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Суммы Мертенса, требующие меньших значений функции Мёбиуса

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Аннотация

Обсудим некоторые тождества с участием $\mu(n)$ и $M(x) = \sum_{n\le x}\mu(n)$, функции Мёбиуса и Мертенса. Они позволяют вычислить $M(N^d)$ для $d = 1, 2, 3, \dots$ как сумму $O_d\left(N^d(\log N)^{2d-2}\right)$ членов, каждое произведение вида $\mu(n_1)\cdots\mu(n_r)$ с $r \le d$ и $n_1, \dots, n_r \le N$. Докажем более общее тождество, в котором $M(N^d)$ заменяется на $M(g, K) = \sum_{n\le K}\mu(n)g(n)$, где $g(n)$ – произвольная полностью мультипликативная функция, тогда как каждое n_j имеет собственный диапазон суммирования $1, \dots, N_j$. Это не ново, за исключением того, что в $N_1, \dots, N_d$ произвольны, но наше доказательство (вдохновленное тождественным равенством Э. Майсселя, 1854) является новым. Мы главным образом заинтересованы в случае $d = 2$, $K = N^2$, $N_1 = N_2 = N$, где тождество имеет вид $M(g, N^2) = 2M(g, N) - \mathbf{m}^{\mathrm{T}}A\mathbf{m}$, при этом A является матрицей $N \times N$ элементов $a_{mn} = \sum_{k\le N^2/(mn)} g(k)$, в то время как $\mathbf{m} = (\mu(1)g(1), \dots, \mu(N)g(N))^{\mathrm{T}}$. Наши результаты в разделах 2 и 3 данной статьи предполагают, что $g(n)$ равно 1 для всех n. Теорема Фробениуса—Перрона применяется в этом случае: мы находим, что A имеет одно большое положительное собственное значение, приблизительно $(\pi^2/6)N^2$, с собственным вектором приблизительно $\mathbf{f} = (1, 1/2, 1/3, \dots, 1/N)^{\mathrm{T}}$ T и что при больших значениях N второе наибольшее собственное значение лежит в $(-0.58N, -0.49N)$. Раздел 2 включает оценки для следов A и A^2 (хотя для $\mathrm{Tr}(A^2)$, мы пропустим часть доказательства). В разделе 3 обсуждаются способы аппроксимации $\mathbf{m}^{\mathrm{T}}A\mathbf{m}$, используя спектральное разложение A или (альтернативно) формулу Перрона: последний подход приводит к контурному интегралу, включающему дзета-функцию Римана. Мы также рассматриваем использование тождества $A = N^2\mathbf{f}\mathbf{f}^T - \frac{1}{2}\mathbf{u}\mathbf{u}^T + Z$, а Z — матрица $N \times N$ элементов $z_{mn} = -\psi(N^2/(mn))$, причем $\psi(x) = x - \lfloor x\rfloor - \frac{1}{2}$. Наши выводы представлены в разделе 4.

Ключевые слова: функция Мёбиуса, функция Мертенса, полностью мультипликативная функция, Майссель, тождество Линника, тождество Вогана, симметричная матрица, теорема Фробениуса-Перрона, собственное значение, собственный вектор, формула Перрона, дзета-функция Римана.

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Mertens Sums requiring Fewer Values of the Möbius Function

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Abstract

We discuss certain identities involving $\mu(n)$ and $M(x) = \sum_{n\le x}\mu(n)$, the functions of Möbius and Mertens. These allow calculation of $M(N^d)$, for $d = 1, 2, 3, \dots$, as a sum of $O_d\left(N^d(\log N)^{2d-2}\right)$ terms, each a product of the form $\mu(n_1)\cdots\mu(n_r)$ with $r \le d$ and $n_1, \dots, n_r \le N$. We prove a more general identity in which $M(N^d)$ is replaced by $M(g, K) = \sum_{n\le K}\mu(n)g(n)$, where $g(n)$ is an arbitrary totally multiplicative function, while each n_j has its own range of summation, $1, \dots, N_j$. This is not new, except perhaps in that $N_1, \dots, N_d$ are arbitrary, but our proof (inspired by an identity of E. Meissel, 1854) is new. We are mainly interested in the case $d = 2$, $K = N^2$, $N_1 = N_2 = N$, where the identity has the form $M(g, N^2) = 2M(g, N) - \mathbf{m}^{\mathrm{T}}A\mathbf{m}$, with A being the $N \times N$ matrix of elements $a_{mn} = \sum_{k\le N^2/(mn)} g(k)$, while $\mathbf{m} = (\mu(1)g(1), \dots, \mu(N)g(N))^{\mathrm{T}}$. Our results in Sections 2 and 3 of the paper assume that $g(n)$ equals 1 for all n. The Perron-Frobenius theorem applies in this case: we find that A has one large positive eigenvalue, approximately $(\pi^2/6)N^2$, with eigenvector approximately $\mathbf{f} = (1, 1/2, 1/3, \dots, 1/N)^{\mathrm{T}}$, and that, for large N, the second-largest eigenvalue lies in $(-0.58N, -0.49N)$. Section 2 includes estimates for the traces of A and A^2 (though, for $\mathrm{Tr}(A^2)$, we omit part of the proof). In Section 3 we discuss ways to approximate $\mathbf{m}^{\mathrm{T}}A\mathbf{m}$, using the spectral decomposition of A, or (alternatively) Perron's formula: the latter approach leads to a contour integral involving the Riemann zeta-function. We also discuss using the identity $A = N^2\mathbf{f}\mathbf{f}^T - \frac{1}{2}\mathbf{u}\mathbf{u}^T + Z$, where $\mathbf{u} = (1, \dots, 1)^{\mathrm{T}}$ and Z is the $N \times N$ matrix of elements $z_{mn} = -\psi(N^2/(mn))$, with $\psi(x) = x - \lfloor x\rfloor - \frac{1}{2}$.

Keywords: Möbius function, Mertens function, completely multiplicative function, Meissel, Linnik's identity, Vaughan's identity, symmetric matrix, Perron-Frobenius, eigenvalue, eigenvector, Perron's formula, Riemann zeta-function.

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Dedicated to the memory of Yu. V. Linnik

1. Introduction

The sieve of Eratosthenes will find the prime numbers in $N+1, \dots, N^2$ provided that we know all the primes in $2, \dots, N$. In particular the sieve gives a relation for the function $\pi(x)$ that counts

the number of primes less than or equal to x:

$$\pi(N^2) = \pi(N) - 1 + \sum_{\substack{d \le N^2 \\ P(d) \le N}} \mu(d) \left[\frac{N^2}{d} \right], \tag{1}$$

where $\mu(d)$ is the Möbius function (which is $(-1)^\nu$ when d has ν prime factors, all different, but 0 when d has any prime factor repeated), while $P(d)$ is the greatest non-composite divisor of d, and $[x] = \max\{m \in \mathbb{Z} : m \le x\}$. The numbers d in (1) are constructed as products of the known primes in $2, \dots, N$, so the values $\mu(d)$ can be read off. In general, given a number n, it is very difficult to factorise n and so find $\mu(n)$. Thus the Mertens sum

$$M(x) = \sum_{n \le x} \mu(n) \tag{2}$$

is difficult to calculate from the definition. The Dirichlet series $\sum \mu(n)/n^s$ is $1/\zeta(s)$ (the reciprocal of the Riemann zeta function), and, according to folklore, the fastest method of calculating $M(x)$ is by Perron's contour integral formula for the sum of the coefficients of a Dirichlet series.

