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AFDELING NUMERIEKE WISKUNDE
(DEPARTMENT OF NUMERICAL MATHEMATICS)

NW 64/78 DECEMBER

H.J.J. TE RIELE

COMPUTATIONS CONCERNING THE CONJECTURE OF MERTENS

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Computations concerning the conjecture of Mertens[*)]

by

H.J.J. te Riele

ABSTRACT

In 1897, F. Mertens conjectured that $|M(x)| < \sqrt{x}$, for all real $x > 1$, where $M(x) = \Sigma_{n \leq x} \mu(n)$, and μ is is the Möbius function. Nowadays, it is generally believed that this conjecture is false. Using a programmable desk calculator W. Jurkat and A. Peyerimhoff recently proved that $|M(x)| > 0.779\sqrt{x}$, for some real $x > 1$, thereby suggesting that one might try to disprove Mertens' conjecture with the aid of a high speed computer. After using several hundreds of hours of CPU-time of a CDC Cyber 73/173 computer system, we proved that $|M(x)| > 0.860\sqrt{x}$, for some real $x > 1$, and we now believe that the Mertens conjecture can not yet be disproved, even with the fastest present day computers.

KEY WORDS & PHRASES: *Mertens' conjecture, zeros of the Riemann zeta function, Diophantine approximation, high precision computation*

*) This paper will be submitted for publication elsewhere.

1. In 1897, F. Mertens ([6], p. 779) conjectured that

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

where $M(x) = \Sigma_{n \le x} \mu(n)$, and μ is the Möbius function. Let

$$\underline{m} = \liminf_{x \to \infty} M(x)x^{-1/2}, \quad \bar{m} = \limsup_{x \to \infty} M(x)x^{-1/2}.$$

Using a programmable desk calculator, W. Jurkat and A. Peyerimhoff [5] recently proved that $\bar{m} > 0.779$ and $\underline{m} < -0.638$ (also compare [8]). They suggested that one might try to disprove the conjecture of Mertens by using a high speed computer. We have followed this suggestion and have implemented their procedure on a CDC Cyber 73/173 system. Our best results (after several hundreds of hours of CPU-time) are $\bar{m} > 0.860$ and $\underline{m} < -0.843$, and we now believe that Mertens' conjecture cannot be disproved by using present day computers (with the method of J. and P., which is probably the best one available). Perhaps $|M(x)| > 0.9\sqrt{x}$ is still attainable.

This short note should be considered as additional to [5]. We describe how we have obtained our new bounds for $\bar{m}$ and $\underline{m}$, with emphasis on some modifications of the method of J. and P. We use the notations of [5].

2. Let n be some (fixed) positive integer and let $\rho_\nu = \frac{1}{2} + i\gamma_\nu$, $\nu = 1,2,\ldots,n$, be the first n nontrivial simple zeros of the Riemann zeta function $\zeta(s)$. In our computations we work with $n \le 15000$, so that these assumptions are certainly justified. (It was shown by R. Brent [3] that the first 70,000,000 nontrivial zeros of $\zeta(s)$ lie on the critical line $\mathrm{Re}\, s = \frac{1}{2}$ and are simple.) Let $\pi\psi_\nu = \arg(\rho_\nu\zeta'(\rho_\nu))$, where $-1 < \psi_\nu \le 1$ and let $\kappa(t) = (1-t)\cos \pi t + \frac{1}{\pi} \sin \pi t$, $0 \le t \le 1$. Figure 1 shows the graph of κ.

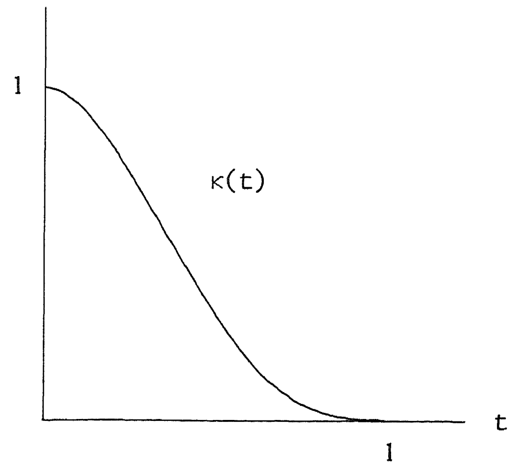

Figure 1.

