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Analytic Functions of M-Matrices and Generalizations

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Dedicated to Ky Fan

We introduce the notion of positivity cone $\mathbf{K}$ of matrices in $\mathbb{C}^{nn}$ and with such a $\mathbf{K}$ we associate sets $\mathbf{Z}$ and $\mathbf{M}$. For suitable choices of $\mathbf{K}$ the set $\mathbf{M}$ consists of the classical (non-singular) M-matrices or of the positive definite (Hermitian) matrices. If $A \in \mathbf{M}$ and $1 \leqslant p \leqslant 3$ we prove that there is a unique $B \in \mathbf{M}$ for which $B^p = A$. If $p > 3$, this uniqueness theorem is false for general $\mathbf{M}$ and we prove a weaker result. We extend the result that for a Z-matrix A we have $A^{-1} \geqslant 0$ if and only if A is an M-matrix. Under an additional hypothesis on the positivity cone, we exhibit a class of entire functions $f(z)$ such that for $A \in \mathbf{Z}$ we have $A \in \mathbf{M}$ if and only if there is a $B \in \mathbf{K}$ for which $f(B) = A^{-1}$.

§1. INTRODUCTION

Since their introduction as objects of study by Ostrowski [9], M-matrices have received a great deal of attention. A summary of the literature may be found in [4] and we choose to mention here just one of several papers by Fan on this topic, [6].

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Here we shall consider some problems on analytic functions of M-matrices and M-matrix will mean *non-singular* M-matrix throughout. We investigate the existence and uniqueness of roots of an M-matrix which are also M-matrices. We find new characterizations of the set of M-matrices as a subset of the set of Z-matrices. We introduce generalization of M-matrices for which our results are proved.

We shall now summarize our paper in greater detail. In §2 we introduce generalizations of Z-matrices and M-matrices associated with certain cones of matrices which we call positivity cones. Thus for each positivity cone $\mathbf{K}$ we define the sets $\mathbf{Z} = \mathbf{Z}(\mathbf{K})$ and $\mathbf{M} = \mathbf{M}(\mathbf{K})$. If $\mathbf{K}$ consists of the (elementwise) nonnegative matrices, then $\mathbf{Z}$ and $\mathbf{M}$ are the sets of Z-matrices and M-matrices, respectively (and we reserve the terms *nonnegative matrix*, *Z-matrix* and *M-matrix* for this classical case). If $\mathbf{K}$ is the set of positive semi-definite (Hermitian) matrices, then $\mathbf{Z}$ is the set of Hermitians and $\mathbf{M}$ is the set of positive definite matrices. Thus we give a unified treatment of results on M-matrices and positive definite matrices and thereby respond to a research problem raised by Olga Taussky [11]. We also use a certain positivity cone to obtain a counterexample in §4.

In §3 we prove some very straightforward results on analytic functions $f(z)$ such that $f(A) \in \mathbf{M}$ or $f(A) \in \mathbf{Z}$ whenever $A \in \mathbf{Z}$. For technical reasons, we confine ourselves to the subset $\mathbf{Z}^*$ of $\mathbf{Z}$ consisting of matrices A for which $A \leqslant I$ in the order induced by $\mathbf{K}$. If $\mathbf{M}$ is the set of M-matrices and all orders of square matrices are considered we have a characterization of analytic functions $f(z)$ with the property described. Examples of such functions $f(z)$ are z^q, $0 < q < 1$ and $\log z$. For these particular functions it is known that $f(A)$ is a Z-matrix when A is an M-matrix. Ando [3] obtained these implications as special cases of very interesting results on Pick functions of M-matrices. However, our class of functions does not coincide with the Pick functions.

The results of §3 show that if $A \in \mathbf{M}$, $p > 1$, and $B = A^{1/p}$ then $B \in \mathbf{M}$. In §4 we investigate uniqueness properties and we show that for $1 \leqslant p \leqslant 3$, $B = A^{1/p}$ is the unique matrix in $\mathbf{M}$ that $B^p = A$. For $p > 3$ we prove a weaker theorem: $B = A^{1/p}$ is the unique matrix for which $B^p = A$ and $B, B^2, \ldots, B^m$ belong to $\mathbf{M}$, where m is the integer satisfying $p/3 \leqslant m < (p/3) + 1$. Let $p > 3$. If $\mathbf{M}$ is the set of positive definite matrices, then roots within $\mathbf{M}$ are unique. However we give an example of a positivity cone $\mathbf{K}$ such that for the corresponding set $\mathbf{M}$ there is an $A \in \mathbf{M}$ with at least $2^{(n-1)}$ matrices $B \in \mathbf{M}$ for which $B^p = A$. We also show that for $n \geqslant 3$ and $p > 12$ there exist distinct M-matrices B_0, B_1 in $\mathbb{R}^n$ such that $B_0^p = B_1^p$ is again an M-matrix.

Let A be a Z-matrix. It is very well known that A is a (nonsingular) M-matrix if and only if $A^{-1} \geqslant 0$. It is easy to find functions $g(z)$ such that $g(A) \geqslant 0$ if A is an M-matrix but where the converse implication may be false, e.g. for $g(z) = z^{-2}$. A class of such functions was introduced by Varga [12], cf. [4, pp. 142–146] (who also obtained a converse by considering the *series expansion* rather than the function itself). We are thus led to §5 to the search for functions $g(z)$ for which $A \in \mathbf{M}$ if and only if $A \in \mathbf{K}$. Our class of functions is described in terms of what we call reciprocating pairs of functions $(f(z), g(z))$. Examples are $(z^p, z^{-1/p})$, p a positive integer and $(e^{k(z-1)}, 1 - k^{-1}\log z)$ where $k > 0$. For M-matrices, the case $g(z) = z^{-1}$ is classical and the special case of $g(z) = z^{-1/2}$ of our result is known, and was recently proved by E. Alefeld and N. Schneider [1] by different methods.