In this paper we discuss a family of identities which allow $M(N^d)$ to be calculated for each positive integer d as a sum of no more than $O_d\left(N^d (\log N)^{2d-2}\right)$ terms, each a product of the form $\mu(n_1) \cdots \mu(n_r)$ with $r \le d$ and $\{n_1, \dots, n_r\} \subseteq \{1, \dots, N\}$. In Theorem 1, below, we state a more complicated form of these identities, in which each of the variables of summation n_j $(j = 1, \dots, r)$ can have its own independent range of summation: $1, \dots, N_j$ (say).

We actually treat the more general Möbius sum

$$M(g, x) = \sum_{n \le x} \mu(n) g(n), \tag{3}$$

where $g(n)$ can be any totally multiplicative arithmetic function, that is, $g(rs) = g(r)g(s)$ holds for any positive integers r and s. The relevant identity when $d = 1$ is (of course) the definition (3). The case $d = 2$ is the next simplest. Let $\mathbf{m}(g, N)$ be the column-matrix $(\mu(1)g(1), \dots, \mu(N)g(N))^{\mathrm{T}}$, and let $A(g, N)$ be the $N \times N$ matrix with elements

$$a_{mn}(g, N) = \sum_{k \le \frac{N^2}{mn}} g(k) \quad (m, n \in \{1, \dots, N\}). \tag{4}$$

Then

$$M(g, N^2) = 2M(g, N) - (\mathbf{m}(g, N))^{\mathrm{T}} A(g, N) \mathbf{m}(g, N) \,. \tag{5}$$

In the general case, when $d, K, N \in \mathbb{N}$ satisfy $d \ge 2$ and $K \ge N > K^{1/d} - 1$, we have:

$$\begin{aligned} M(g, K) = {} & d M(g, N) \\ & - \sum_{r=2}^{d} (-1)^r \, {}_dC_r \sum_{n_1 \le N} \cdots \sum_{n_r \le N} \sum_{k_1} \cdots \sum_{k_{r-1}} g(k_1 \cdots k_{r-1}) \prod_{i=1}^{r} \mu(n_i) g(n_i) \,, \\ & \qquad n_1 n_2 \dots n_r k_1 k_2 \dots k_{r-1} \le K \end{aligned} \tag{6}$$

where ${}_dC_r = d(d-1)\cdots(d-(r-1))/(r!)$.

Note that (5) is just the special case $d = 2$, $K = N^2$ of (6). Moreover, (6) is itself a special case of another identity (that stated in Theorem 1, below), in which the single range of summation

$1, \ldots, N$ is replaced by d independent ranges of summation. In order to state this more general identity we require some more notation.

Let d be a positive integer greater than 1. Let $V = v_1 v_2 \ldots v_d$ be a word of length d in the alphabet $\{0, 1\}$. The support of a word V is the set of indices i for which $v_i = 1$. The weight $w(V)$ of a word V is the size of the support, so that $w(V) = \sum v_i$. The combinatorial Möbius function, which we write as μ^* to distinguish it from the number-theoretic function μ, is $\mu^*(V) = (-1)^{w(V)}$.

Let $N_1, \ldots, N_d$ be positive integers. For each word V, and each $L \in \mathbb{N}$, let the notatation $\sum_1^L(V)$ signify summation over $n_1, \ldots, n_d$ in the ranges $n_i = 1, \ldots, L$ when $v_i = 0$, but $n_i = 1, \ldots, N_i$ when $v_i = 1$. When $L = 1$ and $v_i = 0$, the variable of summation n_i effectively becomes 'frozen', meaning that its range of summation is then just the single-element set $\{1\}$.

Let K be a positive integer that is less than $(1 + N_1)(1 + N_2) \ldots (1 + N_d)$. If $n_1, \ldots, n_d$ are integers satisfying the condition $n_1 n_2 \ldots n_d \le K$, then $n_i \le N_i$ holds for at least one index i. It therefore follows by the inclusion-exclusion principle of combinatorics that if $f : \mathbb{N}^d \to \mathbb{C}$ is such that one has $|f(n_1, \ldots, n_d)| > 0$ only when $n_1 n_2 \cdots n_d \le K$, then

$$\sum_1^K (00\ldots0) f(n_1, \ldots, n_d) = \sum_{r=1}^{d} (-1)^{r-1} \sum_{V\,:\,\omega(V)=r} \sum_1^K (V) f(n_1, \ldots, n_d)\,, \tag{7}$$

or, to put it more elegantly, $\sum_V \mu^*(V) \sum_1^K (V) f(n_1, \ldots, n_d) = 0$.

THEOREM 1. *When $g(n)$ is a totally multiplicative arithmetic function, and d, $N_1, \ldots, N_d$ and K are as above, we have:*

$$\begin{aligned} M(g, K) = &\sum_{i=1}^{d} M(g, \min\{N_i, K\}) \\ &- \sum_{V\,:\,w(V)\ge 2} (-1)^{w(V)} \sum_1^1 (V) \sum_{k_1} \cdots \sum_{\substack{k_{\omega(V)-1} \\ k_1 \ldots k_{\omega(V)-1} \le \frac{K}{n_1 \ldots n_d}}} g(k_1 \cdots k_{\omega(V)-1}) \prod_{i=1}^{d} \mu(n_i) g(n_i)\,. \end{aligned} \tag{8}$$

Proof. We apply (7) with f given by:

$$f(n_1, \ldots, n_d) = \sum_{\substack{k_1 \\ k_1 \ldots k_{d-1} \le \frac{K}{n_1 \ldots n_d}}} \cdots \sum_{k_{d-1}} \mu(n_1) \ldots \mu(n_d) g(k_1 \ldots k_{d-1} n_1 \ldots n_d). \tag{9}$$

For the word $V = 11 \ldots 1$ with $w(V) = d$, we have

$$\sum_1^K (11\ldots1) = \sum_1^1 (11\ldots1).$$

All other words V have $v_j = 0$ for at least one index j, so the corresponding summand n_j runs over the full range from 1 to K. For these words V we carry out the following 'contraction step'. Take an index j for which $v_j = 0$. We sum over n_j and k_{d-1} first, observing that by Möbius inversion we have:

$$\sum_{n_j=1}^{K} \sum_{k_{d-1}\le \frac{K}{n_1\dots n_d k_1\dots k_{d-2}}} \mu(n_j) g(n_j k_{d-1}$$
$$= \sum_{m\le \frac{K}{n_1\dots n_{j-1}n_{j+1}\dots n_d k_1\dots k_{d-2}}} g(m) \sum_{n_j\mid m} \mu(n_j)$$
$$= \begin{cases} g(1)=\mu(1)g(1) & \text{if } n_1\dots n_{j-1}n_{j+1}\dots n_d k_1\dots k_{d-2}\le K,\\ 0 & \text{otherwise.}\end{cases}$$

We thereby find that the value of the relevant sum over $n_1,\dots,n_d$ and $k_1,\dots,k_{d-1}$ is unchanged when we omit k_{d-1} and freeze n_j as the fixed value $n_j=1$.

