INVERSES OF UNIPATHIC M–MATRICES

(SIAM Journal on Matrix Analysis and Applications, 17(4):1025-1036, 1996)

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SUBMITTED OCTOBER 1994

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*Work supported by NSERC grant 6-53120
†Work supported by NSF Grant DMS-8901860 and NSF Grant DMS-9306357.
‡Work supported by NSF Grant DMS-9123318.
§Work supported by NSERC grant 6-53121

Abstract

In this paper we characterize all nonnegative matrices whose inverses are M–matrices with unipathic digraphs. A digraph is called unipathic if there is at most one simple path from any vertex j to any other vertex k. The set of unipathic digraphs on n vertices includes the simple n–cycle and all digraphs whose underlying undirected graphs are trees (or forests). Our results facilitate the construction of nonnegative matrices whose inverses are M–matrices with unipathic digraphs. We highlight this procedure for inverses of tridiagonal M–matrices and of M–matrices whose digraphs are simple n–cycles with loops.

1 Introduction

The inverse of an M–matrix is always a nonnegative matrix, however characterizing the nonnegative matrices whose inverses are M–matrices is a long-standing open problem. In the present article we contribute to the solution of the inverse M–matrix problem by identifying a subclass of the inverse M–matrices. We provide necessary and sufficient conditions for a nonnegative matrix C to be the inverse of an M–matrix whose digraph is unipathic. A digraph is called unipathic if there is at most one simple path from any vertex j to any other vertex k.

Unipathic digraphs were introduced by Harary, Norman, and Cartwright [5], and they were proposed as a new direction of research in combinatorial matrix analysis by Maybee [11]. It is pointed out in [11] that unipathic digraphs can serve as a generalization and a theoretic unification of digraphs whose underlying undirected graphs are trees (or forests) and of directed simple cycles.

The conditions we obtain for a nonnegative matrix to be an inverse of an M–matrix whose digraph is unipathic (see Theorem 3.2) involve positivity of the diagonal entries and certain 2×2 principal minors as well as the zeroness of particular off–diagonal entries and 2×2 almost principal minors (an almost principal minor is the determinant of a submatrix whose row and column index sets differ by only one element). Our proof is based on properties of unipathic digraphs (see Lemmas 2.1 and 2.2) and on a key observation in [12] that connects zero 2×2 almost principal minors of an inverse M–matrix to the digraph of the M–matrix (see Theorem 3.1).

Our results facilitate the construction of nonnegative matrices whose inverses are M–matrices with unipathic digraphs. We illustrate this procedure for inverses of tridiagonal M–matrices and of M–matrices whose digraphs are simple cycles with loops (see Section 5).

For definitions, references, and background on M–matrices and the inverse M–matrix problem the reader is referred to Berman and Plemmons [2] and Johnson [6].

In the following section we introduce the notation necessary to describe our results, summarize the properties of unipathic digraphs, and present some definitions and auxiliary results.

2 Notation and Preliminaries

Throughout the paper we let $\langle n\rangle = \{1, 2, \ldots, n\}$ and $\Gamma = (V, E)$ be a digraph with vertex set $V = \langle n\rangle$ and directed edge set $E = \{(i, j) \mid i, j \in V\}$. A *path* from j to k in Γ is a sequence of vertices $j = r_1, r_2, ..., r_t = k$, with $(r_i, r_{i+1}) \in E$, for $i = 1, ..., t-1$. A path is *simple* if $r_1, r_2, \ldots, r_t$ are distinct. A path $r_1, \ldots, r_t, r_1$ with $t > 1$ is called a *cycle*. It is called a *simple cycle* if the intermediate vertices are distinct.

A digraph is called *unipathic* if there is at most one simple path from any vertex j to any other vertex k.

We adopt the following notation to be used within proofs and in commentary:

$j \rightsquigarrow_\Gamma k$: if there is a path from j to k in Γ ("j has access to k in Γ").
$j \not\rightsquigarrow_\Gamma k$: if there is no path from j to k in Γ.
$j \rightarrow_\Gamma k$: if $(j, k) \in E$.
$j \not\rightarrow_\Gamma k$: if $(j, k) \notin E$.

We denote by Γ_i the digraph obtained from Γ when vertex i and any associated edges are removed (i.e., the subgraph of Γ induced by $\langle n\rangle \setminus i$). We denote by Γ^i the digraph obtained from Γ_i by adding an edge from a vertex j to a vertex k whenever $j \rightarrow_\Gamma i$ and $i \rightarrow_\Gamma k$. The *transitive closure* of Γ, denoted by $\overline{\Gamma}$, is obtained from Γ by adding an edge (i, j) whenever $i \rightsquigarrow_\Gamma j$. If $\Gamma = (V, E)$ and $\Gamma' = (V, E')$ are two digraphs, we let $\Gamma \cup \Gamma' = (V, E \cup E')$.

The *digraph of a matrix* $A = (a_{ij}) \in \mathbb{R}^{nn}$ is denoted by $\mathcal{D}(A) = (V, E)$, with $V = \langle n\rangle$ and $E = \{(i, j) \mid a_{ij} \neq 0\}$. We say that A is *irreducible* if $j \rightsquigarrow_{\mathcal{D}(A)} k$ for all $j, k \in V$. The matrix A is called *unipathic* if $\mathcal{D}(A)$ is a unipathic digraph.

