THE UPPER BOUND OF THE MERTENS FUNCTION FROM THE VIEWPOINT OF STATISTICAL MECHANICS

RONG QIANG WEI

ABSTRACT. We provide some upper bounds for the Mertens function \( M(n) \): the cumulative sum of the Möbius function, by an approach of statistical mechanics, in which the Möbius function is taken as a particular state of a modified one-dimensional (1D) Ising model without the exchange interaction between the spins. Further, based on the assumptions and conclusions of the statistical mechanics, we discuss the problem that \( M(n) \) can be equivalent to the sum of an independent random sequence. It holds in the sense of equivalent probability, from which two upper bounds for the \( M(n) \) can be inferred.

Keywords:
Mertens function upper bound Statistical mechanics Ising model

1. Introduction

The Mertens function \( M(n) \) is defined as the cumulative sum of the Möbius function \( \mu(k) \) for all positive integers \( n \),

\[
M(n) = \sum_{k=1}^{n} \mu(k)
\]

where the Möbius function \( \mu(k) \) is defined as follows for a positive integer \( k \) by

\[
\mu(k) = \begin{cases} 
1 & \text{if } k = 1 \\
0 & \text{if } k \text{ is divisible by a prime square} \\
(-1)^m & \text{if } k \text{ is the product of } m \text{ distinct primes}
\end{cases}
\]

In most cases, \( M(n) \) can be extended to real numbers as follows:

\[
M(x) = \sum_{n\leq x} \mu(n)
\]

The upper bound of \( M(n) \) is always of concern to people, and many results have been presented. The following are just a few examples. The famous one is an old conjecture, "Mertens conjecture", proposed that \(|M(n)| < n^{1/2}\) for all \( n \), which was disproved by Odlyzko and te Riele (1985). Wei (2016) showed that Mertens conjecture is not true in a statistical point of view. Based on an assumption that \( \mu(n) \) is an independent random
sequence, Wei (2016) discussed the upper bound of the $M(n)$, and found that the inequality (4) for $M(n)$ holds with a probability of $1 - \alpha$,

\[ M(n) \leq \sqrt{\frac{6}{\pi^2}} K_{\alpha/2} \sqrt{n} \]

where,

\[ \int_{-K_{\alpha/2}}^{K_{\alpha/2}} \frac{1}{\sqrt{2\pi}} \exp(-\frac{t^2}{2}) dt = 1 - \alpha \]

or, the following inequality (5) holds with a probability $p > 1 - \alpha$

\[ M(n) \leq \frac{\sqrt{6}}{\pi^2} \frac{1}{\sqrt{\alpha}} \sqrt{n} \]

Without taking $\mu(n)$ as an independent random sequence, Wei (2017) conjectured that the upper bound of the $M(n)$ should have a similar formula to (4) or (5) from three facts.

Besides the examples above, MacLeod (1967; 1969) showed that

\[ |M(x)| \leq \frac{x + 1}{80} + \frac{11}{2} \quad (x \geq 1) \]

El Marraki (1995) proved that,

\[ |M(x)| \leq \frac{0.002969}{(\log x)^{1/2}} x \quad (x \geq 142194) \]

and

\[ |M(x)| \leq \frac{0.6437752}{\log x} x \quad (x > 1) \]

Ramaré (2013) showed that,

\[ |M(x)| \leq \frac{0.0146 \log x - 0.1098}{(\log x)^2} x \quad (x \geq 464402) \]

In this paper, the upper bound of the $M(n)$ will be estimated based on a modified 1D Ising model in the statistical mechanics. Although it is possible that the results are not as precise as those mentioned above, we can study the upper bound of $M(n)$ and the similar problems from a new perspective.
2. 1D Ising Model and its partition function

The 1D Ising model in the statistical mechanics is composed of a chain of $n$ spins, in which each spin interacts only with its two nearest neighbors and with an external magnetic field $h$. This nearest-neighbor Ising model is defined in terms of the following Hamiltonian (total energy) (eg., Huang, 1987),

$$H = -\frac{1}{2} J \sum_{(i,j)} s_i s_j - \xi h \sum_i s_i$$

where $(i,j)$ means that the sum is carried out over all the nearest-neighbor pair of spins $(i,j)$. $s_i = +1$, $s_i = -1$ and $s_i = 0$ are the three possible states. $J$ denotes the exchange interaction energy. $\xi$ is the magnetic moment of each spin. It should be pointed out that $s_i = \pm 1$ in the traditional 1D Ising model.