We repeat the contraction step for every index j with $v_j=0$, freezing the corresponding variable as $n_j=1$, and removing the last variable k_i. Exceptionally, when V is $00\dots0$, we can remove $k_{d-1},k_{d-2},\dots,k_1$, and freeze $n_d,n_{d-1},\dots,n_2$, but the sum over n_1 remains over the range $1,\dots,K$, giving the term $M(g,K)$ on the left of (8). The summation identity (7), when applied with f given by (9), contracts to give (8). ■

In (5), (6) and Theorem 1, we require the total multiplicativity of g only in order to 'separate variables' (as, in (6) for example, we separate $k_1,\dots,k_{r-1}$ from $n_1,\dots,n_r$ by means of the identity $g(k_1\cdots k_{r-1}n_1\cdots,n_r)=g(k_1\cdots k_{r-1})g(n_1)\cdots g(n_r)$). Indeed, (8) gives a formula for the Möbius function itself, for we can apply (8) to each term in the difference $M(g,K)-M(g,K-1)=\mu(K)g(K)$, and we can then divide through by $g(K)$ to obtain a formula for $\mu(K)$ that is independent of g. This formula for $\mu(K)$ may also be deduced from the identity

$$\frac{1}{\zeta(s)}\prod_{j=1}^{d}\Big(1-\zeta(s)\sum_{n=1}^{N_j}\frac{\mu(n)}{n^s}\Big)=\zeta^{d-1}(s)\prod_{j=1}^{d}\sum_{n=1+N_j}^{\infty}\frac{\mu(n)}{n^s}\quad(\mathrm{Re}(s)>1),\tag{10}$$

through multiplying out the brackets on the left-hand side, and then computing the coefficient of K^{-s} on each side of the resulting identity, subject to the hypothesis that the product $(1+N_1)\cdots(1+N_d)$ be greater than K. This approach yields a second proof of Theorem 1. We prefer the first proof due to its more obvious connection with Meissel's identity [**8** p 303],

$$\sum_{n\le x}\Big[\frac{x}{n}\Big]\mu(n)=\begin{cases}1 & if\ \ x\ge 1,\\ 0 & if\ \ 1>x>0,\end{cases}\tag{11}$$

which was the initial source of inspiration for our work.

Given any $K\in\mathbb{N}$, any integer $d\ge 2$, and any $\theta_1,\dots,\theta_d>0$ with $\theta_1+\cdots+\theta_d=1$, it follows from Theorem 1 that (8) will hold when one has also $N_j=[K^{\theta_j}]$, for $j=1,\dots,d$. Theorem 1 therefore offers considerably more flexibility of application than (6) does. Although we believe Theorem 1 to be new (in respect of the flexibility in the choice of $N_1,\dots,N_d$), the special cases of it that are displayed in (5) and (6) are known results. The result (5) is contained in Vaughan's (slightly more complicated) identity [**13** equation (18)] (essentially the special case when $u=\sqrt{X}$, and so $S_3=0$), and one can find in equation (13.38) of [**5**], for example, a formula for $\mu(n)$ that is equivalent to what we have in (6). It is, moreover, clear that even our identity in (8) is akin to formulae of Heath-Brown for sums involving $\Lambda(n)$, the von Mangoldt function: compare (10), from which (8) may be deduced, with Lemma 1 of [**2**]. The earliest formula of this type is due to Linnik himself in [**6**,**7**].

We shall refer to the case of (3) (or of (4), (5), (6), or (8)), where the function $g(n)$ takes the constant value 1, as the principal case. The main focus of our work has been on the principal case of the identity (5). Indeed, all subsequent sections of this paper are exclusively devoted to matters connected with this single topic, such as (for example) questions concerning certain properties of the $N \times N$ matrix $A = A(N)$ that occurs in the principal case of (5) and has, by (4), elements $a_{mn} = [N^2/(mn)] \in \mathbb{N}$. In Section 2 we discuss matters related to the spectral decomposition of $A = A(N)$. In the third (and final) section we discuss decompositions (spectral and otherwise) of the quadratic form $\mathbf{m}^T A \mathbf{m}$, where $\mathbf{m} = \mathbf{m}(N)$ is the column-matrix $(\mu(1), \ldots, \mu(N))^{\mathrm{T}}$ that occurs in the principal case of (5).

We consider especially the principal case of (5), in the hope that it (modified as necessary) might lead to a new proof of the prime number theorem, or even some new upper bound for the Mertens sum $|M(x)|$. The following parts of this paper report what we have discovered in the search for such an application of (5).

One of our findings is that the matrix $A(N)$, which (clearly) is real and symmetric, has one exceptionally large positive eigenvalue, approximately $N^2\zeta(2)$, with eigenvector approximately $(1, 1/2, 1/3, \ldots, 1/N)^{\mathrm{T}}$. Calculations by the second author show that the second-largest eigenvalue of $A(N)$ lies in an interval of the form $[d_4 N + o(N), c_4 N + o(N)]$, where c_4 and d_4 are constants that are approximately -0.496 and -0.572, respectively: for more details, see (18), (25), (31) and (32) below. Hence, for N sufficiently large, the quadratic form on the right-hand side of (5) is neither positive definite nor negative definite in the principal case.

By the principal case of (6), we have a sequence of formulae through which each of $M(N^2), M(N^3), M(N^4), \ldots$ is expressed in terms of $\mu(1), \ldots, \mu(N)$. Although the first of these formulae, the principal case of (5), may be considered analogous to the sieve of Eratosthenes (1), there seems to be no version of (1) for $\pi(N^3)$, because unwanted numbers of the form pq, where p and q are both primes greater than N, survive the sieve process ("Gnoggensplatts" in Greaves's lectures on *Sieve Methods*).

A connection between Mertens sums and certain symmetric matrices U_n $(n \in \mathbb{N})$, that bear some resemblance to our matrices $A(N)$ $(N \in \mathbb{N})$ has previously been established by Cardinal [**1**]. To define Cardinal's matrix U_n, one first takes $\sigma_1 < \sigma_2 < \cdots < \sigma_s$ to be the elements of the set $\mathcal{S} = \mathcal{R} \cup \{[n/\rho] : \rho \in \mathcal{R}\}$, where $\mathcal{R} = \{\rho \in \mathbb{N} : \rho \leq \sqrt{n}\}$ (it follows that $0 \leq 2[\sqrt{n}] - s \leq 1$). Then U_n is the $s \times s$ matrix with elements $u_{ij} = [n/(\sigma_i \sigma_j)]$. In Propositions 21 and 22 of [**1**], it is shown that one has $T_n U_n^{-1} T_n = V_n$, where T_n and V_n are the $s \times s$ matrices with elements $t_{ij} = |[2, s+1] \cap \{i+j\}|$ and $v_{ij} = M(u_{ij})$, respectively.

In the cases where n is a perfect square, so that $n = N^2$ for some integer N, then $|\mathcal{R}| = N$, and the $N \times N$ principal submatrix of U_n consisting of the array of elements from the first N rows and first N columns of U_n is our matrix $A(N)$: since $2N - 1 \leq s \leq 2N$, we can say that $A(N)$ constitutes (exactly, or approximately) the top left-hand quarter of Cardinal's matrix U_n. In these same cases, Cardinal's identity $T_n U_n^{-1} T_n = V_n$ implies that v_{11}, which is $M(N^2)$, will be equal to the sum of all s^2 of the elements of the inverse of the matrix $U_n = U_{N^2}$: we obtain a formula for $M(N^2)$ thereby that seems quite different from what we see in the principal case of (5).

