Infinitely Divisible Matrices

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1 INTRODUCTION.

Let A, B, C, and D be $n \times n$ symmetric matrices whose entries are, respectively,

$$\begin{aligned} a_{ij} &= \frac{1}{i+j}, \\ b_{ij} &= \binom{i+j}{i}, \\ c_{ij} &= \min(i,j), \\ d_{ij} &= \gcd(i,j). \end{aligned}$$

Assembling natural numbers in such nice patterns often has interesting consequences, and so it is in this case. Each of the aforementioned matrices is endowed with positive definiteness of a very high order: for every positive real number r the matrices with entries a_{ij}^r, b_{ij}^r, c_{ij}^r, and d_{ij}^r are positive semidefinite. This special property is called *infinite divisibility* and is the subject of this paper.

Positive semidefinite matrices arise in diverse contexts: calculus (Hessians at minima of functions), statistics (correlation matrices), vibrating systems (stiffness matrices), quantum mechanics (density matrices), harmonic analysis (positive definite functions), to name just a few. Many of the test matrices used by numerical analysts are positive definite. One of the interests of this paper might be the variety of examples that are provided in it. The general theorems and methods presented in the context of these examples are, in fact, powerful techniques that could be used elsewhere.

In this introductory section we begin with the basic definitions and notions related to positive semidefinite matrices.

Positive semidefinite matrices. Let $A = [a_{ij}]$ be an $n \times n$ matrix with complex entries. The matrix A is Hermitian if $A = A^*$, where A^* is the conjugate transpose of A (i.e., if $a_{ij} = \overline{a}_{ji}$, a condition that is readily verified by inspection). A Hermitian matrix is *positive semidefinite* if it satisfies any of the following equivalent conditions

(i) for each vector x in $\mathbb{C}^n$, the inner product $\langle x, Ax\rangle$ is nonnegative;

(ii) all principal minors of A are nonnegative;

(iii) all eigenvalues of A are nonnegative;

(iv) $A = BB^*$ for some matrix B;

(v) $A = LL^*$ for some lower triangular matrix L;

(vi) there exist vectors $u_1, \dots, u_n$ in some inner product space such that $a_{ij} = \langle u_i, u_j\rangle$. (The matrix A is then said to be the *Gram matrix* associated with the vectors $\{u_1, \dots, u_n\}$.)

It is not easy to verify any of the conditions (i)–(vi) and a little ingenuity is often needed in proving that a certain matrix is positive semidefinite.

The Hadamard product. Let $A = [a_{ij}]$ and $B = [b_{ij}]$ be $n \times n$ matrices. The *Hadamard product* (or the *entrywise product*) of A and B is the matrix $A \circ B = [a_{ij} b_{ij}]$. The most interesting theorem about Hadamard products was proved by Issai Schur [27]. It says that if A and B are positive semidefinite, then so is $A \circ B$. This theorem is so striking that the product $A \circ B$ is often called the *Schur product.* Note that the usual matrix product AB (of positive semidefinite matrices A and B) is positive semidefinite if and only if $AB = BA$.

For each nonnegative integer m let $A^{\circ m} = \left[a_{ij}^m\right]$ be the mth Hadamard power of A, and A^m its usual mth power. If A is positive semidefinite, then both $A^{\circ m}$ and A^m enjoy that property.

Infinitely divisible matrices. Fractional powers of positive semidefinite matrices are defined via the spectral theorem. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of a positive semidefinite matrix A, and let $v_1, \ldots, v_n$ be a corresponding set of (orthonormal) eigenvectors. Then $A = \sum \lambda_i v_i v_i^*$, and for each r in $[0, \infty)$ the (usual) rth power of A is the positive semidefinite matrix $A = \sum \lambda_i^r v_i v_i^*$. If the entries a_{ij} are nonnegative real numbers, it is natural to define *fractional Hadamard powers* of A. In this case for nonnegative r we write $A^{\circ r} = \left[a_{ij}^r\right]$.

Suppose that A is positive semidefinite and that $a_{ij} \geq 0$ for all i and j. We say that A is *infinitely divisible* if the matrix $A^{\circ r}$ is positive semidefinite for every nonnegative r. A 2×2 Hermitian matrix is positive semidefinite if and only if its diagonal entries and determinant are nonnegative. Using this fact it is easy to see that every 2×2 positive semidefinite matrix with nonnegative entries is infinitely divisible. This is no longer the case when

$n > 2$. The 3×3 matrix

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

is positive semidefinite, whereas $A^{\circ r}$ is positive semidefinite if and only if $r \geq 1$.

Carl FitzGerald and Roger Horn [11] have shown that, if A is an $n \times n$ positive semidefinite matrix with $a_{ij} \geq 0$ for all i and j, then the matrix $A^{\circ r}$ is positive semidefinite for each real numbers $r \geq n-2$. The *critical exponent* $n-2$ is best possible here: if $r < n-2$ one can construct a positive semidefinite matrix A for which $A^{\circ r}$ is not positive semidefinite.