§2. POSITIVITY CONES AND ASSOCIATED SETS

We begin with some definitions. By $\mathbb{R}$ we denote the real field, and by $\mathbb{C}$ the complex field. As usual, $\mathbb{C}^n$ will denote the space of complex n-tuples, and $\mathbb{C}^{nn}$ the set of all $n \times n$ matrices with elements in $\mathbb{C}$. We use $\mathbb{R}^n$ and $\mathbb{R}^{nn}$ similarly.

A *cone* $\mathbf{K}$ is a non-empty subset of a (usually complex) vector space which is closed under addition and multiplication by nonnegative reals. The cone $\mathbf{K}$ is pointed if $P \in \mathbf{K}$ and $P \in -\mathbf{K}$ imply $P = 0$, cf. [4, p. 2]. A pointed cone $\mathbf{K}$ partially orders the vector space, viz. $P \geqslant Q$ defined by $P - Q \in \mathbf{K}$ is a partial order which is compatible with addition and multiplication by nonnegative scalars.

We now introduce a definition which is fundamental for our results.

Definition 2.1 A pointed, closed cone $\mathbf{K}$ in $\mathbb{C}^{nn}$ such that

(a) $I \in \mathbf{K}$,
(b) If $P \in \mathbf{K}$ then $P^r \in \mathbf{K}$, $r = 1, 2, \ldots$,

will be called a *positivity cone of matrices*.

Henceforth $\mathbf{K}$ will always denote a positivity cone of matrices and we partially order $\mathbb{C}^{nn}$ with respect to $\mathbf{K}$. (We may write $P \geqslant 0$ for $P \in \mathbf{K}$ even though we reserve the *words* nonnegative matrix for the classical case.)

Suppose $P \geqslant 0$ and let $\omega(P)$ be the cone of all polynomials $\sum_{r=0}^{m} c_r P^r$ where $c_r \geqslant 0$, $r = 0, 1, \ldots, m$. Then $\omega(P) \subseteq \mathbf{K}$ and hence also $\bar{\omega}(P) \subseteq \mathbf{K}$, where $\bar{\omega}(P)$ is the closure of $\omega(P)$. Hence, $\bar{\omega}(P)$ is pointed and the spectral radius $\rho(P)$ of P belongs to $\operatorname{spec} P$ (the spectrum of P), see [10, Theorem 5.2].

We call $\rho(P)$ the *Perron–Frobenius* root of P. Hence $A = sI - P$, where $s \in \mathbb{R}$ and $P \geqslant 0$ has an eigenvalue $\alpha(A)$ such that $\alpha(A) = \min\{\operatorname{Re}\lambda : \lambda \in \operatorname{spec} A\}$. We call $\alpha(A)$ the *minimal eigenvalue* of $A = sI - P$.

DEFINITION 2.2 Let $\mathbf{K}$ be a positivity cone of matrices. We put

(a) $\mathbf{Z} = \{A \in \mathbb{C}^{nn} : A = sI - P,\ s \in \mathbb{R},\ P \in \mathbf{K}\}$,
(b) $\mathbf{Z}^* = \{A \in \mathbf{Z} : A \leqslant I\}$,
(c) $\mathbf{M} = \{A \in \mathbf{Z} : \alpha(A) > 0\}$,
(d) $\mathbf{M}^* = \mathbf{Z}^* \cap \mathbf{M}$.

Our notation does not indicate the dependence of $\mathbf{Z}$, $\mathbf{M}$, etc. on $\mathbf{K}$. But $\mathbf{K}$ may be considered fixed throughout. Nor do we indicate the order n of our matrices. But here also, n may be considered fixed, except in one theorem. We give some examples of possible choices for $\mathbf{K}$.

Example 2.3 (i) Let $\mathbf{K}_1$ be the cone of all (elementwise) nonnegative matrices in $\mathbb{C}^{nn}$, viz. $P \in \mathbf{K}_1$ if $p_{ij} \geqslant 0$, $i, j = 1, \ldots, n$. Then $\mathbf{Z}_1$ and $\mathbf{M}_1$ are respectively the sets of Z-matrices and (non-singular) M-matrices as defined in Berman–Plemmons [4].

(More generally we could choose $\mathbf{K}$ to be the cone of matrices which map a proper cone in $\mathbb{R}^n$ into itself, see [10] for definition of proper cone.)

(ii) Let $\mathbf{K}_2$ be the cone of positive semi-definite (Hermitian) matrices. Then $\mathbf{Z}_2$ is the set of all Hermitian matrices and $\mathbf{M}_2$ the set of positive definite matrices.

(iii) Let $\mathbf{K}_3 = \mathbf{K}_1 \cap \mathbf{K}_2$.

(iv) Let $n \geqslant 2$. Let $\mathbf{K}_4$ be the cone of all diagonal matrices P with $p_{11} \geqslant |p_{ii}|$, $i = 2, \ldots, n$. (Note that $p_{11} \geqslant 0$). Then $\mathbf{Z}_4$ consists of all diagonal matrices A with $a_{11} \in \mathbb{R}$ and either $a_{11} = a_{ii}$ or $a_{11} < \operatorname{Re} a_{ii}$, $i = 2, \ldots, n$. Also $A \in \mathbf{M}_4$ if and only if $A \in \mathbf{Z}_4$ and $a_{11} > 0$. Observe that $\mathbf{Z}_4$ is not closed in $\mathbb{C}^{nn}$.

