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Further systematic computations on the summatory function of the Möbius function

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In the past, the Mertens function $M(x)$, i.e. the sum of the Möbius function $\mu(n)$ for $1 \le n \le x$, has been computed for $x \le 10^{13}$. We describe the results obtained by extending this range to $x \le 10^{14}$, and discuss the prospects of such computations for even larger ranges.

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In the past, the Mertens function $M(x)$, i.e. the sum of the Möbius function $\mu(n)$ for $1 \le n \le x$, has been computed for $x \le 10^{13}$. We describe the results obtained by extending this range to $x \le 10^{14}$, and discuss the prospects of such computations for even larger ranges.

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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

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

From a table of all $M(n)$ with $1 \le n \le 10^4$, 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

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

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 $\mathrm{li}(x) := \int_0^x \frac{du}{\log u}$. Namely, the absence of zeros of $\zeta(s)$ in the half-plane $\Re(s) > \theta$ would imply that [14, Theorem 30]

$$\pi(x) = \mathrm{li}(x) + O(x^{\theta} \log x). \tag{1.3}$$

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

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

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 ζ-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

$$\pi(x) = \mathrm{li}(x) + O(\sqrt{x}\log x). \tag{1.5}$$

We also have, due to Littlewood [23],

$$\pi(x) = \mathrm{li}(x) + \Omega_{\pm}\left(\sqrt{x}\frac{\log\log\log x}{\log x}\right). \tag{1.6}$$

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 Ω-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

$$\begin{aligned} \frac{1}{\zeta(s)} &= \prod_p \left(1 - \frac{1}{p^s}\right) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n^s} = \sum_{n=1}^{\infty} \frac{M(n) - M(n-1)}{n^s} \\ &= \sum_{n=1}^{\infty} M(n)\left(\frac{1}{n^s} - \frac{1}{(n+1)^s}\right) = s\int_1^{\infty} \frac{M(x)}{x^{s+1}}dx\,. \end{aligned} \tag{1.7}$$

If $M(x) = O(x^{\alpha})$ for some α, 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

$$M(x) = O(x^{1/2+\varepsilon}) \quad \text{for every } \varepsilon > 0 \tag{1.9}$$

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]

$$M(x) = \Omega_{\pm}(x^{1/2}) \tag{1.10}$$

and therefore, also in the case of $M(x)$, a proof of the RH would bring the O- and Ω-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 $M(7\,725\,038\,629) = 43\,947$. 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

$$\liminf_{x\to\infty} \, |M(x)| \, / \sqrt{x} < -1.009 \tag{1.11a}$$

$$\limsup_{x\to\infty} \, |M(x)| \, / \sqrt{x} > 1.06 \tag{1.11b}$$

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 $x \lesssim e^{3.21\times10^{64}} \simeq 10^{1.4\times10^{64}}$. 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

$$\limsup_{x\to\infty} \frac{|M(x)|}{\sqrt{x \log\log x}} = C \tag{1.12}$$

with $C = \frac{6\sqrt{2}}{\pi^2}$ according to Lévy in a comment to Saffari [34], whereas $C = \frac{\sqrt{12}}{\pi}$ 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

$$M(x) = O(x / \log^{236/75} x) \tag{1.13}$$

for which he moreover provided the implied constant, while due to Walfisz [42] we also have

$$M(x) = O\left(x \exp\left(-A \frac{(\log x)^{3/5}}{(\log\log x)^{1/5}}\right)\right) \quad \text{for some } A > 0. \tag{1.14}$$

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 $|M(x)| < \frac{x}{K}$ 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.

