

Nonnegatively Posed Problems and Completely Monotonic Functions*†

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1. INTRODUCTION

If we consider the solution $c(x, t)$ of the simple heat conduction equation

$$c_t(x, t) = c_{xx}(x, t) + K, \quad 0 < x < 1, \quad t > 0, \quad (1.1)$$

where K is a positive constant, subject to the boundary conditions that

$$c(x, 0) \equiv 0, \quad 0 \leq x \leq 1, \quad c(0, t) = c(1, t) = 0, \quad t > 0, \quad (1.2)$$

then $c(x, t)$, for any fixed x in $[0, 1]$, increases *monotonically* in t to the steady state solution $\hat{c}(x) = Kx(1 - x)/2$, i.e.,

$$0 \leq c(x, t) \leq c(x, t + \delta) \leq \hat{c}(x) \quad (1.3)$$

for all $t \geq 0$, all $\delta \geq 0$, any $x \in [0, 1]$.

The problem to be treated here is to what extent semidiscretizations (in which the time variable is left continuous) and full discretizations of (1.1), (1.2) possess a monotone behavior analogous to that of (1.3). One of our results (Theorem 10) shows that this problem is closely related to stability in the uniform norm of matrix approximations of (1.1), (1.2).

Our technique for developing these results is in part based on a connection between completely monotonic functions and nonnegative functions of nonnegative matrices. As this gives rise to new proofs of known results on

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nonnegative matrices (cf. Theorems 3 and 4) as well as some new results (Theorems 1, 2, and 5), this connection may be of interest by itself.

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2. COMPLETELY MONOTONIC FUNCTIONS AND BERNSTEIN'S THEOREM

We begin with

DEFINITION 1. Let $G(x)$ be defined in the interval (a, b) where $-\infty \leq a < b \leq +\infty$. Then, $G(x)$ is said to be *completely monotonic* in (a, b) if and only if

$$(-1)^j G^{(j)}(x) \geq 0 \quad \text{for all } a < x < b \text{ and all } j = 0, 1, 2, \dots \quad (2.1)$$

It is known [12, p. 146] that if $G(x)$ is completely monotonic in (a, b) , then it can be extended to an analytic function in the open disk $|z - b| < b - a$ when b is finite, and when $b = +\infty$, G is analytic in $\text{Re}(z) > a$. Thus, for each y with $a < y < b$, $G(z)$ is analytic in the open disk $|z - y| < R(y)$, where $R(y)$ denotes the radius of convergence of $G(z)$ about the point $z = y$. It is clear that $R(y) \geq y - a$ for $a < y < b$.

We now make the change of variables $z = y - \zeta$. Writing

$$G(y - \zeta) = \sum_{j=0}^{\infty} b_j(y) \zeta^j, \quad |\zeta| < R(y), \quad (2.2)$$

it follows that the coefficients $b_j(y)$ are given by

$$b_j(y) = \frac{(-1)^j G^{(j)}(y)}{j!}, \quad j = 0, 1, 2, \dots \quad (2.3)$$

Thus, if $G(x)$ is completely monotonic in (a, b) and y satisfies $a < y < b$, then the coefficients $b_j(y)$ are, from (2.1), all nonnegative, i.e.,

$$b_j(y) \geq 0 \quad \text{for } j = 0, 1, 2, \dots \quad (2.4)$$

We now make use of some matrix notation. Let $\rho(C)$ denote the spectral radius of any $n \times n$ complex matrix C , i.e., $\rho(C) = \max_{1 \leq i \leq n} |\lambda_i|$ where the λ_i are eigenvalues of C . Next, let $C \geq 0$ ($C > 0$) denote any $n \times n$ matrix with nonnegative (positive) entries. Finally, if $C \geq 0$, let $j(C)$ denote the order of the largest Jordan block for the eigenvalue $\rho(C)$ in

the Jordan normal form for the matrix C . If $C \geq 0$ is irreducible,* then we know that $j(C) = 1$. With this notation, we now prove

THEOREM 1. *Let $G(x)$ be completely monotonic in (a, b) , let C be any $n \times n$ matrix with $C \geq 0$, and let y be any number with $a < y < b$. Then,*

$$G(yI - C) \equiv \sum_{j=0}^{\infty} b_j(y)C^j \tag{2.5}$$

is a convergent as a matrix series and defines a matrix with nonnegative entries if and only if $\rho(C) \leq R(y)$, with $\rho(C) = R(y)$ only if the series

$$(-1)^m G^{(m)}(y - R(y)) = \sum_{j=m}^{\infty} b_j(y) \frac{j!(R(y))^{j-m}}{(j-m)!} \tag{2.5'}$$

are convergent for all $0 \leq m \leq j(C) - 1$.

Proof. If $r > 0$ is the radius of convergence of the power series $f(z) = \sum_{j=0}^{\infty} \alpha_j z^j$, then we make use of the well-known fact (cf. [13, p. 17]) that the matrix series $f(A) = \sum_{j=0}^{\infty} \alpha_j A^j$ for an $n \times n$ matrix A is convergent if and only if $\rho(A) < r$, with $\rho(A) = r$ only if the series for $f(\lambda_i), \dots, f^{(m_i-1)}(\lambda_i)$ are all convergent for any λ_i with $|\lambda_i| = \rho(A) = r$, where m_i is the largest order of the Jordan blocks for the eigenvalue λ_i for the matrix A . If the coefficients α_j of the power series are all nonnegative numbers and if A is itself a nonnegative matrix, it is clear that the above result can be simplified to state that $f(A) = \sum_{j=0}^{\infty} \alpha_j A^j$ is convergent if and only if $\rho(A) < r$, with $\rho(A) = r$ only if the series for $f^{(m)}(r)$ are all convergent for $0 \leq m \leq j(A) - 1$. Now, by the hypotheses of the theorem, it is evident that the coefficients $b_j(y)$ of (2.5) are all nonnegative, and that $C \geq 0$. Thus, to complete the proof, we simply apply the above result, noting that the series of (2.5), when convergent, defines a nonnegative matrix. Q.E.D.

