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NONNEGATIVE SOLUTIONS OF A QUADRATIC MATRIX EQUATION ARISING FROM COMPARISON THEOREMS IN ORDINARY DIFFERENTIAL EQUATIONS*

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Abstract. We study the quadratic matrix equation

$$X^2+\beta X+\gamma A=0,$$

where A is a given elementwise nonnegative (resp. positive semi-definite) matrix and the solution X is required to be an elementwise nonnegative (resp. positive semi-definite) matrix. When $\beta=-1$ and $\gamma=1$, our results may be used, for example, to obtain a simple nonoscillation criterion for the matrix differential equation

$$Y''(t)+Q(t)Y(t)=0,$$

where Y and Q are matrix-valued functions and ′ denotes differentiation. This generalizes a result of Hille for the scalar case. Extensions are given when A and X are nonnegative with respect to more general cone orderings.

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1. Introduction. In this paper we characterize the existence of solutions of the quadratic matrix equation

$$X^2+\beta X+\gamma A=0, \tag{1.1}$$

where γ and β are given real scalars and A is a given "nonnegative" $n\times n$ matrix. We first consider the case when $\gamma>0$, $\beta<0$ and A is either Hermitian positive semi-definite or elementwise nonnegative. The solution X is then restricted to be Hermitian or elementwise nonnegative, respectively. In these cases we completely characterize the existence of a solution in terms of the spectrum of A; see § 2.

In § 3 we use the notion of a positivity cone K, see [9], to unify and extend the results of § 2. Thus, in the case that $\gamma>0$, we characterize the existence of nonnegative or M-matrix (with respect to K) solutions of (1.1) when A is nonnegative (with respect to K).

The problem of the existence of solutions of (1.1) arises in the context of comparison theorems for two matrix-valued ordinary differential equations. Consider the equation

$$Y''(t)+Q(t)Y(t)=0. \tag{1.2}$$

Here Y and Q are continuous $n\times n$ matrix-valued functions and ′ denotes differentiation. Such equations arise both in the self-adjoint case (in the study of Hamiltonian

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systems, for example [7], [8]) and in the nonself-adjoint case [1], [5]. See also the references in [5]. A solution $Y(t)$ of (1.2) is said to be nonoscillatory if for some t_0 it is nonsingular for all $t \geqq t_0$. In that case we may form the so-called Riccati equation

$$Z'(t)+Z^2(t)+Q(t)=0, \qquad t \geqq t_0 \tag{1.3}$$

where $Z(t)=Y'(t)Y^{-1}(t)$.

Of interest are comparison theorems between two equations of the form (1.2) with different coefficients. Thus we consider also the equations

$$Y''(t)+Q_1(t)Y(t)=0, \tag{1.2_1}$$

$$Z'(t)+Z^2(t)+Q_1(t)=0. \tag{1.3_1}$$

In the scalar case ($n=1$), the classical Sturm comparison theorem yields the result that if (1.2) has a nonoscillatory solution (and therefore (1.3) has a solution on some interval $[t_0, \infty)$) and if $Q(t) \geqq Q_1(t)$ for all t, then $(1.2)_1$ will have a nonoscillatory solution (and $(1.3)_1$ will have a solution on $[t_0, \infty)$). There are many other comparison theorems in the scalar case (see [12], for example).

The extension of comparison theorems to the general matrix case requires some kind of ordering on the coefficient matrices $Q(t)$, $Q_1(t)$; hence some form of positivity must be defined. Positive semi-definite is the appropriate concept for studying self-adjoint equations; positive cone versions of positivity are a suitable choice for nonself-adjoint equations.

The idea behind comparison theorems is that the oscillatory or nonoscillatory character of an equation $(1.2)_1$ may be determined by comparison with some equation (1.2) whose behavior is known.

Here we shall confine ourselves to obtaining a simple nonoscillation criterion for $(1.2)_1$, which is a generalization of a well-known result of Hille [10] in the scalar case.

Suppose that

$$P(t)=\lim_{T\to\infty}\int_t^T Q(s)\,ds$$

and

$$P_1(t)=\lim_{T\to\infty}\int_t^T Q_1(s)\,ds$$

both exist, and are finite, and that

$$P(t) \geqq |P_1(t)| \geqq 0 \quad \text{for all } t, \tag{1.4}$$

in the sense that $P(t)-|P_1(t)|$ has nonnegative elements, and where $|P_1(t)|$ is the matrix whose elements are the absolute values of those of $P_1(t)$.