We shall use the subscript 1, 2, 3, 4 to refer to the cones, etc., in the above example. Note that for $\mathbf{K} = \mathbf{K}_i$, $i = 1,2,3,4$ we have a property stronger than (2.1) which will be needed in §5:

Condition 2.4 If P, $Q \in \mathbf{K}$ and P, Q commute then $PQ \in \mathbf{K}$.

We observe that if $P \in \mathbb{C}^{nn}$ and $\bar{\omega}(P)$ is pointed, then $\mathbf{K} = \bar{\omega}(P)$ obviously satisfies the conditions (2.1) and (2.4).

The following lemma is obvious.

LEMMA 2.5 *Let $A \in \mathbf{Z}$ (where $\mathbf{Z}$ corresponds to a positivity cone $\mathbf{K}$). Then the following are equivalent.*

(a) $A \in \mathbf{M}$,
(b) *All eigenvalues of A have positive real part.* ■

§3. PRELIMINARY RESULTS ON ANALYTIC FUNCTIONS

If $g(z)$ is a single-valued function analytic in an open subset V of the complex plane and $A \in \mathbb{C}^{nn}$ has $\operatorname{spec} A \subseteq V$, then we define $g(A)$ as in Dunford–Schwartz [5, p. 557]. Thus we choose any polynomial $p(z)$ with $p^{(r)}(\alpha) = g^{(r)}(\alpha)$ for $\alpha \in \operatorname{spec} A$ and $r = 0, 1, \ldots, n$. For the Jordan form $QAQ^{-1} = \sum_{i=1}^{s} \oplus (\alpha_i I_i + N_i)$ where I_i is an identity matrix and N_i is nilpotent, we define

$$Qg(A)\,Q^{-1} = \sum_{i=1}^{s} \oplus \left(\sum_{r=0}^{\infty} \frac{1}{r!}\, p^r(\alpha_i) N_i^r \right).$$

We shall be particularly interested in analytic functions whose derivatives at 1 satisfy certain properties.

DEFINITION 3.1 Let $f(z)$ be a function analytic at 1.

(a) We call $f(z)$ *totally nonnegative at* 1 if

$$f^{(r)}(1) \geqslant 0, \qquad \text{for} \quad r = 0, 1, \ldots .$$

(b) We call $f(z)$ *totally oscillating at* 1 if

$$(-1)^r f^{(r)}(1) \geqslant 0, \qquad \text{for} \quad r = 0, 1, \ldots .$$

The terms absolutely monotonic have been used in a manner related to our totally nonnegative and totally oscillating cf. Widder [13, p. 144–145], Varga [12] and [4, p. 142].

By U we shall henceforth denote the set

$$U = \{ z \in \mathbb{C} : |z - 1| < 1 \}. \tag{3.2}$$

If $g(z)$ is an analytic function in U then for $|x| < 1$

$$g(1-x) = \sum_{r=0}^{\infty} b_r x^r = g(1) - \sum_{r=1}^{\infty} c_r x^r$$

where

$$-c_r = b_r = (-1)^r \frac{g^{(r)}(1)}{r!}, \qquad r = 1, 2, \ldots . \tag{3.3}$$

Hence $g(z)$ is totally oscillating if and only if $b_r \geqslant 0$, $r = 0, 1, \ldots$. Also, $g'(z)$ is totally oscillating if and only if $c_r \geqslant 0$, $r = 1, 2, \ldots$. If $A \in \mathbf{M}^*$, then $A = I - P$, where $P \geqslant 0$ and $\rho := \rho(P) < 1$. Hence $\sum_{r=1}^{\infty} c_r P^r$ converges and

$$g(A) = g(I) - \sum_{r=0}^{\infty} c_r P^r \tag{3.4}$$

We have proved (i) of the following simple theorem.

THEOREM 3.5 *Let $A \in \mathbf{M}^*$ with minimal eigenvalue α. Let $g(z)$ be function analytic in U such that $g'(z)$ is totally oscillating at* 1. *Then*

(i) $g(A) \in \mathbf{Z}$,
(ii) $g(\alpha)$ *is the minimal eigenvalue of* $g(A)$.
(iii) $g(A) \in \mathbf{M}$ *if and only if* $g(\alpha) > 0$.

Proof (i) was proved before the statement of the theorem.
(ii) We have

$$\operatorname{spec} g(A) = \{ g(\lambda) : \lambda \in \operatorname{spec} A \}.$$

Hence $g(\alpha)$ is an eigenvalue of $g(A)$. If $A = I - P$ and $\lambda = 1 - \mu \in \operatorname{spec} A$, then $\mu \in \operatorname{spec} P$, and so $|\mu| \leqslant \rho < 1$. Hence

$$|g(1) - g(\lambda)| = \left| \sum_{r=1}^{\infty} c_r \mu^r \right| \leqslant \sum_{r=1}^{\infty} c_r \rho^r = g(1) - g(\alpha)$$

since $\alpha = 1 - \rho$. Thus $\operatorname{Re} g(\lambda) \geqslant g(\alpha)$, for $\lambda \in \operatorname{spec} A$, and this proves (ii).

(iii) is an immediate consequence of (ii). ∎

If $z = re^{i\theta}$, where $r \geqslant 0$, $-\pi < \theta = \arg z \leqslant \pi$, we define

$$\log z = \log r + i\theta$$

where $\log r$ is real, and, for $p \in \mathbb{R}$,

$$z^p = r^p e^{ip\theta}.$$

Thus $\log z$ and z^p are analytic in $\mathbb{C}$ with the negative axis and 0 removed. If $0 < q < 1$, then $g(z) = \log z$ and $g(z) = z^q$ have $g'(z)$ totally oscillating at 1 and $g'(1) > 0$. We thus have the following corollaries, which are obtained from Theorem (3.5) by consideration of $s^{-1}A$ where s is sufficiently large to ensure $s^{-1}A \in \mathbf{M}^*$.