Now the "key" function in [5] is

$$\sigma_n(t) = 2 \sum_{\nu=1}^{n} \kappa\left(\frac{\gamma_\nu}{\gamma_n}\right) \frac{\cos(\gamma_\nu t - \pi\psi_\nu)}{|\rho_\nu \zeta'(\rho_\nu)|}, \qquad -\infty < t < \infty, \tag{2}$$

which is shown by J. and P. to satisfy $\underline{m} \le \sigma_n(t) \le \bar{m}$, for all $t \in \mathbb{R}$. In Table 1 we give a selection of values of $|\rho_\nu \zeta'(\rho_\nu)|^{-1}$, in order to give a first impression of the behaviour of the sequence $\{|\rho_\nu \zeta'(\rho_\nu)|^{-1}\}_{\nu \in \mathbb{N}}$.

Table 1.

ν	$\lvert\rho_\nu\zeta'(\rho_\nu)\rvert^{-1}$	ν	$\lvert\rho_\nu\zeta'(\rho_\nu)\rvert^{-1}$	ν	$\lvert\rho_\nu\zeta'(\rho_\nu)\rvert^{-1}$	ν	$\lvert\rho_\nu\zeta'(\rho_\nu)\rvert^{-1}$	ν	$\lvert\rho_\nu\zeta'(\rho_\nu)\rvert^{-1}$
1	$.891_{10}{-1}$	11	$.778_{10}{-2}$	30	$.313_{10}{-2}$	400	$.155_{10}{-3}$	5000	$.190_{10}{-4}$
2	$.418_{10}{-1}$	12	$.748_{10}{-2}$	40	$.522_{10}{-2}$	500	$.323_{10}{-3}$	6000	$.334_{10}{-4}$
3	$.291_{10}{-1}$	13	$.121_{10}{-1}$	50	$.186_{10}{-2}$	600	$.407_{10}{-3}$	7000	$.347_{10}{-5}$
4	$.252_{10}{-1}$	14	$.994_{10}{-2}$	60	$.149_{10}{-2}$	700	$.172_{10}{-3}$	8000	$.145_{10}{-4}$
5	$.220_{10}{-1}$	15	$.671_{10}{-2}$	70	$.110_{10}{-2}$	800	$.175_{10}{-3}$	9000	$.613_{10}{-5}$
6	$.137_{10}{-1}$	16	$.836_{10}{-2}$	80	$.147_{10}{-2}$	900	$.268_{10}{-3}$	10000	$.117_{10}{-4}$
7	$.164_{10}{-1}$	17	$.658_{10}{-2}$	90	$.111_{10}{-2}$	1000	$.253_{10}{-3}$	11000	$.460_{10}{-4}$
8	$.126_{10}{-1}$	18	$.468_{10}{-2}$	100	$.106_{10}{-2}$	2000	$.822_{10}{-4}$	12000	$.671_{10}{-5}$
9	$.133_{10}{-1}$	19	$.742_{10}{-2}$	200	$.103_{10}{-2}$	3000	$.414_{10}{-4}$	13000	$.215_{10}{-4}$
10	$.142_{10}{-1}$	20	$.889_{10}{-2}$	300	$.412_{10}{-3}$	4000	$.203_{10}{-4}$	14000	$.631_{10}{-5}$
								15000	$.620_{10}{-5}$

Since for any fixed t the numbers $\gamma_\nu t - \pi\psi_\nu \pmod{2\pi}$, $\nu \in \mathbb{N}$, have the appearance of a sequence of random numbers, and since the numbers $\kappa(\gamma_\nu/\gamma_n)|\rho_\nu\zeta'(\rho_\nu)|^{-1}$ tend to decrease with increasing ν (although not monotonically), it seems reasonable to expect that the first terms of the sum in (2) give the most significant contribution to the value of $\sigma_n(t)$. This inspired J. and P. to look for values of t, such that $\cos(\gamma_1 t - \pi\psi_1) = 1$ and $\cos(\gamma_\nu t - \pi\psi_\nu) > 1 - \delta$ (e.g. $\delta = \frac{1}{10}$), for $\nu = 2,3,\dots,N+1$, N being as large as possible. It follows that t must have the form $\pi(2k + \psi_1)/\gamma_1$, where k is an integer, such that