As Cardinal observes in Theorem 24 and Remark 25 of [**1**], information about small eigenvalues of the matrix $V_n^{-1} = T_n^{-1} U_n T_n^{-1}$ might lead to new upper bounds on $M(x)$. In this respect, the connection that we have found between $M(x)$ and $A(N)$ is quite different from Cardinal's connection between $M(x)$ and U_n, for it is the larger eigenvalues of $A(N)$ and their eigenvectors that matter most in the principal case of (5): see, for example, equation (35), below.

We have scarcely considered non-principal cases of (5), (6), or (8). Certain non-principal cases of (5) may merit further investigation. The first case is when $g(n) = \chi(n)$, a non-principal Dirichlet character to some modulus $q > 1$. The sums $\sum_{\ell \leq x} \chi(\ell)$ that we use to construct the matrix elements $a_{mn}(\chi, N)$ in (4) are periodic step functions of x, whose period is q or some

proper factor of q. In contrast to the principal case, where the set of elements of the matrix $A(N)$ in (5) contains at least N different integers, namely $[N^2/1], [N^2/2], \dots, [N^2/N]$, there is a single finite set, $\{\sum_{0<\ell\le L}\chi(\ell) : L \in (0,q]\cap\mathbb{Z}\}$, that contains all the elements of all the matrices $A(\chi,1), A(\chi,2), A(\chi,3), \dots$. For χ real, $A(\chi,N)$ will, of course, be real and symmetric just like $A(N)$.

A case of (3) known to be related to the prime number theorem is when $g(n) = 1/n$ (see page 248 of [**9**], for example). More generally, when $g(n) = n^{-s}$ for some fixed complex number s, then the sum $M(g,x)$ in (3) becomes a partial sum for the Dirichlet series for $1/\zeta(s)$. If, for some $\sigma_0 \in [1/2,1)$, the only zeros of $\zeta(s)$ with real parts greater than σ_0 are a pair of simple zeros, ρ and $\overline{\rho}$ (say), and if we put $g(n) = n^{-\rho}$ $(n \in \mathbb{N})$, then the sum $M(g,x)$ in (3) will grow logarithmically in x.

Another interesting case of (3) to (5) is when $g(n) = \lambda(n)$, the Liouville function, which is the projection of the Möbius function μ onto the space of totally multiplicative arithmetic functions. In this case $M(g,x)$ grows like $x/\zeta(2)$.

2. Elementary Estimates for Eigenvalues and an Eigenvector

Let N be a given positive integer. Since the matrix $A = A(N)$, in the principal case of (5), is both real and symmetric, it has eigenvalues $\lambda_1 \le \lambda_2 \le \dots \le \lambda_N$ with corresponding eigen-(column-)vectors of unit length $\mathbf{e}_1, \dots, \mathbf{e}_N$ that form an orthonormal basis of $\mathbb{R}^N$. When $\mathbf{v} \in \mathbb{R}^N$, one has

$$\mathbf{v}^T A\mathbf{v} = \sum_{k=1}^{N} \lambda_k \,(\mathbf{e}_k \cdot \mathbf{v})^2 \tag{12}$$

as a consequence of the spectral decomposition $A = \sum_{k=1}^{N} \lambda_k \mathbf{e}_k \mathbf{e}_k^T$, and Parseval's identity gives

$$\sum_{k=1}^{N} (\mathbf{e}_k \cdot \mathbf{v})^2 = \mathbf{v}\cdot\mathbf{v} = \|\mathbf{v}\|^2. \tag{13}$$

In order to study the terms appearing in (12) and (13), we estimate:

(a) $\mathrm{Tr}(A) = \sum a_{nn}$ (the trace of the matrix A),

(b) $\mathrm{Tr}(A^2) = \mathrm{Tr}(A^T A) = \sum\sum a_{mn}^2$,

(c) $\mathbf{f}^T A\mathbf{f}$, where $\mathbf{f} = (1, \frac{1}{2}, \frac{1}{3}, \dots, \frac{1}{N})^T$,

(d) $\mathbf{w}^T A\mathbf{w}$, where $\mathbf{w} = \mathbf{u} - \|\mathbf{f}\|^{-2}(\mathbf{f}\cdot\mathbf{u})\mathbf{f}$, with $\mathbf{u} = (1,1,\dots,1)^T \in \mathbb{R}^N$.

We use the following notation:

$$\zeta_j = \sum_{m=1}^{N} m^{-j}\,, \quad \delta = \sum_{m\le N}\sum_{n\le N} \frac{\{N^2/(mn)\}}{mn} \quad \text{and} \quad \phi = \frac{1}{N^2}\sum_{m\le N}\sum_{n\le N}\left\{\frac{N^2}{mn}\right\}^2\,,$$

where $\{t\} = t - [t]$ (the fractional part of t). Taking (b) first, we simply observe that

$$\mathrm{Tr}\left(A^2\right) = \sum_{m\le N}\sum_{n\le N}\left[\frac{N^2}{mn}\right]^2 = \sum_{m\le N}\sum_{n\le N}\left(\frac{N^2}{mn} - \left\{\frac{N^2}{mn}\right\}\right)^2 = \zeta_2^2 N^4 + (\phi - 2\delta)\,N^2\,. \tag{14}$$

Since $\mathrm{Tr}(A^2) = \lambda_1^2 + \dots + \lambda_N^2$, and since $\delta \ge 0$ and $\phi < 1$, the identity (14) shows already that $\lambda_N < \zeta_2 N^2 + (2\zeta_2)^{-1}$.

Regarding (c), we are content to note that

$$\mathbf{f}^T A\mathbf{f} = \sum_{m\le N}\sum_{n\le N}\frac{\left[N^2/(mn)\right]}{mn} = \sum_{m\le N}\sum_{n\le N}\frac{\left(N^2/(mn) - \left\{N^2/(mn)\right\}\right)}{mn} = \zeta_2^2 N^2 - \delta\ . \tag{15}$$

We have here $\|\mathbf{f}\|^2 = \zeta_2$, so by Rayleigh's Principle it follows from (15) that

$$\zeta_2 N^2 - \frac{\delta}{\zeta_2} \le \lambda_N\ . \tag{16}$$

By (16) and the point noted immediately below (14), we conclude that

$$-\frac{(1+\log N)^2}{\zeta_2} < \lambda_N - \zeta_2 N^2 < \frac{1}{2\zeta_2}\ . \tag{17}$$

As $0 \le \delta < \zeta_1^2 \le \zeta_0\zeta_2 = N\zeta_2 \le N^2\zeta_2^2$, the lower bound on λ_N in (16) is non-negative, and so we may deduce from it that $\lambda_N^2 \ge (\zeta_2 N^2 - \delta\zeta_2^{-1})^2 = \zeta_2^2 N^4 - 2\delta N^2 + \delta^2\zeta_2^{-2}$: this, together with the evaluation of $\mathrm{Tr}(A^2)$ in (14), is enough to show that

$$\lambda_1^2 + \ \cdots\ + \lambda_{N-1}^2 \le \phi N^2 - \delta^2\zeta_2^{-2} < N^2\ . \tag{18}$$