If $A^{\circ r}$ is positive semidefinite for $r = 1/m$ $(m = 1, 2, \ldots)$, then by Schur's theorem $A^{\circ r}$ is positive semidefinite for all positive rational numbers r. Taking limits, we see that $A^{\circ r}$ is positive semidefinite for all nonnegative real numbers. Thus a positive semidefinite matrix with nonnegative entries is infinitely divisible if and only if for each positive integer m there exists a positive semidefinite matrix B such that $A = B^{\circ m}$. The term infinitely divisible stems from this property.

Some simple facts. Most of our proofs invoke the following facts.

(a) If $A_1, \ldots, A_k$ are positive semidefinite, then so is any linear combination $a_1 A_1 + \cdots + a_k A_k$ with nonnegative coefficients a_j.

(b) If a sequence $\{A_k\}$ of positive semidefinite matrices converges entrywise to A, then A is positive semidefinite.

(c) The $n \times n$ matrix E with $e_{ij} = 1$ for all i and j is called the $n \times n$ *flat matrix.* It is a rank-one positive semidefinite matrix.

(d) If A is positive semidefinite, then the matrix X^*AX is positive semidefinite for every matrix X of the same size as A. In particular, choosing X to be a diagonal matrix with positive diagonal entries λ_i, we see that if A is positive semidefinite (respectively, infinitely divisible), then the matrix $XAX = [\lambda_i \lambda_j a_{ij}]$ is also positive semidefinite (respectively, infinitely divisible). The matrices A and X^*AX are said to be *congruent* to each other if X is invertible.

We will make frequent use of the Schur theorem stated earlier, a result that is easy to prove. One of the several known proofs goes as follows. Every rank-one positive semidefinite matrix A has the form $A = xx^*$ for some vector x; or in other words, $a_{ij} = x_i \overline{x}_j$ for some $x = (x_1, \ldots, x_n)$ in $\mathbb{C}^n$. If $A = xx^*$ and $B = yy^*$ are two such matrices, then $A \circ B = zz^*$, where

$z = (x_1 y_1, \ldots, x_n y_n)$. Thus the Hadamard product of two rank-one positive semidefinite matrices is positive semidefinite. The general case follows from this because every positive semidefinite matrix is a sum of rank-one positive semidefinite matrices.

The point to note is that it is straightforward to show that $A^{\circ m}$ is positive semidefinite if A is positive semidefinite. It is not so easy to decide whether $A^{\circ r}$ is positive semidefinite for every nonnegative real number r.

Chapter 7 of [20] is a rich source of information on positive semidefinite matrices. A very interesting and lively discussion of the nomenclature, the history, and the most important properties of the Hadamard product can be found in the survey article [19] by Roger Horn. Two of the early papers on infinitely divisible matrices, also by Horn, are [17] and [18].

2 EXAMPLES.

The Cauchy matrix. Assume that $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. The matrix C with entries $c_{ij} = 1/(\lambda_i + \lambda_j)$ is called the *Cauchy matrix* associated with $\lambda_1, \lambda_2, \ldots, \lambda_n$. The *Hilbert matrix* H that has $h_{ij} = 1/(i+j-1)$ is an example of a Cauchy matrix.

In 1841 Cauchy gave a formula for the determinant of a matrix C of the type under discussion:

$$\det C = \frac{\Pi_{1\le i<j\le n}\,(\lambda_i-\lambda_j)^2}{\Pi_{1\le i,j\le n}\,(\lambda_i+\lambda_j)}.$$

Since each principal submatrix of a Cauchy matrix is another Cauchy matrix, this formula shows that all principal minors of C are nonnegative, hence that C is positive semidefinite. This latter fact can be proved more easily by showing that C is a Gram matrix.

Consider the Hilbert space $L_2(0,\infty)$. Its elements are the functions on $(0,\infty)$ that are square-integrable with respect to the Lebesgue measure, and the inner product between two elements u_1 and u_2 of this space is defined by

$$\langle u_1, u_2\rangle = \int_0^\infty u_1(t)\overline{u_2(t)}dt.$$

Let $u_i(t) = e^{-t\lambda_i}$ $(1\le i\le n)$. The identity

$$\frac{1}{\lambda_i+\lambda_j} = \int_0^\infty e^{-t(\lambda_i+\lambda_j)}dt = \langle u_i, u_j\rangle \tag{1}$$

establishes that C is a Gram matrix. Hence C is positive semidefinite. Actually C is infinitely divisible. We give two proofs of this fact.

For the first, choose any number ε between 0 and λ_1. If $r>0$ we have

$$\frac{1}{(\lambda_i+\lambda_j-\varepsilon)^r} = \left(\frac{\varepsilon}{\lambda_i\lambda_j}\right)^r \frac{1}{\left(1-\frac{(\lambda_i-\varepsilon)(\lambda_j-\varepsilon)}{\lambda_i\lambda_j}\right)^r}$$

$$= \Big(\frac{\varepsilon}{\lambda_i\lambda_j}\Big)^r \sum_{m=0}^{\infty} a_m \Big(\frac{(\lambda_i-\varepsilon)(\lambda_j-\varepsilon)}{\lambda_i\lambda_j}\Big)^m, \tag{2}$$

where the a_m are the coefficients in the series expansion

$$\frac{1}{(1-x)^r} = \sum_{m=0}^{\infty} a_m x^m \quad (|x|<1).$$

All a_m are positive; namely, $a_0 = 1$ and $a_m = r(r+1)\cdots(r+m+1)/m!$ for $m > 1$.

