



Unital Sums of the Möbius and Mertens Functions

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Abstract

We use standard techniques of linear algebra to construct an infinite family of identities that involve finite weighted sums of the Möbius and Mertens functions, where the weights are equal to -1 , 0 , or 1 . In a related manner, we construct, for each positive integer n , an $n \times n$ symmetric unimodular matrix, and each matrix is used to express an identity that involves a finite weighted sum of the Möbius function. We establish several results on the spectral decomposition of these matrices.

1 Introduction

The Möbius function is defined as

$$\mu(k) := \begin{cases} 1, & \text{if } k \text{ is squarefree and has an even number of prime factors;} \\ -1, & \text{if } k \text{ is squarefree and has an odd number of prime factors;} \\ 0, & \text{otherwise.} \end{cases}$$

Summatory behavior of μ is of great interest, in part due to the close connection that μ has to the distribution of the prime numbers. Indeed, it is known that the Mertens function, which we write as $M(n) := \sum_{k \leq n} \mu(k)$, satisfies $M(n) = o(n)$, and that this asymptotic bound is equivalent to the prime number theorem.

It is the goal of the first part of this paper to state and prove several summatory identities satisfied by μ and M that we have not found in prior work. These identities are stated in Proposition 1 and Corollary 3 of Section 2.1. In Section 3, we employ similar techniques to

construct, for each positive integer n , an $n \times n$ symmetric matrix, Q_n , having integer entries and determinant 1 that satisfies $\sum_{k \leq n} Q_n(j, k) \mu(k) = 0$ when $j > 1$, and the sum equals 1 when $j = 1$. This is the content of Proposition 6. We also obtain asymptotic bounds on the extremal eigenvalues of Q_n . This is the content of Proposition 8. A corollary of these propositions is the asymptotic bound $\sum_{i \leq n} v_n(i) \mu(i) \leq n^{-3/2} C(1 + o(1))$, where v_n is the normalized dominant eigenvector of Q_n , and C is a constant smaller than 3. This is stated in Corollary 9. We conclude with a conjecture about v_n .

We now briefly summarize Proposition 1 and Corollary 3 of the next section. For each $m, n \geq 1$, we construct $(-1, 0, 1)$ -valued functions, $\epsilon^{m,n}$ and $E^{m,n}$, that satisfy the identities

$$\sum_{k \leq n} \epsilon^{m,n}(k) \mu(k) = 1$$

and

$$\sum_{k \leq n} E^{m,n}(k) M(k) = 1.$$

Each function $\epsilon^{m,n}$ is the result of applying the transpose of Dirichlet convolution by the n -term sequence $(1, 1, 1, \dots, 1)$ to a particular $4m$ -periodic function. Each function $E^{m,n}$ is a finite difference operation applied to $\epsilon^{m,n}$. Complete details are presented in Section 2.1. Before proceeding, we state a concise formula for $\epsilon^{m,n}$ in the special case $m = 1$. For all $k \geq 1$,

$$\epsilon^{1,n}(k) = \sum_{jk \leq n} \cos\left(\frac{\pi(jk - 1)}{2}\right). \quad (1)$$

See Section 2.2 for further observations concerning the function $\epsilon^{1,n}$.

Figure 1 displays $\epsilon^{m,n}$ for various choices of m and n . Both $E^{m,n}$ and $\epsilon^{m,n}$ are $4m$ -periodic on the interval $n/3 < k \leq n$. The behavior of $E^{m,n}$ and $\epsilon^{m,n}$ near the origin is more complicated. In general, $\epsilon^{m,n}$ and $E^{m,n}$ are sparse when m is large.

The body of literature on the functions μ and M is vast, and many results on sums with the form

$$\sum_{k \leq n} w(k) \mu(k),$$

are known. Two well-known examples, both of which may be found in Apostol ([1, Theorem 2.1 and Theorem 3.12]), are

$$\sum_{k|n} \mu(k) = \begin{cases} 1, & \text{if } n = 1; \\ 0, & \text{otherwise,} \end{cases} \quad (2)$$

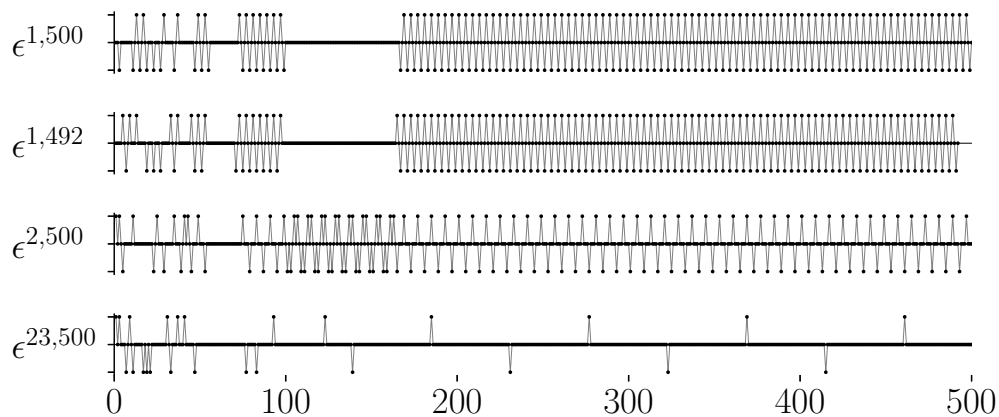


Figure 1: Examples of the function $\epsilon^{m,n}$.

and

$$\sum_{k \leq n} \left\lfloor \frac{n}{k} \right\rfloor \mu(k) = 1. \quad (3)$$

This pair of identities is closely related to Proposition 6 of Section 3. The Mertens function is also known to satisfy similar kinds of identities. One example is

$$\sum_{k \leq n} M\left(\frac{n}{k}\right) = 1.$$

Lehman [5], Deléglise and Rivat [3] and Benito and Varona [2] have all leveraged this and similar identities to find efficient recursive methods of evaluating M and related functions at large values. We state a similar identity in Section 2.3.

