A Notion of Positive Definiteness for Arithmetical Functions

Mika Mattila and Pentti Haukkanen

Abstract In the theory of Fourier transform some functions are said to be positive definite based on the positive definiteness property of a certain class of matrices associated with these functions. In the present article we consider how to define a similar positive definiteness property for arithmetical functions, whose domain is not the set of real numbers but merely the set of positive integers. After finding a suitable definition for this concept we shall use it to construct a partial ordering on the set of arithmetical functions. We shall study some of the basic properties of our newly defined relations and consider a couple of well-known arithmetical functions as examples.

Keywords Arithmetical function · GCD matrix · Positive definite function · Positive semidefinite ordering · Dirichlet convolution · Möbius function

1 Introduction

A complex valued function $f : \mathbb{R} \to \mathbb{C}$ is said to be a *positive definite function* if the matrix $[f(x_i - x_j)]$ is positive semidefinite for all choices of points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}$ and all $n = 1, 2, \ldots$. A positive definite function is under mild restrictions the Fourier transform of a nonnegative real-valued function $g : \mathbb{R} \to \mathbb{R}_{\geq 0}$; see [3] or [5, Article 192B] for Bochner's theorem (note that the notion of a "positive semidefinite function" is not a term usually employed). By using the definition it is possible to prove several basic properties for a positive definite function f:

- $f(-x) = \overline{f(x)}$ for all $x \in \mathbb{R}$
- $f(0) \in \mathbb{R}$ and $f(0) \geq 0$

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- f is a bounded function, and $|f(x)| \leq f(0) \quad \forall x \in \mathbb{R}$
- If f is continuous at 0, then it is continuous everywhere
- If $f_1, f_2, \ldots, f_n$ are positive definite functions and $a_1, a_2, \ldots, a_n$ are nonnegative real numbers, then the function $a_1 f_1 + a_2 f_2 + \cdots + a_n f_n$ is a positive definite function
- If f is a positive definite function, then so are $\overline{f}$ and $|f|^2$

Functions $\cos x$ (but not $\sin x$), e^{aix} $(a \in \mathbb{R})$, $\frac{1}{1-ix}$, $\frac{1}{1+x^2}$ and $\frac{1}{\cosh x}$ are all examples of positive definite functions (for more information, see [9, pp. 400–401] and [3, Section 3]).

In this article we are interested in *arithmetical functions*, which are real-valued (or sometimes complex-valued) functions on $\mathbb{Z}^+ = \{1, 2, 3, \ldots\}$. There are various operations defined on the set of arithmetical functions, see [2, 12]. For our purposes the most important are:

- The usual sum: $(f + g)(m) = f(m) + g(m) \quad \forall m \in \mathbb{Z}^+$
- The usual product: $(fg)(m) = f(m)g(m) \quad \forall m \in \mathbb{Z}^+$
- The Dirichlet convolution: $(f * g)(m) = \sum_{d \mid m} f(d)g\left(\frac{m}{d}\right) \quad \forall m \in \mathbb{Z}^+$

One of the main goals of this article is to consider how to define positive definiteness property for arithmetical functions. The original definition is a bit problematic since it would require the function to be defined on negative integers as well. There are a couple of ways how one may try to get around this problem, and we shall discuss them in Sect. 2. In Sect. 3 we shall introduce our final definition and in Sect. 4 we investigate some of the basic properties of our newly defined positive definiteness concept. In Sect. 5 we use our positive definiteness relation to define a partial order on the set of arithmetical functions and then study the properties of this relation. We also present several examples concerning some fundamental arithmetical functions. In Sect. 6 we give some concluding remarks.

2 Defining Positive Definiteness of Arithmetical Functions by Using the Original Definition

The most obvious way to define positive definiteness for arithmetical functions would be to expand the domain of arithmetical functions and to define the concept by using the matrix $[f(x_i - x_j)]$. First it should be noted that without loss of generality, we may assume that $x_1 < x_2 < \cdots < x_n$. If $x_i = x_j$ for some indices i and j with $i \neq j$, then the respective rows (and respective columns) are identical and the multiplicity of eigenvalue zero is increased by one. After eliminating identical rows and columns we can permute the rows and respective columns of the matrix $[f(x_i - x_j)]$ so that $x_1 < x_2 < \cdots < x_n$ is satisfied and the eigenvalues are still the same (if P is any permutation matrix, then $P^{-1} = P^T$ and the matrices $P^T AP$ and A share the same spectrum).

