Further systematic computations on the summatory function of the Möbius function

Tadej Kotnik, Jan van de Lune

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1. 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 $\mu(n) = 0$ if $n$ is divisible by a prime to a power higher than the first. For reasons which will soon become apparent, Mertens [25] defined

$$M(x) := \sum_{1 \leq n \leq x} \mu(n), \quad (x \in \mathbb{R}). \quad (1.1)$$

From a table of all $M(n)$ with $1 \leq n \leq 10^4$, Mertens [25] conjectured that $|M(n)| < \sqrt{n}$ for all $n > 1$. This is the celebrated Mertens Hypothesis (MH, for short). Extending Mertens’s table up to $n = 5 \times 10^6$, von Sterneck [38] went a step farther and conjectured that $|M(n)| < \frac{1}{2}\sqrt{n}$ for all $n > 200$.

The main reason for Mertens to introduce the function $M(x)$ was its simple relation to the location of the zeros of the Riemann zeta-function, which is, largely due to its consequences for the distribution of the primes, one of the most important unsolved problems in analytic number theory. We first briefly elaborate on this, and then return to $M(x)$.

1.1 The zeros of $\zeta(s)$ and the approximation of $\pi(x)$
The Riemann zeta-function, defined by

$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}, \quad (s \in \mathbb{C}, \quad \Re(s) > 1) \quad (1.2)$$

has an analytic continuation to the whole complex plane, except for a simple pole at $s = 1$. This function was already studied by Euler, but only for real values of $s$, and it was Riemann who, in a seminal paper written in 1859 [33], first treated it as an analytic function of a complex variable.
The principal importance of the location of the zeros of \(\zeta(s)\) lies in their role in the error committed when approximating \(\pi(x)\), the number of primes not exceeding \(x\), by \(\text{li}(x) := \int_0^x \frac{du}{\log u}\). Namely, the absence of zeros of \(\zeta(s)\) in the half-plane \(\Re(s) > \theta\) would imply that [14, Theorem 30]

\[
\pi(x) = \text{li}(x) + O(x^\theta \log x). \tag{1.3}
\]

From the well known Euler product formula, \(\zeta(s) = \prod_p (1 - p^{-s})^{-1}\), with the product taken over all primes and valid in the half-plane \(\Re(s) > 1\), it is clear that \(\zeta(s) \neq 0\) in this half-plane. So, we may take \(\theta = 1\), but this is obviously insufficient to make (1.3) useful. In 1896, Hadamard [13] and de la Vallée Poussin [40] proved independently that \(\zeta(s) \neq 0\) also on the vertical \(\Re(s) = 1\). This is equivalent to the Prime Number Theorem, which states that \(\lim_{x \to \infty} \frac{\pi(x)\log x}{x} = 1\). In 1958, by taking into account that also some region to the left of the vertical \(\Re(s) = 1\) is zero-free, Vinogradov [41] and Korobov [18] developed a method which allows to show that

\[
\pi(x) = \text{li}(x) + O \left( x \exp \left( -0.2098 \frac{(\log x)^{3/5}}{(\log \log x)^{1/5}} \right) \right). \tag{1.4}
\]

Both Vinogradov and Korobov actually claimed a stronger result, and it was Walfisz [42] who obtained the first correct result following from their method. The formula (1.4), due to Ford [10], improves upon Walfisz’s result by providing the value 0.2098 for the previously undetermined constant. This is the strongest result to date, but with \(\theta < 1\), it would obviously be superseded by (1.3).

It was already known to Riemann that \(\zeta(s)\) has zeros on the line \(\Re(s) = \frac{1}{2}\), from which it clearly follows that the value \(\theta = \frac{1}{2}\) is the smallest possible. Riemann conjectured that actually all \(\zeta\)-zeros with \(\Re(s) > 0\) lie on this vertical, and this is the famous Riemann Hypothesis (RH, for short). If true, we may take \(\theta = \frac{1}{2}\) and hence

\[
\pi(x) = \text{li}(x) + O (\sqrt{x} \log x). \tag{1.5}
\]

We also have, due to Littlewood [23],

\[
\pi(x) = \text{li}(x) + \Omega_{\pm} \left( \sqrt{x \log \log x} \right). \tag{1.6}
\]

A comparison between (1.5) and (1.6) shows that even under the RH, some space would remain for improvements of either the \(O\)- or the \(\Omega\)-estimate of the error term, or perhaps both.