To extend Theorem 1, it is convenient to make the following

DEFINITION 2. Let $G(x)$ be defined in the interval (a, b) where $-\infty \leq a < b \leq +\infty$. Then, $G(x)$ is said to be *s-completely monotonic*

* An $n \times n$ matrix A is said to be irreducible if and only if there is no $n \times n$ permutation matrix P such that $PAP^T = \begin{bmatrix} A_{1,1} & A_{1,2} \\ 0 & A_{2,2} \end{bmatrix}$, where $A_{1,1}$ is an $r \times r$ submatrix, $1 \leq r < n$.

in (a, b) if and only if

$$(-1)^j G^{(j)}(x) > 0 \quad \text{for all } a < x < b \text{ and all } j = 0, 1, 2, \dots \quad (2.6)$$

THEOREM 2. Let $G(x)$ be s -completely monotonic in (a, b) , let C be any $n \times n$ matrix with $C \geq 0$, and let y be any number with $a < y < b$. Then, $G(yI - C) = \sum_{j=0}^{\infty} b_j(y)C^j$ is convergent as a matrix series and defines a matrix with positive entries if and only if C is irreducible and $\rho(C) \leq R(y)$, with $\rho(C) = R(y)$ only if the series of (2.5') is convergent for $m = 0$.

Proof. First, assuming that $\rho(C) \leq R(y)$, with $\rho(C) = R(y)$ only if the series of (2.5') are convergent for all $0 \leq m \leq j(C) - 1$, we know from Theorem 1 that the matrix $G(yI - C)$, defined by the convergent power series of (2.5), is a nonnegative matrix. But as $C \geq 0$ and $G(y)$ is s -completely monotonic, there exists a positive constant K such that

$$G(yI - C) = \sum_{j=0}^{\infty} b_j(y)C^j \geq K(I + C)^{n-1}.$$

If C is irreducible, it follows that $j(C) = 1$ and that $(I + C)^{n-1} > 0$ [8, p. 26], whence $G(yI - C) > 0$. Conversely, assume that the matrix series of (2.5) is convergent and defines a positive matrix. Using the result of Theorem 1, it is only necessary to show that C is irreducible. Assume the contrary. Then, there exists a pair of integers i and j , with $i \neq j$ and $1 \leq i, j \leq n$ such that $(C^m)_{i,j} = 0$ for all $m = 0, 1, 2, \dots$. It is clear that this implies that $(G(yI - C))_{i,j} = 0$ also, which contradicts the assumption that $G(yI - C) > 0$. Q.E.D.

Perhaps the simplest way to show that a function is completely monotonic in $(0, \infty)$ is to use a result of Bernstein [1]. Bernstein proved (cf. [12, p. 161]) that $G(x)$ is completely monotonic in $(0, \infty)$ if and only if $G(x)$ is the Laplace-Stieltjes transform of $\alpha(t)$:

$$G(x) = \int_0^{\infty} e^{-xt} d\alpha(t), \quad (2.7)$$

where $\alpha(t)$ is nondecreasing and the integral of (2.7) converges for all $0 < x < \infty$. In this case, $G(z)$ is analytic in $\text{Re}(z) > 0$, and $R(s) \geq s$. Next, if $G(x)$ is completely monotonic on $(0, \infty)$, then $G(x)$ is s -completely monotonic if and only if the nondecreasing function $\alpha(t)$ of (2.7) has at least one positive point of increase, i.e., there exists a $t_0 > 0$ such that

$$\alpha(t_0 + \delta) - \alpha(t_0) > 0 \quad \text{for any } \delta > 0. \tag{2.8}$$

This follows from the inequalities of

$$\begin{aligned} (-1)^j G^{(j)}(x) &= \int_0^\infty e^{-xt} t^j d\alpha(t) \geq \int_{t_0}^{t_0+\delta} e^{-xt} t^j d\alpha(t) \\ &\geq \exp[-x(t_0 + \delta)] t_0^j (\alpha(t_0 + \delta) - \alpha(t_0)) > 0 \end{aligned} \tag{2.9}$$

for all $0 < x < \infty$ and all $j = 0, 1, 2, \dots$. More simply stated, this shows that if $G(x)$ is completely monotonic in $(0, \infty)$, then $G(x)$ is s -completely monotonic there if and only if $G(x)$ does not identically reduce to a constant [14]. Finally, if $G(x)$ is completely monotonic on $(0, \infty)$, suppose that the nondecreasing function $\alpha(t)$ of (2.7) is such that for some $t_1 > 0$, $\alpha(t) = \alpha(t_1)$ for all $t \geq t_1$, where $\alpha(t_1)$ is finite. It then follows from (2.9) that

$$|G^{(j)}(x)| = \int_0^{t_1} e^{-xt} t^j d\alpha(t) \leq t_1^j [\alpha(t_1) - \alpha(0)] \tag{2.10}$$

for $0 \leq x < \infty, j = 0, 1, 2, \dots$.

Thus, since

$$\frac{|G^{(j)}(0)|}{j!} \leq \frac{t_1^j [\alpha(t_1) - \alpha(0)]}{j!} \quad \text{for all } j = 0, 1, 2, \dots, \tag{2.11}$$

it follows that $G(z)$ in this case is an *entire function*, i.e., $G(z)$ is analytic for all complex numbers z . Consequently, for any s with $0 \leq s < \infty$, we have that $R(s) = +\infty$.

The above observations, connected with Bernstein's result on completely monotonic functions, can be used to obtain several known results on functions of nonnegative matrices as simple cases of Theorems 1 and 2. As our first example, we have

THEOREM 3. *Let $C \geq 0$ be an $n \times n$ matrix. If $A \equiv yI - C$ where $0 < y < \infty$, then A is nonsingular and $A^{-1} \geq 0$ if and only if $\rho(C) < y$. Moreover, $A^{-1} > 0$ if and only if $\rho(C) < y$ and C is irreducible.*

Proof. If we write $G_1(x) = (1/x) = \int_0^\infty e^{-xt} d\alpha_1(t)$ for $0 < x < \infty$, where $\alpha_1(t) = t$ for $t \geq 0$, then $G_1(x)$ is s -completely monotonic on $(0, \infty)$, and

$R(y) = y$ for $y > 0$. Since $G_1(x)$ is unbounded for $x = 0$, the series (2.5') for $G_1(0) = G_1(y - R(y))$ is divergent. Then, apply Theorems 1 and 2. Q.E.D.