The matrix with entries $(\lambda_i-\varepsilon)(\lambda_j-\varepsilon)/\lambda_i\lambda_j$ is congruent to the flat matrix. Hence this matrix is positive semidefinite, and by Schur's theorem so are its mth Hadamard powers for $m = 0, 1, 2, \ldots$. Thus the matrix whose entries are given by the infinite series in (2) is positive semidefinite. The matrix with (i,j)th entry $1/(\lambda_i\lambda_j)^r$ is positive semidefinite (it is congruent to the flat matrix). So, again by Schur's theorem the matrix with entries prescribed by (2) is positive semidefinite. Letting $\varepsilon \downarrow 0$ we see that the rth Hadamard power of the Cauchy matrix is positive semidefinite for each positive r.

For our second proof we use the gamma function, which is defined on $(0,\infty)$ by the formula

$$\Gamma(x) = \int_0^{\infty} e^{-t} t^{x-1} dt. \tag{3}$$

Using this definition it is not difficult to see that

$$\frac{1}{(\lambda_i+\lambda_j)^r} = \frac{1}{\Gamma(r)} \int_0^\infty e^{-t(\lambda_i+\lambda_j)} t^{r-1} dt \tag{4}$$

whenever $r > 0$. When $r = 1$ this formula reduces to (1). Once again we observe that the matrix with entries $1/(\lambda_i + \lambda_j)^r$ is the Gram matrix associated with the elements $u_i(t) = e^{-t\lambda_i}$ in the space $L_2(0,\infty)$ relative to the measure

$$d\mu(t) = \frac{t^{r-1}}{\Gamma(r)} dt.$$

For the Hilbert matrix a proof similar to our first proof is given by M.-D. Choi [8].

Generalized Cauchy matrices. The ideas of the preceding section work for certain other matrices. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be positive numbers, and for each real number t different from -2 let Z be the $n \times n$ matrix with entries

$$z_{ij} = \frac{1}{\lambda_i^2 + \lambda_j^2 + t\lambda_i\lambda_j}.$$

When is such a matrix positive semidefinite or infinitely divisible? If $t < -2$, then z_{ii} could be negative in some cases. Accordingly, we need to assume that $t > -2$. When $n = 2$ this condition is also sufficient to ensure that Z is positive semidefinite, hence infinitely divisible. When $n \geq 3$ the condition $t > -2$ is no longer sufficient. If $(\lambda_1, \lambda_2, \lambda_3) = (1, 2, 3)$ and $t = 10$, for example, Z is not positive semidefinite. However, if $-2 < t \le 2$, then the matrix Z is infinitely divisible for $n = 1, 2, 3, \ldots$. When $-2 < t < 2$ and $r > 0$ we have the expansion

$$z_{ij}^r = \frac{1}{(\lambda_i + \lambda_j)^{2r}} \sum_{m=0}^{\infty} a_m (2-t)^m \frac{\lambda_i^m \lambda_j^m}{(\lambda_i + \lambda_j)^{2m}}.$$

This shows that the matrix $Z^{\circ r}$ is a limit of sums of Hadamard products of positive semidefinite matrices. It follows that Z is infinitely divisible for all t in the range $-2 < t < 2$. By continuity this is true also for $t = 2$.

It is known [5] that for each t in $(2, \infty)$ there exists an n for which the $n \times n$ matrix Z is not positive semidefinite for some choice of numbers $\lambda_1, \ldots, \lambda_n$. The proof of this needs somewhat advanced arguments (of the kind discussed later in this paper). The matrix Z was studied by M. K. Kwong [22], who used rather intricate arguments to prove that Z is positive semidefinite for all n whenever $-2 < t \le 2$.

When $t = 1$, the entries of the matrix Z can be rewritten as

$$z_{ij} = \frac{\lambda_i - \lambda_j}{\lambda_i^3 - \lambda_j^3}.$$

The matrix W with entries

$$w_{ij} = \frac{\lambda_i - \lambda_j}{\lambda_i^4 - \lambda_j^4} = \frac{\lambda_i - \lambda_j}{\lambda_i^2 - \lambda_j^2} \frac{1}{\lambda_i^2 + \lambda_j^2}$$

is infinitely divisible, for it is the Hadamard product of infinitely divisible matrices. This argument shows that the matrix V with entries

$$v_{ij} = \frac{\lambda_i - \lambda_j}{\lambda_i^n - \lambda_j^n}$$

is infinitely divisible for positive integers n that can be expressed in the form $n = 2^m$ or $n = 3 \cdot 2^m$. It is known that the matrix V is infinitely divisible for all n. We discuss this in section 3.