$$(3) \qquad \left|\frac{\gamma_{\nu+1}}{\gamma_1} k + \frac{1}{2}\left(\frac{\gamma_{\nu+1}}{\gamma_1} \psi_1 - \psi_{\nu+1}\right)\right| < \varepsilon \pmod 1,$$

for $\nu = 1,2,\dots,N$, $\varepsilon = (2\pi)^{-1}\arccos(1-\delta)$. J. and P. devised an ingenious algorithm for the solution of this inhomogeneous Diophantine approximation problem, and applied it with $\delta = 1 - \cos(\frac{5}{36}\pi)$ (so that $\varepsilon = \frac{5}{72}$), and $N = 12$. Their best result was $\sigma_{536}(t_k) = 0.765$, for $k = 416220432570893$, and some further refinements led them to the result $\bar{m} > 0.779$.

3. We have programmed the method of J. and P. in FORTRAN, using double precision arithmetic (about 28 significant digits) where necessary, together with one modification and one extension.

The *modification* consists of making those cosines in (2) as large as possible, for which the numbers $\kappa(\gamma_\nu/\gamma_n)|\rho_\nu\zeta'(\rho_\nu)|^{-1}$ are as large as possible. If n is large compared with ν, we may assume that the variation of the sequence $\{\kappa(\gamma_\nu/\gamma_n)\}$ for small values of ν is small, compared with the variation of the sequence $\{|\rho_\nu\zeta'(\rho_\nu)|^{-1}\}$ (for $t \to 0$ we have $\kappa(t) \sim 1 - \frac{1}{2}\pi^2t^2$). Therefore, in (3) we replace "$\nu = 1,2,\dots,N$" by "$\nu = \nu_1,\nu_2,\dots$ $\dots,\nu_N$", where $|\rho_{\nu_i}\zeta'(\rho_{\nu_i})|^{-1} \geq |\rho_{\nu_j}\zeta'(\rho_{\nu_j})|^{-1}$ if $i > j$. For $N = 20$ this yields, according to table 1 (and after inspecting *all* 15000 terms of the sequence $\{|\rho_\nu\zeta'(\rho_\nu)|^{-1}\}_{\nu=1}^{\nu=15000}$), $\nu = 1,2,3,4,6,9,5,8,7,12,13,19,15,10,11,18,$ $26,14,16,\dots$. Solving (3) for $N = 12$ and $\varepsilon = \frac{5}{72}$, we obtained new values of k, and hence new values of t, which improved J. and P.'s best result by about 0.01. Although this improvement is not very impressive, the principle is important: from a table of $S_n = 2\,\Sigma_{\nu=1}^{n}\,|\rho_\nu\zeta'(\rho_\nu)|^{-1}$ in [5], J. and P.

concluded that at least 58 terms are required in (2), in order to get $\bar{m} \geq 1$, but *reordering* the values of $|\rho_\nu \zeta'(\rho_\nu)|^{-1}$ in strictly decreasing order shows that the number 58 can be lowered to 54 if one uses the values of $|\rho_\nu \zeta'(\rho_\nu)|^{-1}$ with indices ν = 1-28,30-36,39-41,43-45,48,49,53,54,57,58,63, 64,71,72,91,97,98, instead of those with indices ν = 1-58.

The *extension*, mentioned above, consists of using 15,000 zeros of the Riemann zeta function, instead of 536, as J. and P. did. The zeros were computed in two steps:

(i) separation of the zeros by using the Riemann-Siegel formula [4], and improving the accuracy of the γ_ν's to about 12 digits by means of an algorithm of Brent [2] for finding a zero of a continuous function which changes sign in a given interval;

(ii) improvement of the accuracy of the γ_ν's to about 28 digits (necessitated by the large values of t involved in (2)), by three iteration steps of the Newton process (the last step as a check), using the Euler-Maclaurin formula for the computation of $\zeta(s)$ and $\zeta'(s)$ [4].