The first part of Theorem 3 is due to Frobenius [5], while the second part is known and can be found in [10, p. 84]. Our next example is a known result of [2].

THEOREM 4. *Let B be any essentially nonnegative $n \times n$ matrix, i.e., $B + sI \geq 0$ for all real s sufficiently large. Then, for all $t \geq 0$, $\exp(tB) = \sum_{j=0}^{\infty} (tB)^j / j! \geq 0$. Moreover, $\exp(tB) > 0$ for some (and hence all) $t > 0$ if and only if B is irreducible.*

Proof. Writing $G_2(x) = e^{-x} = \int_0^{\infty} e^{-xt} d\alpha_2(t)$ for $0 < x < \infty$, where $\alpha_2(t) = 0$ for $0 \leq t < 1$, and $\alpha_2(t) = 1$ for $t \geq 1$, then $G_2(x)$ is s -completely monotonic on $(0, \infty)$ and $G_2(z)$ is an entire function. Thus, $R(y) = +\infty$ for any $0 < y < \infty$. By hypothesis, for any $t \geq 0$, $C \equiv tB + sI$ is a nonnegative matrix for all positive s sufficiently large, and thus $G_2(sI - C) = \exp(tB) \geq 0$ from Theorem 1. The remainder follows from Theorem 2. Q.E.D.

While it is true that not *all* results on functions of nonnegative matrices fall out as consequences of Theorems 1 and 2, as is shown by an interesting result of Fan [4, Theorem 6] which involves additional assumptions on the principal submatrices, we nevertheless can generate some apparently new results, such as

THEOREM 5. *Let B be any essentially nonnegative $n \times n$ matrix. Then $\{I - \exp(tB)\}(-B)^{-1} \geq 0$ for all $t \geq 0$. Moreover, $\{I - \exp(tB)\}(-B)^{-1} > 0$ for all $t > 0$ if and only if B is irreducible.*

Proof. Writing $G_3(x) = (1 - e^{-x})/x = \int_0^{\infty} e^{-xt} d\alpha_3(t)$ for $0 < x < \infty$, where $\alpha_3(t) = t$ for $0 \leq t \leq 1$ and $\alpha_3(t) = 1$ for $t \geq 1$, then $G_3(x)$ is s -completely monotonic on $(0, \infty)$ and $G_3(z)$ is an entire function. By hypothesis, for any $t \geq 0$, $C \equiv tB + sI$ is a nonnegative matrix for all positive s sufficiently large, and the conclusions follow from Theorems 1 and 2. Q.E.D.

If $A = (a_{i,j})$ is an $n \times n$ M -matrix, as introduced by Ostrowski [7], i.e., $a_{i,j} \leq 0$ for all $i \neq j$, $1 \leq i, j \leq n$, and A is nonsingular with $A^{-1} \geq 0$, then $-A$ is evidently an essentially nonnegative matrix. Thus, we have from Theorem 5 the

COROLLARY. Let A be an $n \times n$ M -matrix. Then, $\{I - \exp(-tA)\}A^{-1} \geq 0$ for all $t \geq 0$, and $\{I - \exp(-tA)\}A^{-1} > 0$ for all $t > 0$ if and only if A is irreducible.

This last Corollary will be useful in the next section.

3. NONNEGATIVELY AND POSITIVELY POSED SEMIDISCRETE PROBLEMS

We consider the following semidiscrete form of (1.1), (1.2):

$$\frac{d\underline{c}(t)}{dt} = -A\underline{c}(t) + \underline{g}, \quad t > 0, \quad (3.1)$$

subject to the initial condition that

$$\underline{c}(0) = \underline{0}. \quad (3.2)$$

Here, $A = (a_{i,j})$ is an $n \times n$ matrix, and $\underline{c}(t)$ and \underline{g} are column vectors with n components.

DEFINITION 3. Given a nonsingular $n \times n$ matrix A , the semidiscrete problem of (3.1), (3.2) is said to be *nonnegatively posed* if and only if the solution $\underline{c}(t)$ of (3.1), (3.2) satisfies

$$\underline{0} \leq \underline{c}(t) \leq A^{-1}\underline{g} \quad \text{for all real } t \geq 0 \text{ and all vectors } \underline{g} \geq \underline{0}. \quad (3.3)$$

Similarly, the semidiscrete problem of (3.1), (3.2) is said to be *positively posed* if and only if the solution $\underline{c}(t)$ of (3.1), (3.2) satisfies

$$\underline{0} < \underline{c}(t) < A^{-1}\underline{g} \quad (3.4)$$

for all real $t > 0$ and all vectors $\underline{g} \geq \underline{0}$ with $\underline{g} \neq \underline{0}$.

Because $\underline{c}(0) = \underline{0}$ in (3.2), the solution of (3.1), (3.2) can be expressed as

$$\underline{c}(t) = \{I - \exp(-tA)\}A^{-1}\underline{g} \quad \text{for all real } t \geq 0, \quad (3.5)$$

and thus

$$A^{-1}\underline{g} - \underline{c}(t) = \exp(-tA) \cdot A^{-1}\underline{g} \quad \text{for all real } t \geq 0. \quad (3.5')$$

Hence, as the inequalities of (3.3) hold for *all* vectors $\underline{g} \geq \underline{0}$, then necessary

and sufficient conditions that the semidiscrete problem of (3.1), (3.2) be nonnegatively posed are that

$$\{I - \exp(-tA)\}A^{-1} \geq 0 \quad \text{for all real } t \geq 0, \quad (3.6)$$

and

$$\exp(-tA) \cdot A^{-1} \geq 0 \quad \text{for all real } t \geq 0. \quad (3.6')$$

Note that with $t = 0$ in (3.6'), we necessarily have that $A^{-1} \geq 0$, i.e., A is a *monotone matrix*. Similarly, necessary and sufficient conditions that the semidiscrete problem of (3.1), (3.2) be positively posed are that

$$\{I - \exp(-tA)\}A^{-1} > 0 \quad \text{for all real } t > 0, \quad (3.7)$$

and

$$\exp(-tA) \cdot A^{-1} > 0 \quad \text{for all real } t > 0. \quad (3.7')$$

We now examine the conditions of (3.6) and (3.6').