2 The functions $\epsilon^{m,n}$ and $E^{m,n}$

2.1 Notation, statements of the main results, and proofs

The greatest common divisor of positive integers $a, b \in \mathbb{N}$ is written (a, b) . Let D be the matrix

$$D(i, j) := \begin{cases} 1, & \text{if } j|i; \\ 0, & \text{otherwise.} \end{cases}$$

The action of this matrix on vectors corresponds to Dirichlet convolution by $\mathbf{1} := (1, 1, 1, \dots)$. In matrix notation, where the functions μ and $\delta := (1, 0, 0, 0, \dots)$ are treated as a column vectors, and $*$ denotes Dirichlet convolution,

$$\mathbf{1} * \mu = \left(\sum_{d|k} \mu(d) : k \geq 1 \right) = D\mu = \delta. \quad (4)$$

We adopt the convention that the smallest index of sequences, vectors and matrices is 1, and not 0. Thus, the leading entry of δ is $\delta(1) = 1$. Let δ_m be the column vector consisting of the m leading terms of δ and let

$$c^m := (\delta_{2m}, -\delta_{2m}, \delta_{2m}, -\delta_{2m}, \dots). \quad (5)$$

Then c^m is supported on integers $k \equiv 1 \pmod{2m}$ and c^m is $4m$ -periodic. We indicate the transpose operation using a $'$ symbol. The functions of primary interest are now defined.

For each $m, n \geq 1$, set

$$\epsilon^{m,n} := D'_n c^{m,n},$$

where D_n denotes the n th leading principal submatrix of D , D'_n denotes the transpose of D_n and $c^{m,n}$ consists of the n leading terms of c^m . Written explicitly, for $1 \leq j \leq n$,

$$\epsilon^{m,n}(j) = \sum_{\substack{k \\ jk \leq n}} c^m(jk). \quad (6)$$

For example,

$$\epsilon^{1,6} = D'_6 c^{1,6} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

The following proposition describes basic properties of $\epsilon^{m,n}$. When applied to the above example, items 2 and 4 of Proposition 1 imply that $\|\epsilon^{1,6}\|_\infty \leq 1$ and $\sum_{k \leq 6} \epsilon^{1,6}(k)\mu(k) = 1$, which may be verified by inspection.

Proposition 1. *In the established notation,*

1. if $1 \leq k \leq n$ and $(k, 2m) > 1$, then $\epsilon^{m,n}(k) = 0$;
2. $\epsilon^{m,n} \in \{-1, 0, 1\}^n$;
3. if $n \geq 3m$, then $\|\epsilon^{m,n}\|_1 \geq \lfloor n/(3m) \rfloor$ and $\max\{k : \epsilon^{m,n}(k) \neq 0\} = 2m \lfloor (n-1)/(2m) \rfloor + 1$;

$$4. \sum_{k \leq n} \epsilon^{m,n}(k) \mu(k) = 1.$$

Proof. For all $1 \leq j \leq n$,

$$\begin{aligned} \epsilon^{m,n}(j) &= \sum_{\substack{k \\ jk \leq n}} c^m(jk) \\ &= \sum_{\substack{k \leq n \\ k \equiv 0 \pmod{j} \\ k \equiv 1 \pmod{4m}}} 1 - \sum_{\substack{k \leq n \\ k \equiv 0 \pmod{j} \\ k \equiv 2m+1 \pmod{4m}}} 1 \\ &= |A^j| - |B^j|, \end{aligned}$$

where

$$A^j := \{jk \leq n : k \in \mathbb{N}, jk \equiv 1 \pmod{4m}\}$$

and

$$B^j := \{jk \leq n : k \in \mathbb{N}, jk \equiv 2m+1 \pmod{4m}\}.$$

To see item 1 of the proposition, observe that neither $jk \equiv 1 \pmod{4m}$ nor $jk \equiv 2m+1 \pmod{4m}$ has an integer solution when $(j, 2m) > 1$. Consequently, $\epsilon^{m,n}(j) = |A^j| - |B^j| = 0 - 0 = 0$ when $(j, 2m) > 1$.

For item 2, observe that either $\epsilon^{m,n}(j) = 0$, or else $(j, 2m) = 1$ and

$$\epsilon^{m,n}(j) = |A^j| - |B^j| = \sum_{\substack{k \leq n/j \\ k \equiv j^* \pmod{4m}}} 1 - \sum_{\substack{k \leq n/j \\ k \equiv (2m+1)j^* \pmod{4m}}} 1,$$

where j^* is the unique integer satisfying both $1 \leq j^* \leq 4m-1$ and $jj^* \equiv 1 \pmod{4m}$. Then since j^* is necessarily odd, $(2m+1)j^* \equiv 2m+j^* \pmod{4m}$. Therefore,

$$\begin{aligned} \epsilon^{m,n}(j) &= \sum_{\substack{k \\ 0 < j^* + 4mk \leq n/j}} 1 - \sum_{\substack{k \\ 0 < 2m + j^* + 4mk \leq n/j}} 1 \\ &= \sum_{\substack{k \\ 0 < 2k + \frac{j^*}{2m} \leq \frac{n/j}{2m}}} 1 - \sum_{\substack{k \\ 0 < (2k+1) + \frac{j^*}{4m} \leq \frac{n/j}{2m}}} 1. \end{aligned}$$

Hence,

$$\epsilon^{m,n}(j) = \sum_{-\frac{j^*}{2m} < v \leq \frac{n/j}{2m} - \frac{j^*}{2m}} (-1)^v. \quad (7)$$

Consecutive terms in the last expression sum to 0. Since each individual term in the expression is either -1 or $+1$, the total sum is either -1 , 0 , or 1 .