For an arithmetical function f it is customary to assume that $f(x) = 0$ whenever $x \notin \mathbb{Z}^+$. Under this assumption the matrix $[f(x_i - x_j)]$ takes the form

$$\begin{bmatrix} f(x_1 - x_1) & f(x_1 - x_2) & f(x_1 - x_3) & \ldots \\ f(x_2 - x_1) & f(x_2 - x_2) & f(x_2 - x_3) & \ldots \\ f(x_3 - x_1) & f(x_3 - x_2) & f(x_3 - x_3) & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \ldots \\ f(x_2 - x_1) & 0 & 0 \ldots \\ f(x_3 - x_1) & f(x_3 - x_2) & 0 \ldots \\ \vdots & \vdots & \vdots \ddots \end{bmatrix}.$$

But since the concept of positive definiteness is defined only on Hermitian matrices, the positive definiteness of the above matrix actually implies that all the elements of the matrix are equal to zero. Thus f must be the constant function 0, which is the only positive definite function according to this definition. It appears that for the purposes of arithmetical functions the classical definition of positive definite function is quite useless.

If f is a real-valued arithmetical function, then another rather obvious attempt would be to define $f(-m) = f(m)$ for all $m \in \mathbb{Z}^+$, which makes the matrix $[f(x_i - x_j)]$ symmetric. In this case the matrix $[f(x_i - x_j)]$ takes the form

$$\begin{bmatrix} f(0) & f(x_2 - x_1) & f(x_3 - x_1) & \ldots \\ f(x_2 - x_1) & f(0) & f(x_3 - x_2) & \ldots \\ f(x_3 - x_1) & f(x_3 - x_2) & f(0) & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

This is still problematic since $f(0)$ remains undefined. However, the value $f(0)$ is crucial to the positive definiteness of the matrix $[f(x_i - x_j)]$. As was the case with the usual positive definite functions, also this definition implies that $|f(i)| \leq f(0)$ for all $i \in \mathbb{Z}^+$. It becomes quite clear that this approach does not work either, and therefore there seems to be no natural way to define positive definiteness of arithmetical functions by using the matrix $[f(x_i - x_j)]$.

Since the two most natural ways to extend the domain of arithmetical functions do not serve our purposes very well, it seems that we need to use a different class of matrices in order to define positive definiteness for arithmetical functions. It would also make sense to define this concept without extending the domain of arithmetical functions, since many operations such as the Dirichlet convolution are defined intrinsically only on $\mathbb{Z}^+$. These kind of technical difficulties can be avoided if we base our definition on GCD matrices.

3 Defining Positive Definiteness by Using GCD Matrices

Let $\mathscr{A}$ denote the set of arithmetical functions and let $f \in \mathscr{A}$. Let

$$S = \{x_1, x_2, \ldots, x_n\}$$

be a finite subset of $\mathbb{Z}^+$ with $x_1 < x_2 < \cdots < x_n$. The GCD matrix $(S)_f$ of the set S with respect to the function f is the $n \times n$ matrix with $f(\gcd(x_i, x_j))$ as its ij entry. This definition originates from the seminal paper [17] by H. J. S. Smith published in 1876. For more information about GCD and related matrices, see [1, 8, 13, 16].

Definition 1 An arithmetical function $f : \mathbb{Z}^+ \to \mathbb{R}$ is positive definite if the GCD matrix $[f(\gcd(x_i, x_j))]$ is positive semidefinite for all choices of points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{Z}^+$ and all $n = 1, 2, \ldots$

Remark 1 Arithmetical function f is positive definite if and only if the GCD matrix $(S)_f$ succeeds the corresponding zero matrix with respect to the Löwner order for all finite nonempty sets $S \subset \mathbb{Z}$.

Example 1 Let $\delta \in \mathscr{A}$ with $\delta(1) = 1$ and $\delta(m) = 0$ for all $m > 1$ (the function δ is the identity element with respect to the Dirichlet convolution). Let $S = \{1, 2\}$. Then

$$(S)_\delta = \begin{bmatrix} \delta(\gcd(1,1)) & \delta(\gcd(1,2)) \\ \delta(\gcd(2,1)) & \delta(\gcd(2,2)) \end{bmatrix} = \begin{bmatrix} \delta(1) & \delta(1) \\ \delta(1) & \delta(2) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}.$$

This matrix is not positive semidefinite, since $\det(S)_\delta = -1$, and thus δ is not a positive definite function.

Example 2 The Möbius function μ is defined as follows:

- $\mu(m) = (-1)^k$ if $p^2 \nmid m$ for any prime number p and k is the number of the prime factors of m,
- $\mu(m) = 0$ if $p^2 \mid m$ for some prime number p.