The *underlying undirected graph* $\tilde{\Gamma} = (V, \tilde{E})$ of $\Gamma = (V, E)$ has a vertex set V and an edge set $\tilde{E} \subseteq \{\{i, j\} \mid i, j \in V\}$, where $\{i, j\} \in \tilde{E}$ if and only if $i \neq j$ and either $(i, j) \in E$ or $(j, i) \in E$. We define paths, cycles, and simple cycles of a graph to correspond to the definitions for a digraph. A graph with no cycles is called a *forest*. A connected forest is called a *tree*.

We continue with a summary of the characteristics of unipathic digraphs. Clearly in any digraph, if there is a path from j to k, then there is a simple path from j to k. By definition, if Γ is unipathic, then there may be several paths from j to k, but there can only be one simple path. More precisely we have the following lemma.

Lemma 2.1 *Let* Γ *be a unipathic digraph. Let* i, j, k *be distinct vertices such that* $j \rightsquigarrow_\Gamma k$. *Then the following are equivalent:*

(i) *The vertex* j *does not have access to* k *in* Γ_i.

(ii) *Every path in* Γ *from* j *to* k *goes through* i.

(iii) *The simple path from* j *to* k *in* Γ *goes through* i.

Proof:

(i) implies (ii): If $j \not\rightsquigarrow_{\Gamma_i} k$, then every path from j to k must go through i.

(ii) implies (iii): If every path in Γ from j to k goes through i, then the simple path from j to k in Γ goes through i.

(iii) implies (i): Let i be any vertex in the simple path from j to k. Suppose $j \rightsquigarrow_{\Gamma_i} k$. Then there is a simple path from j to k in Γ_i. But then we would have two different simple paths from j to k in Γ. Contradiction. Hence $j \not\rightsquigarrow_{\Gamma_i} k$. □

A unipathic digraph may have loops on its vertices and, unlike a digraph whose underlying undirected graph is a tree, may have cycles of any length. However, no two cycles can have a common edge. As explained in [11], every strongly connected unipathic digraph can be constructed from a tree (by adjoining chords and orienting the resulting cycles, and by replacing edges with directed simple paths). Notice that if the digraph of a combinatorially symmetric matrix $A = (a_{ij})$ (i.e., $a_{ij} \neq 0$ implies $a_{ji} \neq 0$) is strongly connected and unipathic, then its underlying undirected graph must be a tree.

An important property of unipathic digraphs is given next. The *indegree* (resp. *outdegree*) of a vertex i of a digraph is the number of edges entering (resp. issuing from) vertex i.

Lemma 2.2 *Let* $\Gamma = (V, E)$ *be a unipathic digraph. Then there is a vertex with indegree at most 1, and a vertex with outdegree at most 1.*

Proof:

Let $r_1, \ldots, r_t \in V$ be a simple path in Γ of maximal length. Suppose r_1 has indegree greater than 1. Then there exist two distinct edges ending in r_1 and they must be of the form (r_i, r_1) and (r_j, r_1), with $1 < i < j$, by the maximality of the simple path $r_1, \ldots, r_t$. But then there are two simple paths from r_i to r_1, a contradiction. Similarly we can show that r_t has outdegree at most 1. $\square$

We denote an entrywise nonnegative matrix C by $C \geq 0$. If all the entries of C are positive we write $C \gg 0$. Let $S, T \subseteq \langle n \rangle$ and $C \in \mathbb{R}^{nn}$. We write $C[S,T]$ for the submatrix of C whose rows and columns are indexed by S and T, respectively, in their natural order. If S or T is a singleton, e.g., $T = \{\ell\}$, we write $C[S,\ell]$ instead of $C[S,\{\ell\}]$. Let $R \subseteq \langle n \rangle$. The *Schur complement* of C with respect to an invertible principal submatrix $C[R,R]$ is

$$C/C[R,R] = C[Q,Q] - C[Q,R](C[R,R])^{-1}C[R,Q],$$

where $Q = \langle n \rangle \setminus R$.

The following lemma will be used in the proof of Theorem 3.2. It can be obtained by combining formulae from Brualdi and Schneider [3, (10), p. 773] and Watford [14, (4), p. 251].

Lemma 2.3 *Let $C \in \mathbb{R}^{nn}$ and let $R \subseteq \langle n \rangle$, $Q = \langle n \rangle \setminus R$. If all the relevant inverses in the following block matrix exist, then C is invertible and its inverse permutationally similar to*

$$\begin{bmatrix} (C/C[R,R])^{-1} & -(C[Q,Q])^{-1}C[Q,R](C/C[Q,Q])^{-1} \\ -(C[R,R])^{-1}C[R,Q](C/C[R,R])^{-1} & (C/C[Q,Q])^{-1} \end{bmatrix}.$$

We close this section with a characterization for a nonnegative matrix to be an inverse M–matrix. Owing to its generality, it gives less insight than one might wish. However, it can be used to obtain some additional characterizations for inverses of M–matrices.

Lemma 2.4 *Let $A = sI - P$, $P \geq 0$, be a nonsingular M–matrix. Then for all $\beta \geq 0$, $A(A+\beta I)^{-1}$ is a nonsingular M–matrix which is given by*

$$A(A+\beta I)^{-1} \;=\; \frac{s}{s+\beta}I - \frac{\beta}{s+\beta}\sum_{j=1}^{\infty}\frac{P^j}{(s+\beta)^j}. \tag{2.5}$$

Proof:

The proof is essentially to be found in the proof of Theorem 3 of Johnson [6]. □

Lemma 2.4 now yields the following characterization mentioned above.