We now show the third claim. Assume $n \geq k > n/3$. From Eq. (6), and since $c^m(k) = 0$ whenever $k \not\equiv 1 \pmod{2m}$,

$$\epsilon^{m,n}(k) = c^m(k) + c^m(2k) = c^m(k). \quad (8)$$

Consequently,

$$\|\epsilon^{m,n}\|_1 \geq \sum_{n/3 < j \leq n} |\epsilon^{m,n}(j)| = \sum_{n/3 < j \leq n} |c^m(j)| = \sum_{\substack{n/3 < j \leq n \\ j \equiv 1 \pmod{2m}}} 1 = \sum_{n/3 < 1+2ml \leq n} 1 = \sum_{\substack{\frac{n-3}{6m} < l \leq \frac{3n-3}{6m}}} 1.$$

Since $a < b$ implies $\left| (b-a) - \sum_{a < j \leq b} 1 \right| < 1$, it follows that

$$\|\epsilon^{m,n}\|_1 > \frac{n}{3m} - 1.$$

Since $\|\epsilon^{m,n}\|_1$ is integer-valued, the first statement of the third item follows. The second statement of this item follows from the definition of c^m and Eq. (8).

To see the last claim, observe that Eq. (4) implies $D_n \mu_n = \delta_n$, where μ_n represents the leading n terms of μ . Then, by applying the definitions of $c^{m,n}$ and $\epsilon^{m,n}$, it follows that

$$\sum_{1 \leq k \leq n} \epsilon^{m,n}(k) \mu(k) = \mu'_n \epsilon^{m,n} = \mu'_n D'_n c^{m,n} = (D_n \mu_n)' c^{m,n} = \delta'_n c^{m,n} = c^{m,n}(1) = 1. \quad \square$$

Equation (1) of Section 1 follows from the above observations. To see this, let $d^{k,n}$ denote column k of D_n and note that $d^{k,n}$ is supported on integers $jk \leq n$. Next, observe that

$$c^{1,n} = (1, 0, -1, 0, \dots) = \left(\cos \left(\frac{\pi(k-1)}{2} \right) : 1 \leq k \leq n \right).$$

Hence,

$$\epsilon^{1,n}(k) = (d^{k,n})' c^{1,n} = \sum_{jk \leq n} \cos \left(\frac{\pi(jk-1)}{2} \right),$$

which shows the claim.

Corollary 2. *Let $m, n, \in \mathbb{N}$. For each positive integer $k \leq n$ set*

$$\omega^{m,n}(k) := \begin{cases} \epsilon^{m,n}(k), & \text{if } k \text{ is odd;} \\ \epsilon^{m, \lfloor n/2 \rfloor}(k/2), & \text{if } k \text{ is even.} \end{cases}$$

Then $\omega^{m,n} \in \{-1, 0, 1\}^n$. If $n > 1$, then $\sum_{k \leq n} \omega^{m,n}(k) \mu(k) = 0$.

Proof. By Proposition 1 item 1, for all $m, n \geq 1$, the function $\epsilon^{m,n}$ is supported on odd integers. Since $\mu(2k) = -\mu(k)$ when k is odd, it follows by Proposition 1 item 4 that

$$\sum_{k \leq n} \omega^{m,n}(k) \mu(k) = \sum_{2k+1 \leq n} \epsilon^{m,n}(2k+1) \mu(2k+1) + \sum_{2k \leq n} \epsilon^{m, \lfloor n/2 \rfloor}(k) \mu(2k) = 1 - 1 = 0. \quad \square$$

Our next aim is to develop analogous results for the summatory function of μ , i.e., the Mertens function, M . Let $S_n \in \{0, 1\}^{n \times n}$ denote the lower-triangular matrix with $S_n(i, j) = 1$ whenever $j \leq i$. Then S_n is the matrix representation that corresponds to the operation of cumulative summation applied to n -vectors. Let $M_n := (M(1), \dots, M(n))$. Then $M_n = S_n \mu_n$. Let $\Delta_n := (S'_n)^{-1}$. Then

$$\Delta_n = \begin{pmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & 1 & -1 & \\ & & & \ddots & -1 \\ & & & & 1 \end{pmatrix}, \quad (9)$$

which is the matrix representation of a difference operation applied to n -vectors. Set

$$E^{m,n} := \Delta_n \epsilon^{m,n}.$$

The next corollary combines the above observations into a result that parallels Proposition 1.

Corollary 3. *In the established notation,*

1. $E^{m,n} \in \{-1, 0, 1\}^n$;
2. if $n \geq 3m$, then $\|E^{m,n}\|_1 \geq 2 \lfloor n/(3m) \rfloor - 1$;
3. $\sum_{k \leq n} M(k) E^{m,n}(k) = 1$.

Proof. Since $\epsilon^{m,n}(2k) = 0$ for all $k \geq 1$, the difference of adjacent entries of $\epsilon^{m,n}$ is $-1, 0$ or 1 . This shows the first claim.

