν	n	$K_2^*(z)$
397555026 3771598448 1041653607	101	40	0.95691
-722 6978154684 2939759163 4147185898	118	50	0.95819
-11151 3027038161 8358956745 9995538280	119	48	-0.96787
-37511 0582961517 4867934330 9083664217	123	54	0.95999
216072 6803670377 0085698435 1791104824	125	48	0.95237
1027817 3478789657 9893810100 6330785076	130	45	-0.97553
1506726 2403784656 4791444352 3724114901	128	44	0.95720
2652469 4469765372 4513268486 9611582627	127	43	0.97611
3022614 7966641562 9069201852 5628578321	130	52	0.97516
3034722 0578127545 4980254745 7921844038	133	63	-0.96040
-4347188 6716564527 1319537188 1864617970	129	51	0.96901
5258842 4031931376 4577845993 9819416585	129	54	-0.95532
5769991 7802388518 6808949748 7315551326	131	53	-0.98410
12531000 7686655073 6115159801 8094973853	129	45	0.95729
36202340 6640585861 2678465512 2561392001	133	59	0.95589
36351141 6925600240 0926330274 8479207105	133	57	0.98856
48783853 5621928886 3020780579 8685191285	131	49	0.95612
69217225 6310367394 3355689783 5087389701	135	54	0.96118

7. CHOOSING CONSTANTS

From the preceding section, we have a possible counterexample $u = z/1024 \approx 1.00372 \times 10^{33}$. The final conclusion will be drawn from the computation of $K_2(u + k, T_0, k)$ with appropriate values for k and T_0. This computation will be validated provided that the upper bounds of the integrals $J_1, ..., J_6$ are small enough.

In our computations, we set $k = 3 \times 10^{-9}$. For the 37D-integer z of (6.1), we have $K_2(u + k, 1.4 \times 10^4, k) = -1.00738$. It was verified on the first zeros of ζ, that larger values for k would probably give values for $K_2(u + k, T_0, k)$ less than 1 in absolute value. From (4.8), we can easily prove that $|J_6| \leq \exp(-\exp(10^{30}))$ and thus J_6 is infinitesimal.

From what precedes, we have seen that 10379424.827854489 is the maximal admissible value for T_1. Then we set $T_1 = 10^7$. Conditions are then satisfied for J_5 and (4.6) gives $|J_5| \leq \exp(-145000)$. Conditions are also satisfied for J_4 and, from (4.4), we obtain $|J_4| \leq \exp(-297000)$. We have also, necessarily, $T_0 \leq T_1$, so that (4.2) can be used to prove $|J_1| \leq \exp(-10^{30})$.

The previous integrals have extremely small values and thus do not influence the final computation. This is not the case for J_2 and J_3. Moreover, since their upper bounds involve T_0, in order to save computational cost it is better to choose a value for T_0 just large enough to validate the final computation. For $T_0 = 300000$, (5.3) gives $|J_3| \leq 10^{-11}$. The two zeros of ζ around height T_0 have heights 299999.720467800 and 300000.614026284. Thus we have $K \simeq 3.57$. Then (4.3) gives $|J_2| \leq 10^{-90}$.

As a consequence, we see that our choices $k = 3 \times 10^{-9}$, $T_0 = 300000$ should be sufficient for the counterexample we wish to confirm.

8. COMPUTING THE SUMMATION

From (2.1), we see that the exact computation of $K_2(v, T_0, k)$ for $v = u + k$ requires the computation of terms of the form $\cos(\gamma_\nu v - \pi\psi_\nu)$. Because of the large size of candidate v, this implies that the values γ_ν have to be determined with great accuracy. For the values ψ_ν, the required accuracy is smaller because $-1 < \psi_\nu \leq 1$. Then we need to compute the values γ_ν up to T_0 with great accuracy and the values $\zeta'(1/2 + \gamma_\nu)$ with less accuracy, at least in what concerns the numerator.

For the denominator, the values $\zeta'(\rho_\nu)$ are again required. In theory, nothing prevents these values from being arbitrarily close to 0. Thus, the absolute accuracy required for these values is a priori not known. However, in practice, these values are in fact quite far from 0, so a reduced accuracy is sufficient.