Theorem 2.6 *Let* $C = (c_{ij}) \in \mathbb{R}^{nn}$ *be a nonnegative matrix. Then* C *is the inverse of an M–matrix if and only if* $c_{ii} > 0$ *for all* $1 \leq i \leq n$, $C + \alpha I$ *is invertible for all* $\alpha \geq 0$, $\mathcal{D}(C) = \overline{\mathcal{D}(C)}$, *and*

$$\mathcal{D}((C+\alpha I)^{-1}) \;=\; \mathcal{D}(C), \quad \textit{for all} \;\; \alpha > 0. \tag{2.7}$$

Proof:

Assume first that C is the inverse of an M–matrix. Then it is well known that $c_{ii} > 0$, $i = 1, \ldots, n$, $C + \alpha I$ is invertible for all $\alpha \geq 0$, and $\mathcal{D}(C) = \overline{\mathcal{D}(C)}$. Now put $A = C^{-1}$ and observe that

$$(C+\alpha I)^{-1} \;=\; \beta A(A+\beta I)^{-1}, \tag{2.8}$$

where $\beta := 1/\alpha$. Since A is a nonsingular M–matrix, there exists $P \geq 0$ such that $A = sI - P$ and such that $s > \rho(P)$ (the spectral radius of P). But then, by the Neumann expansion,

$$C \;=\; \frac{1}{s} I + \frac{1}{s} \sum_{j=1}^{\infty} \frac{P^j}{s^j}. \tag{2.9}$$

The validity of (2.7) now follows by comparing, for $\alpha > 0$, the expansion for the matrix on the right–hand–side of (2.8) which can be obtained via (2.5) and the expansion in (2.9).

Conversely, suppose that the equality in (2.7) holds for all $\alpha > 0$. If $((C + \alpha I)^{-1})_{ij} = 0$ for some $\alpha > 0$, then by (2.7) it must hold for all $\alpha > 0$ and hence, by continuity arguments, $(C^{-1})_{ij} = 0$. Similarly, if $((C+\alpha I)^{-1})_{ij} < 0$ then, again by (2.7), this entry must be negative for all $\alpha > 0$ so that $(C^{-1})_{ij} \leq 0$. Suppose now that $((C + \alpha I)^{-1})_{ij} > 0$, $i \neq j$, for some $\alpha > 0$ so that this entry is positive for all $\alpha > 0$. Then, for sufficiently large $\alpha > 0$, the Neumann expansion gives us that:

$$((C+\alpha I)^{-1})_{ij} \;=\; \frac{1}{\alpha}\left(\left(I + \frac{C}{\alpha}\right)^{-1}\right)_{ij} \;=\; \frac{1}{\alpha}\left(I - \frac{C}{\alpha} + \frac{C^2}{\alpha^2} - \ldots\right)_{ij}.$$

In particular we see that as α increases, it will attain a value such that beyond this value the (i, j)–th entry of $(C + \alpha I)^{-1}$ will become negative, contradicting the constancy of the sign implied by (2.7). Hence there cannot be a value of $\alpha > 0$ for which $((C + \alpha I)^{-1})_{ij} > 0$ and our proof is done. □

Our theorem has the following two corollaries.

Corollary 2.10 *Let $C = (c_{ij}) \in \mathbb{R}^{nn}$ be nonnegative. Then a necessary and sufficient condition for C to be the inverse of an M–matrix is that $c_{ii} > 0$, the matrix $C + \alpha I$ is invertible for all $\alpha > 0$, $\mathcal{D}(C) = \overline{\mathcal{D}(C)}$, and that for each pair (i, j), the minor of $C + \alpha I$ obtained after deleting the i–th row and j–th column, has a constant sign as a function of $\alpha > 0$.*

Corollary 2.11 *If $A \in \mathbb{R}^{nn}$ is a nonsingular M–matrix, then for any $\alpha > 0$, $\mathcal{D}(A^{-1} + \alpha I)^{-1} = \overline{\mathcal{D}(A)}$.*

The last corollary has the following implication. Suppose that $A \in \mathbb{R}^{nn}$ is a nonsingular irreducible M–matrix, but which has some off–diagonal entries equal to zero. Invert A to obtain the positive matrix C. Now invert $C + \alpha I$. Then $(C + \alpha I)^{-1}$ is an M–matrix and, by the foregoing, all its entries are nonzero.

3 The Inverse of a Unipathic M–matrix

We begin with a theorem on nonsingular M–matrices proved in McDonald, Neumann, Schneider, and Tsatsomeros [12]. It represents a graph–theoretical refinement and generalization of a condition found in Willoughby [15] that is necessary for a matrix to be an inverse M–matrix.

Theorem 3.1 *Let $A \in \mathbb{R}^{nn}$ be a nonsingular M–matrix and $\Gamma = \mathcal{D}(A)$. Let also $C = A^{-1}$ and $\{i, j, k\} \subseteq \langle n \rangle$ be distinct. Then:*

(i) $c_{jk} = \frac{c_{ji}c_{ik}}{c_{ii}}$, *whenever j does not have access to k in Γ_i,*

(ii) $c_{jk} > \frac{c_{ji}c_{ik}}{c_{ii}}$, *whenever j has access to k in Γ_i.*

Notice that Theorem 3.1 refers to the value (zero or positive) of the almost principal minors of C formed from rows $i,\ j$ and columns $i,\ k$.

In the next theorem, our main result, we provide necessary and sufficient conditions for $C \geq 0$ to be the inverse of a unipathic M–matrix. It is well known that if C is an inverse M–matrix then its diagonal entries and 2×2 principal minors are positive, the 2×2 almost principal minors satisfy Theorem 3.1, and $\mathcal{D}(C) = \overline{\mathcal{D}(C)} = \overline{\mathcal{D}(C^{-1})}$. These conditions are not in general sufficient for $C \geq 0$ to be an inverse M–matrix. However, as we will show in Theorem 3.2, a subset of these conditions, dictated by a unipathic digraph, is necessary and sufficient for C to be the inverse of a unipathic M–matrix.