Take any prime number p and set $S = \{p\}$. We obtain $(S)_\mu = [\mu(p)] = [-1]$. Thus the function μ is not positive definite.

Example 3 Let $\alpha \in \mathbb{R}$. We define $N^\alpha(m) = m^\alpha$ for all $m \in \mathbb{Z}^+$.

(a) Let $\alpha > 0$. It is a well-known fact (see, e.g., [4]) that in this case the matrix $(S)_{N^\alpha} = [\gcd(x_i, x_j)^\alpha]$ is positive definite for all finite nonempty sets $S \subset \mathbb{Z}^+$. Thus N^α is a positive definite function for all $\alpha > 0$.

(b) Let $\alpha < 0$ and $S = \{x_1, x_2\}$ with $x_1 \mid x_2$. In this case

$$(S)_{N^\alpha} = \begin{bmatrix} N^\alpha(x_1) & N^\alpha(x_1) \\ N^\alpha(x_1) & N^\alpha(x_2) \end{bmatrix} = \begin{bmatrix} x_1^\alpha & x_1^\alpha \\ x_1^\alpha & x_2^\alpha \end{bmatrix}.$$

Now $\det(S)_{N^\alpha} = (x_1 x_2)^\alpha - (x_1^2)^\alpha < 0$. Thus N^α is not a positive definite function for any $\alpha < 0$.

(c) For $\alpha = 0$ we denote $N^0 = \zeta$ and have $\zeta(m) = 1$ for all $m \in \mathbb{Z}^+$ (the function ζ is the identity element with respect to the usual product). For any finite nonempty set $S \subset \mathbb{Z}$ the matrix $(S)_\zeta$ is an $n \times n$ matrix with all elements equal to 1. It has two distinct eigenvalues: 0 with multiplicity $n-1$ and n with multiplicity 1. The matrix $(S)_\zeta$ is positive semidefinite and thus ζ is a positive definite function.

4 Positive Definiteness Properties for Arithmetical Functions

In this section we investigate various basic properties that follow directly from the definition of a positive definite arithmetical function. We continue to assume that S is ordered as in the previous section: $x_1 < x_2 < \cdots < x_n$.

Theorem 1 *Let $f \in \mathscr{A}$ be a positive definite function. Then*

(a) $f(m) \geq 0$ for all $m \in \mathbb{Z}^+$,
(b) $k \mid m \Rightarrow f(k) \leq f(m)$ for all $k, m \in \mathbb{Z}^+$.

Proof Let $m \in \mathbb{Z}^+$. The part (a) follows by setting $S = \{m\}$, which yields the 1×1 GCD matrix $(S)_f = [f(m)]$. This matrix needs to be positive semidefinite, and therefore $f(m) \geq 0$.

Next we prove part (b). Suppose that $k \mid m$. In this case we choose $S = \{k, m\}$ to obtain the GCD matrix

$$(S)_f = \begin{bmatrix} f(k) & f(k) \\ f(k) & f(m) \end{bmatrix}.$$

The determinant of this matrix is equal to $f(k)f(m) - f(k)^2 = f(k)(f(m) - f(k)) \geq 0$. From this we deduce by distinguishing the cases in which $f(k)$ is 0 and $\neq 0$, that $f(m) \geq f(k)$.

Corollary 1 *If $f \in \mathscr{A}$ is a positive definite function, then $f(m) \geq f(1) \geq 0$ for all $m \in \mathbb{Z}^+$.*

Theorem 2 *A function $f \in \mathscr{A}$ is positive definite if and only if the GCD matrix $(S_m)_f$ of the set $S_m = \{1, 2, \ldots, m\}$ is positive semidefinite for all $m = 1, 2, \ldots$.*

Proof The implication $\Rightarrow$ is trivial, and thus it suffices to show the direction $\Leftarrow$. Suppose that the matrix $(S_m)_f$ of the set $S_m = \{1, 2, \ldots, m\}$ is positive semidefinite for all $m = 1, 2, \ldots$. Let $S = \{x_1, x_2, \ldots, x_n\}$ be an arbitrary subset of $\mathbb{Z}^+$. Let m be a positive integer with $x_n \leq m$. Now the GCD matrix $(S)_f$ of the set S is a principal submatrix of the GCD matrix $(S_m)_f$ of the set $\{1, 2, \ldots, m\}$. Since every principal submatrix of a positive semidefinite matrix is positive semidefinite, see [9, Observation 7.1.2], we may deduce that the matrix $(S)_f$ is positive semidefinite.