COROLLARY 3.6 *Let $A \in \mathbf{M}$. Then $\log A \in \mathbf{Z}$ and $\log A \in \mathbf{M}$ if and only if $\alpha > 1$, where α is the minimal eigenvalue of A.* ∎

COROLLARY 3.7 *Let $A \in \mathbf{M}$ and let $0 < q < 1$. Then $A^q \in \mathbf{M}$.* ∎

For $A \in \mathbf{M}_1$, it was noted by Ando [3] that $\log A \in \mathbf{Z}_1$ and $A^q \in \mathbf{M}_1$, if $0 < q < 1$. As remarked in our introduction, his proof uses Pick functions, though a remark of his suggests he was aware of the above simple argument with Taylor expansions. See also Johnson [8]. Similar results for $\mathbf{M}_2$ are also known, e.g. Ando [2].

In the rest of this section we consider the classical case; viz. $\mathbf{K} = \mathbf{K}_1$. If $A \in \mathbb{R}^{nn}$, we define the (directed) graph $G(A)$ in the normal way, viz. $G(A)$ has as its vertex set $\{1, \ldots, n\}$ and (i, j) is an edge of $G(A)$ if and only if $a_{ij} \neq 0$, cf. [4, p. 29]. (Usually the definition is given for nonnegative A, but here it is convenient to apply it also to other matrices). A *class* of A (or strongly connected component of $G(A)$) is characterized as being a subset of $\{1, \ldots, n\}$ which is maximal with respect to the property that it is either a singleton or else there is a path (directed sequence of edges) from each element of the subset to every other element. The graph $G(A)$ is called *essentially transitive* if, for $i \neq j$, (i, j) is an edge of $G(A)$ whenever there is a path from i to j in $G(A)$. The set of classes of A will be called the *class structure* of A, cf. [4, p. 42]. If $P \geqslant 0$ (elementwise) and $r \geqslant 1$ it is easy to see that (i, j) is an edge of $G(P^r)$ whenever there is a path from i to j in $G(P)$ consisting of r edges. It follows that each class of P^r is contained in a class of P. Hence we can easily prove the following lemma which is related to known results, e.g. Johnson [8].

LEMMA 3.8 *Let P be a nonnegative matrix and let*

$$Q = \sum_{r=0}^{\infty} c_r P^r,$$

where $c_r \geqslant 0$, for $r = 1, 2, \ldots$. If $c_1 > 0$ then P and Q have the same *class structure. If $c_r > 0$, $r = 1, 2, \ldots,$ then $G(Q)$ is essentially transitive.* ■

We have the following completion of Theorem (3.5) and Corollaries (3.6) and (3.7).

THEOREM 3.9 *Let $A \in \mathbf{M}_1^*$. Let $g(z)$ be a function analytic in U such that $g'(z)$ is totally oscillating at 1. If $g'(1) > 0$ then A and $g(A)$ have the same class structures. If $g^{(r)}(1) \neq 0$, $r = 1, 2, \ldots,$ then the graph of $g(A)$ is transitive. In particular* $\log A$ *and A^q, where $0 < q < 1$, have the same class structure as A and their graphs are essentially transitive.*

Proof Follows immediately from Lemma (3.8) since $g(z) = c_0 - \sum_{r=1}^{\infty} c_r$, where $c_r > 0$, $r = 1, 2, \ldots$. ■

We end this section by showing that there is a converse to Theorem (3.5) provided that we consider all orders of square matrices. Thus the totally oscillating functions arise naturally in the type of problem we are considering.

THEOREM 3.10 *Let $g(z)$ be a function analytic in U. Then the following are equivalent*:

(a) *$g'(z)$ is totally oscillating at* 1,
(b) *For all orders of square matrices, $A \in \mathbf{M}_1^*$ implies $g(A) \in \mathbf{Z}_1$.*

Proof In view of Theorem (3.5), we need only prove that (b) implies (a). We assume that $(-1)^s g^{(s)}(1) < 0$ for some s, $s \geqslant 1$, and we shall construct an $A \in \mathbf{M}_1^*$ for which $g(A) \notin \mathbf{Z}_1$. We let $n > s$ and we put $A = I - J$, where J is the matrix with entry 1 everywhere in the first super-diagonal and entry 0 elsewhere. Then we define B by

$$B = g(A) = c_0 I - \sum_{r=1}^{n-1} c_r J^r,$$

where $-c_r = (-1)^r g^{(r)}(1)/(r!)$, $r = 1, \ldots, n-1$ and $c_0 = g(1)$. Hence $b_{1,s} = -c_s > 0$ and so $g(A) \notin \mathbf{Z}_1$. ■

We remark that it is easy to find functions which satisfy the hypothesis of Theorem (3.10) which are not Pick functions, e.g. $g(z) = 1 - (1-z)^3$. Of course, Ando [3] obtains many properties for Pick functions in addition to $g(A) \in \mathbf{Z}_1$.

