

*Dedicated to Marius Iosifescu
on the occasion of his 80th anniversary*

Positive-semidefinite matrices and the Jordan totient function

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ABSTRACT. The aim of the paper is to prove that several classes of matrices, some of them built with the help of the Jordan totient function, are positive semidefinite.

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1. Introduction

Positive-definite matrices are the matrix analogues to positive numbers.

A real square matrix \mathbf{A} of dimension n is called positive-semidefinite (or sometimes nonnegative-definite) if $\mathbf{x}^T \mathbf{A} \mathbf{x} \geq \mathbf{0}$ for every $\mathbf{x} \in \mathbb{R}^n$.

A real square matrix \mathbf{A} of dimension n is called positive-definite if $\mathbf{x}^T \mathbf{A} \mathbf{x} > \mathbf{0}$ for every $\mathbf{x} \in \mathbb{R}^n - \{0\}$.

A real square matrix \mathbf{A} of dimension n is positive-definite if and only if it arises as the Gram matrix of some set of n linearly independent vectors.

A real square matrix \mathbf{A} of dimension n is positive-semidefinite if and only if it arises as the Gram matrix of some set of n vectors. In contrast to the positive-definite case, these vectors need not be linearly independent.

There are many books and research papers that study positive-definite and positive-semidefinite matrices. We recommend the readers Bhatia's book [6] and the paper Bhatia [5].

Positive definite matrices are of both theoretical and computational importance in a wide variety of applications. They are used, for example, in optimization algorithms and in the construction of various linear regression models, machine learning, statistics, and optimization.

Historically, positive definite matrices arise quite naturally in the study of n -ary quadratic forms. They are employed in certain optimization algorithms in mathematical programming, in testing the strict convexity of scalar vector functions (here positive definiteness of the Hessian matrix provides a sufficient condition for strict convexity).

In statistics, the covariance matrix of a multivariate probability distribution is always positive semi-definite. It is positive definite unless one variable is an exact linear combination of the others. Conversely, every positive semi-definite matrix is the covariance matrix of some multivariate distribution.

In the study of document similarity positive semidefinite matrices arise in the text document classification. Let a_{ij} be a measure of similarity between the i -th and j -th document and x_i, x_j be their respective bag-of-words representation (normalized to have Euclidean norm). Then the Gram matrix $G = (\langle x_i, x_j \rangle) = (a_{ij})$ is positive semidefinite.

Similarity based classification methods use positive semidefinite (PSD) similarity matrices. When several data representations (or metrics) are available, they should be combined to build a single similarity matrix. Often the resulting combination is an indefinite matrix and it cannot be used to train the classifier. In Munoz and de Diego [10] new methods to build a positive semidefinite matrix from an indefinite matrix were built. The obtained matrices were used as input kernels to train Support Vector Machines (SVMs) for classification tasks. Experimental results on artificial and real data sets were reported.

Classification methods generally rely on the use of a (symmetric) similarity matrix. In many situations it is convenient to consider more than one similarity measure. For instance, in Web Mining problems we have an asymmetric link matrix among Web pages, $A = (a_{ij})$. a_{ij} is 1 when there is a link between page i and page j and it is 0 when there is not a link. Two different matrices are defined starting from A : the co-citations ($A^T A$) and co-references (AA^T) matrices. Another matrix $D = (d_{ij})$ is defined from the terms by documents (or web pages). $d_{ij} = 1$ if term i appears in web page j and it is 0 when it does not appear. The ‘document by document’ matrix is defined by $D^T D$. The co-citations, co-references and ‘document by document’ matrices correspond to different similarity representations focusing on different data aspects.

For two matrices, $A = (a_{ij})$ and $B = (b_{ij})$ of the same dimension, the Hadamard product $A \circ B = (c_{ij})$, is a matrix, of the same dimension as the operands, with elements given by $c_{ij} = a_{ij} \cdot b_{ij}$. For matrices of different dimensions ($m \times n$ and $p \times q$, where $m \neq p$ or $n \neq q$ or both) the Hadamard product is undefined.