From the way we have ordered the eigenvalues, the bound (18) implies:

$$|\lambda_k| < \frac{N}{\sqrt{\min\{k, N-k\}}} \qquad (k = 1, 2, \dots, N-1). \tag{19}$$

In view of (17) and (19), it is clear that for N large, λ_N will be exceptionally large, compared with all other eigenvalues of A. Accordingly we consider first the corresponding eigenvector $\mathbf{e}_N$, before discussing the estimation (a) of $\mathrm{Tr}(A)$. Putting $F_N = \mathbf{e}_N \cdot \hat{\mathbf{f}}$, where $\hat{\mathbf{f}} = \|\mathbf{f}\|^{-1}\mathbf{f}$, we find by (15) and (17), and (12), (19) and (13), that

$$\lambda_N - \left(\frac{1}{2} + (1+\log N)^2\right) < \hat{\mathbf{f}}^T A\hat{\mathbf{f}} < \lambda_N F_N^2 + N\left(1 - F_N^2\right)\ .$$

For $N > 1$ we have $\lambda_N > N$ (this follows by (17) when $N \ge 3$), and so, by comparison of the upper and lower bounds for $\hat{\mathbf{f}}^T A\hat{\mathbf{f}}$ that were just obtained, we deduce that

$$1 \ge F_N^2 > 1 - \frac{\left(\frac{1}{2} + (1+\log N)^2\right)}{(\lambda_N - N)}\ .$$

Choosing the $\pm$-sign so that $\pm F_N = |F_N|$, we therefore find from (17) that

$$\left\|\mathbf{e}_N - \left(\pm\hat{\mathbf{f}}\right)\right\| = \sqrt{2\left(1 - |F_N|\right)} = \sqrt{\frac{2\left(1-F_N^2\right)}{r1 + |F_N|}} = O\left(\frac{\log N}{rN}\right)\ . \tag{20}$$

We now come to the task mentioned in (a) above, which is the estimation of the sum $S = \mathrm{Tr}(A) = \sum a_{nn}$. We pick a positive integer K, and we divide the original sum S into two parts: S_1, which has the terms with $n^2 \le N^2/(K+1)$, and S_2, which has the terms with $N^2 \ge n^2 > N^2/(K+1)$ (so that $a_{nn} = [N^2/n^2] = k$ for some $k \in \{1, \dots, K\}$). We have

$$\begin{aligned} S_1 = \sum_{n^2 \le N^2/(K+1)} a_{nn} &= \sum_{n \le N/\sqrt{K+1}}\left(\frac{N^2}{n^2} + O(1)\right) \\ &= N^2\left(\zeta_2 - \int_{N/\sqrt{K+1}}^{N} x^{-2}\,\mathrm{d}x + O\left(\frac{K}{N^2}\right)\right) + O\left(\frac{N}{\sqrt{K}}\right) \\ &= \zeta_2 N^2 - N\sqrt{K} + N + O\left(K + \frac{N}{\sqrt{K}}\right). \end{aligned}$$

The sum S_2 is more complicated. We have

$$S_2 = \sum_{k=1}^{K} \sum_{\frac{N}{\sqrt{k+1}}<n\le\frac{N}{\sqrt{k}}} k = \sum_{1\le\ell\le k\le K}\sum \left(\left[\frac{N}{\sqrt{k}}\right] - \left[\frac{N}{\sqrt{k+1}}\right]\right)$$
$$= \sum_{\ell=1}^{K}\left(\left[\frac{N}{r\sqrt{\ell}}\right] - \left[\frac{N}{\sqrt{K+1}}\right]\right) = \sum_{\ell=1}^{K}\frac{N}{\sqrt{\ell}} - \frac{KN}{\sqrt{K+1}} + O(K).$$

Let

$$g(\ell) = 2\sqrt{\ell} - 2\sqrt{\ell-1} - \frac{1}{\sqrt{\ell}} = \frac{1}{\sqrt{\ell}(\sqrt{\ell}+\sqrt{\ell-1})^2} \quad (\ell\in\mathbb{N}) \quad \text{and} \quad \alpha = \sum_{\ell=1}^{\infty} g(\ell).$$

Then

$$\sum_{\ell=1}^{K}\frac{1}{\sqrt{\ell}} = \sum_{\ell=1}^{K}\left(2\sqrt{\ell} - 2\sqrt{\ell-1} - g(\ell)\right) = 2\sqrt{K} - \alpha + O\left(\frac{1}{\sqrt{K}}\right).$$

Hence

$$S_2 = 2N\sqrt{K} - \alpha N - \frac{NK}{\sqrt{K+1}} + O\left(\frac{N}{r\sqrt{K}} + K\right) = N\sqrt{K} - \alpha N + O\left(\frac{N}{\sqrt{K}} + K\right),$$

and so, putting $K = [N^{2/3}]$, we get:

$$\mathrm{Tr}(A) = S_1 + S_2 = \zeta_2 N^2 - (\alpha-1)N + O\left(N^{2/3}\right). \tag{21}$$

By (21) and (17), it follows that

$$\lambda_1 + \cdots + \lambda_{N-1} = -(\alpha-1)N + O\left(N^{2/3}\right). \tag{22}$$

By equations (1.11) to (1.13) of [**4**] and the case $K = 1$ of of equation (B.24) of [**9**] (itself an application of the Euler-Maclaurin summation formula), we find that for $\sigma \in (0,1)\cup(1,\infty)$ and $K\in\mathbb{N}$,

$$\sum_{\ell=1}^{K}\frac{1}{\ell^\sigma} = \frac{K^{1-\sigma}}{1-\sigma} + \zeta(\sigma) + \frac{\theta(K,\sigma)}{K^\sigma} \tag{23}$$
$$= \frac{\theta(K,\sigma)}{K^\sigma} + \frac{K^{1-\sigma}-1}{1-\sigma} + \gamma + \sum_{j=1}^{\infty}\gamma_j(\sigma-1)^j, \tag{24}$$

where $\zeta(s)$ is Riemann's zeta function, each of γ, γ_1, γ_2, ... is a certain (real valued) absolute constant (the first of these, γ, being Euler's constant) and $\theta(K,\sigma)$ is a number lying in the interval $(0,1)$. By (23), we have $\alpha = -\zeta(1/2)$ in (21), and we can calculate that

$$\alpha - 1 = -(\zeta(1/2)+1) = 0.4603545\ldots.$$

Given that $\zeta(2) = \pi^2/6$, we find (similarly) that $\zeta_2 = (\pi^2/6) - N^{-1} + O(N^{-2})$ in (14) to (18). We also note that $\zeta_1 = \log N + \gamma + O(1/N)$ (as follows, for example, by letting $\sigma\to 1$ in (24)).

We remark that, by combining methods similar to those used to obtain (21) with certain applications of the Euler-Maclaurin summation formula, we have been able to determine that the variable $\phi\in[0,1)$ in (14) and (18) satisfies

$$\phi = \beta + O\left(\frac{1+\log N}{N^{1/7}}\right), \tag{25}$$

where $\beta = 1 - \frac{\pi^2}{24} - \frac{1}{2}(\log(2\pi) - 1)^2 + \frac{1}{2}(1-\gamma)^2 = 0.32712\ldots$. We omit our proof of (25), which shows no features that are truly novel (and would require more than just a few pages). By (25), we can sharpen (19) somewhat, for large values of N.