LEMMA 1. *Let $A = (a_{i,j})$ be an $n \times n$ monotone matrix, i.e., A is nonsingular and $A^{-1} \geq 0$. Then, $(I - \exp(-tA)) \cdot A^{-1} \geq 0$ for all $t \geq 0$ if and only if A is an M -matrix. Similarly, $(I - \exp(-tA)) \cdot A^{-1} > 0$ for all $t > 0$ if and only if A is an irreducible M -matrix.*

Proof. Writing $(I - \exp(-tA))A^{-1} \equiv (d_{i,j}(t))$, $1 \leq i, j \leq n$, then

$$d_{i,j}(t) = t \left\{ \delta_{i,j} - \frac{t}{2} a_{i,j} + O(t^2) \right\}, \quad 1 \leq i, j \leq n, \quad \text{as } t \rightarrow 0. \quad (3.8)$$

Thus, if $d_{i,j}(t) \geq 0$ for all $t \geq 0$, it is evident that $a_{i,j} \leq 0$ for all $i \neq j$. But a monotone matrix $A = (a_{i,j})$ with nonpositive off-diagonal entries is by definition an M -matrix (cf. [7] and [10, p. 85]). Conversely, if A is an M -matrix, then, as a consequence of the Corollary of Theorem 5, $(I - \exp(-tA))A^{-1} \geq 0$ for any $t \geq 0$. The second part of this lemma follows similarly from the Corollary of Theorem 5. Q.E.D.

With this lemma, we then prove

THEOREM 6. *The semidiscrete problem (3.1), (3.2) is nonnegatively posed if and only if the matrix A of (3.1) is an M -matrix. Similarly, the*

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semidiscrete problem (3.1), (3.2) is positively posed if and only if A is an irreducible M -matrix.

Proof. If the semidiscrete problem (3.1), (3.2) is nonnegatively posed, then (3.6) is valid for all $t \geq 0$. Hence, from Lemma 1, A is necessarily an $n \times n$ M -matrix. Conversely, if A is an $n \times n$ M -matrix, then $A^{-1} \geq 0$, $\exp(-tA) \geq 0$ for all $t \geq 0$ from Theorem 4, and $(I - \exp(-tA))A^{-1} \geq 0$ for all $t \geq 0$ from the Corollary of Theorem 5. Thus, (3.6) and (3.6') are satisfied, proving that (3.1), (3.2) is nonnegatively posed. The remainder follows in a similar fashion. Q.E.D.

COROLLARY. *If the semidiscrete problem of (3.1), (3.2) is nonnegatively posed, then the solution $\underline{c}(t)$ of (3.1), (3.2) satisfies the following sharpened form of (3.3):*

$$\underline{0} \leq \underline{c}(t) \leq \underline{c}(t + \delta) \leq A^{-1}\underline{g} \quad (3.9)$$

for all $t \geq 0$, all $\delta \geq 0$, and all vectors $\underline{g} \geq \underline{0}$.

Similarly, if the semidiscrete problem of (3.1), (3.2) is positively posed, then the solution $\underline{c}(t)$ of (3.1), (3.2) satisfies

$$\underline{0} < \underline{c}(t) < \underline{c}(t + \delta) < A^{-1}\underline{g} \quad (3.10)$$

for all $t > 0$, all $\delta > 0$, and all vectors $\underline{g} \geq \underline{0}$ with $\underline{g} \neq \underline{0}$.

Proof. If (3.1), (3.2) is nonnegatively posed, then A is an M -matrix from Theorem 6, and consequently $\exp(-tA) \geq 0$ and $\{I - \exp(-\delta A)\}A^{-1} \geq 0$ for all $t \geq 0$ and $\delta \geq 0$. Hence, from (3.5), $\underline{c}(t + \delta) - \underline{c}(t) = \exp(-tA)\{I - \exp(-\delta A)\}A^{-1}\underline{g} \geq 0$ for all $t \geq 0$, $\delta \geq 0$, and all vectors $\underline{g} \geq \underline{0}$, which establishes (3.9). The proof of the second part follows in a similar fashion. Q.E.D.

4. NONNEGATIVELY AND POSITIVELY POSED FULLY DISCRETE PROBLEMS

We now consider general matrix approximations $S(t)$ of $\exp(-tA)$. For any fixed $t_0 \geq 0$, the fully discrete problem corresponding to (3.1), (3.2) is defined by the sequence of vectors $\{\underline{w}(mt_0)\}_{m=0}^{\infty}$, where

$$\underline{w}((m+1)t_0) \equiv S(t_0)\underline{w}(mt_0) + (I - S(t_0))A^{-1}\underline{g}, \quad m = 0, 1, 2, \dots, \quad (4.1)$$

and where, in analogy with (3.2), we put

$$\underline{w}(0) = \underline{0}. \quad (4.2)$$

DEFINITION 4. Given a nonsingular $n \times n$ matrix A , the fully discrete problem of (4.1), (4.2) is said to be *nonnegatively posed* for $0 \leq t_0 \leq T$ ($0 < T \leq \infty$) if and only if the sequence of vectors $\{\underline{w}(mt_0)\}_{m=0}^{\infty}$ defined by (4.1), (4.2) satisfies

$$\underline{0} \leq \underline{w}(mt_0) \leq A^{-1}\underline{g} \quad (4.3)$$

for all $m = 0, 1, 2, \dots$, all $0 \leq t_0 \leq T$, and all vectors $\underline{g} \geq \underline{0}$.

Similarly, the fully discrete problem of (4.1), (4.2) is said to be *positively posed* for $0 < t_0 < T$ ($0 < T \leq \infty$) if and only if the sequence of vectors $\{\underline{w}(mt_0)\}_{m=0}^{\infty}$ defined by (4.1), (4.2) satisfies

$$\underline{0} < \underline{w}(mt_0) < A^{-1}\underline{g} \quad (4.4)$$

for all $m = 1, 2, \dots$, all $0 < t_0 < T$, and all vectors $\underline{g} \geq \underline{0}$, $\underline{g} \neq \underline{0}$.