For $1 \leq k < n$,

$$|E^{m,n}(k)| = |\epsilon^{m,n}(k)| + |\epsilon^{m,n}(k+1)|.$$

This fact, when combined with items 2 and 3 of Proposition 1 implies

$$\begin{aligned} \|E^{m,n}\|_1 &= \sum_{k < n} (|\epsilon^{m,n}(k)| + |\epsilon^{m,n}(k+1)|) + |\epsilon^{m,n}(n)| \\ &= \|\epsilon^{m,n}\|_1 + \|\epsilon^{m,n}\|_1 - |\epsilon^{m,n}(1)| \geq 2 \left\lfloor \frac{n}{3m} \right\rfloor - 1. \end{aligned}$$

This shows the second claim.

Finally, apply Proposition 1 and the respective definitions to find

$$M'_n E^{m,n} = (S_n \mu_n)' \Delta_n \epsilon^{m,n} = \mu'_n S'_n (S'_n)^{-1} \epsilon^{m,n} = \mu'_n \epsilon^{m,n} = 1. \quad \square$$

2.2 Remarks on Eq. (1)

It follows from (1), that for all positive integers n and $k \in \mathbb{N}$ satisfying $k \leq n$, the value of $\epsilon^{1,n}(k)$ equals the real part of the sum, $\sum_{1 \leq j \leq \lfloor n/k \rfloor} i^{jk-1}$, where $i := \sqrt{-1}$. This leads to a closed-form expression for $\epsilon^{1,n}(k)$. When k is even, it follows by Proposition 1 item 1 that $\epsilon^{1,n}(k) = 0$. Now assume k is odd. One has

$$\sum_{1 \leq j \leq \lfloor n/k \rfloor} i^{jk-1} = i^{k-1} \frac{1 - i^{k \lfloor n/k \rfloor}}{1 - i^k} = (-1)^{\lfloor k/2 \rfloor} \frac{(1 - i^{k \lfloor n/k \rfloor})(1 + i^k)}{2}.$$

Since $i^{k \lfloor n/k \rfloor} = (i^{\lfloor n/k \rfloor})^k$, the above expression vanishes when $\lfloor n/k \rfloor \equiv 0 \pmod{4}$. Next, when $\lfloor n/k \rfloor$ is odd, and since k is assumed odd, the real part of the above expression equals $(-1)^{\lfloor k/2 \rfloor} (1 - i^{k(\lfloor n/k \rfloor + 1)}) / 2$, which vanishes when $\lfloor n/k \rfloor \equiv -1 \pmod{4}$. When $\lfloor n/k \rfloor \equiv 1 \pmod{4}$, one has $i^{\lfloor n/k \rfloor} = i$ so that the right-hand side of the above sum reduces to

$$(-1)^{\lfloor k/2 \rfloor} \frac{(1 - i^k)(1 + i^k)}{2} = (-1)^{\lfloor k/2 \rfloor} \frac{1 - i^{2k}}{2} = (-1)^{\lfloor k/2 \rfloor}.$$

Finally, when $\lfloor n/k \rfloor \equiv 2 \pmod{4}$, $i^{\lfloor n/k \rfloor} = -1$, and (recalling that k is assumed odd) the right-hand side of the above sum reduces to

$$(-1)^{\lfloor k/2 \rfloor} \frac{(1 - (-1)^k)(1 + i^k)}{2} = (-1)^{\lfloor k/2 \rfloor} (1 + i^k),$$

the real part of which is $(-1)^{\lfloor k/2 \rfloor}$.

Therefore, for all positive integers n and k that satisfy $k \leq n$,

$$\epsilon^{1,n}(k) = \begin{cases} 0, & \text{if } \lfloor n/k \rfloor \equiv r \pmod{4} \text{ for some } r \in \{0, -1\}; \\ \sin(k\pi/2), & \text{otherwise.} \end{cases} \quad (10)$$

When $1 \leq k \leq n$, an explicit formula for $\epsilon^{m,n}(k)$ is possible to derive. The case where $(k, 2m) > 1$ is discussed in Proposition 1 item 1, so we now assume $(k, 2m) = 1$. Let k^* be

any integer satisfying $kk^* = 1 \pmod{4m}$. By Eq. (7), one has

$$\begin{aligned}
\epsilon^{m,n}(k) &= \sum_{\substack{j \\ \frac{-k^*}{2m} < 2j \leq \frac{\lfloor n/k \rfloor - k^*}{2m}}} 1 - \sum_{\substack{j \\ \frac{-k^*}{2m} < 2j+1 \leq \frac{\lfloor n/k \rfloor - k^*}{2m}}} 1 \\
&= \sum_{\substack{j \\ \frac{-k^*}{4m} < j \leq \frac{\lfloor n/k \rfloor - k^*}{4m}}} 1 - \sum_{\substack{j \\ \frac{-k^*}{4m} - \frac{1}{2} < j \leq \frac{\lfloor n/k \rfloor - k^*}{4m} - \frac{1}{2}}} 1 \\
&= \left(\left\lfloor \frac{\lfloor n/k \rfloor - k^*}{4m} \right\rfloor - \left\lfloor \frac{-k^*}{4m} \right\rfloor \right) - \left(\left\lfloor \frac{\lfloor n/k \rfloor - k^*}{4m} - \frac{1}{2} \right\rfloor - \left\lfloor \frac{-k^*}{4m} - \frac{1}{2} \right\rfloor \right) \\
&= \left(\left\lfloor \frac{\lfloor n/k \rfloor - k^*}{4m} \right\rfloor - \left\lfloor \frac{\lfloor n/k \rfloor - k^*}{4m} - \frac{1}{2} \right\rfloor \right) - \left(\left\lfloor \frac{-k^*}{4m} \right\rfloor - \left\lfloor \frac{-k^*}{4m} - \frac{1}{2} \right\rfloor \right) \\
&= \sum_{\substack{j \\ \frac{\lfloor n/k \rfloor - k^*}{4m} - \frac{1}{2} < j \leq \frac{\lfloor n/k \rfloor - k^*}{4m}}} 1 - \sum_{\substack{j \\ \frac{-k^*}{4m} - \frac{1}{2} < j \leq \frac{-k^*}{4m}}} 1.
\end{aligned}$$

