

# A NEW UPPER BOUND ON THE SMALLEST COUNTEREXAMPLE TO THE MERTENS CONJECTURE

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ABSTRACT. We report the finding of the new upper bound on the lowest positive integer  $x$  for which the Mertens conjecture

$$\left| \sum_{1 \leq n \leq x} \mu(n) \right| < \sqrt{x}$$

fails to hold:  $x < \exp(1.017 \times 10^{29})$ , an improvement over previously known  $\exp(1.59 \times 10^{40})$  due to Kotnik and te Riele [7].

## 1. INTRODUCTION

Perhaps one of the most striking application of the LLL reduction algorithm ([9]; also see [13]) to number theory is the disproof of the Mertens conjecture by Odlyzko and te Riele [14] in 1985. It is a conjecture made by Mertens [10] in 1897 stating that

$$M(x) := \left| \sum_{1 \leq n \leq x} \mu(n) \right| < \sqrt{x} \text{ for any } x > 1,$$

where  $\mu(n)$  is the usual Möbius function.

This conjecture lasted for nearly a century, until in [14] the authors solved the associated problem in simultaneous diophantine approximation, by reformulating it as a lattice reduction problem and applying the then-cutting-edge LLL algorithm. There are two natural follow-up questions to ask, both still open today:

- (i) What is the correct asymptotic growth rate of  $M(x)$ ?
- (ii) What is the smallest  $x$  for which  $|M(x)| \geq \sqrt{x}$ ?

The present paper focuses on the latter question. A theorem of Pintz [15] provides an approach via diophantine approximation again, based on which Kotnik and te Riele [7] showed in 2006

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

which remains the best known bound to this date. A numerical study of Kotnik and van de Lune [8] conjectures that the smallest counterexample should be of size about  $\exp(5.15 \times 10^{23})$ .

Meanwhile, there have been huge and rapid improvements in the art of lattice reduction, largely motivated by post-quantum cryptography. LLL itself has seen several improvements which led to substantial speedups in practice (e.g. [11]; see also [17]). Furthermore, much stronger algorithms have been proposed. Especially noteworthy is the BKZ algorithm, originally due to Schnorr and Euchner [18], that has undergone a series of optimizations in both output quality and complexity since the last decade (e.g. [4], [1]). Nowadays, fpLLL's implementation [5] of BKZ yields a result of strength — e.g. the

quality of the diophantine approximation — unachievable by LLL in the blink of an eye on a personal laptop.

Our idea was simply to adopt the more recent and powerful lattice reduction in place of LLL. By randomized runs of BKZ on a personal laptop, guided by some common-sense knowledge on lattices, we obtained the bound

$$x < \exp(1.017 \times 10^{29})$$

on the smallest counterexample to the Mertens conjecture, bringing us closer to the conjectured  $x \approx \exp(5.15 \times 10^{23})$ . Furthermore, we found a number of suggestive data points in this conjectured range — see Section 3 below.

This paper demonstrates only a tiny portion of the current art of lattice reduction. In a forthcoming work, we employ much more powerful tools and techniques for the goal of attaining the conjectured bound of [8] and perhaps even further. We hope our work motivates more applications of the recent advances in the computational lattice problems to number theory.

**Acknowledgments.** Both authors acknowledge support from the NSF grant CNS-2034176. We thank Yuntao Wang for his help with the powerful progressive BKZ, and Phong Nguyen for helpful discussions.

## 2. OUTLINE OF THE APPROACH

We denote by  $\mu(n)$  and  $\zeta(s)$  the usual Möbius function and the Riemann zeta function, respectively.  $\rho$  denotes a zero of  $\zeta(s)$  with  $\operatorname{Re} \rho = \frac{1}{2}$ , and for a given  $\rho$  we denote  $\gamma := \operatorname{Im} \rho, \alpha := |\rho \zeta'(\rho)|^{-1}, \psi := \arg(\rho \zeta'(\rho))$ . There are two different ways in the literature to index the zeroes and the associated quantities:  $\{\rho_i\}, \{\gamma_i\}, \{\alpha_i\}, \{\psi_i\}$  are ordered so that  $\gamma_i < \gamma_{i+1}$  for all  $i$ , and  $\{\rho_i^*\}, \{\gamma_i^*\}, \{\alpha_i^*\}, \{\psi_i^*\}$  are ordered so that  $\alpha_i^* > \alpha_{i+1}^*$  for all  $i$ .

Our approach, as with [7], is based on the following result.