The Pascal matrix. The $n \times n$ *Pascal matrix* is the matrix P with entries

$$p_{ij} = \binom{i+j}{i} \quad (i, j = 0, 1, \ldots, n-1).$$

The rows of the Pascal triangle occupy the anti-diagonals of P. Thus the 4×4 Pascal matrix is

$$P = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 6 & 10 \\ 1 & 4 & 10 & 20 \end{bmatrix}.$$

Let $\triangle$ be the $n \times n$ lower triangular matrix whose rows are occupied by the rows of the Pascal triangle. For instance, when $n = 4$ we have

$$\triangle = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 1 & 3 & 3 & 1 \end{bmatrix}.$$

The Pascal matrix P is positive semidefinite. This can be proved by showing that $P = \triangle\triangle^\star$. In [10], Alan Edelman and Gilbert Strang have given four different proofs for this factorization. Two of these proofs employ the interesting combinatorial identity

$$\binom{i+j}{i} = \sum_{k=0}^{\min(i,j)} \binom{i}{k}\binom{j}{k}.$$

Positive definiteness of the Pascal matrix can also be demonstrated by representing it as a Gram matrix. One such representation is

$$p_{rs} = \frac{1}{2\pi}\int_0^{2\pi}(1+e^{i\theta})^r(1+e^{-i\theta})^s d\theta. \tag{5}$$

A second representation derives from the gamma function (3). If $x > 0$ and $y > 0$, then

$$\Gamma(x+y+1) = \int_0^\infty e^{-t}t^x t^y dt. \tag{6}$$

Since $\Gamma(n+1) = n!$ for every nonnegative integer n, this shows that the matrix G with entries

$$g_{ij} = (i+j)! = \Gamma(i+j+1)$$

is a Gram matrix. The Pascal matrix, which has

$$p_{ij} = \frac{(i+j)!}{i!\ j!},$$

is congruent to G and is therefore positive semidefinite.

Our argument shows that for any positive numbers $\lambda_1, \ldots, \lambda_n$ the matrix K with entries

$$k_{ij} = \frac{\Gamma(\lambda_i + \lambda_j + 1)}{\Gamma(\lambda_i + 1)\Gamma(\lambda_j + 1)} \tag{7}$$

is positive semidefinite. When $\lambda_j = j$, this matrix is the Pascal matrix.

In fact, the matrix K is infinitely divisible. (This seems not to have been noticed before, even for the Pascal matrix.) Using Gauss's formula

$$\Gamma(z) = \lim_{m \to \infty} \frac{m! m^z}{z(z+1)\cdots(z+m)} \quad (z \neq 0, -1, -2, \ldots) \tag{8}$$

we see that

$$k_{ij} = \lim_{m \to \infty} \frac{1}{m \cdot m!} \prod_{p=1}^{m+1} \frac{(\lambda_i + p)(\lambda_j + p)}{(\lambda_i + \lambda_j + p)}. \tag{9}$$

For each p the matrix

$$\left[\frac{(\lambda_i + p)(\lambda_j + p)}{\lambda_i + \lambda_j + p}\right]$$

is congruent to the Cauchy matrix

$$\left[\frac{1}{\lambda_i + \lambda_j + p}\right],$$

so is infinitely divisible. The expression (9) demonstrates that K is a limit of Hadamard products of infinitely divisible matrices. Hence, by Schur's theorem and continuity, K is infinitely divisible.

A small aside may be of interest here. If $\lambda_1, \ldots, \lambda_n$ are complex numbers with positive real parts, then the matrix C with entries

$$c_{ij} = \frac{1}{\lambda_i + \overline{\lambda}_j}$$

is positive semidefinite. This can be established by representing C as a Gram matrix as in (1). The condition $\operatorname{Re} \lambda_i > 0$ guarantees that the integral

$$\int_0^\infty e^{-t(\lambda_i + \overline{\lambda}_j)} dt$$

is convergent. Our arguments show that with this restriction on λ_i the matrix K with entries

$$k_{ij} = \frac{\Gamma(\lambda_i + \overline{\lambda}_j)}{\Gamma(\lambda_i)\Gamma(\overline{\lambda}_j)}$$

is a positive semidefinite matrix.

"Min" matrices. Consider the $n \times n$ matrix M with entries $m_{ij} = \min(i, j)$. The idea behind the discussion that follows is captured by the equation

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}$$

$$+\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&1&1\\0&0&1&1\end{bmatrix}+\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{bmatrix}$$

Each of the matrices in this sum is positive semidefinite. Therefore, M is positive semidefinite.

This idea can be taken further. Let $\lambda_1, \dots, \lambda_n$ be arbitrary positive numbers, and let M be the $n \times n$ matrix with entries $m_{ij} = \min(\lambda_i, \lambda_j)$. We can write M as a sum of matrices each of which is plainly positive semidefinite. First, by applying a permutation similarity, we may assume that $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. Thus

$$M = \begin{bmatrix}\lambda_1 & \lambda_1 & \dots & \lambda_1\\ \lambda_1 & \lambda_2 & \dots & \lambda_2\\ \vdots & \vdots & & \vdots\\ \lambda_1 & \lambda_2 & & \lambda_n\end{bmatrix}.$$

For each k with $1 \leq k \leq n$ let $\tilde{E}_k$ be the $n \times n$ matrix whose bottom right corner is occupied by the $k \times k$ flat matrix and whose remaining entries are zeros. Then we can express M as

$$M = \lambda_1 \tilde{E}_n + (\lambda_2 - \lambda_1)\tilde{E}_{n-1} + (\lambda_3 - \lambda_2)\tilde{E}_{n-2} + \cdots + (\lambda_n - \lambda_{n-1})\tilde{E}_1,$$

revealing that M is a positive semidefinite matrix.