Theorem 3 *A function $f \in \mathscr{A}$ is positive definite if and only if $(f * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$.*

Proof By Theorem 2, it suffices to show that the GCD matrix $(S_m)_f$ of the set $S_m = \{1, 2, \ldots, m\}$ is positive semidefinite for all $m \in \mathbb{Z}^+$ if and only if $(f * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$. Let $m \in \mathbb{Z}^+$. First we recall the well-known factorization

$$(S_m)_f = EDE^T,$$

where E is the $m \times m$ matrix with

$$e_{ij} = \begin{cases} 1 & \text{if } j \mid i, \\ 0 & \text{otherwise} \end{cases}$$

and $D = \mathrm{diag}((f*\mu)(1), (f*\mu)(2), \ldots, (f*\mu)(m))$. Since E is a triangular matrix with all of its diagonal elements equal to 1, by Sylvester's Law of Inertia (see [9, Theorem 4.5.8]) we may deduce that the matrix $(S_m)_f$ is positive semidefinite if and only if the matrix D is positive semidefinite. The claim follows from this.

Remark 2 Neither the argument used in the proof of Theorem 2 nor the idea of using LDL^T factorization in determining the inertias of GCD type matrices is entirely new—both of them appear in the article [14] from the year 2004 by J. S. Ovall. The LDL^T factorization itself originates from [15] and [4]. The factorization has also other applications, see, e.g., [11].

Theorem 4 *Let $f, g \in \mathscr{A}$ be positive definite functions. Then*

(a) af is a positive definite function for all $a \geq 0$,
(b) $f + g$ is a positive definite function,
(c) fg is a positive definite function,
(d) $f * g$ is a positive definite function.

Proof It is clear that $(S)_{af} = a(S)_f$ and $(S)_{f+g} = (S)_f + (S)_g$. Thus parts (a) and (b) follow from the fact that every nonnegative linear combination of positive semidefinite matrices is positive semidefinite. Since $(S)_{fg} = (S)_f \circ (S)_g$, the part (c) follows from the observation that the Hadamard product of two positive semidefinite matrices is positive semidefinite—see [9, Theorem 7.5.3]. We prove part (d) by showing that $((f * g) * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$. The associativity of the Dirichlet convolution yields

$$((f * g) * \mu)(k) = (f * (g * \mu))(k) = \sum_{d \mid k} \underbrace{f(d)}_{\geq 0} \underbrace{(g * \mu)\left(\frac{k}{d}\right)}_{\geq 0} \geq 0.$$

Remark 3 It is easy to see that in the proof of Theorem 4 (d) it suffices that one of the functions f and g is positive definite and the values of the other are nonnegative.

The following corollary is an immediate consequence of Theorem 4.

Corollary 2 *Suppose that $f \in \mathscr{A}$ is positive definite. Then the functions*

$$f^r = \underbrace{f \cdot f \cdots f}_{r\ times} \qquad and \qquad f^{*r} = \underbrace{f * f * \cdots * f}_{r\ times}$$

are positive definite for all $r = 1, 2, 3, \ldots$.

It is also interesting to consider how positive definiteness of arithmetical functions behaves with respect to different inverse operations.

Theorem 5 *Let $f \in \mathscr{A}$ be a positive definite function.*

(a) If $-f$ is also a positive definite function, then $f(m) = 0$ for all $m \in \mathbb{Z}^+$.
(b) If $f^{-1} = \frac{1}{f}$ exists and is also a positive definite function, then there exists $a \in \mathbb{R}$ such that $f(m) = a$ for all $m \in \mathbb{Z}^+$.
(c) If $f^{*(-1)}$ (the Dirichlet inverse of f) exists, then it cannot be positive definite.

Proof

(a) The first part follows directly from the simple fact that if both A and $-A$ are positive definite, then A must be equal to the zero matrix. And if the GCD matrix of any finite nonempty set $S \subset \mathbb{Z}^+$ with respect to the function f is the zero matrix, then f must be the constant function zero.
(b) If the function $\frac{1}{f}$ exists and is positive definite, then we must have $f(m) > 0$ for all $m \in \mathbb{Z}^+$. Let m be an arbitrary integer greater than 1 and let $S = \{1, m\}$. Since f and $\frac{1}{f}$ are positive definite, both of the GCD matrices

$$(S)_f = \begin{bmatrix} f(1) & f(1) \\ f(1) & f(m) \end{bmatrix} \quad \text{and} \quad (S)_{\frac{1}{f}} = \begin{bmatrix} \frac{1}{f(1)} & \frac{1}{f(1)} \\ \frac{1}{f(1)} & \frac{1}{f(m)} \end{bmatrix}$$

are positive semidefinite. The determinants of these matrices must be nonnegative, in other words,

$$f(1)(f(m) - f(1)) \geq 0 \quad \text{and} \quad \frac{1}{f(1)}\left(\frac{1}{f(m)} - \frac{1}{f(1)}\right) \geq 0.$$