Because $\underline{w}(0) = \underline{0}$ from (4.2), the solution of (4.1), (4.2) can be expressed as

$$\underline{w}(mt_0) = (I - S^m(t_0))A^{-1}\underline{g} \quad \text{for all } m = 0, 1, 2, \dots, \quad (4.5)$$

and thus,

$$A^{-1}\underline{g} - \underline{w}(mt_0) = S^m(t_0)A^{-1}\underline{g} \quad \text{for all } m = 0, 1, 2, \dots \quad (4.5')$$

Since the vectors of (4.5) and (4.5') are to be nonnegative for any vector $\underline{g} \geq \underline{0}$, it is clear that necessary and sufficient conditions that the fully discrete problem (4.1), (4.2) be nonnegatively posed for $0 \leq t_0 \leq T$ are that

$$(I - S^m(t_0))A^{-1} \geq 0 \quad (4.6)$$

for all $m = 0, 1, 2, \dots$, and all $0 \leq t_0 \leq T$,

and

$$S^m(t_0)A^{-1} \geq 0 \quad (4.6')$$

for all $m = 0, 1, 2, \dots$, and all $0 \leq t_0 \leq T$,

which are the discrete analogs of (3.6) and (3.6'). Notice again that the particular case $m = 0$ of (4.6') necessarily gives that A is a monotone matrix. Similarly, necessary and sufficient conditions that the fully discrete problem (4.1), (4.2) be positively posed for $0 < t_0 < T$ are that

$$(I - S^m(t_0))A^{-1} > 0 \quad (4.7)$$

for all $m = 1, 2, \dots$, and all $0 < t_0 < T$,

and

$$S^m(t_0)A^{-1} > 0 \quad (4.7')$$

for all $m = 0, 1, 2, \dots$, and all $0 < t_0 < T$,

which are the discrete analogs of (3.7) and (3.7').

If A is an $n \times n$ M -matrix, then $S(t_0) = \exp(-t_0A)$ satisfies (4.6), (4.6') for all $t_0 \geq 0$, and consequently the existence of matrices in this case for which (4.1), (4.2) is nonnegatively posed is obviously guaranteed. To determine other solutions, suppose that $S(t)$ is a *consistent* approximation of $\exp(-tA)$, i.e., if we write

$$S(t) \equiv I - tA + B(t) \quad \text{for all } 0 \leq t \leq T \quad (T > 0), \quad (4.8)$$

then $S(t)$ is a consistent approximation of $\exp(-tA)$ if and only if $\|B(t)\| = o(t)$ as $t \rightarrow 0$, i.e., for any matrix norm,

$$\lim_{t \rightarrow 0} \frac{\|B(t)\|}{t} = 0. \quad (4.9)$$

The analog of Theorem 6 is

THEOREM 7. *The fully discrete problem (4.1), (4.2) is nonnegatively posed for some consistent approximation $S(t)$ of $\exp(-tA)$ for $0 \leq t \leq T$ ($T > 0$) if and only if A is an M -matrix. Similarly, the fully discrete problem is positively posed for some consistent approximation of $\exp(-tA)$ for $0 < t < T$ if and only if A is an irreducible M -matrix.*

Proof. If A is an $n \times n$ M -matrix, then $S(t) \equiv \exp(-tA)$ is a trivially consistent approximation of $\exp(-tA)$ for all $0 \leq t < \infty$, and (4.1), (4.2) is obviously nonnegatively posed for all $0 \leq t_0 < \infty$. Conversely, assume that (4.1), (4.2) is nonnegatively posed for some consistent approximation

$S(t)$ of $\exp(-tA)$ for $0 \leq t \leq T$ ($T > 0$). It then follows from (4.6) that for any $t_0 \geq 0$,

$$\left(I - S^m\left(\frac{t_0}{m}\right)\right)A^{-1} \geq 0 \quad \text{for all positive integers } m \text{ sufficiently large.} \quad (4.10)$$

Since $S(t)$ is a consistent approximation of $\exp(-tA)$, it can be verified from (4.8), (4.9) that

$$S^m\left(\frac{t_0}{m}\right) \rightarrow \exp(-t_0A) \quad \text{as } m \rightarrow \infty. \quad (4.11)$$

Thus, letting $m \rightarrow \infty$ in (4.10) yields $(I - \exp(-t_0A))A^{-1} \geq 0$ for any $t_0 \geq 0$. But then, it follows from Lemma 1 that A is an M -matrix. Similarly, the second part of this result follows from (4.7) and Lemma 1. Q.E.D.

We now give sufficient conditions for a particular matrix approximation $S(t)$ of $\exp(-tA)$ to be nonnegatively or positively posed.

THEOREM 8. *Let A be an $n \times n$ monotone matrix. If the $n \times n$ matrix $S(t_0)$ satisfies $S(t_0) \geq 0$ and $(I - S(t_0))A^{-1} \geq 0$ for all $0 \leq t_0 \leq T$ ($T > 0$), then the fully discrete problem (4.1), (4.2) is nonnegatively posed for $0 \leq t_0 \leq T$. Similarly, let A be an $n \times n$ matrix with $A^{-1} > 0$. If the $n \times n$ matrix $S(t_0)$ satisfies $S(t_0) > 0$ and $(I - S(t_0))A^{-1} > 0$ for all $0 < t_0 < T$, then the fully discrete problem of (4.1), (4.2) is positively posed for $0 < t_0 < T$.*

Proof. If A is a monotone matrix, then $A^{-1} \geq 0$. Thus, if $S(t_0) \geq 0$ for $0 \leq t_0 \leq T$, so are the products $S^m(t_0)A^{-1}$. If, in addition, $(I - S(t_0))A^{-1} \geq 0$ for $0 \leq t_0 \leq T$, then so are the products $S^m(t_0) \cdot (I - S(t_0))A^{-1}$. But, as

$$\begin{aligned} (I - S^m(t_0))A^{-1} &= (I - S(t_0))A^{-1} + S(I - S(t_0))A^{-1} \\ &\quad + \cdots + S^{m-1}(t_0)(I - S(t_0))A^{-1} \end{aligned} \quad (4.12)$$

is the sum of nonnegative matrices, then $(I - S^m(t_0))A^{-1} \geq 0$ for all $m \geq 0$, and all $0 \leq t_0 \leq T$. Hence, from (4.6), (4.6'), the fully discrete problem (4.1), (4.2) is nonnegatively posed for $0 \leq t_0 \leq T$. The second part follows similarly from (4.12) and (4.7), (4.7'). Q.E.D.