The classical way to perform these kinds of computations is to use the Euler-Maclaurin summation formula. For $k \leq 0$, we respectively denote B_k and $B_k(x)$ the k-th Bernoulli number and the k-th Bernoulli polynomial. We also introduce the Pochhammer symbol $(s)_m = \Gamma(s + m)/\Gamma(m)$ and $(s)_0 = 1$ for m an integer and s a complex number. For any s such that $\mathrm{Re}(s) > 1 - 2m$, for m an integer with $m \geq 2$, and any integer $n \geq 1$, we then have, from [Cho95],

$$(8.1) \quad \zeta(s) = \sum_{j=1}^{n} \frac{1}{j^s} + \frac{n^{1-s}}{s-1} - \frac{1}{2}n^{-s} + \sum_{k=1}^{m-1} (s)_{2k-1} \frac{B_{2k}}{(2k)!} n^{-s-2k+1} + R_m(s, n)$$

where

$$(8.2) \quad R_m(s, n) = (s)_{2m} \int_n^{+\infty} \frac{B_{2m} - B_{2m}(x - [x])}{(2m)!} x^{-s-2m} dx$$

and

$$(8.3)$$
$$\zeta'(s) = -\sum_{j=1}^{n} \frac{\log j}{j^s} - \frac{n^{1-s}}{(s-1)^2} - \frac{n^{1-s}}{s-1}\left(1 - \frac{s-1}{2n}\right)\log n$$
$$- \sum_{k=1}^{m-1} (s+1)_{2k-2} \frac{B_{2k}}{(2k)!} n^{-s-2k+1} \left\{ s\log n - 1 - \sum_{i=1}^{2k-2} \frac{s}{s+i} \right\} + R'_m(s, n)$$

where

$$(8.4)$$
$$R'_m(s, n) = -(s+1)_{2m-1} \int_n^{+\infty} \frac{B_{2m} - B_{2m}(x - [x])}{(2m)!}$$
$$\cdot \left\{ s\log x - 1 - \sum_{i=1}^{2k-1} \frac{s}{s+i} \right\} x^{-s-2m} dx.$$

These equations will be used for values on the critical line, i.e., for $s = \frac{1}{2} + it$, $t > 0$. Using this fact and properties of Bernoulli polynomials, with some computations it is possible to prove that in this case, we have

$$(8.5) \quad |R_m(s, n)| \leq \frac{\pi^2}{3} \frac{(2m-1+t)^{2m-1} n^{-2m+1/2}}{(2\pi)^{2m}}$$

and

$$(8.6) \qquad |R'_m(s,n)| \leq \frac{8(t+2m)^{2m-1}}{(2\pi)^{2m}(2m-1/2)n^{2m-1/2}}$$
$$. \left((t+1)\left(\log n - \frac{1}{(2m+1/2)n}\right) + 2m\right).$$

Given (8.5) and (8.6) and a desired accuracy $\eta > 0$, it is then possible to choose values for m and n for practical computations. The strategy we used is the following. If $t \leq 5000$, then we fix $m = 100$, else we put $m = \lfloor(t+1)/50\rfloor$. Then n is computed by dichotomy so that the right-hand side of (8.5) or (8.6) is less than η. This strategy gives a near optimal complexity in the sense that the number of terms to be considered in (8.1) and (8.3) grows nearly as $t/(2\pi)$.

In [SD10], we already computed values of the first 22 million zeros of ζ to at least 9 correct decimal places of accuracy. First, we extended the accuracy of our zeros to at least 100 decimal places. For this purpose, we used the secant method. To reach this precision, 5 or 6 iterations of the secant method were generally sufficient. After this was done, we finally verified that at least 100 decimal places were indeed correct. To that end, we computed the values of $\zeta(s)$ with an offset of 5×10^{-101} above and below the computed value to check the sign change. These values were then used to compute values for the derivative of ζ with (8.6). In this second computation, the final required accuracy was set to only 30 decimal places.

These computations had a high cost. Indeed, computing all the zeros ρ and values $\zeta'(\rho)$ up to height T by Euler-Maclaurin summation has a complexity of $T^2 \log(T)$, independently of the precision. Moreover, for the computation of the zeros, several summations are necessary. The cost is also linear with the required number of decimal places. These facts led us to realize that the direct computation of $K_2(u+k, T_0, k)$ with $T_0 = 300000$ would have been very lengthy.

Fortunately, it is possible to make shortcuts in the computations. Indeed, from (2.1), for $T'_0 < T_0$, we have:

$$(8.7) \qquad |K_2(v, T_0, k) - K_2(v, T'_0, k)| \leq 2 \sum_{T'_0 \leq \gamma_\nu < T_0} \frac{e^{-k\gamma_\nu^2}}{|\rho_\nu \zeta'(\rho_\nu)|}.$$

The right-hand side of (8.7), that we denote by $K'_2(T'_0, T_0, k)$, is easier to compute since it does not require a large accuracy in the values of ρ and $\zeta'(\rho)$, provided that T'_0 is large enough. Indeed, as said previously, the value of $\zeta'(\rho)$ for ρ being a zero of ζ is generally away from 0. Thus the denominator of the fraction can be computed to several significant decimal places even if the precision of $\zeta'(\rho)$ is not great, and the value of $|\rho\zeta'(\rho)|$ can be expected to be large. On the contrary, the denominator for $\gamma > T'_0$ is expected to be very small. As a consequence, the value of $K'_2(T'_0, T_0, k)$ is also expected to be small and it should be easily computed to, say, 8 or 9 digits of accuracy with limited computational cost.