Mertens [25]	1897	$n \le 10^4$
von Sterneck [36]	1897	$n \le 1.5 \times 10^5$
von Sterneck [37]	1901	$n \le 5 \times 10^5$
von Sterneck [38]	1912	$n \le 5 \times 10^6$
Neubauer [27]	1963	$n \le 10^8$ and several isolated values up to $n = 10^{10}$; gives an $n > 200$ with $M(n) > \frac{\sqrt{n}}{2}$
Yorinaga [43]	1979	$n \le 4 \times 10^8$
Cohen and Dress [2]	1979	$n \le 7.8 \times 10^9$; gives the smallest $n > 200$ with $M(n) > \frac{\sqrt{n}}{2}$
Dress [7]	1993	$n \le 10^{12}$; gives the smallest $n > 200$ with $M(n) < -\frac{\sqrt{n}}{2}$
Lioen and van de Lune [22]	1994	$n \le 10^{13}$

Our main goal was to extend these results by computing $M(n)$ for $10^{13} < n \le 10^{14}$. In doing so, our strategy has been very similar to the one described in detail in Lioen and van de Lune [22]. Our approach differred 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:

set $M[N_0 - 1] \leftarrow M(N_0 - 1)$
precompute all primes $p \le \sqrt{N}$
for $n = N_0$ to N : set $\mu[n] \leftarrow 1$ $\{$*initialization*$\}$
for all $p \le \sqrt{N}$: for all n such that $p^2|n$ set $\mu[n] \leftarrow 0$ $\{$*sieve with* $p^2\}$
for all $p \le \sqrt{N}$: for all n such that $p|n$ set $\mu[n] \leftarrow -p \times \mu[n]$ $\{$*sieve with* $p\}$
for $n = N_0$ to N : if $|\mu[n]| \ne n$ then set $\mu[n] \leftarrow -\mu[n]$ $\{$*change sign if factorization is incomplete*$\}$
for $n = N_0$ to N : set $\mu[n] \leftarrow \operatorname{sign}\mu[n]$ $\{$*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 $1 \le n \le 10^{14}$.
- 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 $\mu[.]$ (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 3.07×10^6 (resp. 2.93×10^6) values of μ 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 $10^{13} < n \le 10^{14}$ 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 $n < 10^{1.4\times 10^{64}}$. A rather free interpretation of the conjecture of Good and Churchhouse, and of the one by Lévy, leads us to $n \simeq 10$ and $n \simeq 48$, 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 $n < 10^{30}$. 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, $k \le T_k \le k+1$, 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 $n \simeq 10^{2.3\times 10^{23}}$ 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.

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Table 1. Some selected values of $M(n)$ and $M(n)/\sqrt{n}$ in the range $10^4 < n \le 10^{14}$. 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*)

n	$M(n)$	$\frac{M(n)}{\sqrt{n}}$	n	$M(n)$	$\frac{M(n)}{\sqrt{n}}$	n	$M(n)$	$\frac{M(n)}{\sqrt{n}}$
11 759	36	0.332	119 545	132	0.382	991 297	265	0.266
19 291	51	0.367	141 866	−133	−0.353	1 066 854	432	0.418
23 833	−44	−0.285	230 399	−154	−0.321	1 496 299	−369	−0.302
24 185	−72	−0.463	288 894	133	0.247	1 497 305	−388	−0.317
31 530	52	0.293	300 551	240	$\boxed{0.438}$	1 761 366	433	0.326
31 989	72	$\boxed{0.403}$	335 702	−155	−0.268	1 793 918	550	0.411
31 990	73	$\boxed{0.408}$	355 733	−258	−0.433	2 015 141	−389	−0.274
42 578	−73	−0.354	463 129	241	0.354	3 239 797	−683	−0.380
42 961	−88	−0.425	463 139	244	0.359	4 321 553	551	0.265
48 151	74	0.337	598 053	−259	−0.335	4 549 130	633	0.297
48 405	90	$\boxed{0.409}$	603 151	−278	−0.358	4 956 581	−684	−0.307
48 433	96	$\boxed{0.436}$	668 557	245	0.300	5 343 761	−847	−0.366
59 023	−89	−0.366	693 255	264	0.317	6 392 954	634	0.251
96 014	−132	−0.426	897 162	−279	−0.295	6 481 601	1 060	0.416
114 701	97	0.286	926 265	−368	−0.382	7 081 861	−848	−0.319