Theorem 3.2 *Let Γ be a unipathic digraph on n vertices and $C \in \mathbb{R}^{nn}$. Then the following are equivalent:*

(i) *C is nonsingular and C^{-1} is an M–matrix such that $\mathcal{D}(C^{-1}) = \Gamma$.*

(ii) *$C \geq 0$ and satisfies:*

- **(a)** *$c_{ii} > 0$, for all $i \in \langle n \rangle$.*
- **(b)** *$c_{jj}c_{kk} > c_{jk}c_{kj}$, for all distinct j and k such that there is an edge from j to k in Γ.*
- **(c)** *$c_{jk} = 0$, whenever there is no path from j to k in Γ.*
- **(d)** *$c_{jk} = \frac{c_{ji}c_{ik}}{c_{ii}}$, for all distinct i, j, k, such that there is a path from j to k in Γ, but there is no path from j to k in Γ_i.*

Proof:

(i) implies (ii): Since C^{-1} is an M–matrix, $C \geq 0$ and (ii)(a),(b) follow from well known facts about M–matrices (see e.g., [2]). Property (ii)(c) follows from the fact that the digraph of an inverse M–matrix is the transitive closure of the digraph of its inverse (see Lewin and Neumann [8] and Schneider [13]). Property (ii)(d) follows from Theorem 3.1.

(ii) implies (i): We proceed by induction on n. For $n = 1$, the result follows trivially. Assume $n \geq 2$ and that (ii) implies (i) for all $(n-1) \times (n-1)$ matrices.

Using the inductive hypothesis we will establish three claims which, combined with Lemma 2.3, will allow us to show that C is invertible and that its inverse is a Z–matrix (i.e., it has nonpositive off–diagonal entries) with digraph Γ.

Claim 1 $c_{jj}c_{kk} > c_{jk}c_{kj}$, *for all distinct* $j, k \in \langle n \rangle$.

Proof of Claim 1: If $j \not\rightsquigarrow_\Gamma k$ or $k \not\rightsquigarrow_\Gamma j$ then by (c), $c_{jk}c_{kj} = 0$, and the claim follows. Assume $j \rightsquigarrow_\Gamma k$ and $k \rightsquigarrow_\Gamma j$. We induct on the length, r, of the simple path from j to k. If $r = 1$, the claim follows from (b). Assume $r > 1$ and that the claim holds for any two vertices connected by a simple path with length less than r. Either the simple path from j to k has no vertices, other than j and k, in common with the simple path from k to j, or there is an additional vertex i which is common to both paths. In the latter case, by (d), Lemma 2.1, and the induction hypothesis on the path length,

$$\frac{c_{jk}c_{kj}}{c_{jj}c_{kk}} = \frac{c_{ji}c_{ik}c_{ki}c_{ij}}{c_{jj}c_{ii}c_{kk}c_{ii}} = (\frac{c_{ji}c_{ij}}{c_{jj}c_{ii}})(\frac{c_{ik}c_{ki}}{c_{kk}c_{ii}}) < 1.$$

In the former case, for any i in the simple path from j to k, there is a simple path from i to j through k. Hence by (d), Lemma 2.1, and the induction hypothesis on the path length,

$$\frac{c_{jk}c_{kj}}{c_{jj}c_{kk}} = \frac{c_{ji}c_{ik}c_{kj}}{c_{jj}c_{ii}c_{kk}} = \frac{c_{ji}c_{ij}}{c_{jj}c_{ii}} < 1.$$

This establishes Claim 1.

Claim 2 *For any* $\ell \in \langle n \rangle$, *let* $B = C/C[\ell, \ell]$. *Then* B *is invertible and* B^{-1} *is an M–matrix with* $\mathcal{D}(B^{-1}) = \Gamma_\ell$.

Proof of Claim 2: By the induction hypothesis, it is enough to show B satisfies (ii) for the digraph Γ_ℓ. For ease of notation, we will assume that the indices of the entries of B correspond to those of C, i.e.,

$$b_{jk} = c_{jk} - \frac{c_{j\ell}c_{\ell k}}{c_{\ell\ell}}.$$

First we show that B is nonnegative. If $b_{jk} = 0$, we are done. So suppose that $b_{jk} \neq 0$. Then either $c_{jk} \neq 0$ or $c_{j\ell}c_{\ell k} \neq 0$.

If $c_{j\ell}c_{\ell k} = 0$, then $b_{jk} = c_{jk} > 0$.