**Theorem 1** (Pintz [15]). *Let*

$$(1) \quad h_P(y) := 2 \sum_{\gamma < 14000} \alpha \exp(-1.5 \cdot 10^{-6} \gamma^2) \cos(\gamma y - \psi).$$

*If there exists  $y \in [e^7, e^{50000}]$  with  $|h_P(y)| > 1 + e^{-40}$ , then  $M(x) > \sqrt{x}$  for some  $x < \exp(y + \sqrt{y})$ .*

The idea, due to [14], is that, to make  $h_P$  as large as possible, one tries to minimize those  $\gamma y - \psi \pmod{2\pi}$  with large weights, since (1) is approximately

$$(2) \quad 2 \sum_{i=1}^n \alpha_i^* \left(1 - (\gamma_i^* y - \psi_i^* \pmod{2\pi})^2\right) + (\text{“error”})$$

for some  $n \leq 100$ , say. This leads them to consider the lattice in  $\mathbb{R}^{n+2}$  generated by the columns of the matrix

$$(3) \quad \begin{pmatrix} -\lfloor \sqrt{\alpha_1^*} \psi_1^* 2^\nu \rfloor & \lfloor \sqrt{\alpha_1^*} \gamma_1^* 2^{\nu-10} \rfloor & \lfloor 2\pi \sqrt{\alpha_1^*} 2^\nu \rfloor & 0 & \cdots & 0 \\ -\lfloor \sqrt{\alpha_2^*} \psi_2^* 2^\nu \rfloor & \lfloor \sqrt{\alpha_2^*} \gamma_2^* 2^{\nu-10} \rfloor & 0 & \lfloor 2\pi \sqrt{\alpha_2^*} 2^\nu \rfloor & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\lfloor \sqrt{\alpha_n^*} \psi_n^* 2^\nu \rfloor & \lfloor \sqrt{\alpha_n^*} \gamma_n^* 2^{\nu-10} \rfloor & 0 & 0 & \cdots & \lfloor 2\pi \sqrt{\alpha_n^*} 2^\nu \rfloor \\ 2^\nu n^4 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

where  $n$  is as earlier, and  $\nu$  is the parameter controlling the round-off of the involved quantities. In a reduced (by LLL or other algorithms) basis of (3), one finds a vector, for some integers  $p_i$ 's and  $z$ ,

$$(p_1 \lfloor 2\pi \sqrt{\alpha_1^*} 2^\nu \rfloor + z \lfloor \sqrt{\alpha_1^*} \gamma_1^* 2^{\nu-10} \rfloor - \lfloor \sqrt{\alpha_1^*} \psi_1^* 2^\nu \rfloor, \dots \\ \dots, p_n \lfloor 2\pi \sqrt{\alpha_n^*} 2^\nu \rfloor + z \lfloor \sqrt{\alpha_n^*} \gamma_n^* 2^{\nu-10} \rfloor - \lfloor \sqrt{\alpha_n^*} \psi_n^* 2^\nu \rfloor, \pm 2^\nu n^4, z)^{\text{tr}},$$

since  $2^\nu n^4$  was chosen to be much larger than the rest of the entries of (3). We let  $y = \pm z 2^{-10}$ , the sign being that of the second last entry; then the first  $n$  entries can be seen to provide the minimizations of  $\gamma_i^* y - \psi_i^* \pmod{2\pi}$  weighted by  $\sqrt{\alpha_i^*}$ .

One can also aim for a large negative value of  $h_P$  by a similar construction, in which we replace  $\psi^*$  in (3) by  $\psi^* + \pi$ .

From a slightly different perspective, what the reduction of (3) achieves is a solution to a certain *approximate closest vector problem* (aCVP), that is, finding a vector of the lattice in  $\mathbb{R}^{n+1}$  generated by the columns of

$$(4) \quad \begin{pmatrix} \lfloor \sqrt{\alpha_1^*} \gamma_1^* 2^{\nu-10} \rfloor & \lfloor 2\pi \sqrt{\alpha_1^*} 2^\nu \rfloor & 0 & \dots & 0 \\ \lfloor \sqrt{\alpha_2^*} \gamma_2^* 2^{\nu-10} \rfloor & 0 & \lfloor 2\pi \sqrt{\alpha_2^*} 2^\nu \rfloor & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \lfloor \sqrt{\alpha_n^*} \gamma_n^* 2^{\nu-10} \rfloor & 0 & 0 & \dots & \lfloor 2\pi \sqrt{\alpha_n^*} 2^\nu \rfloor \\ 1 & 0 & 0 & \dots & 0 \end{pmatrix}$$

that is very close to the ‘‘target vector’’

$$\mathbf{t} := (-\lfloor \sqrt{\alpha_1^*} \psi_1^* 2^\nu \rfloor, \dots, -\lfloor \sqrt{\alpha_n^*} \psi_n^* 2^\nu \rfloor, 0)^{\text{tr}} \in \mathbb{R}^{n+1}.$$

The matrix (3) is designed so that reducing it will execute what is nowadays known as *Babai's nearest plane algorithm* [2] (see also [16, Chapter 2]), one of the main approaches to aCVP to this day. The output quality, i.e. the distance from the found lattice vector to  $\mathbf{t}$ , is affected by the strength of the reduction algorithm used.