Then, letting $\{x\} := x - \lfloor x \rfloor$ denote the fractional part of x ,

$$\epsilon^{m,n}(k) = \begin{cases} 1, & \text{if } (k, 2m) = 1, \left\{ \frac{k^*}{4m} \right\} \in (0, \frac{1}{2}] \text{ and } \left\{ \frac{k^* - \lfloor n/k \rfloor}{4m} \right\} \notin (0, \frac{1}{2}]; \\ -1, & \text{if } (k, 2m) = 1, \left\{ \frac{k^*}{4m} \right\} \notin (0, \frac{1}{2}] \text{ and } \left\{ \frac{k^* - \lfloor n/k \rfloor}{4m} \right\} \in (0, \frac{1}{2}]; \\ 0, & \text{otherwise.} \end{cases}$$

2.3 An identity involving a sparse sum

Benito and Varona ([2, Theorem 9]) establish the identity,

$$2M(n) + 3 = g(n, 1) + \sum_{3 \leq a \leq n-1} h(a) \left(M\left(\frac{n}{a}\right) - M\left(\frac{n}{a+1}\right) \right),$$

where $g(x, 1)$ and $h(x)$ depend on the value of $x \pmod{6}$, and the values of both g and h are tabulated. The utility of this formula is that it leads to an efficient and recursive means of evaluating M . In Proposition 4 of this section, we establish a similar identity.

Before stating the identity, we introduce notation. The unique non-principal Dirichlet character mod 4 is

$$\chi(k) = \begin{cases} 1, & \text{if } k \equiv 1 \pmod{4}; \\ -1, & \text{if } k \equiv -1 \pmod{4}; \\ 0, & \text{otherwise.} \end{cases}$$

The sine-factor in the non-vanishing case of (10) satisfies $\sin(k\pi/2) = \chi(k)$ for all integers k . Next, we define

$$M(x, \chi) := \sum_{k \leq x} \mu(k) \chi(k),$$

and set

$$\eta(k) := \begin{cases} 1, & \text{if } k \equiv r \pmod{4} \text{ for some } r \in \{1, 2\}; \\ 0, & \text{otherwise.} \end{cases}$$

We are now ready to state the identity.

Proposition 4. *For all $n \geq 1$,*

$$\sum_{1 \leq k \leq n} \eta(k) \left(M\left(\frac{n}{k}, \chi\right) - M\left(\frac{n}{k+1}, \chi\right) \right) = 1.$$

Proof. One has

$$\begin{aligned} \sum_{1 \leq k \leq n} \eta(k) \left(M\left(\frac{n}{k}, \chi\right) - M\left(\frac{n}{k+1}, \chi\right) \right) &= \sum_{\substack{k, j \\ k \equiv r \pmod{4}, r \in \{1, 2\} \\ \frac{n}{k+1} < j \leq \frac{n}{k}}} \mu(j) \chi(j) \\ &= \sum_{4l+3 > \lfloor n/j \rfloor \geq 4l+1} \mu(j) \chi(j) \\ &= \sum_j \epsilon^{1, n}(j) \mu(j) \\ &= 1, \end{aligned}$$

where the third equality follows from Eq. (10) and the definition of χ , and the last equality from Proposition 1 item 4. \square

3 A family of unimodular matrices

The classical identities expressed in Eq. (2) and Eq. (3) of the introduction are equivalent. Indeed, for any integer $n \in \mathbb{N}$, Eq. (2) states $D_n \mu_n = \delta_n$. Multiplication of both sides by S_n yields, $S_n D_n \mu_n = S_n \delta_n = \mathbf{1}_n$, which is (3). Equivalence follows by observing that S_n is invertible. This observation generalizes to yield the infinite family of identities, $S_n^k D_n \mu_n = S_n^k \delta_n$, where $k, n \in \mathbb{N}$ are arbitrary. The next proposition describes a closely-related family of identities. We first state a lemma that generalizes the identity, $\sum_{d|n} \phi(d) = n$, where ϕ is Euler's totient function.

Lemma 5. *For positive $j, k \in \mathbb{N}$, write $\phi^k(j) := \sum_{\ell \leq j/k, (\ell, j)=1} 1$. Let $R_n := D_n^{-1} S_n D_n$. Then for all $1 \leq j, k \leq n$, $R_n(j, k) = \phi^k(j)$.*

Proof. Column k of $S_n D_n$ equals $(\lfloor 1/k \rfloor, \lfloor 2/k \rfloor, \dots, \lfloor n/k \rfloor)$. Let ϕ_n^k denote the column vector consisting of the n leading terms of ϕ^k . Our aim is to demonstrate that

$$(D_n \phi_n^k)(j) = \sum_{d|j} \phi^k(d) = \lfloor j/k \rfloor \quad (11)$$

holds when $1 \leq j, k \leq n$. Once this has been shown, one arrives at $(D_n^{-1} S_n D_n)(j, k) = \phi^k(j)$ by applying D_n^{-1} to both sides. Fix j and k . For each integer d with $d|j$, define the set

$$S_d := \{s \in \mathbb{N} : 1 \leq s \leq j/k \text{ and } (s, j) = j/d\}.$$

Then S_d consists of all integers with the form $(t)(j/d)$, where $1 \leq t \leq d/k$ and $(t, d) = 1$. Then $|S_d| = \phi^k(d)$. Each integer between 1 and $\lfloor j/k \rfloor$ belongs to a unique S_d . Summing over d , one has (11). \square