The same argument shows that if f is a monotonically increasing function from $(0, \infty)$ into itself, then the matrix $[f(m_{ij})]$ is positive semidefinite. The special choice $f(t) = t^r$ with $r > 0$ shows that M is infinitely divisible.

We could have started the discussion in this section with the factorization

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Building on this, alternate proofs of other results in this section can be obtained.

The Lehmer matrix. For positive numbers x and y we have

$$\frac{\min(x, y)}{xy} = \frac{1}{\max(x, y)}.$$

It follows from earlier results in this section that for positive numbers $\lambda_1, \ldots, \lambda_n$ the $n \times n$ matrix W with entries

$$w_{ij} = \frac{1}{\max(\lambda_i, \lambda_j)}$$

is infinitely divisible.

If $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and L is the matrix with entries

$$l_{ij} = \frac{\min(\lambda_i, \lambda_j)}{\max(\lambda_i, \lambda_j)},$$

then as the Hadamard product of two infinitely divisible matrices L is infinitely divisible. We have $l_{ij} = \lambda_i/\lambda_j$ $(1 \leq i \leq j \leq n)$. For the special choice $\lambda_j = j$ $(1 \leq j \leq n)$ the matrix L is called the *Lehmer matrix.*

Suppose that $\lambda_1, \ldots, \lambda_n$ are positive numbers and that N is the matrix with entries

$$n_{ij} = \exp(-|\lambda_i - \lambda_j|).$$

It follows from our discussion of the matrix L that N is an infinitely divisible matrix. This property is equivalent to the fact that the function $f(x) = e^{-|x|}$ is a positive definite function on $\mathbb{R}$ (see section 3).

Some of the special matrices studied in this section are frequently used for testing the stability of numerical algorithms and are available in MATLAB through the function `(gallery)`. We refer the reader to [14] and [15].

3 Other proofs and connections.

Positive definite functions. The concept of infinite divisibility is important in the theory of characteristic functions of probability distributions. Infinitely divisible distributions are exactly the class of limit distributions for sums of independent random variables (see [7, pp.190–196] and [12, chap.

9]). General techniques from this subject can be used to prove special results on matrices.

A complex-valued function f on $\mathbb{R}$ is a *positive definite function* if for every positive integer n and for every choice of points $x_1, \ldots, x_n$ in $\mathbb{R}$ the $n \times n$ matrix $[f(x_i - x_j)]$ is positive semidefinite. A theorem of Salomon Bochner (see [7, p.174]) states that a function $f : \mathbb{R} \to \mathbb{C}$ that is continuous at 0 is positive definite if and only if there exists a finite positive Borel measure μ on $\mathbb{R}$ such that

$$f(x) = \int_{-\infty}^{\infty} e^{-itx} d\mu(t). \tag{10}$$

We say that f is the *Fourier transform* of μ and express this relationship with the notation $f = \hat{\mu}$.

The measure μ is *absolutely continuous* if there exists a nonnegative integrable function g on $\mathbb{R}$ such that $d\mu(t) = g(t)dt$. In this case the relation (10) can be expressed as

$$f(x) = \int_{-\infty}^{\infty} e^{-itx} g(t) dt. \tag{11}$$

We use the notation $f = \hat{g}$ to express the relation (11), and say that f is the *Fourier transform of the function* g. If f is integrable, then g can be obtained from f by the *Fourier inversion formula*

$$g(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{itx} f(x)dx. \tag{12}$$

If ν_1 and ν_2 are two Borel measures on $\mathbb{R}$, then there exists a unique Borel measure ν on $\mathbb{R}$ such that

$$\int_{-\infty}^{\infty} f(t)d\nu(t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x-y)d\nu_1(x)d\nu_2(y) \tag{13}$$

for every bounded Borel function f. This measure ν is called the *convolution* of ν_1 and ν_2, and we use the notation $\nu_1 * \nu_2$ for it (see [26, p.149]).

If the Fourier transforms of ν_1 and ν_2 are f_1 and f_2, respectively, then $\widehat{\nu_1 * \nu_2} = f_1 f_2$. A measure μ on $\mathbb{R}$ is called *infinitely divisible* if for each positive integer m there exists a measure ν on $\mathbb{R}$ such that $\mu = \nu * \nu * \cdots * \nu$ (an m-fold convolution).

Bochner's theorem and the Fourier inversion formula lead to a useful criterion for positive definiteness. When a function $f : \mathbb{R} \to \mathbb{C}$ is continuous and integrable, then it is positive definite if and only if $\hat{f}(t) \geq 0$ for almost all t.