We used again our database of zeros of ζ to compute values of $|\zeta'(\rho)|$ up to $T = 300000$. Since the precision in our database is certified to be at least 9 decimal digits after the decimal point, the precision of computed values is at least 3 decimal digits. The smallest value of $|\zeta'(\rho)|$ was encountered for $\rho = \frac{1}{2} + i\, 78974.793348246$ and was evaluated to be equal to 0.121 when rounded to nearest. We can then affirm that $1/|\zeta'(\rho)| \leq 9$ for ρ being a zero of ζ whose height is between 74000 and 300000. This upper bound was used in (8.7) in order to obtain a safe upper bound

of the remainder sum. We finally obtain:

$$(8.8) \qquad |K_2'(74000, 300000, k)| \leq 5.69 \times 10^{-8}.$$

On the other hand, using full precision computation of the zeros of ζ below $T_0' = 74000$ in (2.1), we obtain:

$$(8.9) \qquad K_2(v, 74000, k) \simeq -1.008867.$$

Thus we can finally assert the main result of this paper:

Theorem L.

$$(8.10) \qquad \max_{x \leq X} \frac{|M(x)|}{\sqrt{x}} > 1.0088 \text{ for } X = \exp(1.004 \times 10^{33}).$$

9. Discussion

In this paper, we have revisited the original explicit disproof of the Mertens conjecture given by Pintz [Pin87]. As a result, we obtained a new lower bound for the first violation of the Mertens conjecture. This result has been obtained thanks to a better knowledge of zeros of the Riemann ζ function but also by the use of refined techniques to limit the required computational cost. Moreover, the bounds we used for the remainder terms of our computations are generic and can be used for further work on this topic.

A natural question arises: Is it still possible to improve on this result? In the authors' opinion, it is quite certain. As we have seen in Section 6, the new counterexample has been obtained by the use of the L^3 algorithm [LLL82]. The principle of the search is to seek values of v for which $\cos(\gamma_\nu v - \pi \psi_\nu)$ is close to 1 for as many as possible indices ν for which $|\rho_\nu \zeta'(\rho_\nu)|^{-1}$ is large. This can be formulated as a problem of finding a shortest vector in a lattice. It is then solved with the use of the L^3 algorithm.

The counterexamples provided by the L^3 algorithm are extremely large. The exact growth of the Mertens function $M(x)$ is unknown but some conjectures have been made. For instance, Good and Churchhouse conjectured that

$$\limsup |M(x)|(x \log \log x)^{-1/2} = \sqrt{12}/\pi.$$

Independently, Kotnik and te Riele [KtR06] conjectured that

$$\limsup |M(x)|(x \log \log \log x)^{-1/2} = 1/2.$$

The first conjecture would place the first counterexample at $x \simeq 10^{10}$, which has been disproved. The second conjecture predicts the first counterexample to be at $x \simeq \exp(5 \times 10^{23})$. Another conjecture was recently made. In [Kac07], Kaczorowski gives some theoretical arguments that we could have in fact $|M(x)| = \Omega(x^{1/2} \log \log \log x)$. By extrapolating from known values of $M(x)$, this latter conjecture would imply that the first violation occurs near $x \simeq 10^{703}$. These conjectures, although giving very different estimates, agree at least on the point that our counterexample is probably not the smallest one.

A further avenue of improvement would be to obtain stronger final results. Indeed, while we have obtained a new violation of Mertens conjecture, it should be emphasized that no numerical information is available for the smallest x value such that $M(x) > \sqrt{x}$, or on the opposite side $M(x) < -\sqrt{x}$. It has yet to be noted that by virtue of the work of Odlyzko and te Riele [OtR85], such values are known

to exist in both cases. Because of the dichotomic structure of the proof, we have information only about $|M(x)|$. For the same reason, although we can determine an upper bound, we cannot obtain a lower bound, while we would like to say that in fact $x \geq \exp(v - \sqrt{v})$. These two points might be treated if we were able to modify the path L_5 in such a way that it globally reaches the line $\sigma = 2$ at a very high height but also makes detours to keep zeros of function ζ on its left even if they are not on the critical line. In order to avoid dramatic growth of the integrand, any detour to the right should be balanced by an almost identical detour to the left. We would then have to deal with huge cancellation between integrals. Although this approach is likely to pose tedious technical problems, it could produce unconditional, accurate results.

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