Finally we consider the estimation problem (d), stated earlier. Noting firstly that $\mathbf{w} = \mathbf{u} - -(\zeta_1/\zeta_2)\mathbf{f}$, we are able to deduce that

$$\|\mathbf{w}\|^2 = N - \frac{\zeta_1^2}{\zeta_2} = N + O\left((1+\log N)^2\right) \tag{26}$$

and that

$$\mathbf{w}^T A\mathbf{w} = \mathbf{u}^T A\mathbf{u} - 2\left(\zeta_1/\zeta_2\right)\mathbf{u}^T A\mathbf{f} + \left(\zeta_1/\zeta_2\right)^2 \mathbf{f}^T A\mathbf{f}\ . \tag{27}$$

We have, moreover,

$$\mathbf{u}^T A\mathbf{u} = \sum_{m\le N}\sum_{n\le N}\left[\frac{N^2}{mn}\right] = \sum_m\sum_n\left[\frac{N^2}{mn}\right] - 2\sum_{m>N}\sum_n\left[\frac{N^2}{mn}\right] = D_1 - 2D_2 \quad \text{(say)}. \tag{28}$$

Here

$$D_1 = \sum_{\ell\le N^2}\tau_3(\ell) = \left(\frac{1}{2}\log^2\left(N^2\right) + (3\gamma-1)\log\left(N^2\right) + c_1\right)N^2 + O\left(N^{\varepsilon+43/48}\right)\ , \tag{29}$$

where $c_1 = 3\gamma^2 - 3\gamma + 3\gamma_1 + 1$; see pages 352-4 of [**4**] for the second equality in (29).

Regarding the sum D_2 in (28), we have:

$$\begin{aligned} D_2 = \sum_{m>N}\sum_{\substack{n\\(nk)m\le N^2}}\sum_k 1 &= \sum_{\ell<N}\left(\sum_{n|\ell}1\right)\sum_{N<m\le N^2/\ell}1 \\ &= N^2\sum_{\ell<N}\frac{\tau_2(\ell)}{\ell} - N\sum_{\ell<N}\tau_2(\ell) + O\left(\sum_{\ell<N}\tau_2(\ell)\right)\ . \end{aligned}$$

By partial summation and Huxley's estimate on page 593 of [**3**] for the remainder term in Dirichlet's divisor problem (namely $\Delta(x) = \sum_{\ell\le x}\tau_2(\ell) - (\log x + 2\gamma - 1)x$), we deduce from the above that

$$D_2 = \left(\frac{1}{2}\log^2 N + (2\gamma-1)\log N + c_2\right)N^2 + O\left(N^{547/416}(\log N)^{3.26}\right)\ ,$$

where

$$c_2 = \int_1^\infty \frac{\Delta(x)\mathrm{d}x}{x^2} = \lim_{\sigma\to 2+}\left(\frac{\zeta^2(\sigma-1)}{\sigma-1} - \frac{1}{(\sigma-2)^2} - \frac{2\gamma-1}{\sigma-2}\right) = \gamma^2 - 2\gamma + 2\gamma_1 + 1$$

(with γ and γ_1 as in (24)). Using this, (28), and (19), we have

$$\mathbf{u}^T A\mathbf{u} = \left(\log^2 N + 2\gamma\log N + c_3\right)N^2 + O\left(N^{547/416}(\log N)^{3.26}\right)\ , \tag{30}$$

where $c_3 = c_1 - 2c_2 = \gamma^2 + \gamma - \gamma_1 - 1$. Trivial estimates show that one has

$$\mathbf{u}^T A\mathbf{f} = \zeta_1\zeta_2 N^2 + O((1+\log N)N).$$

Using this, (15), (30), (27), and estimates already obtained for ζ_1 and ζ_2, we find that

$$\begin{aligned} \mathbf{w}^T A\mathbf{w} &= \left(\log^2 N + 2\gamma\log N + c_3 - \zeta_1^2\right)N^2 + O\left(N^{547/416}(\log N)^{3.26}\right) \\ &= c_4 N^2 + O\left(N^{547/416}(\log N)^{3.26}\right)\ , \end{aligned} \tag{31}$$

where $c_4 = c_3 - \gamma^2 = \gamma - \gamma_1 - 1 = 0.57721566\ldots - 0.07281584\ldots - 1 = -0.495600\ldots$ (see [**10**].

Since (26) implies $N > \|\mathbf{w}\|^2 \geq N/10$, we find, using (26), (31), and Rayleigh's principle that:

$$\lambda_1 \leq \frac{\mathbf{w}^T A \mathbf{w}}{\|\mathbf{w}\|^2} < c_4 N + O\left(N^{131/416}(\log N)^{3.26}\right) \quad (N \geq 2). \tag{32}$$

The coefficient of N in this upper bound may well be close to optimal: when $N = 10321$, for example, computations done with the 'GNU Octave' software package returned $-0.493678\ldots$ as an estimate of the value of λ_1/N in this case. By reasoning similar to that which gives (20), we may deduce from (18), (25) and (32) that, as $N \to \infty$, we have $|\lambda_2|/N < (1 + o(1))(\beta - c_4^2)^{1/2} \sim \sim 0.2855539\ldots$ and $(\mathbf{e}_1 \cdot \hat{\mathbf{w}})^2 \geq (0.5 + o(1))(1 + (2c_4^2\beta^{-1} - 1)^{1/2}) \sim 0.8540699\ldots$. Therefore, for N sufficiently large, the lines $\{t\mathbf{w} : t \in \mathbb{R}\}$ and $\{t\mathbf{e}_1 : t \in \mathbb{R}\}$ will meet at an angle of less than $\pi/8$ radians.

We end this section with some speculations driven by certain numerical evidence, gathered with the help of 'GNU Octave'. We omit the detailed evidence, and instead just summarise what it suggests. Let k be any fixed non-zero integer, and let N now be free to vary in the range $N > |k|$. Our numerical evidence suggests that $\lambda_{\{-k/N\}N} \sim \Lambda_k N$ as $N \to \infty$, where Λ_k is a real number that depends only on k, and where each of the two associated sequences, $\Lambda_1, \Lambda_2, \Lambda_3, \ldots$ and $-\Lambda_{-1}, -\Lambda_{-2}, -\Lambda_{-3}, \ldots$, decreases monotonically, and converges to 0. Further numerical evidence suggests that if $\theta \in (0,1)$ is fixed, and if $e_{j,\ell}$ denotes the ℓ-th component of the normalised eigenvector $\mathbf{e}_j$, so that $\mathbf{e}_j = (e_{j,1}, e_{j,2}, \ldots, e_{j,N})^{\mathrm{T}}$ for $j = 1, \ldots, N$, then as $N \to \infty$ we appear to see that

$$e_{\{-k/N\}N,\ell} \sim (-1)^{b(N,k)} N^{-1/2} E_k(\ell/N) \quad \text{for } \ell = [\theta N] + 1, [\theta N] + 2, \ldots, N,$$

with E_k here being a certain real function independent of ℓ and N that is continuous on $(0,1]$, and with an integer exponent $b(N,k)$ independent of ℓ. The occurrence of the functions $E_{\pm 1}, E_{\pm 2}, E_{\pm 3}, \ldots$ in this might be explained if they were eigenfunctions of a suitable linear operator $\mathcal{A} : L^2[0,1] \to L^2[0,1]$.