Proposition 6. *For positive $n \in \mathbb{N}$, set $Q_n := R'_n R_n$. Then Q_n is a positive definite matrix, both Q_n and $(Q_n)^{-1} \in \mathbb{Z}^{n \times n}$, and $\det Q_n = \det (Q_n)^{-1} = 1$. Additionally,*

1. $Q_n \mu_n = \delta_n$;
2. $Q_n(i, j) > 0$ for all $1 \leq i, j \leq n$;
3. $Q_n(1, 1) = \sum_{1 \leq k \leq n} \phi(k)^2$.

Proof. Recall that D is the matrix representation of Dirichlet convolution by $\mathbf{1}$, and the inverse operation is Dirichlet convolution by μ . In particular, the matrix D_n^{-1} is $(-1, 0, 1)$ -valued. Since each of D_n , D_n^{-1} and S_n live in $\mathbb{Z}^{n \times n}$, it follows that $Q_n \in \mathbb{Z}^{n \times n}$.

Also, each of D_n , D_n^{-1} and S_n are lower-triangular with 1 along the main diagonal, so each has determinant equal to 1, as do their transposes. Since \det is multiplicative, $\det Q_n = 1$, from which it follows (by Cramer's rule) that $(Q_n)^{-1} \in \mathbb{Z}^{n \times n}$. Additionally, since for all $x \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ one has $x' Q_n x = \|(D_n^{-1} S_n D_n)x\|^2 \geq 0$, Q_n is nonnegative definite. But $\det Q_n = 1 > 0$, so it has full rank. In particular, $x' Q_n x > 0$, which implies, since $x \neq \mathbf{0}$ is arbitrary, that Q_n is positive definite.

We now establish item 1 of the proposition's statement. The first column of S_n equals the first column of D_n , both of which equal $\mathbf{1}_n$. Thus, recalling Eq. (4),

$$R_n \mu_n = D_n^{-1} S_n D_n \mu_n = D_n^{-1} S_n \delta_n = D_n^{-1} \mathbf{1}_n = \delta_n.$$

The first column of each of the upper-triangular matrices $(D_n^{-1})'$, D'_n and S'_n equals δ_n , so

$$Q_n \mu_n = R'_n R_n \mu_n = D'_n S'_n (D_n^{-1})' \delta_n = D'_n S'_n \delta_n = D'_n \delta_n = \delta_n.$$

For the proof of item 2, note that ϕ^k of Lemma 5 satisfies $\phi^k(l) > 0$ whenever $l \geq k$. Therefore $Q_n(j, k) = \sum_{l \leq n} \phi^j(l) \phi^k(l) \geq \phi^j(n) \phi^k(n) > 0$ when $1 \leq j, k \leq n$. Item 3 is also immediate from Lemma 5. Indeed, $Q_n(1, 1) = \sum_{j \leq n} (\phi^1(j))^2 = \sum_{j \leq n} (\phi(j))^2$. \square

In the discussion below, it may be helpful to have a reference example of R_n , Q_n and Q_n^{-1} :

$$R_7 = \begin{pmatrix} 1 & & & & & & \\ 1 & 1 & & & & & \\ 2 & 1 & 1 & & & & \\ 2 & 1 & 1 & 1 & & & \\ 4 & 2 & 1 & 1 & 1 & & \\ 2 & 1 & 1 & 1 & 1 & 1 & \\ 6 & 3 & 2 & 1 & 1 & 1 & 1 \end{pmatrix}, \quad Q_7 = \begin{pmatrix} 66 & 33 & 22 & 14 & 12 & 8 & 6 \\ 33 & 17 & 11 & 7 & 6 & 4 & 3 \\ 22 & 11 & 8 & 5 & 4 & 3 & 2 \\ 14 & 7 & 5 & 4 & 3 & 2 & 1 \\ 12 & 6 & 4 & 3 & 3 & 2 & 1 \\ 8 & 4 & 3 & 2 & 2 & 2 & 1 \\ 6 & 3 & 2 & 1 & 1 & 1 & 1 \end{pmatrix},$$

and

$$(Q_7)^{-1} = \begin{pmatrix} 1 & -1 & -1 & & -1 & 1 & -1 \\ -1 & 2 & & & & & \\ -1 & & 3 & -1 & 2 & -2 & 1 \\ & & -1 & 2 & -1 & & 1 \\ -1 & & 2 & -1 & 4 & -3 & 2 \\ 1 & & -2 & & -3 & 4 & -3 \\ -1 & & 1 & 1 & 2 & -3 & 5 \end{pmatrix}.$$

Item 1 of the proposition states that μ_n is the first column of $(Q_n)^{-1}$. The second column of $(Q_n)^{-1}$ has a far simpler form, namely $q := (-1, 2, 0, 0, 0, \dots, 0)$. To see this, observe that $R_n(2, 1) = R_n(2, 2) = 1$. When $j > 2$, $R_n(j, 2) = \lfloor R_n(j, 1)/2 \rfloor$, and since $R_n(j, 1) = \phi^1(j) = \phi(j)$ is even, $\lfloor R_n(j, 1)/2 \rfloor = R_n(j, 1)/2$. Noting that R'_n is upper-triangular and $R(1, 1) = 1$, one has

$$R'_n R_n q = R'_n \begin{pmatrix} -1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

Since Q_n is Hermitian, the eigenvalues of Q_n are real. Let $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ denote the eigenvalues of Q_n . By item 2, we may invoke the Perron-Frobenius theorem to conclude that λ_n is simple and that the eigenvector associated with λ_n , denoted v_n , satisfies $v_n(j) > 0$ for $1 \leq j \leq n$.