In the same program the values of $\pi\psi_\nu$ and $|\rho_\nu \zeta'(\rho_\nu)|^{-1}$, needed in (2), were computed with an accuracy of about 14 digits. As far as possible, the computed zeros were compared with existing tables ([4], and a list of the first 650 zeros, the first 400 accurate to at least 62 digits and the remaining 250 to at least 28 digits, kindly sent to the author by Prof. Peyerimhoff), and they were found to be in perfect agreement. More details about our computations, and a table of γ_ν, $|\rho_\nu \zeta'(\rho_\nu)|^{-1}$ and $\pi\psi_\nu$, $1 \leq \nu \leq 15000$, may be found in [7].

4. We have run the algorithm of J. and P. with $\varepsilon = 5/36$ and ν = 1,2,3,4, 6,9,5,8,7,12,13,19 in (3). This yielded many values of k for which (3) holds true, and the best three are given in the first column of table 2a. The second column gives a value of t, close to $\pi(2k+\psi_1)/\gamma_1$, for which $\sigma_{15000}(t)$ has a local maximum, and the last column shows the corresponding value of $\sigma_{15000}(t)$. For comparison, we have also listed the corresponding results for the best value of k found by J. and P. Our best result for $\bar{m}$ is $\bar{m} > 0.860$.

In table 2b we list three values of k such that $\sigma_{15000}(t)$ is very *small*, for t near $\pi(2k+1+\psi_1)/\gamma_1$. These k could be very cheaply computed from the results obtained for $\bar{m}$. This is caused by the fact that the (finite) set of *differences* of consecutive elements of the set of numbers k for which (3) holds depends *only* on the numbers $\gamma_{\nu+1}/\gamma_1$, and *not* on the numbers in the inhomogeneous part of (3), *provided* that the numbers $1, \gamma_{\nu_1}/\gamma_1, \gamma_{\nu_2}/\gamma_1, \ldots, \gamma_{\nu_N}/\gamma_1$ and ε are rationally independent (cf. Theorem 3 in [5]). Although it is not known whether this hypothesis is true, its correctness is generally considered as very probable (cf. [1]). If we now look for values of t such that $\cos(\gamma_1 t - \pi\psi_1) = -1$ and $\cos(\gamma_\nu t - \pi\psi_\nu) < -1 + \delta$, for $\nu = \nu_1, \ldots, \nu_N$, then it follows that $t = \pi(2k + 1 + \psi_1)/\gamma_1$, where k is such that

$$(4) \qquad \left| \frac{\gamma_{\nu+1}}{\gamma_1} k + \frac{1}{2}\left(\frac{\gamma_{\nu+1}}{\gamma_1}\psi_1 - \psi_{\nu+1} + \frac{\gamma_{\nu+1}}{\gamma_1} + 1\right)\right| < \varepsilon \pmod 1,$$

for $\nu = \nu_1, \nu_2, \ldots, \nu_N$, $\varepsilon = (2\pi)^{-1} \arccos(1 - \delta)$. This again is an inhomogeneous Diophantine approximation problem with the same homogeneous part as (3). Assuming the rational independence of the numbers $1, \gamma_{\nu_1}/\gamma_1, \ldots, \gamma_{\nu_N}/\gamma_1$ and ε (which will be justified by the results), we could use the difference set computed for problem (3), in order to compute many numbers k satisfying (4). The three best values of k are given in table 2b, and from the third column we infer that $\underline{m} < -0.843$.

Table 2a

k	t(near $\pi(2k+\psi_1)/\gamma_1$)	$\sigma_{15000}(t)$
106857751982468	47500538601353.0955	0.8326
257965757930993	114671254215031.9656	0.8353
770305562634443	342417170808137.1055	0.8601
416220432570893 (J. and P.)	185018815735982.3572	0.8185

Table 2b

k	t(near $\pi(2k+1+\psi_1)/\gamma_1$)	$\sigma_{15000}(t)$
285460779943741	126893375027342.2209	-0.8433
1513345501403836	672714193149139.5329	-0.8300
2763987636623953	1228651164668513.8647	-0.8337

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