Since $f(1) > 0$, the first inequality yields $f(m) \geq f(1)$ and the second implies that $f(1) \geq f(m)$. Thus we must have $f(m) = f(1)$ for any positive integer m.
(c) If $f^{*(-1)}$ exists and f is positive definite, then we have $f(1) > 0$ and $f^{*(-1)}(1) = \frac{1}{f(1)} > 0$. If $f(m) = 0$ for all $m > 1$, then there exists a positive real number a such that $f = a\delta$, where δ is the arithmetical function defined in Example 1. Like the function δ, the function f is not positive definite.

Assume next that $f(m) > 0$ for some $m > 1$. Let m_0 be the smallest positive integer such that $m_0 > 1$ and $f(m_0) > 0$. We obtain

$$0 = \delta(m_0) = (f * f^{*(-1)})(m_0) = \sum_{d \mid m_0} f(d) f^{*(-1)}\left(\frac{m_0}{d}\right)$$
$$= \underbrace{f(1)}_{>0} f^{*(-1)}(m_0) + \underbrace{f(m_0)}_{>0}\underbrace{f^{*(-1)}(1)}_{>0}.$$

This means that we must have $f^{*(-1)}(m_0) < 0$, and therefore $f^{*(-1)}$ cannot be positive definite.

5 A Partial Order on the Set of Arithmetical Functions

Notation 1 *Let f and g be arithmetical functions. If the function $g - f$ is positive definite, we shall write $f \preceq g$.*

Theorem 6 *$f \preceq g$ if and only if the matrix $(S)_g - (S)_f$ is positive semidefinite for all finite nonempty sets $S \subset \mathbb{Z}^+$ (in other words, $f \preceq g$ if and only if $(S)_f \leqslant (S)_g$ for all finite nonempty sets $S \subset \mathbb{Z}^+$, where $\leqslant$ is the Löwner order).*

Proof By definition, $g - f$ is positive definite if and only if the matrix $(S)_{g-f} = (S)_g - (S)_f$ is positive semidefinite for all sets $S = \{x_1, x_2, \ldots, x_n\} \subset \mathbb{Z}^+$ and for all $n = 1, 2, \ldots$. Furthermore, this is equivalent to the statement that the matrix $(S)_f$ precedes the matrix $(S)_g$ in the sense of the Löwner order.

Theorem 7 *The relation $\preceq$ is a partial order.*

Proof

- For any $f \in \mathscr{A}$ the matrix $(S)_f - (S)_f = \mathbf{0}$ is positive semidefinite for all finite nonempty sets $S \subset \mathbb{Z}^+$. Thus $\preceq$ is reflexive.
- Suppose that $f \preceq g$ and $g \preceq f$. Thus for any finite nonempty set $S \subset \mathbb{Z}^+$ both of the matrices $(S)_g - (S)_f$ and $(S)_f - (S)_g$ are positive semidefinite, which implies that $(S)_f = (S)_g$. Therefore $f(x_i) = g(x_i)$ for all $x_i \in S$ and we must have $f = g$ (since S is an arbitrary set). Thus $\preceq$ is symmetric.
- Suppose that $f \preceq g$ and $g \preceq h$. Let $S \subset \mathbb{Z}^+$. Now the matrices $(S)_g - (S)_f$ and $(S)_h - (S)_g$ are positive semidefinite and

$$(S)_h - (S)_f = ((S)_h - (S)_g) + ((S)_g - (S)_f).$$

Thus $(S)_h - (S)_f$ is positive semidefinite and we must have $f \preceq h$. Thus $\preceq$ is transitive.

The following results now follow directly from Theorems 1 and 3.

Corollary 3 *Suppose that* $f \preceq g$. *Then*

(a) $f(m) \le g(m)$ *for all* $m \in \mathbb{Z}^+$,
(b) $k \mid m \Rightarrow g(k) - f(k) \le g(m) - f(m)$ *for all* $k, m \in \mathbb{Z}^+$.