Under these assumptions, it was shown in [5] that if (1.3) has a positive solution $Z(t)$ on $[t_0, \infty)$, then $(1.3)_1$ has a positive solution $Z_1(t)$, where $0 \leqq Z_1(t) \leqq Z(t)$, $t \geqq t_0$. (This is a generalization of the Hille–Wintner theorem in the scalar case [10], [12]).

To apply this result, we look for a suitable candidate for $Q(t)$.

If $Q(t)=t^{-2}A$, where A is a constant $n\times n$ matrix, we can try to find a solution of (1.3) of the form $Z(t)=t^{-1}X$, where X is a constant $n \times n$ matrix. This leads to the quadratic matrix equation

$$X^2-X+A=0. \tag{1.5}$$

To use the comparison theorem quoted above we require that A and X are positive.

Then the solvability of (1.5) reduces to that of (1.1) with $\beta=-1$, $\gamma=1$. Let $\rho(A)$ be the spectral radius of A. Theorem 2.3 of § 2 will show that (1.5) has a nonnegative solution X if and only if

$$\rho(A)<\tfrac{1}{4}, \text{ or } \rho(A)=\tfrac{1}{4} \text{ and the eigenvalues of } A \text{ which have modulus } \tfrac{1}{4} \text{ have degree equal to } 1, \tag{1.6}$$

where the degree is the size of the largest Jordan block. Denoting the set of nonnegative matrices A satisfying (1.6) by $\mathscr{A}$, we have:

THEOREM 1.1. *Let $Q_1(t)$ be continuous, such that*

$$t\left|\int_t^\infty Q_1(s)\,ds\right|\leqq A$$

for all sufficiently large t, for some $A\in\mathscr{A}$.

Then $(1.2)_1$ *has a nonoscillatory solution Y_1 whose associated Riccati variable Z_1 satisfies $|Z_1(t)|\leqq t^{-1}X$, t sufficiently large, where X is the unique positive solution of* (1.5).

In the scalar case, A can be any constant $\leqq\frac{1}{4}$, and we have Hille's result.

2. Existence of solutions. By using the substitution $X=-\beta Y$, we may consider the equation

$$X^2-X+A=0 \tag{2.1}$$

rather than (1.1), and this we choose to do.

We answer the following two questions concerning existence of solutions:

1. A is given Hermitian, positive semi-definite (psd) and we require X to be Hermitian;
2. A is given real and nonnegative (elementwise) and we require X to be real and nonnegative.

The Hermitian case essentially reduces to a scalar problem, and we have:

THEOREM 2.1. *Suppose that A is a given Hermitian matrix. Then* (2.1) *has a Hermitian solution X if and only if*

$$\sigma(A)\subset(-\infty,\tfrac{1}{4}] \tag{2.2}$$

where $\sigma(A)$ is the spectrum of A.

Proof. Since $A=X-X^2$ is a polynomial in X, A commutes with any solution X and so A and X can be simultaneously diagonalized by some unitary matrix U. Thus X is a Hermitian solution of (2.1) if and only if

$$D^2-D+\Lambda=0 \tag{2.3}$$

has a solution, where $D=UXU^*$ and $\Lambda=UAU^*$ are the diagonal matrices of eigenvalues of X and A, respectively. Thus the diagonal elements satisfy

$$d_i^2-d_i+\lambda_i=0,\qquad i=1,\cdots,n.$$

Since $d_i=\frac{1}{2}(1\pm\sqrt{1-4\lambda_i})$ is real if and only if $1-4\lambda_i\geqq0$, the result follows.

COROLLARY 2.1. *Let A be psd. Then* (2.1) *has a Hermitian solution X if and only if $\sigma(A)\subset[0,\frac{1}{4}]$, and in this case $\sigma(X)\subset[0,1]$, i.e. all Hermitian solutions are psd.*

Proof. The result follows since we need $1+\sqrt{1-4\lambda_i}\geqq0$ for all i.

Now we consider the case that $0\neq A\geqq0$ elementwise, and we seek $X\geqq0$ (elementwise) to solve (2.1). The solution of this problem again rests upon the spectrum of A.