In view of this criterion, the integral representation

$$e^{-|x|} = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{e^{-itx}}{1+t^2}dt$$

shows that for every $r > 0$ the function $e^{-r|x|}$ is positive definite. This, in turn, furnishes another proof of the infinite divisibility of the matrix N from section 2.

One proof of the infinite divisibility of the Cauchy matrix reads as follows. If $\lambda_j = e^{x_j}$ for $j = 1, 2, \ldots, n$, then

$$\frac{1}{\lambda_i + \lambda_j} = \frac{1}{e^{x_i/2} \;\; 2\cosh\left(\frac{x_i - x_j}{2}\right) e^{x_j/2}}.$$

Thus the Cauchy matrix is congruent to the matrix whose (i, j)th entry is

$$\frac{1}{\cosh\left(\frac{x_i - x_j}{2}\right)}.$$

Since congruence is an equivalence relation that preserves positive semidefiniteness, the following two statements are equivalent:

(i) For every n and for every choice of positive numbers $\lambda_1, \ldots, \lambda_n$ the $n \times n$ Cauchy matrix $\left[\frac{1}{\lambda_i + \lambda_j}\right]$ is positive semidefinite.

(ii) The function $f(x) = 1/\cosh\; x$ is positive definite.

The second of these statements can be proved by calculating the Fourier transform of f. This turns out to be

$$\hat{f}(t) = \frac{1}{\cosh\;\left(\frac{t\pi}{2}\right)}.$$

Since $\hat{f}(t) > 0$ for all t, the function f is positive definite by Bochner's theorem.

For positive r let $g(x) = (\cosh\ x)^{-r}$. A calculation involving contour integrals shows that the Fourier transform of g is

$$\hat{g}(t) = 2^{r-2}\frac{1}{\Gamma(r)}\left|\Gamma\Big(\frac{r+it}{2}\Big)\right|^2.$$

This reveals that g is a positive definite function. We conclude that the Cauchy matrix is infinitely divisible.

A proof along these lines is given in [5] and in [13]. Positive definiteness of several other matrices is proved there. This method is especially useful in showing that certain functions are *not* positive definite, hence that certain matrices are not positive semidefinite.

The kernel $M(x,y) = \min(x,y)$ with $x > 0$ and $y > 0$ is known to be the covariance kernel of the standard Brownian motion [7]. By what we said at the begining of this section, this kernel is infinitely divisible in the following sense: if φ is any integrable function defined on an interval $[a,b]$ contained in $[0,\infty)$, then for all positive r

$$\int_a^b\int_a^b M^r(x,y)\varphi(x)\overline{\varphi(y)}dxdy \geq 0.$$

This gives another way of looking at the matrix M in section 2.

Conditionally positive definite matrices. A Hermitian matrix A is *conditionally positive semidefinite* if $x^*Ax \geq 0$ for all vectors x in $\mathbb{C}^n$ such that $\sum_{j=1}^n x_j = 0$.

Charles Loewner showed that if A is a symmetric matrix with positive entries, then A is infinitely divisible if and only if its *Hadamard logarithm* $\log^\circ(A) = [\log\ a_{ij}]$ is a conditionally positive semidefinite matrix (see [21, Theorem 6.3.13]). Good necessary and sufficient conditions for a matrix to be conditionally positive semidefinite are also known. One of them asserts that an $n \times n$ Hermitian matrix $B = [b_{ij}]$ is conditionally positive semidefinite if and only if the $(n-1) \times (n-1)$ matrix D with entries

$$d_{ij} = b_{ij} + b_{i+1,j+1} - b_{i,j+1} - b_{i+1,j}$$

is positive semidefinite. A reference is [21, pp. 457-458], where these criteria are used to prove the infinite divisibility of some matrices.

We illustrate how these ideas can be applied by considering the Pascal matrix. From the foregoing discussion we know that the $n \times n$ Pascal matrix P is infinitely divisible if and only if the $(n-1) \times (n-1)$ matrix D with entries

$$d_{ij} = \log \frac{i+j+2}{i+j+1} = \log \left(1 + \frac{1}{i+j+1}\right) \tag{14}$$

is positive semidefinite. For $x \geq 0$ we have

$$\log(1+x) = \int_1^\infty \frac{tx}{t+x} d\mu(t),$$

where μ is the probability measure on $[1, \infty)$ defined by $d\mu(t) = dt/t^2$. (see [4, p. 145]). We exploit this representation to express d_{ij} in (14) as

$$d_{ij} = \int_1^\infty \frac{1}{i+j+1+\frac{1}{t}} d\mu(t).$$

This implies that D is a limit of positive linear combinations of matrices $C(t) = [c_{ij}(t)]$, where

$$c_{ij}(t) = \frac{1}{i+j+1+\frac{1}{t}} \quad (t \geq 1).$$

If we put $\lambda_i = i + \frac{1}{2}\left(1+\frac{1}{t}\right)$, then

$$c_{ij}(t) = \frac{1}{\lambda_i + \lambda_j}.$$

Thus for each t in $[1, \infty)$ the matrix $C(t)$ is a Cauchy matrix. Accordingly, D is positive semidefinite.