§4. UNIQUENESS OF ROOTS OF MATRICES IN M

In the last section we showed that $A^{1/p} \in \mathbf{M}$ if $A \in \mathbf{M}$ and $p > 1$. In this section we investigate the uniqueness of the solution of $B^p = A$ for $B \in \mathbf{M}$. If B and C are commuting matrices satisfying certain conditions, we have $(BC)^p = B^pC^p$. Some restrictions are clearly necessary in this identity for, according to our definition in §3, the corresponding result does not even hold for all complex numbers β, γ, e.g. if $\beta = \gamma = e^{4i\pi/5}$ and $p = 5/2$ then $\beta^p = \gamma^p = 1$, but $(\beta, \gamma)^p = -1$. However $(\beta\gamma)^p = \beta^p\gamma^p$ if $|\arg \beta + \arg \gamma| < \pi$ and so it is natural to assume a restriction on the spectra of B and C. However, even then the identity is not self evident, and we supply a proof in the form of a sequence of two lemmas. The proof of the first of these is based on a suggestion of H. W. Knobloch.

For commuting indeterminates x, y, z, we let $\mathbb{C}[\![x]\!]$ or, $\mathbb{C}[\![x, y]\!]$ or $\mathbb{C}[\![x, y, z]\!]$ be the rings of formal powers series in x, or x, y or x, y, z respectively, with coefficients in $\mathbb{C}$. If $F(x) \in \mathbb{C}[\![x]\!]$, we say that $F(x)$ represents the analytic function $\alpha \to F(\alpha)$ if for α in some neighborhood of the origin $F(\alpha)$ converges.

LEMMA 4.1 *Let x and y be commuting indeterminates and let* $F(x) = 1 + \binom{p}{1}x + \binom{p}{2}x^2 + \cdots$ *in* $\mathbb{C}[\![x, y]\!]$. *Then*

$$F(x)F(y) = F(x + y + xy).$$

Proof Let z be an indeterminate which commutes with x and y. In $\mathbb{C}ax, y, zb$ define

$$F(xz)F(yz) = \sum_{r=0}^{\infty} P_r(x, y)z^r,$$

$$F(xz + yz + xyz^2) = \sum_{r=0}^{\infty} Q_r(x, y)z^r,$$

where the $P_r(x, y)$ and $Q_r(x, y)$ are in $\mathbb{C}[\![x, y]\!]$. Evidently the $P_r(x, y)$ and $Q_r(x, y)$ are polynomials. Let α, β, γ be in the neighborhood $V = \{z \in \mathbb{C} : |z| < 1/4\}$ of 0. Since $F(\delta) = (1 + \delta)^p$ $\delta = \alpha\gamma$, $\delta = \beta\gamma$ or $\delta = \alpha\gamma + \beta\gamma + \alpha\beta\gamma^2$ we have

$$F(\alpha\gamma)F(\beta\gamma) = F(\alpha\gamma + \beta\gamma + \alpha\beta\gamma^2).$$

But the corresponding series converge absolutely and hence we may rearrange terms to obtain

$$\sum_{r=0}^{\infty} P_r(\alpha, \beta)\gamma^r = \sum_{r=0}^{\infty} Q_r(\alpha, \beta)\gamma^r.$$

Thus $\sum_{r=0}^{\infty} P_r(\alpha, \beta)z^r$ and $\sum_{r=0}^{\infty} Q_r(\alpha, \beta)z^r$ represent the same analytic function. Since this holds for all $\alpha, \beta \in V$, we now deduce that $P_r(x, y) = Q_r(x, y)$. Hence $F(xz)F(yz) = F(xz + yz + xyz^2)$. The lemma follows on replacing z by 1. ∎

LEMMA 4.2 *Let B, C be commuting nonsingular matrices in $\mathbb{C}^{nn}$ and suppose, that for $\beta \in \operatorname{spec} B$, $\gamma \in \operatorname{spec} C$. $|\arg \beta + \arg \gamma| < \pi$. Let $p \in \mathbb{R}$. Then $B^p C^p = (BC)^p$.*

Proof Since B and C commute there is a nonsingular $Q \in \mathbb{C}^{nn}$ such that

$$QBQ^{-1} = \sum_{i=1}^{s} \oplus \beta_i (I_i + X_i)$$

$$QCQ^{-1} = \sum_{i=1}^{s} \oplus \gamma_i (I_i + Y_i)$$

where $\beta_i \in \operatorname{spec} B$, $\gamma_i \in \operatorname{spec} C$, I_i is an identity matrix and X_i, Y_i are commuting strictly upper triangular matrices of the same order as I_i, $i = 1, \dots, s$. Since

$$QB^pQ^{-1} = (QBQ^{-1})^p = \sum_{i=1}^{s} \oplus \beta_i^p (I_i + X_i)^p,$$

$$QC^pQ^{-1} = (QCQ^{-1})^p = \sum_{i=1}^{s} \oplus \gamma_i^p (I_i + Y_i)^p,$$

it is enough to prove the lemma for matrices of form $B = I + X$, $C = I + Y$ where X, Y are commuting strictly upper triangular matrices. Evidently $BC = I + U$, where $U = X + Y + XY$ and U is also nilpotent. But then

$$B^p = I + \binom{p}{1} X + \binom{p}{2} X^2 + \cdots$$

since X is nilpotent, and a similar expansion holds for C^p and $(BC)^p$. The lemma now follows immediately from Lemma (4.1). ∎

For $0 < \theta \leqslant \pi$, we define a sector in the complex plane

$$S(\theta) = \{0 \neq z \in \mathbb{C} : -\theta < \arg z < \theta\}.$$

A matrix A is called *positively stable* if $\operatorname{spec} A \subseteq S(\pi/2)$, the open right half plane.