If X solves (2.1), then

$$0=X^2-X+A=(X-\tfrac{1}{2}I)^2-\tfrac{1}{4}I+A,$$

so

(2.4) $$X=\tfrac{1}{2}(I\pm S),$$

where

(2.5) $$S=(I-4A)^{1/2}.$$

If S should admit a series expansion, then

(2.6) $$X=\frac{1}{2}I\pm\frac{1}{2}\sum_{i=0}^{\infty}(-1)^i\binom{\frac{1}{2}}{i}(4A)^i,$$

so

(2.7) $$X=-\frac{1}{2}\sum_{i=1}^{\infty}(-1)^i\binom{\frac{1}{2}}{i}(4A)^i,$$

choosing the negative sign in (2.6), so that $X\geqq 0$. This series will converge if $4\rho<1$ and diverge if $4\rho>1$.

Now consider the following iterative scheme:

(2.8) $$X_1=A,\qquad X_{n+1}=A+X_n^2,\quad n=1,2,\cdots.$$

If X_n converges to X as $n\to\infty$, we shall have $X=A+X^2$; clearly $X\geqq 0$, and so will be a nonnegative solution of (2.1). The iterative scheme has the following properties.

LEMMA 2.1. *Suppose that* $X\geqq 0$ *solves* (2.1). *Then the sequence of iterates in* (2.8) *satisfies*

(2.9) $$0\leqq X_n\leqq X_{n+1}\leqq X,\qquad n=1,2,\cdots,$$

and

(2.10) $$S_n\leqq X_n\leqq S_{2^n-1},\qquad n=1,2,\cdots,$$

where S_k *denotes the partial sum of degree* k *of the series in* (2.7).

Proof. $X_1=A\leqq A+X^2=X$, and

$$X_1=A\leqq A+A^2=X_2=A+X_1^2\leqq A+X^2=X,$$

i.e. (2.9) holds for $n=1$. Assume that (2.9) holds for a particular value of n. Then

$$X_{n+1}-X_n=(X_n^2-X_{n-1}^2)\geqq 0,$$

and similarly, $X-X_{n+1}\geqq 0$. Thus (2.9) follows by induction.

To obtain (2.10), observe that the power series X defined by (2.7) formally satisfies

(2.11) $$X=X^2+A.$$

Denote the partial sum of degree k of the formal series for X^2 by T_k. Since X has no constant term, formally squaring the power series shows that $T_{n+1}\leqq S_n^2$, $n=1,2,\cdots$.

From (2.11), we have $S_{n+1}=T_{n+1}+A$, and so

(2.12) $$S_{n+1}\leqq S_n^2+A,\qquad n=1,2,\cdots.$$

Again, we see that $T_{2^n}\geqq S_{2^{n-1}}^2$, and so

(2.13) $$S_{2^n}\geqq S_{2^{n-1}}^2+A,\qquad n=1,2,\cdots.$$

Since $S_1 = S_{2^0} = X_1 = A$, a simple induction argument with (2.12) and (2.13) gives (2.10), which completes the proof of the lemma.

In fact, by considering the case when A is a scalar, we see that the infinite series, obtained by expanding the iteration (2.8), must be the same as (2.7).

Now we can obtain the following existence result.

THEOREM 2.3. (i) $4\rho < 1$ *implies that there is a nonnegative solution to* (2.1).

(ii) $4\rho > 1$ *implies that there is no nonnegative solution to* (2.1).

(iii) *If* $4\rho = 1$, *then* (2.1) *has a nonnegative solution if and only if the eigenvalues of A which are equal to the spectral radius in modulus, have degree* 1, *that is,*

$$|\lambda_i| = \rho \Rightarrow \lambda_i \text{ has degree } 1. \tag{2.14}$$

Proof. If $4\rho < 1$, the nonnegative solution X is given explicitly by (2.7).

Now suppose that $4\rho > 1$ and that $X \geqq 0$ is a solution of (2.1). By (2.9) of Lemma 2.1, the iterates of (2.8) are monotone increasing and bounded above by X. Without loss of generality, we may assume that $X_n \to X$, X a positive solution of (2.1). But then (2.10) of Lemma 2.1 shows that X satisfies (2.6), which will be a divergent power series when $4\rho < 1$. This is a contradiction and gives (ii).

Finally suppose that $4\rho = 1$. Suppose that (2.14) holds, and let

$$A = PJP^{-1} \tag{2.15}$$

where J is the Jordan canonical form of A. Convergence of the power series in (2.7) depends only on the individual blocks of J. Since these blocks have spectral radius less than or equal to $\frac{1}{4}$, with equality only if they have degree 1, the power series converges and yields a nonnegative solution to (2.1).