Table 1. (*continued*)

n	$M(n)$	$\frac{M(n)}{\sqrt{n}}$
7 109 110	−1 078	−0.404
9 986 806	1 061	0.336
10 194 458	1 240	0.388
12 395 031	−1 079	−0.307
12 874 814	−1 447	−0.403
25 433 706	1 241	0.246
25 734 597	1 419	0.280
30 095 923	−1 448	−0.264
30 919 091	−2 573	−0.463
34 750 986	1 420	0.241
61 913 863	2 845	0.362
70 497 103	−2 574	−0.307
76 015 339	−3 448	−0.395
90 702 782	2 846	0.299
92 418 127	3 290	0.342
109 528 655	−3 449	−0.330
110 103 729	−4 610	−0.439
141 244 329	3 291	0.277
152 353 222	4 279	0.347
179 545 614	−4 611	−0.344
179 919 749	−6 226	−0.464
216 794 087	4 280	0.291
360 718 458	6 695	0.353
455 297 339	−6 227	−0.292
456 877 618	−8 565	−0.401
514 440 542	6 696	0.295
903 087 703	10 246	0.341
1 029 223 105	−8 566	−0.267
1 109 331 447	−15 335	−0.460
1 228 644 631	10 247	0.292
2 218 670 635	15 182	0.322
2 586 387 614	−15 336	−0.302
2 597 217 086	−17 334	−0.340
3 061 169 989	15 183	0.274
3 314 385 678	21 777	0.378
3 724 183 273	−17 335	−0.284
3 773 166 681	−25 071	−0.408
5 439 294 226	21 778	0.295
5 439 294 781	21 791	0.295
6 600 456 626	−25 072	−0.309
6 631 245 058	−31 206	−0.383
7 544 459 107	21 792	0.251
7 660 684 541	38 317	0.438
7 725 038 629	43 947	0.500
7 766 842 813	50 286	0.571
9 826 066 363	−31 207	−0.315
15 578 669 387	−51 116	−0.410
18 835 808 417	50 287	0.366
19 890 188 718	60 442	0.429
22 745 271 553	−51 117	−0.339
38 066 335 279	−81 220	−0.416
48 201 938 615	60 443	0.275
48 638 777 062	76 946	0.349
56 794 153 135	−81 221	−0.341
101 246 135 617	−129 332	−0.406
106 512 264 731	76 947	0.236
108 924 543 546	170 358	0.516
148 449 169 741	−129 333	−0.336
217 309 283 735	−190 936	−0.410
295 766 642 409	170 359	0.313
297 193 839 495	207 478	0.381
325 813 026 298	−190 937	−0.335
330 138 494 149	−271 317	−0.472
330 486 258 610	−287 440	−0.500
330 508 686 218	−294 816	−0.513
400 005 203 086	207 479	0.328
661 066 575 037	331 302	0.407
1 246 597 697 210	−294 817	−0.264
1 440 355 022 306	−368 527	−0.307
1 600 597 184 945	331 303	0.262
1 653 435 193 541	546 666	0.425
2 008 701 330 005	−368 528	−0.260
2 087 416 003 490	−625 681	−0.433
2 319 251 110 865	546 667	0.359
2 343 412 610 499	594 442	0.388
3 268 855 616 262	−625 682	−0.346
3 270 926 424 607	−635 558	−0.351
3 754 810 967 055	594 443	0.307
4 098 484 181 477	780 932	0.386
5 184 088 665 413	−635 559	−0.279
5 197 159 385 733	−689 688	−0.303
6 202 507 744 370	780 933	0.314
10 236 053 505 745	1 451 233	0.454
11 117 998 183 091	−689 689	−0.207
21 036 453 134 939	−1 745 524	−0.381
23 254 799 760 197	1 451 234	0.301
23 431 878 209 318	1 903 157	0.393
30 320 933 480 917	−1 745 525	−0.317
30 501 639 884 098	−1 930 205	−0.349
35 616 279 861 345	1 903 158	0.319
36 213 976 311 781	2 783 777	0.463
67 146 354 233 351	−1 930 206	−0.236
71 538 179 378 429	−4 337 391	−0.513
71 578 936 427 177	−4 440 015	−0.525

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