The Hadamard product is commutative, associative and distributive over addition. That is,

$$\begin{aligned} A \circ B &= B \circ A \\ A \circ (B \circ C) &= (A \circ B) \circ C \\ A \circ (B + C) &= A \circ B + A \circ C \end{aligned}$$

The Hadamard product of two positive semidefinite matrices is positive semidefinite. This is known as the Schur product theorem, after the German mathematician Issai Schur. See Schur [11]. For positive-semidefinite matrices A and B , it is also known that

$$\det(A \circ B) \geq \det(A) \det(B)$$

One of the consequences of the Schur Product Theorem is the fact that all the positive integer Hadamard powers $A^{(k)} = (a_{ij}^{(k)})$, $k = 1, 2, \dots$ of a positive semidefinite matrix A must be positive definite. It is natural to ask whether the same is true for the noninteger Hadamard powers $A^{(\alpha)} = (a_{ij}^{(\alpha)})$, $\alpha > 0$. The answer is in the affirmative only for $n = 1$ and $n = 2$. It is known Horn [9, p. 270] that if $f : (0, \infty) \rightarrow \mathbb{R}$ is a smooth function such that the matrix $(f(a_{ij}))$ is positive definite whenever $A = (a_{ij})$ is a positive definite $n \times n$ matrix with positive entries, then $f, f', f'', \dots, f^{(n-1)}$ are all

nonnegative on $(0, \infty)$. Applying this criterion to $f(x) = x^\alpha$ shows that α must be a nonnegative integer or α must be a real number greater or equal than $n-2$. Fitzgerald and R. Horn proved in [8] that the latter necessary condition is also sufficient. More precisely they proved that if $\alpha < n-2$ then one can construct a positive semidefinite matrix $A = (a_{ij})$ such that the matrix $A^{(\alpha)} = (a_{ij}^{(\alpha)})$ is not positive semidefinite.

The fact that the Schur (that is, element wise) product of two positive semidefinite matrices is positive semidefinite immediately implies (using the convexity of the positive semidefinite cone) that if $A = (a_{ij})$ is positive semidefinite, then so is $B = (b_{ij})$ where $b_{ij} = f(a_{ij})$, where f is an analytic function all of whose coefficients are positive. As a consequence if $A = (a_{ij})$ is positive semidefinite, then the matrix $B = (\exp(a_{ij}))$ is also positive semidefinite. A converse result that clarifies the connection between positive definite matrices and absolutely monotonic functions can be found in Vasudeva [14].

An arithmetic function generalizing the well-known Euler totient function ϕ is the Jordan's function of order k , where k is a positive integer. This function is denoted by J_k and it is defined by $J_k(n)$ = the number of all vectors $(a_1, a_2, \dots, a_k) \in \mathbb{N}^k$ with the properties $a_i \leq n$, $i = 1, 2, \dots, k$ and $\gcd(a_1, a_2, \dots, a_k, n) = 1$.

It is clear that $J_1 = \phi$. Jordan's totient function is multiplicative and may be evaluated as follows:

If the unique prime decomposition of the natural number n is $n = p_1^{\alpha_1} p_2^{\alpha_2} \dots p_m^{\alpha_m}$ then

$$J_k(n) = n^k \left(1 - \frac{1}{p_1^k}\right) \left(1 - \frac{1}{p_2^k}\right) \dots \left(1 - \frac{1}{p_m^k}\right)$$

An easy argument for this formula is the inclusion-exclusion principle. (Gauss' type formula) The following Gauss' type formula holds

$$\sum_{d/n} J_k(d) = n^k$$

The early history of the function J_k is presented in Dickson [7]. Properties of the Jordan's totient function can be found in Sándor et al. [12] and Andrica and Piticari [1]. Let a_1, a_2, \dots, a_n be natural numbers greater or equal than 1 and consider the GCD matrix $A = (f(a_{ij}))$ where $a_{ij} = \gcd(a_i, a_j)$. In the case $a_i = i$ for every $i \in \{1, 2, \dots, n\}$ and $f(x) = x$ for all x then the matrix A is positive semidefinite. Smith in [13] proved that

$$\det A = \phi(1) \phi(2) \dots \phi(n)$$

Interesting results about GCD matrices can be found in Beslin and Ligh [3], Beslin [4], and Bege [2].

In the second section of the paper we shall prove that several classes of matrices, some of them built with the help of the Jordan totient function, are positive semidefinite.

2. Main results

Theorem 2.1. *Let (X, Σ, μ) be a space with measure and A_1, A_2, \dots, A_n be sets from Σ of finite measure. For every $i, j \in \{1, 2, \dots, n\}$ define*

$$a_{ij} = \mu(A_i \cap A_j), \quad b_{ij} = \exp(-\mu(A_i \cup A_j)), \quad c_{ij} = \exp(-\mu(A_i \Delta A_j)).$$

Then the matrices $A = (a_{ij}), B = (b_{ij})$ and $C = (c_{ij})$ are positive semidefinite. Here we used the notation $A\Delta B = (A \cup B) - (A \cap B)$.