Conversely, suppose that $X \geqq 0$ is a solution of (2.1) and that (2.14) fails to hold. First assume that there is exactly one defective Jordan block corresponding to an eigenvalue equal to ρ. X satisfies (2.4) and S satisfies (2.5). This contradicts the criterion in [2] for the existence of a square root of a singular matrix, which states that the defective Jordan blocks must come in pairs. This then implies that the series in (2.7) diverges if J is replaced by a single defective Jordan block $\hat{J}$. Since the convergence of the series in (2.7) depends only on the individual Jordan blocks, it follows that A cannot have any defective blocks corresponding to an eigenvalue equal to ρ. (We have already seen that the existence of a positive solution of (2.1) implies convergence of the series in (2.7) as the limit of the iterates X_n of (2.8).)

The result now follows, since $|\lambda_i| = \rho$ implies that the degree of λ_i, i.e. the size of the largest block in the Jordan canonical form of A that contains λ_i, is not larger than the degree of the eigenvalue equal to ρ, see e.g. [6]. Thus there can be no defective blocks, and (2.14) must hold.

The above results are related to the notion of an M-matrix. Recall that A is an M-matrix if $A = rI - P$, where $P \geqq 0$ and $\rho(P) \leqq r$. If $\rho(P) = r$, then A is a singular M-matrix. Note that if A is an M-matrix then A has the Z-matrix sign pattern, i.e. $a_{ij} \leqq 0$ if $i \neq j$. If A is an invertible M-matrix, then $A^{-1} \geqq 0$ and moreover, A has a square root $A^{1/2}$ which is also an M-matrix. See e.g. [3]. The M-matrix property arises in (2.5), for if $4\rho < 1$, then S^2 is an invertible M-matrix and so has a square root S which is also an M-matrix. This implies that $X = \frac{1}{2}(-\beta I + S) \geqq 0$. Our proofs yield the following for singular M-matrices.

COROLLARY 2.1. *The (singular) M-matrix* $\rho I - A$ *has a square root if and only if* (2.4) *holds.*

The series (2.6) yields two solutions to (2.1). Choosing the negative sign yields

$$X_1 = -\frac{1}{2}\left(\sum_{i=1}^{\infty}(-1)^i\binom{\frac{1}{2}}{i}(4A)^i\right) \geqq 0.$$

The second solution is

$$X_2 = -I + \frac{1}{2}\left(\sum_{i=1}^{\infty}(-1)^i\binom{\frac{1}{2}}{i}(4A)^i\right).$$

Thus $X_2 = I - P$, where $P \geqq 0$, and so is a Z-matrix. But, if $\rho < \frac{1}{4}$, then $\rho(P) < 1$ which implies that X_2 is in fact an M-matrix. The case $\rho = \frac{1}{4}$ is similar. In fact, we have a nonnegative solution if and only if we have an M-matrix solution. For if X is an M-matrix solution, then $X = \frac{1}{2}(I - S)$ with $\rho(S) \leqq 1$, see (2.4). But then $\frac{1}{2}(I - S)$ is a nonnegative solution.

3. Extension to positivity cones. The notion of a positivity cone was introduced in [9] to give a unified treatment of results on M-matrices and positive definite matrices. We now extend our results to such cones. Following [9], we define $\mathbf{K}$ to be a positivity cone of matrices if $\mathbf{K}$ is a pointed, closed, convex cone, i.e. if $K \cap -K = \{0\}$, $\mathbf{K} + \mathbf{K} \subset \mathbf{K}$ and $\lambda\mathbf{K} \subset \mathbf{K}$, for all $\lambda \geqq 0$, and if

$$P \in \mathbf{K} \text{ implies } P^i \in \mathbf{K}, \qquad i = 0, 1, 2, \cdots. \tag{3.1}$$

The cones $\mathbf{K}_1$, of all nonnegative (elementwise) matrices, and $\mathbf{K}_2$, the cone of positive semi-definite Hermitian matrices to which we addressed ourselves in § 2, are examples of positivity cones, as is $\mathbf{K}_1 \cap \mathbf{K}_2$. Additional examples are given in [9].