Corollary 4 *Function* $f \preceq g$ *if and only if*

$$((g - f) * \mu)(k) = (g * \mu)(k) - (f * \mu)(k) \ge 0$$

for all $k \in \mathbb{Z}$.

At this point it is natural to consider how our newly defined relation $\preceq$ relates to different function operations.

Theorem 8 *Suppose that* $0 \preceq f_1 \preceq g_1$ *and* $0 \preceq f_2 \preceq g_2$. *Then*

(a) $0 \preceq f_1 f_2 \preceq g_1 g_2$,
(b) $0 \preceq f_1 * f_2 \preceq g_1 * g_2$.

Proof

(a) We need to show that for any finite nonempty set $S \subset \mathbb{Z}^+$ the matrix

$$(S)_{f_1 f_2} - (S)_{g_1 g_2} = (S)_{f_1} \circ (S)_{f_2} - (S)_{g_1} \circ (S)_{g_2}$$

is positive semidefinite. Since $\mathbf{0} \preceq (S)_{f_1} \preceq (S)_{g_1}$ and $\mathbf{0} \preceq (S)_{f_2} \preceq (S)_{g_2}$, the claim follows from [9, p. 475, Problem 4].

(b) In the second case it is more convenient to use Corollary 4 and show that for all $k \in \mathbb{Z}^+$ we have

$$((f_1 * f_2) * \mu)(k) \le ((g_1 * g_2) * \mu)(k).$$

Let $k \in \mathbb{Z}^+$. By using the associativity of the Dirichlet convolution and Corollaries 3 and 4 we obtain

$$((f_1 * f_2) * \mu)(k) = (f_1 * (f_2 * \mu))(k) = \sum_{d \mid k} \underbrace{\overbrace{f_1(d)}^{\ge 0}}_{\le g_1(d)} \underbrace{\overbrace{(f_2 * \mu)\left(\frac{k}{d}\right)}^{\ge 0}}_{\le (g_2 * \mu)\left(\frac{k}{d}\right)}$$

$$\le \sum_{d \mid k} g_1(d)(g_2 * \mu)\left(\frac{k}{d}\right) = (g_1 * (g_2 * \mu))(k) = ((g_1 * g_2) * \mu)(k).$$

Thus we have shown that $f_1 * f_2 \preceq g_1 * g_2$. The property $0 \preceq f_1 * f_2$ follows from Theorem 4.

Corollary 5 *Suppose that* $0 \preceq f \preceq g$. *Then for all* $r = 1, 2, \ldots$ *we have*

(a) $0 \preceq f^r \preceq g^r$,
(b) $0 \preceq f^{*r} \preceq g^{*r}$.

Example 4 Recall that $\delta(1) = 1$ and $\delta(m) = 0$ for all $m > 1$ and that $\zeta(m) = 1$ for all $m \in \mathbb{Z}^+$. Since $\zeta(2) = 1 > 0 = \delta(2)$, clearly $\zeta \not\preceq \delta$. Let us show that also $\delta \not\preceq \zeta$. Consider the set $S = \{2, 3, 6\}$. We obtain

$$(S)_{\zeta-\delta} = (S)_\zeta - (S)_\delta = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

The eigenvalues of this matrix are 1, $1 + \sqrt{2}$, and $1 - \sqrt{2} < 0$. Therefore the matrix $(S)_{\zeta-\delta}$ is not positive semidefinite and thus we cannot have $\delta \preceq \zeta$. It is also possible to consider the set $S = \{1, 2, 3, 4, 5, 6\}$. In this case

$$(S)_{\zeta-\delta} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \end{bmatrix}.$$

The smallest eigenvalue of this matrix is approximately -0.4812, and therefore the matrix is not positive semidefinite and we may deduce that $\delta \not\preceq \zeta$.

Definition 2 Arithmetical function f is said to be multiplicative if

$$f(km) = f(k)f(m)$$

for all $k, m \in \mathbb{Z}^+$ with $\gcd(k, m) = 1$.

The values of a multiplicative function are completely determined by the values on prime powers. In fact, if $m = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}$, then

$$f(m) = f(p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}) = f(p_1^{a_1}) f(p_2^{a_2}) \cdots f(p_r^{a_r}).$$

The Möbius function μ is multiplicative, and the Dirichlet convolution of multiplicative functions is also multiplicative, see, e.g., [2, Section 2.10] and [12, Chapter 1]. Thus if $f \in \mathscr{A}$ is multiplicative and we wish to show that f is positive definite, i.e. that $(f * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$, then it suffices to show that $(f * \mu)(p^a) \geq 0$ for any prime number p and for all $a \in \mathbb{Z}^+$.