LEMMA 4.3 *Let $A \in \mathbb{C}^{nn}$ be positively stable and let $p \geqslant 1$. Then* $\operatorname{spec} A^{1/p} \subseteq S(\pi/2p)$ *and $B = A^{1/p}$ is the unique matrix such that $B^p = A$ and* $\operatorname{spec} B \subseteq S(c\pi/2p)$ *where* $c = \min(3, 2p-1)$.

Proof Let $B = A^{1/p}$. Clearly $\operatorname{spec} B \subseteq S(\pi/2p)$. Let $C \in \mathbb{C}^{nn}$ satisfy $\operatorname{spec} C \subseteq S(c\pi/2p)$ and $C^p = A$. Then C commutes with A and hence also with B. Since C is non-singular we may put $D = C^{-1}B$. Since B and C commute and

$$|\arg\beta - \arg\gamma| < \frac{\pi}{2p} + \frac{(2p-1)\pi}{2p} = \pi$$

it follows by Lemma 4.2 that $D^p = (C^{-1})^p B^p = (C^p)^{-1} B^p = I$. Further every eigenvalue of D is of form $\delta = \gamma^{-1}\beta$, where $\beta \in \operatorname{spec} B$ and $\gamma \in \operatorname{spec} C$. Since $\delta^p = 1$ and

$$|\arg\delta| = |\arg\beta - \arg\gamma| < \frac{\pi}{2p} + \frac{3\pi}{2p} = \frac{2\pi}{p}$$

we must have $\delta = 1$. Next, every matrix satisfying $D^p = 1$ is similar to a diagonal matrix [7, p. 100]. Hence $D = I$ and we deduce that $C = B$. ∎

THEOREM 4.4 *Let $A \in \mathbf{M}$ and let $1 \leqslant p \leqslant 3$. Then $B = A^{1/p}$ is the unique matrix in $\mathbf{M}$ satisfying $B^p = A$.*

Proof By Corollary (3.7), $B \in \mathbf{M}$. From the definition of c it follows that $c\pi/2p \geqslant \pi/2$. Hence uniqueness follows from Lemma (4.3). ∎

THEOREM 4.5 *Let $A \in \mathbf{M}$ and let $p > 3$. Then $B = A^{1/p}$ is the unique matrix in $\mathbf{M}$ satisfying*

(a) $B^p = A$,

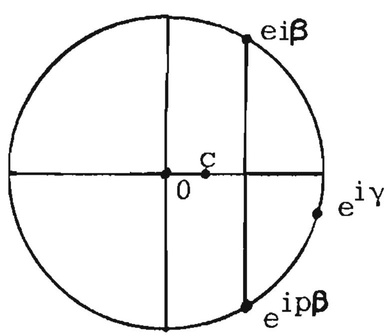
(b) $B, B^2, \ldots, B^m$ *are in* $\mathbf{M}$, *where m is the integer satisfying* $p/3 \leqslant m < (p/3) + 1$.

Proof We repeat the first part of the proof of Theorem (4.4) Thus $B = A^{1/p}$ satisfies $B^p = A$. Further, by Corollary (3.7), $B^k = A^{kq} \in \mathbf{M}$, $k = 1, \dots, m$, since $mq < (1/3) + q < 1$, where $q = 1/p$. Now suppose that $C \in \mathbb{R}^{nn}$ satisfies (a) and (b). From (b) we obtain successively $\operatorname{spec} C \subseteq S(\pi/2)$, $\operatorname{spec} C \subseteq S(\pi/4), \dots,$ $\operatorname{spec} C \subseteq S(\pi/2m)$. Since $m \geqslant p/3$, clearly $\pi/2m \leqslant 3\pi/2p$. Thus $\operatorname{spec} C \subseteq S(c\pi/2p)$, where $c = \min(3, 2p - 1) = 3$. It now follows from Lemma (4.3) that $C = B$. ∎

The question arises to what extent $B \in \mathbf{M}$ and $B^p = A \in \mathbf{M}$ is sufficient to ensure $B = A^{1/p}$ even when $p > 3$. When $\mathbf{K} = \mathbf{K}_2$ the result is true and well known. (The proof depends on the observation that if D is a diagonal matrix with positive diagonal elements, then $UD^pU^{-1} = VD^pV^{-1}$ implies $UDU^{-1} = VDV^{-1}$). By considering the case $\mathbf{K} = \mathbf{K}_3$ we thus have the following corollary.

COROLLARY 4.6 *Let A be a positive definite Z-matrix and let $p > 1$. Then the unique positive definite matrix B satisfying $B^p = A$ is $B = A^{1/p}$ and B is also a Z-matrix.* ∎

For general $\mathbf{K}$ some further conditions are required for uniqueness. We show this by means of an example which is easily understood from the diagram below.



Example 4.7 (i) Let $n \geqslant 2$ and $p > 3$. We put $\beta = 2\pi/(1 + p)$ and $\gamma = -2\pi/p(1 + p)$. Then it is easy to show that $0 < \beta < \pi/2$, $3\pi/2 < p\beta = 2\pi - \beta < 2\pi$. Hence $0 < \cos\beta = \cos p\beta$. Also $0 < -\gamma < \beta$

and so $\cos\gamma > \cos\beta$. Now choose c so that $0 < c < \cos\beta$. Let B be a diagonal matrix in $\mathbb{R}^{nn}$ for which $b_{11} = c$ and either $b_{ii} = e^{i\beta}$ or $b_{ii} = e^{i\gamma}$, $i = 2, \ldots, n$. Then $B \in \mathbf{M}_4$. Let A be the diagonal matrix given by $a_{11} = c^p < \cos\beta$, and $a_{ii} = e^{ip\beta}$, $i = 2, \ldots, n$. Thus $A \in \mathbf{M}_4$. Since $e^{ip\beta} = e^{ip\gamma}$, there are at least $2^{(n-1)}$ matrices B in $\mathbf{M}_4$ such that $B^p = A$.