Proof. For every $A \subset X$ we consider the characteristic function of A

$$\chi_A(x) = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \in X - A \end{cases}$$

Then $a_{ij} = \int_X \chi_{A_i}(x)\chi_{A_j}(x)d\mu(x) = \mu(A_i \cap A_j)$.

Note that A is a Gram matrix associated to the system of $L^2(\mu)$ functions $\chi_{A_i}, i \in \{1, 2, \dots, n\}$. Hence A is positive semidefinite.

Note that

$$\begin{aligned} b_{ij} &= \exp(-\mu(A_i \cup A_j)) = \\ &= \exp(\mu(A_i \cap A_j))\exp(-\mu(A_i))\exp(-\mu(A_j)) = \\ &= \exp(a_{ij})\exp(-\mu(A_i))\exp(-\mu(A_j)). \end{aligned}$$

Let $b_{ij}^{(1)} = \exp(a_{ij}), b_{ij}^{(2)} = \exp(-\mu(A_i))\exp(-\mu(A_j)), B_1 = (b_{ij}^{(1)}), B_2 = (b_{ij}^{(2)})$.

Note that B_1 and B_2 are positive semidefinite and $B = B_1 \circ B_2$. Hence B is positive semidefinite.

Since $\mu(A_i \Delta A_j) = \mu(A_i) + \mu(A_j) - 2\mu(A_i \cap A_j)$ it follows that

$$\begin{aligned} c_{ij} &= \exp(2\mu(A_i \cap A_j))\exp(-\mu(A_i))\exp(-\mu(A_j)) \\ &= \exp(2a_{ij})\exp(-\mu(A_i))\exp(-\mu(A_j)). \end{aligned}$$

Let $c_{ij}^{(1)} = \exp(2a_{ij}), C_1 = (c_{ij}^{(1)})$. Note that $C = C_1 \circ B_2$ hence C is positive semidefinite. □

Corollary 2.2. Let $a_1, a_2, \dots, a_n, b_1, b_2, \dots, b_n \in \mathbb{R}, a_i \leq b_i, i = 1, 2, \dots, n$. For every $i, j \in \{1, 2, \dots, n\}$ let

$$a_{ij} = (\min(b_i, b_j) - \max(a_i, a_j))_+, b_{ij} = \min(b_i, b_j)$$

Then the following assertions hold:

- (1) If $b_i \geq 0, i = 1, 2, \dots, n$ then the matrix $B = (b_{ij})$ is positive semidefinite.
- (2) The matrix $A = (a_{ij})$ is positive semidefinite.

Proof. Let μ be the Lebesgue measure in \mathbb{R} .

Note that $\mu([a_i, b_i] \cap [a_j, b_j]) = (\min(b_i, b_j) - \max(a_i, a_j))_+$. By the preceding theorem it follows that A is positive semidefinite.

If $b_i \geq 0$, and $a_i = 0$ for every $i \in \{1, 2, \dots, n\}$ then $B = A$. Hence B is positive semidefinite. □

Corollary 2.3. Let $x_1, x_2, \dots, x_m \in [1, \infty)$ and $A_1, A_2, \dots, A_n \subseteq \{1, 2, \dots, m\}, a_{ij} = \prod_{k \in A_i \cap A_j} x_k, i, j \in \{1, 2, \dots, n\}$. Then the matrix $A = (a_{ij})$ is positive semidefinite.

Proof. Let $\mu : \mathcal{P}(\{1, 2, \dots, m\}) \rightarrow \mathbb{R}, \mu(M) = \sum_{k \in M} \ln x_k, M \in \mathcal{P}(\{1, 2, \dots, m\})$. Then μ is a positive measure on $\{1, 2, \dots, m\}$. □

Note that $a_{ij} = \exp(\mu(A_i \cap A_j))$ hence the matrix A is positive semidefinite.

Corollary 2.4. Let $x_1, x_2, \dots, x_m \in (0, 1)$ and $A_1, A_2, \dots, A_n \subseteq \{1, 2, \dots, m\}$

$$a_{ij} = \prod_{k \in A_i \cup A_j} x_k, \quad i, j \in \{1, 2, \dots, n\}, \quad b_{ij} = \prod_{k \in A_i \Delta A_j} x_k.$$

Then $A = (a_{ij}), B = (b_{ij})$ are positive semidefinite matrices.