1.2 The order of \(M(x)\) and the zeros of \(\zeta(s)\)

By introducing \(M(x)\), Mertens provided a new approach to the analysis of the location of the zeros of \(\zeta(s)\). For \(\Re(s) > 1\) we have

\[
\frac{1}{\zeta(s)} = \prod_p \left( 1 - \frac{1}{p^s} \right) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n^s} = \sum_{n=1}^{\infty} \frac{M(n) - M(n-1)}{n^s} = \sum_{n=1}^{\infty} M(n) \left( \frac{1}{n^s} - \frac{1}{(n+1)^s} \right) = s \int_1^\infty \frac{M(x)}{x^{s+1}} dx. \tag{1.7}
\]

If \(M(x) = O(x^\alpha)\) for some \(\alpha\), then the integral in (1.7) represents an analytic function in the half-plane \(\Re(s) > \alpha\), and hence \(\frac{1}{\zeta(s)}\) must also be analytic in that half-plane. Consequently, \(\zeta(s)\) cannot have any zero there, so that we may take \(\theta = \alpha\) in (1.3), which explains the interest in the order of \(M(x)\). In particular, the RH would clearly follow from the MH, as well as from its generalized form

\[
M(x) = O(x^{1/2}). \tag{1.8}
\]
A slightly more involved treatment [39, Theorem 14.25C] shows that even
\[ M(x) = O(x^{1/2 + \varepsilon}) \] for every \( \varepsilon > 0 \) \hspace{1cm} (1.9)
would imply the RH, and that the converse is true as well, so that the RH would also imply (1.9).

It is known that [39, Theorem 14.26B]
\[ M(x) = \Omega_{\pm}(x^{1/2}) \] \hspace{1cm} (1.10)
and therefore, also in the case of \( M(x) \), a proof of the RH would bring the \( O \)- and \( \Omega \)-estimates rather close together, but some space would still remain for improvements.

### 1.3 The main results and conjectures on the order of \( M(x) \)

In 1963, Neubauer [27] computed four isolated \( M \)-values for which von Sterneck’s conjecture is violated; among these values, the one with the smallest \( n \) is \( M(7,760,000,000) = 47,465 \). In 1979, Cohen and Dress [2] showed that the first violation of von Sterneck’s conjecture in the positive direction is \( M(7,725,083,629) = 43,947 \). In 1993, Dress [7] discovered that the first such violation in the negative direction is \( M(330,486,258,610) = -287,440 \).

In 1985, Odlyzko and te Riele [28] were able to show that
\[
\liminf_{x \to \infty} \frac{|M(x)|}{\sqrt{x}} < -1.009 \hspace{1cm} (1.11a)
\]
\[
\limsup_{x \to \infty} \frac{|M(x)|}{\sqrt{x}} > 1.06 \hspace{1cm} (1.11b)
\]
thereby refuting the MH in both the negative and the positive direction. Their method did not yield a specific \( x \) for which the MH is violated, but Pintz [29] proved in 1987 that such a violation occurs for some \( x \leq 6.21 \times 10^{64} \approx 10^{14} \times 10^{64} \). For other attempts to refute von Sterneck’s conjecture and/or the MH, we refer to Jurkat [15], [16], Spira [35], Jurkat and Peyerimhoff [17], te Riele [30], Möller [26], and Anderson [1].

Today, many experts suppose that the RH, and hence (1.9), are true, but that even the generalized form of the MH, given by (1.8), is false. In this vein, some authors have proposed conjectures weaker than (1.8), yet stronger than (1.9), such as
\[
\limsup_{x \to \infty} \frac{|M(x)|}{\sqrt{x} \log \log x} = C \hspace{1cm} (1.12)
\]
with \( C = \frac{6\sqrt{2}}{\pi} \) according to Lévy in a comment to Saffari [34], whereas \( C = \frac{\sqrt{2\pi}}{\pi} \) according to Good and Churchhouse [11].