3. Various Decompositions of $\mathbf{m}^T A\mathbf{m}$ in the principal case

It is our hope (as yet unrealised) that a study of the quadratic form $\mathbf{v}^T A\mathbf{v}$ (particularly when $\mathbf{v}$ is the vector $\mathbf{m} = (\mu(1), \ldots, \mu(N))^T$), in the principal case of (5), might lead to new results about the Mertens function $M(x)$. In this section we briefly describe (and compare) several different approaches to such an investigation, each involving a different decomposition of the quadratic form. We find it convenient to modify the earlier notation $M(g,x)$ in (3): we use $M(s,x)$, where s is a complex number, (rather than a function), to mean $M(g,x)$ for the power function $g(n) = n^{-s}$.

We consider firstly (12) with $\mathbf{v} = \mathbf{m}$. We assume throughout that N is large. As the eigenvalue λ_N is exceptionally large among all the eigenvalues of A, we handle the term $\lambda_N(\mathbf{e}_N \cdot \mathbf{m})^2$ with some care. As substitution of $-\mathbf{e}_N$ for $\mathbf{e}_N$ does not alter this term, we can take the ambiguous sign in (20) to be $+$. We note that

$$(\mathbf{e}_N \cdot \mathbf{m})^2 = \Big((\mathbf{e}_N - \hat{\mathbf{f}}) \cdot \mathbf{m}\Big)^2 + 2\Big((\mathbf{e}_N - \hat{\mathbf{f}}) \cdot \mathbf{m}\Big)(\hat{\mathbf{f}} \cdot \mathbf{m}) + (\hat{\mathbf{f}} \cdot \mathbf{m})^2 \,. \tag{33}$$

Here

$$\hat{\mathbf{f}} \cdot \mathbf{m} = \|\mathbf{f}\|^{-1}\mathbf{f} \cdot \mathbf{m} = \frac{1}{\sqrt{\zeta_2}} \sum_{n \leq N} \frac{\mu(n)}{n} = \frac{M(1,N)}{\sqrt{\zeta_2}} \ll \log N$$

and, by the Cauchy-Schwarz inequality and (20),

$$|(\mathbf{e}_N - \hat{\mathbf{f}}) \cdot \mathbf{m}| \leq \|\mathbf{e}_N - \hat{\mathbf{f}}\| \cdot \|\mathbf{m}\| = O\left(\frac{\log N}{N}\right) \cdot \sqrt{\sum_{n \leq N} \mu^2(n)} \ll \frac{\log N}{\sqrt{N}} \,.$$

By these results, together with (33) and (17), we have:

$$\lambda_N(\mathbf{e}_N \cdot \mathbf{m})^2 = O\left(N \log^2 N\right) + O\left(N^{3/2}(\log N)|M(1,N)|\right) + N^2(M(1,N))^2 \,. \tag{34}$$

Small eigenvalues make a relatively insignificant contribution here, for (13) and (19) imply that if $1 \le K \le N/2$, then

$$\sum_{k=K}^{N-K} |\lambda_k| \, (\mathbf{e}_k \cdot \mathbf{m})^2 < \frac{N}{\sqrt{K}} \sum_{n=1}^{N} (\mathbf{e}_k \cdot \mathbf{m})^2 = \frac{N}{\sqrt{K}} \|\mathbf{m}\|^2 \le \frac{N^2}{\sqrt{K}} \,.$$

By this, and by (34) and (12) (for $\mathbf{v} = \mathbf{m}$), we find that

$$\begin{aligned} \frac{\mathbf{m}^T A \mathbf{m}}{N^2} = (M(1,N))^2 \; + \; \left(\|\mathbf{m}\|^2/N\right) \sum_{\substack{1 \le k < N \\ \min\{k, N-k\} < K}} (\lambda_k/N) \, (\mathbf{e}_k \cdot \hat{\mathbf{m}})^2 \\ + O\left(K^{-1/2} + N^{-1/2}(\log N)|M(1,N)| + N^{-1} \log^2 N\right) \,, \end{aligned} \tag{35}$$

for $K = 1, 2, \ldots, N^2$. We remark that, if the second of the three terms on the right-hand side of (35) is considered in isolation, then we observe trivially from (19) that the absolute value of this term is $O(\sqrt{K}\,)$. Taking account of the context here (the relation (35) and the principal case of (5) and (3)), and noting also that $|M(1,N)| \le \|\mathbf{m}\|^2/N$ (a consequence of (11), the trivial bound $|[y] - y| < 1$, and the fact that $[N/1] - (N/1) = 0$), it is clear that this term is a bounded function of the pair $(N, K) \in \mathbb{N}^2$. This gives some idea of the gap that must be bridged if (35) is to help in the study of $M(x)$.

To reach (35) we have used the work of Section 2, on λ_N and $\mathbf{e}_N$. Our next decomposition of $\mathbf{m}^T A \mathbf{m}$ avoids such results, but nevertheless has much in common with (35).

First we use $[x] = x - \frac{1}{2} - \psi(x)$, where $\psi(x) = \{x\} - \frac{1}{2}$. We have

$$A = N^2 \mathbf{f}\mathbf{f}^T - \frac{1}{2}\mathbf{u}\mathbf{u}^T + Z \,, \tag{36}$$

where Z is the $N \times N$ matrix of elements $z_{mn} = -\psi(N^2/(mn))$, whilst $\mathbf{f}$ and $\mathbf{u}$ are as in Section 2. We have trivially $\mathrm{Tr}(Z^2) < N^2/4$; with the help of (25), (30), and an estimate for ζ_1, we obtain the sharper result that $\mathrm{Tr}(Z^2) \sim c_5 N^2$ as $N \to \infty$, where $c_5 = \beta + \frac{1}{4} + c_3 - \gamma^2 = 0.0815206\ldots$. Reasoning as in the derivation of (35), we see from (36) that, for $K = 1, 2, \ldots, N^2$ (say), one has

$$\frac{\mathbf{m}^T A \mathbf{m}}{N^2} = (\mathbf{m} \cdot \mathbf{f})^2 - \frac{(\mathbf{m} \cdot \mathbf{u})^2}{2N^2} + \frac{\mathbf{m}^T Z \mathbf{m}}{N^2} \tag{37}$$

$$\begin{aligned} &= (M(1,N))^2 \; - \frac{(M(N))^2}{2N^2} \\ &\quad + \; \left(\|\mathbf{m}\|^2/N\right) \sum_{\substack{1 \le k \le N \\ \min\{k, N+1-k\} < K}} \left(\widetilde{\lambda}_k/N\right) (\widetilde{\mathbf{e}}_k \cdot \hat{\mathbf{m}})^2 + O\left(K^{-1/2}\right) \,, \end{aligned} \tag{38}$$

where $\widetilde{\lambda}_1 \le \widetilde{\lambda}_2 \le \; \cdots \; \le \widetilde{\lambda}_N$ are the eigenvalues of Z, while $\widetilde{\mathbf{e}}_1, \ldots, \widetilde{\mathbf{e}}_N$ form the corresponding orthonormal basis of eigenvectors. We note the presence of the term $-\frac{1}{2}N^{-2}(M(N))^2$ in (38), which is not apparent in (35): in view of our results on Problem (d) of Section 2, one may regard this term as being an approximation to the term $(\|\mathbf{m}\|^2/N)(\lambda_1/N)(\mathbf{e}_1 \cdot \hat{\mathbf{m}})^2 = N^{-2}\lambda_1(\mathbf{e}_1 \cdot \mathbf{m})^2$, which is present in (35) for $K > 1$.