Proof. Let $\mu : \mathcal{P}(\{1, 2, \dots, m\}) \rightarrow \mathbb{R}$, $\mu(M) = - \sum_{k \in M} \ln x_k$, μ is a positive finite measure on $\{1, 2, \dots, m\}$.

Note that $a_{ij} = \exp(-\mu(A_i \cup A_j))$, $b_{ij} = \exp(-\mu(A_i \Delta A_j))$. □

Theorem 2.5. Let a_1, a_2, \dots, a_n , $r \in \mathbb{N}^*$, $a_{ij} = J_r(a_i a_j)$.

Then $A = (a_{ij})$ is positive semidefinite.

Proof. If $a \in \mathbb{N}^*$ denote $M(a) = \{i \in \mathbb{N}^* : p_i | a\}$, $a = \prod_{k \in M(a)} p_k^{\alpha_k(a)}$

$$a_{ij} = J_r(a_i a_j) = a_i^r a_j^r \prod_{k \in M(a_i) \cup M(a_j)} \left(1 - \frac{1}{p_k^r}\right)$$

$$b_{ij} = a_i^r a_j^r, \quad c_{ij} = \prod_{k \in M(a_i) \cup M(a_j)} \left(1 - \frac{1}{p_k^r}\right), \quad B = (b_{ij}), \quad C = (c_{ij}).$$

Note that the matrix C is positive semidefinite of Corollary 2.4. □

Since $A = B \circ C$ and the matrices B and C are positive semidefinite it follows that A is also positive semidefinite.

Theorem 2.6. Let a_1, a_2, \dots, a_n , $r \in \mathbb{N}^*$, $a_{ij} = J_r(\gcd(a_i, a_j))$. Then $A = (a_{ij})$ is positive semidefinite.

Proof. With notation

$$u(a) = \prod_{k \in M(a)} p_k$$

we have

$$\begin{aligned} \gcd(a_i, a_j) &= \prod_{k \in M(a_i) \cap M(a_j)} p_k^{\alpha_k(a_i) \wedge \alpha_k(a_j)} \\ J_r(\gcd(a_i, a_j)) &= J_r \left(\prod_{k \in M(a_i) \cap M(a_j)} p_k^{\alpha_k(a_i) \wedge \alpha_k(a_j)} \right) \\ &= [\gcd(a_i, a_j)]^r \prod_{k \in M(a_i) \cap M(a_j)} \left(1 - \frac{1}{p_k^r}\right) \\ &= [\gcd(a_i, a_j)]^r \cdot \frac{1}{u(\gcd(a_i, a_j))^r} \prod_{k \in M(a_i) \cap M(a_j)} (p_k^r - 1) \\ &= \left[\gcd \left(\frac{a_i}{u(a_i)}, \frac{a_j}{u(a_j)} \right) \right]^r \cdot \prod_{k \in M(a_i) \cap M(a_j)} (p_k^r - 1). \end{aligned}$$

□

Theorem 2.7. Let a_1, a_2, \dots, a_n , $r \in \mathbb{N}^*$, $a_{ij} = [\gcd(a_i, a_j)]^{2r} \cdot J_r \left(\frac{a_i a_j}{[\gcd(a_i, a_j)]^2} \right)$. Then $A = (a_{ij})$ is positive semidefinite.

Proof. Note that

$$\begin{aligned} a_{ij} &= [\gcd(a_i, a_j)]^{2r} \cdot J_r \left(\frac{a_i a_j}{[\gcd(a_i, a_j)]^2} \right) \\ &= [\gcd(a_i, a_j)]^{2r} \frac{a_i^r a_j^r}{[\gcd(a_i, a_j)]^{2r}} \prod_{k \in M(a_i) \Delta M(a_j)} \left(1 - \frac{1}{p_k^r} \right) \\ &= a_i^r a_j^r \prod_{k \in M(a_i) \Delta M(a_j)} \left(1 - \frac{1}{p_k^r} \right). \end{aligned}$$

□

Theorem 2.8. *Let a_1, a_2, \dots, a_n , $r, s, t \in \mathbb{N}^*$, $a_{ij} = J_r(a_i^s a_j^s [\gcd(a_i, a_j)]^t)$. Then $A = (a_{ij})$ is positive semidefinite.*

Proof.

$$a_{ij} = J_r(a_i^s a_j^s [\gcd(a_i, a_j)]^t) = a_i^{rs} a_j^{rs} [\gcd(a_i, a_j)]^{rt} \cdot \prod_{k \in M(a_i) \cup M(a_j)} \left(1 - \frac{1}{p_k^r} \right).$$

□

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