The following two propositions concern the spectrum of Q_n . Table 1 illustrates these propositions.

Proposition 7. *The eigenvalues of Q_n interlace the eigenvalues of Q_{n+1} . That is, if λ_i is the i th eigenvalue of Q_n and γ_i the i th eigenvalue of Q_{n+1} , then*

$$\gamma_1 \leq \lambda_1 \leq \gamma_2 \leq \dots \leq \gamma_n \leq \lambda_n \leq \gamma_{n+1}.$$

Table 1: Eigenvalue λ_i of Q_n .

i	$n = 999$	$n = 1000$	$n = 1001$
1	4.588×10^{-4}	4.580×10^{-4}	4.573×10^{-4}
2	6.887×10^{-4}	6.879×10^{-4}	6.859×10^{-4}
...			
$n - 1$	4.458×10^4	4.471×10^4	4.487×10^4
n	2.344×10^8	2.346×10^8	2.355×10^8

Proof. We claim that $(Q_n)^{-1}$ is a leading principal submatrix of $(Q_{n+1})^{-1}$. Assume, for the moment, that this has been established. Then by Cauchy's interlacing theorem, the eigenvalues of $(Q_n)^{-1}$ interlace those of $(Q_{n+1})^{-1}$. That is, letting λ_i^{-1} and γ_i^{-1} denote the eigenvalues of $(Q_n)^{-1}$ and $(Q_{n+1})^{-1}$, respectively,

$$\gamma_{n+1}^{-1} \leq \lambda_n^{-1} \leq \gamma_n^{-1} \leq \dots \leq \gamma_2^{-1} \leq \lambda_1^{-1} \leq \gamma_1^{-1}.$$

Since all quantities in this expression are positive scalars, the proposition follows.

We now show that $(Q_n)^{-1}$ is a leading principal submatrix of $(Q_{n+1})^{-1}$. From the definition of Q_n , we have that

$$Q_n^{-1} = (R'_n R_n)^{-1} = (R_n)^{-1} (R'_n)^{-1} = (R_n)^{-1} (R_n^{-1})'. \quad (12)$$

Recall from Lemma 5 the entrywise equality, $R_n(j, k) = \phi^k(j)$. Since the right-hand side does not depend on n , the (j, k) entry of R_n does not depend on n . Therefore, R_n is a leading principal submatrix of R_m whenever $m \geq n$. Since R_n is lower-triangular, it follows (by consideration of block matrix inversion, for example) that $(R_n)^{-1}$ is a leading principal submatrix of $(R_m)^{-1}$ for all $m \geq n$. This also shows that $(R_n^{-1})'$ is a leading principal submatrix of $(R_m^{-1})'$ whenever $m \geq n$.

For $1 \leq j \leq n$, define r^j as the j th column of $(R_{n+1}^{-1})'$. Since $(R_n^{-1})'$ is a leading principal submatrix of $(R_{n+1}^{-1})'$, the first n entries of r^j agree with the j th column of $(R_n^{-1})'$. This, combined with Eq. (12) and the fact that R_n^{-1} is lower-triangular, implies that the j th column of $(Q_n)^{-1}$ equals the column vector that is comprised of the first n entries of $(R_{n+1})^{-1} r^j$. Eq. (12) also implies that the j th column of $(Q_{n+1})^{-1}$ equals $(R_{n+1})^{-1} r^j$. This applies to all $1 \leq j \leq n$, so it follows that $(Q_n)^{-1}$ is a leading principal submatrix of $(Q_{n+1})^{-1}$. \square

The next proposition establishes bounds on the extremal eigenvalues of Q_n .

Proposition 8. *Let λ_n denote the dominant eigenvalue of Q_n . Then*

$$(c + o(1)) n^3 \leq \lambda_n \leq \frac{\pi^2}{18} n^3 + O(n^2),$$

where c is a constant that is approximately equal to 0.1427. Let λ_1 denote the smallest eigenvalue of Q_n . Then

$$\lambda_1 \leq \frac{\pi^2}{6}n^{-1} + O(n^{-3/2}).$$

Proof. We first show the lower bound on λ_n . Since λ_n is the dominant eigenvalue of Q_n , applying item 3 of Proposition 6 one has,

$$\lambda_n \geq \frac{\delta'_n Q_n \delta_n}{\|\delta_n\|^2} = Q_n(1, 1) = \sum_{k \leq n} (\phi(k))^2.$$