Example 5 The Jordan totient function J_α is defined as

$$J_\alpha(m) = m^\alpha \prod_{p\,|\,m} \left(1 - \frac{1}{p^\alpha}\right),$$

where $m = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}$. If $\alpha \geq 1$, then for any $a \geq 2$ we have

$$\begin{aligned}(J_\alpha * \mu)(p^a) &= \sum_{d\,|\,p^a} J_\alpha(d)\mu\left(\frac{p^a}{d}\right) = J_\alpha(p^a) - J_\alpha(p^{a-1}) \\ &= p^{\alpha a} - p^{\alpha(a-1)} - p^{\alpha(a-1)} + p^{\alpha(a-2)} = p^{\alpha(a-2)}(p^{2\alpha} - 2p^\alpha + 1) \\ &= p^{\alpha(a-2)}(p^\alpha - 1)^2 \geq 0\end{aligned}$$

and for $a = 1$ we obtain

$$(J_\alpha * \mu)(p) = J_\alpha(p) - 1 = p^\alpha - 1 - 1 = p^\alpha - 2 \geq 0.$$

By multiplicativity this shows that J_α is positive definite for $\alpha \geq 1$. In particular, the Euler totient function $\phi = J_1$ is positive definite. Since $(J_\alpha * \mu)(2) = 2^\alpha - 2 < 0$ for $\alpha < 1$, we see that J_α is not positive definite for $\alpha < 1$.

By utilizing multiplicativity in a similar manner it is possible to show that for $\alpha, \beta \geq 0$,

$$J_\alpha \preceq J_\beta \Leftrightarrow (J_\alpha * \mu)(k) \leq (J_\beta * \mu)(k)\ \forall k \in \mathbb{Z}^+ \Leftrightarrow \alpha \leq \beta.$$

Example 6 In Example 3 it was shown that the power function N^α is positive definite for all $\alpha \geq 0$. With the aid of multiplicativity (as in Example 5) it is possible to show that for $\alpha, \beta \geq 0$,

$$N^\alpha \preceq N^\beta \Leftrightarrow \alpha \leq \beta.$$

Example 7 The divisor function σ_α is defined as $\sigma_\alpha(m) := \sum_{d\,|\,m} d^\alpha$, or alternatively $\sigma_\alpha = N^\alpha * \zeta$. The function σ_α is positive definite for all $\alpha \in \mathbb{R}$, and for any $\alpha, \beta \in \mathbb{R}$ we have

$$\sigma_\alpha \preceq \sigma_\beta \Leftrightarrow \alpha \leq \beta.$$

The positive definiteness of the function σ_α can easily be shown by using Theorem 3, since

$$\sigma_\alpha * \mu = (N^\alpha * \zeta) * \mu = N^\alpha * (\zeta * \mu) = N^\alpha$$

and $N^\alpha(k) \geq 0$ for all $\alpha \in \mathbb{R}$ and $k \in \mathbb{Z}^+$. The other claim follows similarly, since

$$(\sigma_\beta - \sigma_\alpha) * \mu = (\sigma_\beta * \mu) - (\sigma_\alpha * \mu) = N^\beta - N^\alpha$$

and the values of this function are nonnegative if and only if $\alpha \leq \beta$.

Example 8 Let $\Omega(m)$ denote the total number of prime divisors of m each counted according to its multiplicity (note that $\Omega(1) = 0$). We prove the positive definiteness of the function Ω by showing that $(\Omega * \mu)(k) \geq 0$ for all $k \in \mathbb{Z}^+$.

If $k = 1$, then $(\Omega * \mu)(k) = 0$. Let $k = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r} \neq 1$ $(r \geq 1)$ be the canonical factorization of k. Then

$$\begin{aligned}(\Omega * \mu)(k) = (\mu * \Omega)(k) &= \sum_{d \mid k} \mu(d) \Omega\left(\frac{k}{d}\right) \\ &= (a_1 + a_2 + \cdots + a_r) \\ &\quad - ((a_1 - 1) + a_2 + \cdots + a_r) - (a_1 + (a_2 - 1) + \cdots + a_r) - \cdots \\ &\qquad - (a_1 + a_2 + \cdots + (a_r - 1)) \\ &\quad + ((a_1 - 1) + (a_2 - 1) + a_3 + \cdots + a_r) + \cdots \\ &\qquad + (a_1 + \cdots + a_{r-2} + (a_{r-1} - 1) + (a_r - 1)) \\ &\quad - \cdots\end{aligned}$$