Several applications of conditionally positive semidefinite matrices can be found in the book [2]. Continuous analogues and their applications are discussed in the monograph [24].

Operator monotone functions. If A and B are Hermitian matrices and $A - B$ is positive semidefinite, then we say that $A \geq B$. Let f be any map of the positive half-line $[0, \infty)$ into itself. The function f is *matrix monotone of order* n if $f(A) \geq f(B)$ whenever A and B are $n \times n$ positive semidefinite matrices with $A \geq B$. If f is matrix monotone of order n for $n = 1, 2, \ldots,$ then f is called *operator monotone.*

Two famous theorems of Loewner characterise operator monotone functions. The first states that (a differentiable function) $f : [0, \infty) \to [0, \infty)$ is matrix monotone of order n if and only if for all positive numbers $\lambda_1, \ldots, \lambda_n$ the $n \times n$ matrix

$$\left[\frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j} \right] \tag{15}$$

is positive semidefinite. (If $\lambda_i = \lambda_j$, the difference quotient in (15) is understood to mean $f'(\lambda_i)$.) The matrix (15) is called the *Loewner matrix* associated with f and $\lambda_1, \ldots, \lambda_n$.

The second theorem of Loewner asserts that f is operator monotone if and only if it has an analytic continuation to a mapping of the upper half-plane into itself. It was shown by Horn [16] that this analytic continuation is a one-to-one (also called *univalent* or *schlicht*) map if and only if every Loewner matrix associated with f is infinitely divisible.

From Loewner's second theorem it is clear that the function $f(t) = t^\nu$ is operator monotone when $0 < \nu \leq 1$. Since the function $f(z) = z^\nu$ (principal branch) is univalent in the upper half-plane it follows from Horn's theorem that for every n and for all positive numbers $\lambda_1, \ldots, \lambda_n$ the $n \times n$ matrix

$$\left[\frac{\lambda_i^\nu - \lambda_j^\nu}{\lambda_i - \lambda_j}\right]$$

is infinitely divisible if $0 < \nu \leq 1$. In section 2 we proved this for special values of ν.

The reader can consult [9] and [4, chap. 5] for the theory of operator monotone functions.

4 MORE EXAMPLES.

GCD-matrices. The matrix $m_{ij} = \min(i, j)$ studied in section 2 is a cousin, in spirit, of another matrix. For a given set $S = \{x_1, \ldots, x_n\}$ of distinct positive integers the *GCD-matrix associated with* S is the matrix A with entries $a_{ij} = (x_i, x_j)$, the greatest common divisor of x_i and x_j. This matrix is infinitely divisible. We outline a proof of this fact. To make for easier reading we first prove that A is positive semidefinite. The proofs are borrowed from papers by Beslin and Ligh [3] and Bourque and Ligh [6]. The elementary concepts from number theory that we need can be found in a basic text such as [1].

Let φ signify the *Euler totient function.* For each positive integer n the value $\varphi(n)$ registers the number of integers m less than or equal to n such that $(m,n) = 1$. One has the identity

$$\sum_{d|n} \varphi(d) = n. \tag{16}$$

Here, as usual, $d|n$ means that $1 \leq d \leq n$ and n is divisible by d.

A set F of positive integers is *factor-closed* if d belongs to F whenever x is in F and $d|x$. The smallest factor-closed set F containing a set S is called the *factor-closure* of S. Thus, for example, the set $\{2,3,5,6,10\}$ is the factor-closure of the set $\{2,6,10\}$.

Let $S = \{x_1, \ldots, x_n\}$ be an arbitrary set of distinct positive integers, and let $F = \{d_1, \ldots, d_t\}$ be its factor-closure. Define $n \times t$ matrices E and B as follows:

$$\begin{aligned} e_{ij} &= \begin{cases} 1 & \text{if } d_j | x_i, \\ 0 & \text{otherwise}; \end{cases} \\ b_{ij} &= e_{ij}\sqrt{\varphi(d_j)}. \end{aligned} \tag{17}$$

Then the (i,j)th entry of the matrix BB^* is

$$\sum_{k=1}^{t} b_{ik}b_{jk} \;=\; \sum_{\substack{d_k|x_i \\ d_k|x_j}} \sqrt{\varphi(d_k)}\sqrt{\varphi(d_k)} = \sum_{d_k|(x_i,x_j)} \varphi(d_k) = (x_i, x_j).$$

This verifies that the GCD-matrix $a_{ij} = (x_i, x_j)$ is positive semidefinite.

A (complex-valued) function f on $\mathbb{N}$ is *multiplicative* if $f(mn) = f(m)f(n)$ whenever $(m, n) = 1$. For example, the Euler φ-function is multiplicative. The *Dirichlet convolution* $f * g$ of two multiplicative functions f and g is defined by

$$(f * g)(n) = \sum_{d|n} f(d)g\left(\frac{n}{d}\right).$$

With this binary operation, the collection of multiplicative functions is an Abelian group. The identity element of this group is the function ε such that $\varepsilon(1) = 1$ and $\varepsilon(1) = 0$ when $n > 1$.