The strongest unconditional \( O \)-results on \( M(x) \) are slight improvements of \( M(x) = o(x) \). El Marraki [9] has shown that
\[
M(x) = O(x/\log^{236/75} x) \hspace{1cm} (1.13)
\]
for which he moreover provided the implied constant, while due to Walfisz [42] we also have
\[
M(x) = O\left( x \exp\left( -A \frac{(\log x)^{3/5}}{\log \log x} \right) \right) \quad \text{for some } A > 0. \hspace{1cm} (1.14)
\]
From Ford’s recent result [10] it follows that we may take \( A = 0.2098 \).

Some authors have also focused on estimates of the type \( |M(x)| < \frac{x}{A} \) for all \( x > x_0 \). For these, we refer to Hackel [12], MacLeod [24], Dress [6], Diamond and McCurley [5], Costa Pereira [3], and Dress and El Marraki [8].

More historical details about \( M(x) \) can be found in Landau [20], [21], te Riele [31], [32], and Odlyzko and te Riele [28].
2. Computations

In the past, \(M(n)\) has been computed for various ranges of \(n\). We list some authors and their progress.

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<th>Year</th>
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<td>von Sterneck [36]</td>
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<td>von Sterneck [38]</td>
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<td>Neubauer [27]</td>
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<td>(n \leq 10^8) and several isolated values up to (n = 10^{10}); gives an (n &gt; 200) with (M(n) &gt; \frac{2\pi}{2})</td>
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<td>Yorinaga [43]</td>
<td>1979</td>
<td>(n \leq 4 \times 10^8)</td>
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<tr>
<td>Cohen and Dress [2]</td>
<td>1979</td>
<td>(n \leq 7.8 \times 10^9); gives the smallest (n &gt; 200) with (M(n) &gt; \frac{\sqrt{n}}{2})</td>
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<td>Dress [7]</td>
<td>1993</td>
<td>(n \leq 10^{12}); gives the smallest (n &gt; 200) with (M(n) &lt; -\frac{\sqrt{n}}{2})</td>
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<tr>
<td>Lioen and van de Lune [22]</td>
<td>1994</td>
<td>(n \leq 10^{13})</td>
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Our main goal was to extend these results by computing \(M(n)\) for \(10^{13} < n \leq 10^{14}\). In doing so, our strategy has been very similar to the one described in detail in Lioen and van de Lune [22]. Our approach differed only in using scalar instead of vector programming, and in a slightly improved use of the “small prime variation”. A schematic description of our algorithm, starting from a known value of \(M(N_0 - 1)\), reads as follows:

1. set \(M[N_0 - 1] \leftarrow M(N_0 - 1)\)
2. precompute all primes \(p \leq \sqrt{N}\)
3. for \(n = N_0\) to \(N\):
   - set \(\mu[n] \leftarrow 1\) \{initialization\}
   - for all \(p \leq \sqrt{N}\):
     - for all \(n\) such that \(p^n|n\) set \(\mu[n] \leftarrow 0\) \{sieve with \(p^2\)\}
     - for all \(p \leq \sqrt{N}\):
       - for all \(n\) such that \(p^n|n\) set \(\mu[n] \leftarrow -p \times \mu[n]\) \{sieve with \(p\)\}
   - for \(n = N_0\) to \(N\):
     - if \(|\mu[n]| \neq n\) then set \(\mu[n] \leftarrow -\mu[n]\) \{change sign if factorization is incomplete\}
   - for \(n = N_0\) to \(N\): set \(\mu[n] \leftarrow \text{sign}(\mu[n])\) \{compute true \(\mu(n)\)\}
   - for \(n = N_0\) to \(N\):
     - set \(M[n] \leftarrow M[n - 1] + \mu[n]\) and test \(M[n]\) \{compute \(M(n)\) and test its size\}

For details of the partitioning of the above sieving process and an application of the small prime variation, we refer to Lioen and van de Lune [22]. We add some remarks about the implementation of our program:

- The above sieving process was worked out in detail in Delphi 6 (Object Pascal), and the resulting program was executed on a PC equipped with a 2.4 GHz Intel Pentium 4 processor and 1 GB RAM. It took 13 months to compute all the values of \(M(n)\) in the range \(1 \leq n \leq 10^{14}\).
- Starting our computations at \(n = 1\) allowed us to compare our results with some of the values of \(M(n)\) reported previously (see the list above). No discrepancies were detected.
- It was favorable to the speed of execution to use a rather long sieve block \(\mu[\cdot]\) (several millions of elements).
- As \(n\) increased, the speed of the algorithm gradually decreased, mainly because more and more primes took part in the sieving process. At \(n = 10^{13}\) (resp. \(n = 10^{14}\)), the speed amounted to computing about \(3.07 \times 10^8\) (resp. \(2.93 \times 10^9\)) values of \(\mu\) and \(M\) per second.
- Using the method for computation of isolated values of \(M(x)\) developed by Deléglise and Rivat [4], we checked the output periodically. The final value of our computations, \(M(10^{14})\), took about 75 minutes to evaluate.

In Table 1 we present some selected values of \(M(n)\) and \(M(n)/\sqrt{n}\). The table shows that up to \(n = 10^{14}\) there is no counterexample to the MH, but in the range \(10^{13} < n \leq 10^{14}\) there are several new highs and lows of \(M(n)\), and one new low for \(M(n)/\sqrt{n}\).
3. Discussion and Prospects

With the MH known to be false, the main remaining problem related to this conjecture is to find the smallest \( n \) for which it is violated. We recall once more that due to Pintz we have \( n < 10^{1.4 \times 10^{44}} \). A rather free interpretation of the conjecture of Good and Churchhouse, and of the one by Lévy, leads us to \( n \approx 10 \) and \( n \approx 48 \), respectively. Clearly, these are way off the mark, since the computations show that \( n > 10^{14} \). Odlyzko and te Riele [28] express their opinion that the first violation of the MH will not occur for \( n < 10^{20} \), and perhaps not even for \( n < 10^{10} \). In this context, we recall the following

**Theorem (Titchmarsh [39, Th. 14.27]).** Assume the RH, denote the zeros of \( \zeta(s) \) on the line \( \Re(s) = \frac{1}{2} \) by \( \rho = \frac{1}{2} + i\gamma \), and assume that all these zeros are simple. Then there exists a sequence \( T_k \), \( k \leq T_k \leq k + 1 \), such that

\[
M(x) = 2 \lim_{k \to \infty} \sum_{0 < \gamma < T_k} \Re \left( \frac{x^\rho}{\rho \zeta(\rho)} \right) + O(1). \tag{3.1}
\]

In a forthcoming paper of a more tentative nature [19], we describe an experiment based on the evaluation of partial sums of the “series” in (3.1), which seems to suggest that

\[
\limsup_{x \to \infty} \frac{|M(x)|}{\sqrt{x} \log \log \log x} = C \tag{3.2}
\]

with \( C \approx \frac{1}{2} \). This points in the direction of roughly \( n \approx 10^{2.3 \times 10^{23}} \) for the first violation of the MH. This tentative estimate is substantially smaller than Pintz’s bound, yet still much too large to allow for a violation of the MH to be found by direct computation. In view of this, it occurs to us that it would be futile to continue the search for such a violation by computing \( M(n) \) systematically.

**Acknowledgements**

We wish to thank Dr. ir. Herman J. J. te Riele (CWI, Amsterdam) for his valuable comments and suggestions.

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**Table 1.** Some selected values of \( M(n) \) and \( M(n)/\sqrt{n} \) in the range \( 10^4 < n \leq 10^{14} \). A listed \( M(n) \)-value assures the corresponding \( n \) to be the smallest for which \( M(n) \) assumes this value. Consecutive \( M(n) \)-entries of the same sign assure the absence of new extremal \( M(n) \)-values of the opposite sign between these entries. A framed \( M(n)/\sqrt{n} \)-value assures the corresponding \( n \) to be the smallest \( n > 200 \) for which \( M(n)/\sqrt{n} \) assumes this value. (continued on the next page)

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