As is easily seen, the converse of Theorem 8 is false, i.e., there exist $n \times n$ matrices $S(t_0)$ with *negative* entries for all $t_0 > 0$ sufficiently small such that (4.1), (4.2) is nonnegatively posed.

The conditions $S(t_0) \geq 0$ and $(I - S(t_0))A^{-1} \geq 0$ for $0 \leq t_0 \leq T$ ($T > 0$) can be connected with the results of Section 2 by

THEOREM 9. *Let A be any $n \times n$ M -matrix, and let $h(x)$ and $(1 - h(x))/x$ be both completely monotonic in $(0, \delta]$ where $\delta > 0$. Then, if $S(t_0) \equiv h(t_0A)$, there exists a $T > 0$ such that (4.1), (4.2) is nonnegatively posed for $0 \leq t_0 \leq T$. Similarly, let A be any irreducible $n \times n$ M -matrix, and let $h(x)$ and $(1 - h(x))/x$ be both s -completely monotonic in $(0, \delta)$ where $\delta > 0$. Then, if $S(t_0) \equiv h(t_0A)$, there exists a $T > 0$ such that (4.1), (4.2) is positively posed for $0 < t_0 < T$.*

Proof. If $A = (a_{i,j})$ is an $n \times n$ M -matrix, then $a_{i,i} > 0$ for all $1 \leq i \leq n$. Thus, if $C \equiv \delta I - t_0A$, then $C \geq 0$ for all $0 \leq t_0 \leq \min_{1 \leq i \leq n} (\delta/a_{i,i})$. Next, since $h(x)$ and $(1 - h(x))/x$ are both by hypothesis completely monotonic on $(0, \delta]$, their associated radii of convergence $R_1(y)$ and $R_2(y)$ satisfy $R_i(y) \geq y$ for $0 < y \leq \delta$, $i = 1, 2$. Thus, if $\rho(C) < \delta$, we can apply Theorem I with $y = \delta$ to both $h(x)$ and $(1 - h(x))/x$. But, as A is an M -matrix, its eigenvalues μ_i satisfy $\operatorname{Re}(\mu_i) > 0$ for all $1 \leq i \leq n$ [10, p. 87]. Thus, it can be verified that $\rho(C) < \delta$ if

$$0 < t_0 < \min_{1 \leq i \leq n} \left\{ \frac{2\delta \operatorname{Re}(\mu_i)}{|\mu_i|^2} \right\}.$$

If we define

$$T = \delta \min_{1 \leq i \leq n} \left\{ \frac{1}{a_{i,i}} ; \frac{2 \operatorname{Re}(\mu_i)}{|\mu_i|^2} \right\} > 0, \quad (4.13)$$

then Theorem I with $y = \delta$ gives us that $(I - h(t_0A))A^{-1} \geq 0$ and $h(t_0A) \geq 0$ for all $0 < t_0 < T$. We now show that $(I - h(t_0A))A^{-1} \geq 0$ and $h(t_0A) \geq 0$ for the closed interval $0 \leq t_0 \leq T$. By hypothesis, $h(x)$ and $(1 - h(x))/x$ are both completely monotonic in $(0, \delta]$. Thus, we know that $h(z)$ is analytic in $|z - \delta| < \delta$, and that for $|z| < \delta$,

$$h(\delta - z) = \sum_{j=0}^{\infty} b_j(\delta)z^j \quad \text{where } b_j(\delta) \geq 0 \text{ for all } j \geq 0.$$

If the radius of convergence $R_1(\delta)$ of this series were δ , then the fact that the $b_j(\delta)$'s are nonnegative would imply that the above series *diverges*

for $z = \delta$, i.e., $\lim_{\varepsilon \downarrow 0} h(\varepsilon) = +\infty$, and hence $1 - h(x)$ would be negative for all $x > 0$ sufficiently small. But $(1 - h(x))/x$ is completely monotonic in $(0, \delta]$, and hence $1 - h(x) \geq 0$ for all $0 < x \leq \delta$. Consequently, $R_1(\delta) > \delta$ and Theorem 1 can be applied with $\rho(C) \leq \delta$. This argument incidentally shows that $h(x)$ is completely monotonic in $[0, \delta]$. Thus, $h(t_0 A)$ is continuous as a function of t_0 for $0 \leq t_0 \leq T$, and consequently $(I - h(t_0 A))A^{-1} \geq 0$ and $h(t_0 A) \geq 0$ for all $0 \leq t_0 \leq T$. The desired conclusion for the first part then follows from Theorem 8. In a similar fashion, the second part follows from Theorems 2 and 8. Q.E.D.

The next result, an extension of Theorem 8, establishes the stability of the matrix $S(t_0)$ in the uniform norm.