The *Möbius function* μ is defined as follows. First, $\mu(1) = 1$. If $n > 1$, write

$$n = p_1^{k_1} p_2^{k_2} \dots p_m^{k_m},$$

in which $p_1, \dots, p_m$ are distinct primes. If $k_1 = k_2 = \cdots = k_m = 1$ (i.e., if n is square-free), define $\mu(n) = (-1)^m$; otherwise set $\mu(n) = 0$.

The Möbius function is multiplicative. Its inverse in the group of multiplicative functions is the function $u \equiv 1$; (i.e., $\mu * u = \varepsilon$). Hence $(f * \mu) * u = f$, or stated differently,

$$\sum_{d|n} (f * \mu)(d) = f(n) \tag{18}$$

for every multiplicative function f.

We prove that the matrix $\left[f\Big((x_i, x_j)\Big)\right]$ is positive semidefinite for every multiplicative function f such that $f * \mu > 0$. Instead of B defined by (17) we now consider the matrix B with entries

$$b_{ij} = e_{ij}\sqrt{(f * \mu)(d_j)}. \tag{19}$$

The same calculation as before, with the equality (18) replacing (16), shows that

$$BB^* = \left[f\Big((x_i, x_j)\Big)\right].$$

Choosing $f(n) = n^r$ with $r > 0$ we see that the GCD-matrix $[(x_i, x_j)]$ is infinitely divisible. If l_{ij} is the least common multiple of x_i and x_j, then the argument given in section 2 in conjunction with the Lehmer matrix shows that the matrix A with entries $a_{ij} = 1/l_{ij}$ is likewise infinitely divisible.

Characteristic matrices. Let $x_1, \ldots, x_n$ be vectors in the space $\mathbb{R}^k$. Associate with them an $n \times n$ matrix A as follows. If exactly m coordinates of the vector x_i are equal to the corresponding coordinates of the vector x_j, then $a_{ij} = m$. Note that $0 \leq m \leq k$. The matrix A is called the *characteristic matrix* associated with $x_1, \ldots, x_n$. If A' is the characteristic matrix associated with a rearrangement $x'_1, \ldots, x'_n$ of the vectors $x_1, \ldots, x_n$, then $A' = S^*AS$ for some permutation matrix S. Every characteristic matrix is positive semidefinite. One proof of this fact goes as follows.

First consider the case $k = 1$. We may arrange the numbers $x_1, \ldots, x_n$ in such a way that they are grouped into disjoint classes $S_1, S_2, \ldots, S_\ell$, where x_i and x_j belong to the same class if and only if they are equal. If $\ell = n$, then all the x_i are distinct and the characteristic matrix A is equal to the identity matrix. If $\ell = 1$, then all the x_i are equal to each other and A is the flat matrix. If $1 < \ell < n$, let n_j be the number of elements in the class S_j $(j = 1, 2, \ldots, \ell)$. The matrix A is then an $\ell \times \ell$ block-diagonal matrix whose diagonal blocks are flat matrices of sizes $n_1, n_2, \ldots, n_\ell$. Evidently, A is positive semidefinite.

Now consider the case $k > 1$. Let A_p $(1 \leq p \leq k)$ be the $n \times n$ matrix whose (i, j)th entry is 1 if the pth coordinate of x_i is equal to the pth coordinate of x_j, and 0 otherwise. Then $A = A_1 + \cdots + A_k$ and each of the summands is positive semidefinite.

A characteristic matrix is not always infinitely divisible. For example, let $x_1 = (1, 1)$, $x_2 = (2, 1)$, and $x_3 = (1, 2)$. In this case we obtain the characteristic matrix

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{bmatrix},$$

which is not infinitely divisible.

Two comments are in order here. Our discussion suggests that there might be something special about the pattern of zero entries in an infinitely divisible matrix. The *incidence matrix* of an arbitrary matrix A is the matrix $G(A) = [g_{ij}]$, where $g_{ij} = 1$ if $a_{ij} \neq 0$ and $g_{ij} = 0$ if $a_{ij} = 0$. If $a_{ij} > 0$, then $\lim_{r \to 0^+} a_{ij}^r = 1$. This shows that $G(A)$ is positive semidefinite if A is infinitely divisible. The argument we gave in conjunction with characteristic matrices reveals that the condition that $G(A)$ be positive semidefinite is equivalent to the existence of a permutation matrix S such that $S^*G(A)S$ is a block-diagonal matrix in which each of the nonzero blocks is a flat matrix (see [18], [21, p.457]). This gives a good necessary condition for infinite divisibility.

Our second remark points to a connection between characteristic matrices and positive definite functions. Let G be any additive subgroup of $\mathbb{R}$. Then the characteristic function χ_G is a positive definite function. Using this fact one can see that if A is the matrix with $a_{ij} = m$ if exactly m coordinates of the vector $x_i - x_j$ are in G, then A is positive semidefinite. The special case $G = \{0\}$ corresponds to the characteristic matrix.

Characteristic matrices arise in diverse contexts. See [25] for their use in the study of distance matrices and interpolation problems.

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