Let

$$D = \prod_{i=1}^n \lfloor 2\pi \sqrt{\alpha_i^*} 2^\nu \rfloor,$$

the determinant of (4). We expect a cube in  $\mathbb{R}^{n+1}$  of volume  $D$  to contain one lattice vector on average. Hence one expects a lattice vector  $\mathbf{v}$  whose  $L^\infty$ -norm distance from  $\mathbf{t}$  is at most about  $\frac{1}{2} D^{\frac{1}{n+1}}$ . Since the mass of a cube in a large dimension is concentrated on its corners, we expect each coordinate of  $\mathbf{v} - \mathbf{t}$  to be of size  $\approx \frac{1}{2} D^{\frac{1}{n+1}}$ . Provided our reduction algorithm is strong enough, such  $\mathbf{v}$  can indeed be found. In our experiments, we observed this heuristic to be correct up to a factor of a few hundreds, while  $D^{\frac{1}{n+1}}$  is of magnitude  $10^{30}$  to  $10^{40}$ .

This observation leads to an estimate on the expected size of the intended main term in (2): each term is of size  $O_n(2^{-\frac{2\nu}{n+1}})$ . This partially explains the first inequality in the condition  $2n \leq \nu \leq 4n$  that [14] imposed in their experiments. (The second inequality seems unnecessary to us though.) It also gives a heuristic estimate on the size of  $y$  as a function of  $\nu$ ; a convenient simple rule we found to work well in practice is  $\log_{10} y \sim \log_{10} \nu - 5$  or  $-6$ .

### 3. EXPERIMENT AND RESULT

In search of the smallest  $y$  for which  $h_P(y) > 1 + e^{-40}$ , we reduced lattices of the form (3) for  $105 \leq \nu \leq 125$ ,  $2n \leq \nu \leq 4n$ , using BKZ- $\beta$  for  $\beta = 20, 30, 40$  — briefly speaking,

higher  $\beta$  makes the algorithm stronger and costlier. For each of these parameter choices, we took 500 randomized bases of (3) to reduce, and for the randomization, we used the method of [12] (see also [3] for more on basis randomization). For each  $\nu$  and  $\beta$ , the computations took about one to two days on a personal laptop. We also ran the same experiment looking for a large negative value of  $h_P$ .

Randomizing the input also randomizes the output to some extent, and the hope is that at least one of them yields  $|h_P(y)| > 1 + e^{-40}$ . In fact, this turned out to be a far more efficient strategy than applying a single high-quality (and high-cost) reduction to (3). The reason is that a near-optimal solution to the associated aCVP problem, while taking a disproportionately longer time to compute, does not necessarily lead to a higher value of  $h_P$ . While the sum in (2) is controllable by lattice reduction, the “error” part is not, and yet its size may fluctuate large enough to affect the outcome, either in or against our favor.

The values  $\gamma, \alpha, \psi$  are taken from the data made public by Hurst [6] who computed them up to almost 10000 decimal digits of precision, for which we are grateful. Our computations were made with 1024 binary digits of precision; it is easy to show that this is more than enough to estimate (1) well enough for our purpose. For the values presented below, they were checked again with 16384 binary digits of precision. The source code is made available on the second-named author’s website: <https://sites.google.com/view/seungki/>

The lowest working value of  $y$  is found with  $\nu = 112, n = 53, \beta = 20$ , in which

$$y = 1017256208\ 7569945816\ 8018857216.806640625, h_P(y) = 1.0034372 \dots$$

By Theorem 1, this shows that the first counterexample  $x$  to the Mertens conjecture satisfies  $x < \exp(1.017 \times 10^{29})$ .

The conjecture of [8] that  $x \approx \exp(5.15 \times 10^{23})$  corresponds to  $\nu \approx 95$ . We also found several very suggestive data points in this range (all with  $\beta = 40$ ):

$$y = 7272\ 5861306259\ 2936179649.8388671875, h_P(y) = 9.6027706 \dots \text{ for } \nu = 95, n = 50$$

$$y = 3276\ 1262680303\ 1941538273.2919921875, h_P(y) = 9.6084449 \dots \text{ for } \nu = 95, n = 56$$

$$y = 258\ 4924462692\ 5200109819.8173828125, h_P(y) = -9.5313433 \dots \text{ for } \nu = 95, n = 61$$

$$y = 5714\ 9077379396\ 8420303581, h_P(y) = -9.6006767 \dots \text{ for } \nu = 95, n = 64$$

$$y = -81\ 4638194152\ 4511993798.2373046875, h_P(y) = -9.7588934 \dots \text{ for } \nu = 96, n = 58$$

These examples encourage a further investigation; it is currently in progress.

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