If $c_{j\ell}c_{\ell k} \neq 0$, then, by (c), $j \rightsquigarrow_\Gamma \ell$ and $\ell \rightsquigarrow_\Gamma k$ and the following cases have to be considered:

If $j \not\rightsquigarrow_{\Gamma_\ell} k$, then by (d)

$$b_{jk} = c_{jk} - \frac{c_{j\ell}c_{\ell k}}{c_{\ell\ell}} = c_{jk} - c_{jk} = 0.$$

If $j \rightsquigarrow_{\Gamma_\ell} k$, then joining the simple paths from j to ℓ and from ℓ to k forms a path from j to k through ℓ, which therefore cannot be simple. So let i be the first vertex in the simple path from j to ℓ which is also in the simple path from ℓ to k. Then the (sub)path from j to i and then from i to k, forms a simple path from j to k. Hence $j \not\rightsquigarrow_{\Gamma_i} k$, $j \not\rightsquigarrow_{\Gamma_i} \ell$, and $\ell \not\rightsquigarrow_{\Gamma_i} k$. By Theorem 3.1,

$$b_{jk} = c_{jk} - \frac{c_{j\ell}c_{\ell k}}{c_{\ell\ell}} = c_{jk} - \frac{c_{ji}c_{i\ell}c_{\ell i}c_{ik}}{c_{ii}c_{ii}c_{\ell\ell}}$$

$$= c_{jk} - c_{jk}\frac{c_{i\ell}c_{\ell i}}{c_{ii}c_{\ell\ell}} = c_{jk}(1 - \frac{c_{i\ell}c_{\ell i}}{c_{ii}c_{\ell\ell}}) > 0 \quad \text{(by Claim 1)}.$$

Hence B is a nonnegative matrix.

We now show that conditions (ii)(a)–(d), labeled here as (a')–(d'), also hold for the matrix B with the digraph Γ_ℓ.

(a') By Claim 1,

$$b_{jj} = c_{jj} - \frac{c_{j\ell}c_{\ell j}}{c_{\ell\ell}} > 0.$$

(b') Suppose $j \rightarrow_{\Gamma_\ell} k$.

If $k \not\rightsquigarrow_\Gamma \ell$, then either $k \not\rightsquigarrow_\Gamma j$ or $j \not\rightsquigarrow_\Gamma \ell$, so by (c),

$$c_{k\ell} = 0 = \frac{c_{kj}c_{j\ell}}{c_{jj}}. \tag{3.3}$$

If $k \rightsquigarrow_\Gamma \ell$, then $j \rightsquigarrow_\Gamma \ell$. It follows that either j is in the simple path from k to ℓ in Γ, in which case, by (d) and Lemma 2.1, we have that

$$c_{k\ell} \;=\; \frac{c_{kj}c_{j\ell}}{c_{jj}} \;\geq\; 0, \tag{3.4}$$

or the edge from j to k combined with the simple path from k to ℓ forms a simple path from j to ℓ which includes k. In this case we have, again by (d) and Lemma 2.1, that

$$c_{j\ell} = \frac{c_{jk}c_{k\ell}}{c_{kk}}. \tag{3.5}$$

If (3.3) or (3.4) holds then by replacing $c_{k\ell}$ in the following expression we get:

$$b_{jj}b_{kk} - b_{jk}b_{kj} = (c_{jj} - \frac{c_{j\ell}c_{\ell j}}{c_{\ell\ell}})(c_{kk} - \frac{c_{k\ell}c_{\ell k}}{c_{\ell\ell}}) - (c_{jk} - \frac{c_{j\ell}c_{\ell k}}{c_{\ell\ell}})(c_{kj} - \frac{c_{k\ell}c_{\ell j}}{c_{\ell\ell}})$$

$$= (c_{jj}c_{kk} - c_{jk}c_{kj}) - \frac{c_{jj}c_{kk}c_{j\ell}c_{\ell j} - c_{jk}c_{kj}c_{j\ell}c_{\ell j}}{c_{jj}c_{\ell\ell}} - \frac{c_{kj}c_{j\ell}c_{\ell k} - c_{kj}c_{j\ell}c_{\ell k}}{c_{\ell\ell}}$$

$$= (c_{jj}c_{kk} - c_{jk}c_{kj})(1 - \frac{c_{j\ell}c_{\ell j}}{c_{jj}c_{\ell\ell}}) > 0 \quad \text{(by Claim 1).}$$

If equation (3.5) holds, then the above inequality follows in a similar manner, by replacing c_{jl}.

(c') If $j \not\rightsquigarrow_{\Gamma_\ell} k$, then by (c) or (d),

$$b_{jk} = c_{jk} - \frac{c_{j\ell}c_{\ell k}}{c_{\ell\ell}} = c_{jk} - c_{jk} = 0.$$

(d') Let $i, j, k \in S$ be distinct. Assume $j \rightsquigarrow_{\Gamma_\ell} k$, but $j \not\rightsquigarrow_{(\Gamma_\ell)_i} k$. Then $j \not\rightsquigarrow_{\Gamma_i} k$. Hence by (d),

$$c_{jk} = \frac{c_{ji}c_{ik}}{c_{ii}}. \tag{3.6}$$

If $j \rightsquigarrow_\Gamma \ell$ and $\ell \rightsquigarrow_\Gamma k$, then by Lemma 2.1 either i is in the simple path from j to ℓ, or i is in the simple path from ℓ to k. Hence by (d) and Lemma 2.1,

$$c_{j\ell} = \frac{c_{ji}c_{i\ell}}{c_{ii}} \tag{3.7}$$

or

$$c_{\ell k} = \frac{c_{\ell i}c_{ik}}{c_{ii}}. \tag{3.8}$$

If $j \not\rightsquigarrow_\Gamma \ell$, then $i \not\rightsquigarrow_\Gamma \ell$, and hence by (c), equation (3.7) is satisfied.

If $\ell \not\rightsquigarrow_\Gamma k$, then $\ell \not\rightsquigarrow_\Gamma i$, and hence by (c), equation (3.8) is satisfied.

Hence either (3.7) holds, or (3.8) holds.