Denote $s = a_1 + a_2 + \cdots + a_r$. Then

$$\begin{aligned}(\Omega * \mu)(k) &= s - \binom{r}{1}(s-1) + \binom{r}{2}(s-2) + \cdots + (-1)^r \binom{r}{r}(s-r) \\ &= \sum_{i=0}^{r} (-1)^i \binom{r}{i}(s-i) = s \sum_{i=0}^{r} (-1)^i \binom{r}{i} - \sum_{i=0}^{r} (-1)^i \binom{r}{i} i.\end{aligned}$$

By the binomial theorem, $\sum_{i=0}^{r} (-1)^i \binom{r}{i} = 0$ $(r \geq 1)$ and by formula (1.69) of [7],

$$\sum_{i=0}^{r} (-1)^i \binom{r}{i} i = \begin{cases} -1 & \text{if } r = 1, \\ 0 & \text{if } r \geq 2 \end{cases}$$

(this can also be shown by utilizing formula (5.6) of [6]). Thus $(\Omega * \mu)(k) = 1$ if $r = 1$ (i.e., k is a prime power ($\neq 1$)), and $(\Omega * \mu)(k) = 0$ otherwise.

Example 9 Also for the generalized Liouville function $\lambda_\alpha(m) = \alpha^{\Omega(m)}$ it is possible to show that λ_α is positive definite if and only if $\alpha \geq 1$ and that for $\alpha, \beta \geq 1$,

$$\alpha \leq \beta \Leftrightarrow \lambda_\alpha \preceq \lambda_\beta.$$

In particular, the usual Liouville function $\lambda = \lambda_{-1}$ is not positive definite. These results can be proved by utilizing multiplicativity. Since the function Ω is positive definite by the previous example, the positive definiteness of λ_α for $\alpha \geq 1$ can also be deduced from the results of [10, Section 6.3]. The Liouville function λ gives the parity of the number of prime factors and is related, e.g., to the Riemann hypothesis.

Example 10 For the generalized Dedekind function $\Psi_\alpha = N^\alpha * \mu^2$, where $\mu^2 = \mu \cdot \mu = |\mu|$, it can be shown that Ψ_α is positive definite if and only if $\alpha \geq 0$ and that for $\alpha, \beta \geq 0$,

$$\alpha \leq \beta \Leftrightarrow \Psi_\alpha \preceq \Psi_\beta.$$

In particular, the usual Dedekind function $\Psi = \Psi_1$ is positive definite. Also these results can be shown by using multiplicativity. The function Ψ was introduced by Richard Dedekind in connection with modular functions. It has also connections to the Riemann hypothesis.

Example 11 For $\alpha \geq 0$, we have

$$J_\alpha \preceq N^\alpha \preceq \Psi_\alpha \preceq \sigma_\alpha.$$

For $\alpha \geq 1$, we obtain

$$\lambda_\alpha \preceq J_\alpha \preceq N^\alpha \preceq \Psi_\alpha \preceq \sigma_\alpha.$$

These can be verified by applying the multiplicativity of the functions $\lambda_\alpha * \mu$, $J_\alpha * \mu$, $N^\alpha * \mu = J_\alpha$, $\Psi_\alpha * \mu$ and $\sigma_\alpha * \mu$. In particular (for $\alpha = 1$),

$$\phi(= J_1) \preceq N(= N^1) \preceq \Psi(= \Psi_1) \preceq \sigma(= \sigma_1).$$

6 Conclusions

As we saw in Sect. 2, defining positive definiteness of arithmetical functions by using GCD matrices appears to be the best way to proceed. Positive definite arithmetical functions seem to possess several properties that one could expect them to have. For example, addition, usual multiplication, and Dirichlet convolution all preserve positive definiteness. On the other hand, in some cases positive definiteness of arithmetical functions behaves quite unexpectedly (for example, the function δ is not positive definite, although it is the identity element with respect to the Dirichlet convolution). Positive definiteness also makes it possible to define a partial order on the set of arithmetical functions, and by making use of multiplicativity we are able to compare various fundamental arithmetical functions with each other.

The study of positive definiteness of arithmetical functions offers many possibilities for further research. One could analyze thoroughly the properties of positive definite arithmetical functions, and there might still be a possibility to utilize some other matrix class and find an alternative definition for positive definite arithmetical functions. Yet another possibility would be to generalize the concept of positive definiteness on real-valued functions defined on any meet semilattice P. In this case one only needs to consider the so-called meet matrix of the set S with respect to the function f (instead of GCD matrix).

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