When the periodic boundary condition ($s_0 = s_n$) is imposed, the partition function for such a statistical mechanics model is,

$$Q_n = \sum_{s_i = +1,0,-1} \exp\left(-\frac{H}{kT}\right) = \sum_{s_i = +1,0,-1} \exp\left[\frac{1}{kT} \left(\frac{1}{2} J \sum_{(i,j)} s_i s_j + \xi h \sum_i s_i\right)\right]$$

where $\sum_{(i,j)} s_i s_j = s_0 s_1 + s_1 s_2 + s_2 s_3 + \ldots + s_{n-1} s_n$, and $\sum_i s_i = s_1 + s_2 + s_3 + \ldots + s_n$. $\sum_{s_i = +1,0,-1}$ is to be understood to extend over all possible states of the model system, namely,

$$\sum_{s_i = +1,0,-1} \sim \sum_{s_1 = +1,0,-1} \sum_{s_2 = +1,0,-1} \sum_{s_3 = +1,0,-1} \ldots \sum_{s_n = +1,0,-1}$$

To evaluate $Q_n$, we define a matrix $P$ as follows referring to Huang (1987),

$$P = \begin{pmatrix} 1 & 1 & 1 \\ 1 & x y & \frac{x}{y} \\ \frac{1}{y} & \frac{1}{x y} & \frac{y}{x} \end{pmatrix}$$

where $x = \exp(\frac{J}{kT})$, $y = \exp(\frac{\xi h}{kT})$.

Similar to Huang (1987), it can also be proven the following eq. (14),

$$Q_n = \text{tr} \: P^n = \lambda_1^n + \lambda_2^n + \lambda_3^n$$

where $\lambda_1, \lambda_2$, and $\lambda_3$ are the three eigenvalues of $P$ which are the three roots of the equation $\det(P - \lambda) = 0$.

In our case as follows, the exchange interaction energy is not taken into account, i.e., $J = 0$, and $x = 1$. Then we have
\[ P = \begin{pmatrix} 1 & 1 & 1 \\ y & y & y \\ y & y & y \end{pmatrix} \]

From eq. (15), we can obtain \( \lambda_1 = \lambda_2 = 0 \), and \( \lambda_3 = (1 + y + \frac{1}{y}) \) from \( \det (P - \lambda) = 0 \).

Finally,

\[ Q_n = (1 + y + \frac{1}{y})^n = \left[ 1 + \exp\left( \frac{\xi_h kT}{y} \right) + \exp\left( -\frac{\xi_h kT}{y} \right) \right]^n \]

3. The upper bound of the \( M(n) \)

Here we investigate a particular state of the 1D Ising model system in the section 2, namely the arrangement of spins is: \( s_0 = s_n = \mu(n) \), \( s_1 = \mu(1) = +1 \), \( s_2 = \mu(2) = -1 \), \( s_3 = \mu(3) = -1 \), \( s_4 = \mu(4) = 0 \), \ldots, \( s_{n-1} = \mu(n-1) \). In the case of \( x = 1 \), the Hamiltonian \( \mathcal{H}' \) for this arrangement is,

\[ \mathcal{H}' = -\xi_h \sum_i s_i \]

According to the statistical mechanics, the probability \( p \) for this special state is,

\[ p = \frac{\exp(-\mathcal{H}')}{Q_n} = \frac{\exp(\xi_h \sum_i s_i)}{Q_n} = \frac{\exp(\beta \sum_i s_i)}{Q_n} = \frac{\exp[\beta M(n)]}{Q_n} \]

Since \( p \leq 1 \), we can obtain an upper bound for \( M(n) \) as the follows,

\[ M(n) \leq \frac{1}{\beta} \log Q_n = \left\{ \frac{1}{\beta} \log [1 + \exp(\beta) + \exp(-\beta)] \right\}^n \]

If \( \mu(i) = 0 \) is not taken into account, that is, \( s_i = \pm 1 \), then according to Kramers and Wannier (1941) or Huang (1987),

\[ Q_n = (y + \frac{1}{y})^n = [\exp(\beta) + \exp(-\beta)]^n \]

and,

\[ M(n) \leq \frac{1}{\beta} \log Q_n = \left\{ \frac{1}{\beta} \log [\exp(\beta) + \exp(-\beta)] \right\}^n \]

On the other hand, if \( p \) can be calculated by other methods, we have,

\[ M(n) \leq \frac{1}{\beta} \log p Q_n = \frac{1}{\beta} \log p [1 + \exp(\beta) + \exp(-\beta)]^n \]
and

\begin{equation}
M(n) \leq \frac{1}{\beta} \log p Q_n = \frac{1}{\beta} \log p \left[ \exp(\beta) + \exp(-\beta) \right]^n
\end{equation}