(ii) In the above example it is possible to choose p and c so that $A \in \mathbf{M}_4^*$, $B \in \mathbf{M}_4$, but $B \notin \mathbf{M}_4^*$. Let $p > 5$. Then $0 < \beta < \pi/3$. Choose c such that $\sqrt{2}\sqrt{1-\cos\beta} < c < \cos\beta$ but $c^p < \sqrt{2}\sqrt{1-\cos\beta}$. Then define B by $b \quad = c$, $b \quad = e^{i\beta}$, $i = 2, \ldots, n$ and A as above.

We shall show that for $n \geqslant 3$ and real p, $p > 12$, there exist two different M-matrices (viz. in $\mathbf{M}_1$) B_0, B_1 and an M-matrix A such that $B_0^p = B_1^p = A$. It is enough to consider the case $n = 3$.

Example 4.8 Let

$$X = \frac{1}{\sqrt{3}}\begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix}.$$

Then

$$X^2 = -\frac{1}{3}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}.$$

Let $p > 12$ and put $e^{2\pi i/p} = c + is$, where $c, s \in \mathbb{R}$. Since X is similar to the diagonal matrix $\operatorname{diag}(0, i, -i)$, it is easy to prove that

$$W = I + sX + (1-c)X^2$$

satisfies $W^p = I$. Let $\epsilon > 0$ and

$$B_0 = \epsilon I - X^2,$$
$$B_1 = B_0 w = \epsilon I + s(1+\epsilon)X - (c + \epsilon c - \epsilon)X^2.$$

Then

$$A = B_0^p = B_1^p = \epsilon^p I + \left((1+\epsilon)^p - \epsilon^p\right)X^2.$$

Thus B_0 and A are M-matrices and so is B_1 provided that

$$\frac{s(1+\epsilon)}{\sqrt{3}} \leqslant \frac{c(1+\epsilon) - \epsilon}{3}.$$

Since $s/c = \tan(2\pi/p) < 1/\sqrt{3}$, the inequality holds for sufficiently small positive ϵ.

C. R. Johnson (private communication) has informed us that he has found a similar example. He has also shown that a 3×3 M-matrix has a unique pth root which is an M-matrix when $p \leqslant 12$.

§5. CHARACTERIZATIONS OF M

In this entire section we suppose that the positivity cone $\mathbf{K}$ of matrices satisfies condition (2.4). We shall extend the well-known result that for $A \in \mathbf{Z}_1$ we have $A \in \mathbf{M}_1$ if and only if $A^{-1} \in \mathbf{K}_1$. We first show that this result holds for general $\mathbf{K}$.

LEMMA 5.1 *Let $A \in \mathbf{Z}$. Then $A \in \mathbf{M}$ if and only if A^{-1} exists and $A^{-1} \in \mathbf{K}$.*

Proof Let $A \in \mathbf{M}$. Then $A = t(I - P)$, where $t > 0$, $P \geqslant 0$ and $\rho(P) < 1$. Hence $A^{-1} = t^{-1}\sum_{r=0}^{\infty} P^r \geqslant 0$. Conversely, let $A = (sI - P)$ and $A^{-1} \geqslant 0$. By [10, Thm. 5.2], there exists an F, $0 \neq F \subseteq \overline{\omega}(P) \subseteq \mathbf{K}$ such that $AF = (sI - P)F = (s - \rho)F$. Thus $F = (s - \rho)A^{-1}F$ where $\rho = \rho(P)$. Since $AF = FA$, the matrices A^{-1} and F commute and hence $A^{-1}F \in \mathbf{K}$. But $\mathbf{K}$ is pointed, and so $s - \rho > 0$. Hence $A \in \mathbf{M}$. ∎

We have actually shown the stronger result that $A \in \mathbf{M}$ implies that $A^{-1} \geqslant \epsilon I$ for some $\epsilon > 0$. We may now use the results of §3 to characterize $\mathbf{M}$ as a subset of $\mathbf{Z}$. We shall write $A^{-1/p} \in \mathbf{M}$ to mean that $A^{-1/p}$ is defined and $A^{-1/p} \in \mathbf{M}$, etc.

THEOREM 5.2 *Let $A \in \mathbf{Z}$ and let p be a positive integer. Then the following are equivalent:*

(a) $A \in \mathbf{M}$,
(b) $A^{1/p} \in \mathbf{M}$,
(c) *There is a $B \in \mathbf{M}$ for which $B^p = A$,*
(d) *There is an $\epsilon > 0$ for which $A^{-1/p} \geqslant \epsilon I$,*
(e) *There is an $\epsilon > 0$ and a $C \geqslant \epsilon I$ for which $C^p = A^{-1}$,*
(f) $A^{-1/p} \geqslant 0$,
(g) *There is a $C \geqslant 0$ for which $C^p = A^{-1}$.*

Proof First we prove (a)$\Rightarrow$(b)$\Rightarrow$(d)$\Rightarrow$(f)$\Rightarrow$(g)$\Rightarrow$(a):

(a)$\Rightarrow$(b) By Corollary (3.7).

(b)$\Rightarrow$(d) Apply Lemma (5.1) and the remark following its proof to $A^{1/p}$.

(d)$\Rightarrow$(f)$\Rightarrow$(g) Trivial.

(g)$\Rightarrow$(a) Since p is a positive integer $A^{-1} = C^p \geqslant 0$. Then use Lemma (5.1).