THEOREM 10. *Let A be an $n \times n$ monotone matrix, and let the $n \times n$ matrix $S(t_0)$ satisfy $S(t_0) \geq 0$ and $(I - S(t_0))A^{-1} \geq 0$ for all $0 \leq t_0 \leq T$ ($T > 0$). If $\underline{e} = (1, 1, \dots, 1)^T$ and $A\underline{e} = \underline{\eta} \geq \underline{0}$, then the fully discrete problem (4.1), (4.2) is nonnegatively posed, and*

$$\|S(t_0)\|_\infty \leq 1 \quad \text{for all } 0 \leq t_0 \leq T. \quad (4.14)$$

Proof. The first part, of course, follows from Theorem 8. Next, we recall that if $B = (b_{i,j})$ is any $n \times n$ complex matrix, then $\|B\|_\infty = \max_{1 \leq i \leq n} \sum_{j=1}^n |b_{i,j}| = \max_{1 \leq i \leq n} (|B|\underline{e})_i$, where $|B|$ denotes the $n \times n$ matrix with entries $|b_{i,j}|$. We can write $S(t_0) = I - [(I - S(t_0))A^{-1}]A$, and thus, as $S(t_0) \geq 0$ and $(I - S(t_0))A^{-1} \geq 0$, then

$$\underline{0} \leq S(t_0)\underline{e} = \underline{e} - [(I - S(t_0))A^{-1}]\underline{\eta} \leq \underline{e},$$

since $\underline{\eta} \geq \underline{0}$ by hypothesis. Hence, $\|S(t_0)\|_\infty \leq 1$ for all $0 \leq t_0 \leq T$. Q.E.D.

With the hypotheses of this theorem, we see that we obtain stability of the matrix $S(t_0)$ in the uniform or maximum norm. In this regard, see also Thomée [9], who has established similar results for general pure initial value problems with no boundaries.

5. APPLICATIONS

To give some concrete applications of the previous results, we consider first the partial sums of e^{-x} :

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$$E_{0,n}(x) \equiv \sum_{k=0}^n \frac{(-x)^k}{k!}, \quad n = 0, 1, 2, \dots \quad (5.1)$$

LEMMA 2. For each nonnegative integer n , $E_{0,n}(x)$ and $(1 - E_{0,n}(x))/x$ are both completely monotonic in $(-\infty, +1]$.

Proof. We recall [12, p. 145] that a function $f(x)$ defined on the interval (a, b) , $a < b$, is said to be *absolutely monotonic* in (a, b) if and only if $f(-x)$ is completely monotonic in $(-b, -a)$. As is readily verified, $f(x)$ is absolutely monotonic in $[0, R)$ if and only if $f(x)$ can be extended to an analytic function, expressed by the power series $f(z) = \sum_{k=0}^{\infty} \gamma_k z^k$, in $|z| < R$ and $\gamma_k \geq 0$ for all $k \geq 0$. Hence, to establish this lemma, we must equivalently show that $E_{0,n}(1 - \zeta)$ and $(E_{0,n}(1 - \zeta) - 1)/(\zeta - 1)$ are, as functions of ζ , both absolutely monotonic in $[0, +\infty)$. If we write

$$\{E_{0,n}(1 - \zeta) - 1\}/(\zeta - 1) \equiv \sum_{r=0}^{n-1} c_r(n) \zeta^r, \quad (5.2)$$

$$\text{where } c_r(n) = \sum_{l=0}^{n-r-1} \binom{r+l}{r} \frac{(-1)^l}{(l+r+1)!},$$

then $(1 - E_{0,n}(x))/x$ is completely monotonic in $(-\infty, +1]$ if and only if $c_r(n) \geq 0$ for all $0 \leq r \leq n-1$. Now, group successive pairs of terms in the sum for $c_r(n)$ in (5.2). A representative pair, corresponding to $l = 2j$ and $l = 2j + 1$ in (5.2), where $r + 2j + 1 \leq n - 1$, is

$$\begin{aligned} & \binom{r+2j}{r} \frac{1}{(r+2j+1)!} - \binom{r+2j+1}{r} \frac{1}{(r+2j+2)!} \\ &= \frac{1}{r!(2j+1)!} \left\{ \frac{2j+1}{(r+2j+1)} - \frac{1}{(r+2j+2)} \right\}, \end{aligned} \quad (5.3)$$

which is always positive. Thus, if the number of terms for $c_r(n)$ in (5.2) is even, then $c_r(n)$ is positive. Similarly, if this sum has an odd number of terms, the last term which is not paired off is also always positive, and hence $c_r(n) \geq 0$ for all $0 \leq r \leq n-1$ and all $n \geq 1$. As the case $n = 0$ is trivial, this proves that $(1 - E_{0,n}(x))/x$ is completely monotonic in $(-\infty, +1]$ for all $n \geq 0$. The proof showing that $E_{0,n}(x)$ is completely monotonic in $(-\infty, +1]$ is similar. Q.E.D.

By considering $E_{0,1}(x) = 1 - x$, we see that the result of Lemma 2 is sharp, i.e., the functions $E_{0,n}(x)$ for $n \geq 0$ cannot all be completely monotonic in a larger interval.

Next, consider the rational functions

$$E_{1,n}(x) = \frac{\sum_{k=0}^n \frac{(n+1-k)!n!}{k!(n-k)!} (-x)^k}{(n+1)! + n!x}, \quad n = 0, 1, 2, \dots \quad (5.4)$$

In a similar but more tedious way, we can establish the following analog of Lemma 2.

LEMMA 3. *For each nonnegative integer n , $E_{1,n}(x)$ and $(1 - E_{1,n}(x))/x$ are both s -completely monotonic in $(-n-1, +1)$. For the special cases $n = 0$, and 1, $E_{1,0}(x)$ and $(1 - E_{1,0}(x))/x$ are both s -completely monotonic in $(-1, +\infty)$, and $E_{1,1}(x)$ and $(1 - E_{1,1}(x))/x$ are both s -completely monotonic in $(-2, +2)$.*

With these lemmas, we have immediately from Theorem 9 the result of

THEOREM 11. *Let A be any $n \times n$ M -matrix. Then, with $S(t_0) \equiv E_{i,n}(t_0A)$ where $i = 0$ or 1 and $n \geq 0$, there exists a $T_{i,n} > 0$ such that (4.1), (4.2) is nonnegatively posed for $0 \leq t_0 \leq T_{i,n}$. If A is in addition irreducible, and $S(t_0) = E_{1,n}(t_0A)$ where $n \geq 0$, then (4.1), (4.2) is positively posed for $0 < t_0 < T_{1,n}$.*

We remark that the quantities $E_{i,n}(x)$ as defined in (5.1) and (5.4) are special cases of Padé approximation of e^{-x} (cf. [10, p. 266] and [11]); consequently the matrices $E_{i,n}(t_0A)$ of Theorem 11 are *consistent* approximations of $\exp(-t_0A)$. Since e^{-x} and $(1 - e^{-x})/x$ are both completely monotonic in $(-\infty, +\infty)$, one might expect the general Padé approximation $E_{p,q}(x)$ of e^{-x} to be such that $E_{p,q}(x)$ and $(1 - E_{p,q}(x))/x$ are both completely monotonic in some interval containing the origin. This, however, is not the case, as it can be shown in particular that $E_{2,2}(x)$ gives a counterexample. The problem of which Padé approximations $E_{p,q}(x)$ are such that $E_{p,q}(x)$ and $(1 - E_{p,q}(x))/x$ are completely monotonic in some interval containing the origin is open.