We remark that (37) permits an alternative, non-spectral, decomposition of $\mathbf{m}^T A\mathbf{m}$, through substituting the usual truncated Fourier expansion of the function ψ into each element of the matrix Z in (37):

$$-\psi(x) = \sum_{0<h\le H} \frac{\sin(2\pi hx)}{\pi h} + O\left(\frac{\eta}{\eta + \min\{|x-\ell| \,:\, \ell\in\mathbb{Z}\}}\right) \qquad (H = 1/\eta \ge 1).$$

This leads (via estimates from [**11**]) to the decompositions

$$\mathbf{m}^T Z\mathbf{m} = \sum_{h=1}^{H} \frac{\mathbf{m}^T Z(h)\mathbf{m}}{\pi h} + O\left(\frac{N^2(\log N)^2\log H}{H}\right) \qquad (\text{for } H = 1, 2, \dots, N \text{ (say)}),$$

where $Z(h)$ is the $N\times N$ matrix with elements $z_{mn}(h) = \sin(2\pi hN^2/(mn))$. We have yet to explore making proper use of this truncation idea.

One further approach to the decomposition of $\mathbf{m}^T A\mathbf{m}$ uses Perron's formula, Theorem 5.1 of [**9**], equation (A.8) of [**4**]. We apply Perron's formula as in Lemma 3.12 of [**12**], adapting the proof to sharpen certain error terms (parts of the improvement come from results of Shiu [**11**]). We find that if, whenever $\mathrm{Re}(s) > 1$, one has

$$F(s) = \sum_{\ell=1}^{\infty} \frac{a_\ell}{\ell^s} = \left(\sum_{m\le y} \frac{\alpha_m}{m^s}\right)\left(\sum_{n\le z} \frac{\beta_n}{n^s}\right)\zeta(s) = A(s)B(s)\zeta(s) \qquad (\text{say}), \tag{39}$$

where $y, z \ge 1$ and α_m, β_n denote complex constants of modulus less than or equal to 1, then, for any fixed $\varepsilon > 0$, when $x = yz$, in the ranges $1 < c \le 2$ and $3 \le T \le x^{1-\varepsilon}$, we have

$$\frac{1}{2\pi i}\int_{c-iT}^{c+iT} F(s)x^s\,\frac{\mathrm{d}s}{s} = \sum_{\ell\le x} a_\ell + O\left(\frac{x^c\log^2 x}{(c-1)T}\right) + O_\varepsilon\left(\frac{x(\log x)^2(\log T)}{T}\right). \tag{40}$$

To link this to our matrix A, we observe that (39) implies

$$\sum_{\ell\le x} a_\ell = \sum_{\ell\le x}\sum_{m\le y}\sum_{\substack{n\le z\\ mnk=\ell}}\sum_{k} \alpha_m\beta_n = \sum_{m\le y}\sum_{\substack{n\le z\\ mnk\le x}}\sum_{k} \alpha_m\beta_n = \sum_{m\le y}\sum_{n\le z}\left[\frac{x}{mn}\right]\alpha_m\beta_n\,.$$

Setting $c = 1 + (\log x)^{-1}$ in (40), we shift the contour of integration there until it aligns with the line $\mathrm{Re}(s) = \frac12$: in so doing, we pick up a contribution from the residue of $\zeta(s)$ at its pole, $s = 1$, and also some remainder terms, which are integrals along the line segments joining $\frac12 + iT$ to $c + iT$, and $\frac12 - iT$ to $c - iT$. By Theorem 7.2 (A) of Titchmarsh [**12**], we deduce that these remainder term integrals are of size $O(x(\log x)^2\sqrt{\log T}/T)$ for almost all values of T (in a certain sense) lying in any given 'dyadic interval' $[T_0, 2T_0] \subseteq [3, 2x^{1-\varepsilon}]$. Hence we arrive at the conclusion that, for any given $\varepsilon > 0$ when $x = yz$ and $3 \le T_0 \le x^{1-\varepsilon}$, we have

$$\sum_{m\le y}\sum_{n\le z}\left[\frac{x}{mn}\right]\alpha_m\beta_n = A(1)B(1)x + \frac{1}{2\pi i}\int_{\frac12-iT}^{\frac12+iT} A(s)B(s)\zeta(s)x^s\,\frac{\mathrm{d}s}{s} + O_\varepsilon\left(\frac{x\log^3 x}{T}\right),$$

for some $T \in [T_0, 2T_0]$. We specialise this to the case $\varepsilon = 1/2$, $y = z = N$, where N is a positive integer, so that $x = N^2$, and $\alpha_n = \beta_n = \mu(n)$. We find that when $3 \le T_0 \le N$, there exists some $T \in [T_0, 2T_0]$ such that

$$\begin{aligned}\frac{\mathbf{m}^T A\mathbf{m}}{N^2} = (M(1,N))^2 + \frac{\|\mathbf{m}\|^2}{N}\int_{-T}^{T} \frac{\zeta_1 N^{2it}\zeta\left(\frac12+it\right)}{(\pi + 2\pi it)}\left(\frac{M\left(\frac12+it, N\right)}{\sqrt{\zeta_1}\|\mathbf{m}\|}\right)^2 \mathrm{d}t \\ + O\left(T_0^{-1}\log^3 N\right)\,.\end{aligned} \tag{41}$$

If we put $\mathbf{E}(s) = (1^{-s}, 2^{-s}, \ldots, N^{-s})^T$ for a fixed complex number s, then the factor $M(\frac{1}{2} + it, N)/(\sqrt{\zeta_1}\|\mathbf{m}\|)$ here may be written as $\hat{\mathbf{E}}(\frac{1}{2} + it) \cdot \hat{\mathbf{m}}$: the decomposition in (41) may therefore be considered similar in form to that in (35), although (41) involves an integration over the range $[-T, T]$, instead of the summation over a subset of the (discrete) spectrum of A that we had in (35).

4. Conclusions

Using the principal case of (5), and results such as (35), (38), or (41), we are able to approximate $M(N^2)$ by an expression involving only certain limited data: the numbers $\mu(1), \mu(2), \ldots, \mu(N)$ and either the relevant eigenvalues and eigenvectors, or else values of $\zeta(\frac{1}{2} + it)$ and $g_t(n) = n^{-\frac{1}{2}-it}$. It remains to be seen whether or not such approximations for $M(N^2)$ can be an effective tool in studying the function $M(x)$. With regard to (35) and (38), it would be helpful to find out more about the relevant eigenvalues and eigenvectors, since that might clarify the possible uses of those results. More generally, it may be worthwhile to study the eigenvalues and eigenvectors of certain submatrices of $A = A(N)$, and also (in certain non-principal cases) those of $A(g, N)$ and certain of its submatrices.

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