If (3.7) holds, then using (3.6) to replace c_{jk} and (3.7) to replace $c_{j\ell}$ in the following expression we get:

$$\begin{aligned} b_{jk}b_{ii} - b_{ji}b_{ik} &= (c_{jk} - \frac{c_{j\ell}c_{\ell k}}{c_{\ell\ell}})(c_{ii} - \frac{c_{i\ell}c_{\ell i}}{c_{\ell\ell}}) - (c_{ji} - \frac{c_{j\ell}c_{\ell i}}{c_{\ell\ell}})(c_{ik} - \frac{c_{i\ell}c_{\ell k}}{c_{\ell\ell}}) \\ &= (c_{jk}c_{ii} - c_{ji}c_{ik}) - (\frac{c_{ji}c_{ik}c_{i\ell}c_{\ell i} - c_{ji}c_{i\ell}c_{\ell i}c_{ik}}{c_{ii}c_{\ell\ell}}) \\ &\quad -(\frac{c_{ii}c_{ji}c_{i\ell}c_{\ell k} - c_{ii}c_{i\ell}c_{\ell k}c_{ji}}{c_{ii}c_{\ell\ell}}) = 0. \end{aligned}$$

If (3.8) holds, then the above equality follows in a similar manner.

This establishes Claim 2.

By Lemma 2.2, there is a vertex with indegree at most 1. Without loss of generality, we can assume this vertex is labeled by n (otherwise we can work with a permutation similarity of C). Let $T = \langle n-1 \rangle$.

Claim 3: *The matrix $C[T,T]$ is invertible and its inverse is an M-matrix with digraph Γ^n. Moreover, $C/C[T,T] > 0$.*

Proof of Claim 3: Let $i, j \in T$. Since $i \rightsquigarrow_{\Gamma^n} j$ if and only if $i \rightsquigarrow_\Gamma j$, (a), (c) and (d) of (ii) must hold for $C[T,T]$. Also (ii)(b) follows from Claim 1. Hence, by the induction hypothesis, $C[T,T]$ is invertible and its inverse is an M–matrix with digraph Γ^n. To show that $C/C[T,T] > 0$, if the indegree of n is one choose m such that $m \rightarrow_\Gamma n$, otherwise choose any $m \in \langle n-1 \rangle$. Then by (c) and (d):

$$C[T,n] = \begin{bmatrix} c_{1n} \\ c_{2n} \\ \vdots \\ c_{n-1,n} \end{bmatrix} \tag{3.9}$$

$$= \begin{bmatrix} \frac{c_{1m}c_{mn}}{c_{mm}} \\ \frac{c_{2m}c_{mn}}{c_{mm}} \\ \vdots \\ \frac{c_{n-1,m}c_{mn}}{c_{mm}} \end{bmatrix} = \frac{c_{mn}}{c_{mm}} \begin{bmatrix} c_{1m} \\ c_{2m} \\ \vdots \\ c_{n-1,m} \end{bmatrix} = \frac{c_{mn}}{c_{mm}} C[T,m]$$

Thus, letting $e_m \in \mathbb{R}^{n-1}$ be the m–th standard basis vector, by (3.9) we get:

$$C/C[T,T] = c_{nn} - C[n,T](C[T,T])^{-1}C[T,n]$$
$$= c_{nn} - \frac{c_{mn}}{c_{mm}} C[n,T](C[T,T])^{-1}C[T,m] = c_{nn} - \frac{c_{mn}}{c_{mm}} C[n,T]e_m$$
$$= c_{nn} - \frac{c_{mn}c_{nm}}{c_{mm}} > 0 \ \text{ (by Claim 1).}$$

This establishes Claim 3.

Recall now that, since by Claims 2 and 3, $C/C[n,n]$, $C[T,T]$, and $C/C[T,T]$ are invertible, C has to be invertible and its inverse is, from Lemma 2.3 with $R = \{n\}$ and $Q = T$,

$$\begin{bmatrix} (C/C[n,n])^{-1} & -(C[T,T])^{-1}C[T,n](C/C[T,T])^{-1} \\ -(C[n,n])^{-1}C[n,T](C/C[n,n])^{-1} & (C/C[T,T])^{-1} \end{bmatrix}.$$

Moreover, by Claim 2, for all $\ell \in \langle n \rangle$ and for $S = \langle n \rangle \setminus \ell$, $C^{-1}[S,S] = (C/C[\ell,\ell])^{-1}$ is an M–matrix with digraph Γ_ℓ. It follows that C^{-1} is a Z–matrix with digraph Γ, whose inverse is a nonnegative matrix. This implies that C^{-1} is an M–matrix with digraph Γ. □

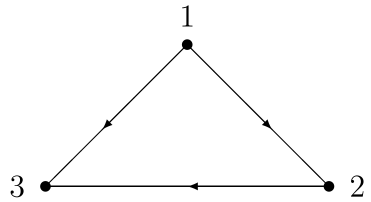
The contents of Claims 2 and 3 within the inductive proof of Theorem 3.2 can now be stated separately.

Corollary 3.10 *Let $C \in \mathbb{R}^{nn}$ be the inverse of a unipathic M–matrix whose digraph is Γ.*

(i) *For any $\ell \in \langle n \rangle$ and $S = \langle n \rangle \setminus \ell$, $C/C[\ell,\ell]$ is the inverse of a unipathic M–matrix whose digraph Γ_ℓ.*

(ii) *For any $\ell \in \langle n \rangle$ of indegree at most 1 and $T = \langle n \rangle \setminus \ell$, $C[T,T]$ is the inverse of a unipathic M–matrix whose digraph is Γ^ℓ. Moreover, $C/C[T,T] > 0$.*

Example 3.11 The assumption in Theorem 3.2 that the digraph Γ is unipathic is critical for condition (ii) of the theorem to imply that the inverse of C is an M–matrix. For example consider

$\Gamma =$ 

Notice that Γ is not unipathic (but if any edge is removed the digraph becomes unipathic). The matrix

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

satisfies condition (ii) of Theorem 3.2 for the digraph Γ, but its inverse

$$C^{-1} = \begin{bmatrix} 1 & -2 & 1 \\ 0 & 1 & -2 \\ 0 & 0 & 1 \end{bmatrix}$$

is not an M–matrix. In particular, this example shows that condition (ii) is not in general sufficient to imply that C^{-1} is an M–matrix when Γ belongs to the classes of digraphs discussed in [4] and [9].