Next we show (b)$\Rightarrow$(c)$\Rightarrow$(e)$\Rightarrow$(g):

(c)$\Rightarrow$(e) Apply Lemma (5.1) and the remark following to B. The other implications are obvious. ■

Technically $A^{-1/p}$ has not been defined if A has a negative eigenvalue, for the function $z^{-1/p}$ is not analytic on the negative axis, cf. our definition in §3. However, given any nonsingular A, by cutting the complex plane along the ray $\arg z = \pi + \epsilon$, where $\epsilon \geqslant 0$ and ϵ is sufficiently small, we may assume that $z^{-1/p}$ is analytic for all $\lambda \in \operatorname{spec} A$ and coincides there with our previous definition. Thus in Theorem 5.2 we may regard $A^{-1/p}$ to be well defined for all nonsingular $A \in \mathbb{C}^{nn}$. Similar remarks apply to $\log A$ in the next theorem.

THEOREM 5.3 *Let $A \in \mathbf{Z}$. Then the following are equivalent*:

(a) $A \in \mathbf{M}$,

(b) $\log A \in \mathbf{Z}$,

(b) *There is a $B \in \mathbf{Z}$ for which $e^B = A$.*

Proof Corollary (3.6) yields (a)$\Rightarrow$(b) and since (b)$\Rightarrow$(c) is trivial, we need only prove that (c)$\Rightarrow$(a).

So let (c) hold for some $B \in \mathbf{Z}$.

Put $B = tI - P$ where $t \in \mathbb{R}$ and $P \geqslant 0$. Then

$$A^{-1} = e^{-B} = e^{-t}e^{P} \geqslant 0,$$

and $A \in \mathbf{M}$ by Lemma (5.1). ■

The substance of Theorems (5.2) and (5.3) will now be generalized. The function $z^{-1/p}$ and $\log z$ which occur there are totally oscillating at 1 and (as will shortly be shown) $A \in \mathbf{M}^*$ implies $g(A) \geqslant 0$ for every function $g(z)$ analytic in U which is totally oscillating at 1. But the desired converse implication may fail. For example let $A = -I$ and $g(z) = z^{-2}$. Then $A \in \mathbf{Z}^*$ and $g(z)$ is totally oscillating at 1. Also $g(A) \geqslant 0$ but $A \notin \mathbf{M}^*$. Thus we are led to the following concept.

DEFINITION 5.4 Let V be an open set in $\mathbb{C}$ which contains the set $U = \{z \in \mathbb{C} : |z - 1| < 1\}$. We call $(f(z), g(z))$ a *reciprocating pair of* *functions* (on V) if

(a) $f(z)$ is an entire function which is totally nonnegative at 1,

(b) $g(z)$ is a function analytic in V which is totally oscillating at 1 and $g(1) = 1$,

(c) $f(g(z)) = z^{-1}$, for $z \in V$.

(Observe that (b) and (c) imply that $f(1) = 1$).

Examples 5.5

(a) Let p be a positive integer. Then (z^p, z^{-p}) where $q = 1/p$, are a reciprocating pair on $\mathbb{C}\backslash\mathbb{R}_-$.

(b) Let $k > 0$ and let $f(z) = e^{k(z-1)}$ and $g(z) = 1 - k^{-1}\log z$. Then $(f(z), g(z))$ are a reciprocating pair on $\mathbb{C}\backslash\mathbb{R}_-$.

THEOREM 5.6 *Let $(f(z), g(z))$ be a reciprocating pair of functions. Let $A \in \mathbf{Z}^*$. Then the following are equivalent:*

(a) $A \in \mathbf{M}^*$,

(b) *($g(A)$ is defined and) $g(A) \geqslant I$,*

(c) *there is a $B \geqslant I$ for which $f(B) = A^{-1}$.*

Proof (a)$\Rightarrow$(b). Since $\operatorname{spec} A \subseteq U \subseteq V$ the function $g(A)$ is defined. Since $g(1) = 1$, we have $g(A) = I + \sum_{r=1}^{\infty} b_r P^r$, where $b_r = (-1)^r g^{(r)}(1)/r! \geqslant 0$, cf. (3.3) and (3.4). Hence $g(A) \geqslant 1$.

(b)$\Rightarrow$(c). By (5.4c), $f(g(A)) = A^{-1}$ cf. [5, Theorem 5, p. 602].

(c)$\Rightarrow$(a). Suppose that $B = I + Q$, $Q \geqslant 0$, and $f(B) = A^{-1}$. Then $A^{-1} = f(I + Q) = \sum_{r=0}^{\infty} d_r Q^r$, where $d_r = f(r)(1)/r! \geqslant 0$, $r = 0, 1, \ldots$. Hence $A^{-1} \geqslant 0$. By Lemma (5.1) it follows that $A \in \mathbf{M}$. ∎

Our proof shows that the implications (a)$\Rightarrow$(b)$\Rightarrow$(c) hold for functions $g(z)$ satisfying (5.4b) and that the implication (c)$\Rightarrow$(a) holds for functions $f(z)$ satisfying (5.4a) and $f(1) = 1$.

The assumption that $f(z)$ is entire cannot be omitted from the hypotheses of Theorem (5.6). For the pair $((2-z)^{-1}, 2-z)$ satisfies all other conditions for a reciprocating pair and if $A = I - P$, where $P \geqslant 0$, then $B \equiv g(A) = I + P \geqslant I$. Clearly $f(B) = A^{-1}$, if A is nonsingular. Thus no conclusion on $\rho(P)$ can be drawn.

Note added in proof. As an application of a spectral theorem in two variables Hartwig [14] has obtained a general result which contains our Lemma 4.2 as a special case.

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