Consider now the numerical solution of

$$u_t(x, t) = a(x)u_{xx}(x, t) + 2b(x)u_x(x, t) - c(x)u(x, t) + d(x), \quad (5.5)$$

$$0 < x < 1, \quad t > 0,$$

with boundary conditions

$$u(0, t) = \alpha \geq 0, \quad u(1, t) = \beta \geq 0, \quad t > 0, \quad u(x, 0) \equiv 0 \quad (5.6)$$

for $0 \leq x \leq 1$.

We assume that the functions $a(x)$, $b(x)$, $c(x)$, and $d(x)$ are continuous in $[0, 1]$, and

$$a(x) \geq \omega > 0, \quad c(x) \geq 0, \quad d(x) \geq 0 \quad \text{in } [0, 1]. \quad (5.7)$$

Choosing a uniform mesh of size $h = 1/(N + 1)$ on the interval $[0, 1]$, a standard three-point semidiscrete difference approximation to (5.5), (5.6):

$$\frac{d\underline{c}(t)}{dt} = -A\underline{c}(t) + \underline{g}, \quad t > 0, \quad (5.8)$$

subject to

$$\underline{c}(0) = \underline{0}, \quad (5.9)$$

can be readily derived. Here, A is a real tridiagonal $N \times N$ matrix and \underline{g} is a column vector with N components, explicitly given by

$$A = \frac{1}{h^2} \begin{bmatrix} 2a_1 + c_1 h^2 & -a_1 - b_1 h & & & 0 \\ & -a_2 + b_2 h & 2a_2 + c_2 h^2 & -a_2 - b_2 h & \\ & & & & -a_{n-1} - b_{n-1} h \\ 0 & & & -a_n + b_n h & 2a_n + c_n h^2 \end{bmatrix}; \quad (5.10)$$

$$\underline{g} = \begin{bmatrix} d_1 + \alpha/h^2 \\ d_2 \\ \vdots \\ d_{n-1} \\ d_n + \beta/h^2 \end{bmatrix},$$

where in general $f_i \equiv f(ih)$. It follows from (5.7) that for all h sufficiently small, A is an irreducible M -matrix (cf. [10, p. 85]), and as the vector \underline{g} of (5.10) is a nonnegative vector from (5.6), (5.7), then the semidiscrete problem of (5.8) is *positively posed* (cf. Theorem 6).

For the fully discrete problem corresponding to (5.8), (5.9), consider the matrix approximations $E_{0,1}(t_0A)$, $E_{1,0}(t_0A)$, and $E_{1,1}(t_0A)$ of $\exp(-t_0A)$, where $E_{0,n}(x)$, and $E_{1,n}(x)$ are defined in (5.1) and (5.4). These correspond to the well-known *forward explicit*, *backward implicit*, and *Crank-Nicolson* methods, respectively. From Theorem 10, we know that each possesses an interval $0 \leq t_0 \leq T_{i,n}$ such that (4.1), (4.2) with $S(t_0) \equiv E_{i,n}(t_0A)$ is *nonnegatively posed* in this interval. Moreover, from (5.10) we see for all h sufficiently small that $A \underline{e} = \underline{\eta} \geq 0$, where $\underline{e} = (1, 1, \dots, 1)^T$. Thus, each of these matrices, viz. $E_{0,1}(t_0A)$, $E_{1,0}(t_0A)$, and $E_{1,1}(t_0A)$, is *stable* in the uniform norm in its interval $0 \leq t_0 \leq T_{i,n}$ (cf. Theorem 10).

To show connections with other related works, let us calculate the quantities $T_{i,n}$ for the special case of the heat conduction problem: $a(x) \equiv 1$, $b(x) \equiv 0$, $c(x) \equiv 0$ in $[0, 1]$. In this case, the eigenvalues μ_i of A all satisfy $0 < \mu_i < 4/h^2$, and thus as $a_{i,i} = 2/h^2$ where $A = (a_{i,j})$, then

$$\min_{1 \leq i \leq N} \left\{ \frac{1}{a_{i,i}} ; \frac{2}{\mu_i} \right\} = \frac{h^2}{2}.$$

Next, as Lemmas 2 and 3 determine δ in Theorem 9, then from (4.13) of Theorem 9, we deduce that

$$T_{0,1} = \frac{h^2}{2}, \quad T_{1,0} = +\infty, \quad T_{1,1} = h^2. \quad (5.11)$$

In other words, for the heat conduction problem, the forward difference method is nonnegatively posed and consequently stable in the uniform norm for $0 \leq t_0/h^2 \leq \frac{1}{2}$, which is the Courant-Friedrichs-Lewy stability condition [3], the backward difference method is nonnegatively posed for any $t_0 \geq 0$ and is hence *unconditionally* stable in the uniform norm, and the Crank-Nicolson method is nonnegatively posed and stable in the uniform norm for $0 \leq t_0/h^2 \leq 1$. The latter statements are well known for the heat equation, and can be derived from a maximum principle [6, 8].

Finally, we mention that similar applications can obviously be made to parabolic problems in *higher dimensions*, and the unconditional stability in the uniform norm of the backward implicit method is immediate,

provided that the matrix A of (4.1) is derived to be an M -matrix. That one similarly obtains conditional stability in the uniform norm of the Padé approximations $E_{i,n}(t_0 A)$ with $i = 0$ or 1 , and $n \geq 0$, is believed to be new.

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