Remark 3.12 It follows by Corollary 2.10 that if C is a nonnegative matrix that satisfies one and hence both of the equivalent conditions of Theorem 3.2, then for each pair $1 \leq i, j \leq n$, the minor of $C + \alpha I$ which is obtained by deleting the i–th row and j–th column has a constant sign as a function of $\alpha > 0$.

4 Construction of Inverses of Unipathic M–matrices

Theorem 3.2 enables us to construct a matrix C which is the inverse of an M–matrix with a given unipathic digraph. The process is as follows. Given a unipathic digraph Γ, first fill the diagonal entries with positive values. Then, for any simple cycle $r_1 \to \ldots \to r_t \to r_1$, choose $c_{r_i r_{i+1}}$ and $c_{r_t r_1}$ so that they are positive and

$$\frac{c_{r_1 r_1} c_{r_2 r_2} \ldots c_{r_t r_t}}{c_{r_1 r_2} c_{r_2 r_3} \ldots c_{r_t r_1}} > 1.$$

Since Γ is unipathic, no two simple cycles share a common edge so making the above choices can proceed without overlap. If there is an edge from j to k in Γ, with $j \neq k$, but this edge is not part of any simple cycle, assign any positive value to c_{jk}. If j does not have access to k in Γ, then set $c_{jk} = 0$. The remaining entries of C are uniquely determined by Theorem 3.2 (ii)(d).

We highlight this procedure for the inverse of a tridiagonal M–matrix and of an M–matrix whose digraph is the simple n–cycle with loops.

We begin with the inverse of a tridiagonal M–matrix. Conditions (ii)(c), (iii)(c), and (iii)(d) of the following theorem also appear in Barrett [1], who characterizes inverses of tridiagonal matrices in general.

Theorem 4.1 *The following are equivalent for $C \in \mathbb{R}^{nn}$.*

(i) *C is nonsingular and C^{-1} is a tridiagonal M–matrix.*

(ii) *$C \geq 0$ and satisfies*

- **(a)** $c_{ii} > 0$, *for all $i \in \langle n \rangle$.*
- **(b)** $c_{ii} c_{i+1,i+1} - c_{i+1,i} c_{i,i+1} > 0$, *for all $i \in \langle n-1 \rangle$.*
- **(c)** $c_{jk} = \frac{c_{ji} c_{ik}}{c_{ii}}$, *for all $j > i > k$ and for all $k > i > j$.*

(iii) *$C \geq 0$ and satisfies*

- **(a)** $c_{ii} > 0$, *for all $i \in \langle n \rangle$.*
- **(b)** $c_{ii} c_{i+1,i+1} - c_{i+1,i} c_{i,i+1} > 0$, *for all $i \in \langle n-1 \rangle$.*
- **(c)** $c_{ij} = \frac{c_{i,i+1} c_{i+1,i+2} \cdots c_{j-1,j}}{c_{i+1,i+1} c_{i+2,i+2} \cdots c_{j-1,j-1}}$, *for all $j > i+1$.*
- **(d)** $c_{ij} = \frac{c_{j,j+1} c_{j+1,j+2} \cdots c_{i-1,i}}{c_{j+1,j+1} c_{j+2,j+2} \cdots c_{i-1,i-1}}$, *for all $i > j+1$.*

(iv) *C is a nonsingular matrix which is totally nonnegative (i.e., all the minors of C are nonnegative) and whose inverse is an M–matrix.*

Proof:

The equivalence of (i) and (ii) follows directly from Theorem 3.2 applied to the digraph of a tridiagonal matrix.
The equivalence of (ii) and (iii) is also straightforward.
The equivalence of (i) and (iv) is a result due to Lewin [7]. □

We remark that in [10], Markham introduces a class of matrices which he calls of type D. A real $n \times n$ matrix $C = (c_{ij})$ is of *type D* if

$$c_{ij} = \begin{cases} c_i & \text{if } i \leq j \\ c_j & \text{if } j < i \end{cases}$$

and if $c_n > c_{n-1} > \ldots > c_1$. Markham shows that if $c_1 > 0$, then C is nonsingular and C^{-1} is a tridiagonal M–matrix. It can be readily checked that if $c_{11} > 0$ and C is a matrix of type D, then its entries satisfy the conditions (ii)(a)–(c) stipulated in the above theorem. Thus the class of matrices characterized in Theorem 4.1 contains the positive matrices of type D as a subclass.

Note that if the entries of the first superdiagonal, first subdiagonal and the diagonal of $C = (c_{ij})$ satisfy (ii)(a) and (ii)(b) of Theorem 4.1, then (ii)(c) (or (iii)(c) and (iii)(d)) uniquely determine the remaining entries of C. This is illustrated in the following example.