We let $\mathbf{K}$ denote a positivity cone and partially order $\mathbf{C}^{nn}$ with respect to $\mathbf{K}$, i.e. $P \geqq 0$ if $P \in \mathbf{K}$. Associated with $\mathbf{K}$ are the sets

$$\mathbf{Z} = \{A \in \mathbf{C}^{nn} : A = sI - P, s \in R, P \in K\}, \tag{3.2}$$

$$\mathbf{M} = \{A \in \mathbf{Z} : \operatorname{Re}\lambda \geqq 0, \text{for all eigenvalues } \lambda \text{ of } A\}. \tag{3.3}$$

Corresponding to $\mathbf{K}_1$ and $\mathbf{K}_2$ above, $\mathbf{Z} = \mathbf{Z}_1$ is the set of Z-matrices, $\mathbf{M} = \mathbf{M}_1$ is the set of M-matrices, $\mathbf{Z} = \mathbf{Z}_2$ is the set of Hermitian matrices and $\mathbf{M} = \mathbf{M}_2$ is the set of positive semi-definite matrices.

We would like to unify our results from § 2 as well as extend them to general positivity cones. We shall require the series solution defined by (2.6) and a result corresponding to Lemma 2.1 concerning the iterative scheme (2.8). For the lemma to hold in the new partial order, we need an additional condition, (3.4) below.

LEMMA 3.1. *Lemma* 2.1 *holds if the partial order induced by a positivity cone* $\mathbf{K}$ *is closed under commuting products, i.e.* $\mathbf{K}$ *satisfies*

$$B_1, B_2 \in \mathbf{K}, \qquad B_1B_2 = B_2B_1 \Rightarrow B_1B_2 \in \mathbf{K}. \tag{3.4}$$

(*this is condition* (2.4) *in* [9]).

Proof. Since $A \in \mathbf{K}$ and (3.1) holds for a positivity cone, it follows inductively that the iterates X_n of (2.8) are in $\mathbf{K}$ and are polynomials in A with nonnegative coefficients. Thus we have

$$X_{n+1} - X_n = (X_n^2 - X_{n-1}^2) = (X_n - X_{n-1})(X_n + X_{n-1}), \tag{3.5}$$

since the two factors on the right-hand side commute. It follows inductively from (3.5) that $0 \leqq X_n \leqq X_{n+1}$, $n = 1, 2, \cdots$.

Now suppose that $X \geqq 0$ solves (2.1). Then $X = X^2 + A$, so

$$X^2 = X^3 + AX = X^3 + XA,$$

so X commutes with A. Since the X_n are polynomials in A, it follows that X commutes with each X_n. It is now easy to show that $X_n \leqq X$ for all n, and we have (2.9) of Lemma 2.1.

The proof of (2.10) proceeds as before.

We remark that $\mathbf{K}_1$ and $\mathbf{K}_2$ are both positivity cones that satisfy (3.4).

Next we prove the following result which includes a generalization of Theorem 2.3 to positivity cones satisfying (3.4).

THEOREM 3.1. *Let* $\mathbf{K}$ *be a positivity cone satisfying* (3.4) *and let* $A \geqq 0$ (*with respect to* $\mathbf{K}$). *Then* (2.1) *has a solution* $X \in \mathbf{K}$ *if and only if*

$$4\rho \leqq 1, \tag{3.6}$$

with (2.13) *holding if* $4\rho = 1$.

Proof. If $4\rho < 1$, then the series in (2.7) converges to X, which is a solution to (2.1). From the definition of the positivity cone, $\sum_{i=0}^{\infty} (-1)^i \binom{1/2}{i} (4A)^i \in -\mathbf{K}$. Thus $X \geqq 0$. If $4\rho = 1$ and (2.3) holds, then we still obtain convergence. (See the argument in the proof of Theorem 2.3.) Conversely, suppose that X solves (2.1) and $X \geqq 0$. To complete the proof we need only show that the existence of a solution $X \geqq 0$ of (2.1) implies that the series in (2.7) converges. First we show that the order interval $[0, X] = \{Y: 0 \leqq Y \leqq X\}$ is compact. Suppose not. Then there is a sequence $\{Y_n\} \subset [0, X]$ with $\|Y_n\| \to \infty$. We may assume that $Y_n/\|Y_n\| \to Y \in \mathbf{K}$. But then $(X - Y_n)/\|Y_n\| \in \mathbf{K}$, and upon taking the limit as $n \to \infty$, we find that $-Y \in \mathbf{K}$, a contradiction, since $\mathbf{K}$ is pointed. It follows that $[0, X]$ is compact. Using Lemma 3.1, we deduce that $X_n \to Y$, a solution of (2.1), which implies that the series in (2.7) converges.

Note that an M-matrix solution (with respect to $\mathbf{K}$) is obtained by using the positive sign in the expansion (2.6).

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