We estimate the right-hand sum by applying the Wiener-Ikehara Theorem to the function $H(s) := \sum_{k \geq 1} \phi(k)^2 k^{-s}$. A comment associated with the sequence [A127473](#) asserts that $H(s) = \zeta(s-2) \prod_{p \text{ prime}} (1 - 2p^{1-s} + p^{-s})$. Since this is a known fact, but no proof is provided in the citation, we sketch a proof here. To start, if $n = \prod_p p^r$, then $\phi(n) = \prod_{p|n} p^r - p^{r-1}$. Since $n \mapsto \phi(n)n^{-s}$ is a multiplicative function, one has the Euler product,

$$\begin{aligned} H(s) &= \prod_{p \text{ prime}} \left(1 + \sum_{r \geq 1} \frac{(p^r - p^{r-1})^2}{p^{rs}} \right) \\ &= \prod_{p \text{ prime}} \left(1 + \sum_{r \geq 1} \frac{p^{2r}}{p^{rs}} - 2 \frac{p^{2r-1}}{p^{rs}} + \frac{p^{2r-2}}{p^{rs}} \right) \\ &= \prod_{p \text{ prime}} \left(1 + \left(1 - \frac{2}{p} + \frac{1}{p^2} \right) \frac{p^{2-s}}{1 - p^{2-s}} \right) \\ &= \prod_{p \text{ prime}} (1 - p^{2-s} + p^{2-s} - 2p^{1-s} + p^{-s}) \left(\frac{1}{1 - p^{2-s}} \right) \\ &= \zeta(s-2) \prod_{p \text{ prime}} (1 - 2p^{1-s} + p^{-s}). \end{aligned}$$

At $s = 3$, the infinite product converges and $\zeta(s-2)$ has a simple pole with residue equal to 1. Therefore, H has a simple pole at $s = 3$, with residue equal to the product of the right-hand side. We now apply the Wiener-Ikehara Theorem to conclude that

$$\sum_{k \leq n} (\phi(x))^2 \sim \frac{n^3}{3} \prod_{p \text{ prime}} (1 - 2p^{-2} + p^{-3}) = \left(\frac{n^3}{3} \right) (0.42824950\dots)$$

We now show the upper bound on λ_n . Indeed,

$$\begin{aligned}
\text{Trace}(Q_n) &= \sum_{k=1}^n Q_n(k, k) \\
&= \sum_{k=1}^n \sum_{j=1}^n (\phi^k(j))^2 \\
&\leq \sum_{k=1}^{\infty} \sum_{j=1}^n \left(\frac{j}{k}\right)^2 \\
&= \frac{n(n+1)(2n+1)}{6} \sum_{k=1}^{\infty} k^{-2} \\
&= \frac{\pi^2}{18} n^3 + O(n^2),
\end{aligned}$$

where we have used the elementary identity $\sum_{j=1}^n j^2 = n(n+1)(2n+1)/6$ and Euler's identity $\sum_{i=1}^{\infty} i^{-2} = \pi^2/6$. Finally, recall that Q_n is positive definite and $\text{Trace}(Q_n) = \sum_{i=1}^n \lambda_i \geq \lambda_n$.

We now show the upper bound on λ_1 . We have by item 1 of Proposition 6 that

$$\frac{\mu'_n Q_n \mu_n}{\|\mu_n\|^2} = \frac{\mu'_n \delta_n}{\|\mu_n\|^2} = \frac{\mu(1)}{\sum_{k \leq n} \mu_n(k)^2} = \frac{1}{\sum_{k \leq n} |\mu_n(k)|} \geq \lambda_1.$$

The penultimate expression is the reciprocal of the number of squarefree integers not exceeding n . The desired bound is a consequence of this, combined with an application of Gegenbauer's estimate [4, p. 47],

$$\sum_{k \leq n} |\mu_n(k)| = \frac{6}{\pi^2} n + O(n^{1/2}).$$

That is,

$$\lambda_1 \leq \left(\sum_{k \leq n} |\mu_n(k)| \right)^{-1} = \frac{\pi^2}{6} n^{-1} + O(n^{-3/2}). \quad \square$$

Corollary 9. *In the established notation, $|v'_n \mu_n| \leq n^{-3/2} C(1 + o(1))$, where the constant C is approximately 2.6467.*

Proof. For $1 \leq i \leq n$, let v_i satisfy $Q_n v_i = \lambda_i v_i$. We may assume that $v'_i v_j = 0$ whenever $i \neq j$, that $v'_i v_i = 1$ for all $1 \leq i \leq n$ and that the space spanned by $\{v_i : 1 \leq i \leq n\}$ has dimension n . Then $\mu_n = \sum_{1 \leq i \leq n} (v'_i \mu_n) v_i$. By item 1 of Proposition 6, $\mu'_n Q_n \mu_n = 1$. Since $\lambda_i > 0$ for all i ,

$$1 = \mu'_n Q_n \mu_n = \sum_{1 \leq i \leq n} \lambda_i |v'_i \mu_n|^2 \geq \lambda_n |v'_n \mu_n|^2 \geq n^3 (c + o(1)) |v'_n \mu_n|^2,$$

where the last inequality is from Proposition 8. The constant C in the Corollary statement is $c^{-1/2}$. \square

We conclude with a conjecture. Recall that the dominant eigenvector of Q_n , which is denoted v_n , was shown to satisfy $v_n(j) > 0$, for all $1 \leq j \leq n$. Assume we have normalized v_n , so that $\|v_n\|_2 = 1$. Let $h(k) := k^{-1}$ and let h_n denote the n th truncation of h . Then

$$\lim_{n \rightarrow \infty} n \|h_n - (v_n' h_n) v_n\|_\infty = 1. \quad (\text{Conjecture})$$

The sequence h_n arises in combination with μ_n in the asymptotic estimate,

$$h_n' \mu_n = \sum_{k=1}^n \frac{\mu(k)}{k} = o(1),$$

which is equivalent to the prime number theorem [6].

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(Concerned with sequences [A002321](#), [A008683](#), [A056594](#), [A127473](#), and [A327580](#).)

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