Example 4.2 We construct inverses of tridiagonal M–matrices as follows. Begin by filling in the tridiagonal structure of $C = (c_{ij})$ so that (ii)(a) and (ii)(b) of Theorem 4.1 are satisfied. For example let

$$C = \begin{bmatrix} 4 & 2 & * & * & * & * \\ 2 & 2 & 2 & * & * & * \\ * & 1 & 2 & 6 & * & * \\ * & * & 0 & 1 & 1 & * \\ * & * & * & 1 & 3 & 4 \\ * & * & * & * & 2 & 4 \end{bmatrix}.$$

Then use (ii)(c) (or (iii)(c) and (iii)(d)) to (uniquely) fill in the *'s, one (sub–) superdiagonal at a time:

$$C = \begin{bmatrix} 4 & 2 & 2 & 6 & 6 & 8 \\ 2 & 2 & 2 & 6 & 6 & 8 \\ 1 & 1 & 2 & 6 & 6 & 8 \\ 0 & 0 & 0 & 1 & 1 & 4/3 \\ 0 & 0 & 0 & 1 & 3 & 4 \\ 0 & 0 & 0 & 2/3 & 2 & 4 \end{bmatrix}.$$

Then

$$C^{-1} = \begin{bmatrix} 1/2 & -1/2 & 0 & 0 & 0 & 0 \\ -1/2 & 3/2 & -1 & 0 & 0 & 0 \\ 0 & -1/2 & 1 & -3 & 0 & 0 \\ 0 & 0 & 0 & 3/2 & -1/2 & 0 \\ 0 & 0 & 0 & -1/2 & 7/6 & -1 \\ 0 & 0 & 0 & 0 & -1/2 & 3/4 \end{bmatrix}.$$

Next we consider the case where the digraph is a simple cycle with loops.

Theorem 4.3 *The following are equivalent for $C \in \mathbb{R}^{\mathrm{nn}}$.*

(i) *The matrix C is nonsingular and C^{-1} is an M–matrix whose digraph is the simple n–cycle $1 \to 2 \to \ldots \to n \to 1$, with loops.*

(ii) *$C \gg 0$ and satisfies*

- **(a)** $\frac{c_{11}c_{22}\ldots c_{nn}}{c_{12}c_{23}\ldots c_{n-1,n}c_{n1}} > 1$,
- **(b)** $c_{jk} = \frac{c_{ji}c_{ik}}{c_{ii}}$, *for all* $i > j > k$, $k > i > j$, *and* $j > k > i$, *(i.e., for all distinct vertices i, j, k such that i lies on the path from j to k).*

Example 4.4 We construct an inverse of an M–matrix whose digraph is a simple cycle with loops as follows. Begin by filling in the cycle of $\mathcal{D}(C)$ so that Theorem 4.3 (ii)(a) is satisfied. For example let

$$C = \begin{bmatrix} 4 & 2 & * & * & * & * \\ * & 2 & 2 & * & * & * \\ * & * & 2 & 6 & * & * \\ * & * & * & 1 & 1 & * \\ * & * & * & * & 3 & 4 \\ 1 & * & * & * & * & 4 \end{bmatrix}.$$

Then use (ii)(b) to (uniquely) fill in the *'s:

$$C = \begin{bmatrix} 4 & 2 & 2 & 6 & 6 & 8 \\ 2 & 2 & 2 & 6 & 6 & 8 \\ 2 & 1 & 2 & 6 & 6 & 8 \\ 1/3 & 1/6 & 1/6 & 1 & 1 & 4/3 \\ 1 & 1/2 & 1/2 & 3/2 & 3 & 4 \\ 1 & 1/2 & 1/2 & 3/2 & 3/2 & 4 \end{bmatrix}.$$

Then

$$C^{-1} = \begin{bmatrix} 1/2 & -1/2 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -6 & 0 & 0 \\ 0 & 0 & 0 & 2 & -2/3 & 0 \\ 0 & 0 & 0 & 0 & 2/3 & -2/3 \\ -1/8 & 0 & 0 & 0 & 0 & 1/2 \end{bmatrix}.$$

Let Z denote the $n \times n$ simple cycle permutation matrix. We can apply Theorem 4.3 to characterize all nonnegative matrices which are polynomials in Z and which are inverses of M–matrices whose digraph is a simple n–cycle with loops.

Corollary 4.5 *Let Z be the $n \times n$ simple cycle permutation matrix. Let $k_1, \ldots, k_n$ be nonnegative numbers and consider the matrix*

$$C \;=\; p(Z) \;=\; k_1 I + k_2 Z + \ldots k_n Z^{n-1}.$$

Then necessary and sufficient conditions for C to be the inverse of an M–matrix whose digraph is the simple cycle $1 \rightarrow 2 \rightarrow \ldots \rightarrow n \rightarrow 1$, with loops, are that:

(i) $k_1 \;>\; k_2 \;>\; 0.$

(ii) $k_j \;=\; (k_2)^{j-1} \,/\, (k_1)^{j-2}, \;\; j = 3, \ldots, n.$

Proof:

Notice that

$$C = \begin{bmatrix} k_1 & k_2 & \cdots & k_{n-1} & k_n \\ k_n & k_1 & k_2 & \cdots & k_{n-1} \\ \vdots & k_n & k_1 & \ddots & \vdots \\ k_3 & \vdots & \ddots & k_1 & k_2 \\ k_2 & k_3 & \cdots & k_n & k_1 \end{bmatrix}.$$

The result now follows by applying Theorem 4.3 to C.

ACKNOWLEDGEMENTS

The authors would like to thank Professor Bjarne Toft for providing us with the simple proof of Lemma 2.2. We also thank Professor Miroslav Fiedler for drawing our attention to [4].

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