4. Discussion

It can be seen from the section 3 that \( \mu(n) \) is a particular state of 1D Ising model system in the case of \( x = 1 \), that is, \( s_0 = s_n = \mu(n) \), \( s_1 = \mu(1) = +1 \), \( s_2 = \mu(2) = -1 \), \( s_3 = \mu(3) = -1 \), \( s_4 = \mu(4) = 0 \), \ldots, \( s_{n-1} = \mu(n-1) \). Its Hamiltonian (total energy) is \( \beta \sum_i \mu(i) = \beta M(n) \), and the probability \( p \) for this special can be obtained by eq. (18). When this Hamiltonian (or \( M(n) \)) is given or fixed, it can be obtained by numerous ways rather than the sequence of \( \mu(n) \) above only, since \( s_i \) is an independent random sequence according to the definition of the 1D Ising model. For example, \( s_0 = s_n = \mu(n) \), \( s_1 = \mu(10) = +1 \), \( s_2 = \mu(20) = 0 \), \( s_3 = \mu(30) = -1 \), \( s_4 = \mu(17) = -1 \), \ldots, \( s_{n-1} = \mu(n-3) \), or, \( s_0 = s_n = -1 \), \( s_1 = +1 \), \( s_2 = -1 \), \( s_3 = -1 \), \( s_4 = 0 \), \ldots, \( s_{n-1} = 0 \), \ldots (\( \sum_i s_i = M(n) \)), and so on. Therefore, \( M(n) \) is equivalent to the sum of an independent random sequence but results in an equal probability \( p \) to that from the sequence of \( \mu(n) \), i.e.,

\begin{equation}
p = \frac{\exp[\beta M(n)]}{Q_n} = \frac{\exp[\beta \sum_i \mu(i)]}{Q_n} = \frac{\exp(\beta \sum_i s_i)}{Q_n}
\end{equation}

Thus,

\begin{equation}
M(n) = \sum_i \mu(i) = \sum_i s_i
\end{equation}

Eq. (24) and (25) show that \( M(n) = \sum_i \mu(i) \) is equivalent to \( \sum_i s_i \) in the sense of equivalent probability in statistical mechanics.

Therefore, we can estimate the upper bound of the \( M(n) \) by the independent random sequence \( s_i \) with an expectation \( u = 0 \) and with a standard variance \( \sigma = \sqrt{2/3} \). Similar to Wei (2016), we have two inequality eq. (26) and (27) hold with a probability of \( 1 - \alpha \).

\begin{equation}
M(n) \leq \sqrt{2/3} K_{\alpha/2} \sqrt{n}
\end{equation}

where,

\begin{equation}
\int_{-K_{\alpha/2}}^{K_{\alpha/2}} \frac{1}{\sqrt{2\pi}} \exp(-t^2/2) dt = 1 - \alpha
\end{equation}

(27)

\begin{equation}
M(n) \leq \frac{\sqrt{2/3}}{\sqrt{\alpha}} \sqrt{n}
\end{equation}

Eq. (26) and (27) are more precise than those in section 3. However, the prerequisite is that we first acknowledge the all assumptions and results of statistical physics.
5. Conclusions

The upper bound for the Mertens function can be estimated by the way of statistical mechanics, from which the Mertens function can be studied from a physical and statistical perspective. Some new upper bounds, which are shown in the inequality of (19), (21), (22) and (23) are presented.

References

[1] El Marraki, M., 1995. Fonction sommatoire de la fonction $\mu$ de Möbius, majorations effectives fortes, J. Théorie Nombres Bordeaux 7: 407-433.
[2] Huang K., 1987. Statistical Mechanics (2nd Edition), John Wiley & Sons, Inc.
[3] Kramers, H. A., Wannier, G. H., 1941. Statistics of the Two-Dimensional Ferromagnet. Part I. Phys. Rev., 60: 252-262.
[4] MacLeod, R. A., 1967. A new estimate for the sum $M(x) = \sum_{n \leq x} \mu(n)$, Acta Arith. 13: 49-59. Corrigendum: Acta Arith. 16 (1969): 99-100.
[5] Odlyzko A M, te Riele H J J. Disproof of the Mertens conjecture, J. reine angew. Math, 1985, 357: 138-160.
[6] Ramaré, O., 2013. From explicit estimates for primes to explicit estimates for the Möbius function, Acta Arithmetica, 157 (4): 365-379.
[7] Wei RQ, 2016. A recursive relation and some statistical properties for the Möbius function, International Journal of Mathematics and Computer Science, 11(2): 215-248.
[8] Wei RQ, 2017. Two elementary formulae and some complicated properties for Mertens function, Journal of Algebra, Number Theory: Advances and Applications, 18(1-2): 15-33.

College of Earth and Planetary Sciences, University of Chinese Academy of Sciences, Beijing, PRC, 100049
E-mail address: wrq1973@ucas.ac.cn