# Orthogonal Bases which Lead to Symmetric Nonnegative Matrices

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**Abstract**

In a paper dating back to 1983, Soules constructs from a positive vector $x$ an orthogonal matrix $R$ which has the property that for any nonnegative diagonal matrix $\Lambda$, with nonincreasing diagonal entries, the matrix $R\Lambda R^T$ has all its entries nonnegative. Independently, Fiedler in 1988 showed that any symmetric irreducible nonsingular matrix, whose powers are all M–matrices (and hence an MMA–matrix in the language of Friedland, Hershkowitz, and Schneider) must have an orthogonal matrix of eigenvectors $\tilde{R}$ which has similar properties to those of $R$.

Here, for a given positive $n$–vector $x$, we investigate the structure of **all** orthogonal matrices $R$ for which, for any nonnegative diagonal matrix $\Lambda$ as above, the matrices $R\Lambda R^T$ are nonnegative. Up to a permutation of its columns, each such $R$ corresponds to a binary tree whose vertices are subsets of the set $\{1, 2, \ldots, n\}$ with the property that each vertex has either no successor or exactly two disjoint successors.

For such orthogonal matrices $R$ and such nonsingular diagonal matrices $\Lambda$, we show that the set of matrices of the form $R\Lambda R^T$ and the set of inverse MMA–matrices (i.e. matrices whose inverses are MMA–matrices) coincide. Using this result we establish a relation between strictly ultrametric matrices and inverse MMA–matrices. Finally, we show that the QR–factorization of $R\Lambda R^T$, for certain such $R$'s, has a special sign pattern.

# 1 INTRODUCTION

In a 1983 paper, [10], Soules creates a remarkable matrix. Beginning with a positive $n$–vector $x$, he generates an $n \times n$ **orthogonal matrix** $R_x$ such that for any nonnegative diagonal matrix $\Lambda$ =diag($\lambda_1, \ldots,\ \lambda_n$), with $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, the **symmetric** matrix $A_\Lambda = R\Lambda R^T$ has nonnegative entries only. This motivates the following definition:

**DEFINITION 1.1** Let $R \in \mathbb{R}^{\mathrm{n,n}}$ be an orthogonal matrix with columns $(r_1, \ldots, r_n)$. The set $\{r_1, \ldots, r_n\}$ is called a Soules basis and $R$ is called a Soules matrix if $r_1$ is positive and if for every diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \geq 0$, the matrix $A_\Lambda = R\Lambda R^T$ is nonnegative.

One principal aim of this paper is to **refine** Soules' results by showing precisely how to construct, from a given positive normalized vector $r_1$, **all possible** Soules bases. This we do beginning with a simple, but essential, observation, implicit already in the work of Soules, characterizing when the sum of two rank one matrices that are mutually orthogonal is a nonnegative matrix.

Continuing, we shall exhibit that each Soules basis can, essentially, be associated with a rooted binary tree $\mathcal{F}$ on the nonempty subsets of $\{1, 2, \ldots, n\}$. Each vertex $v$ of the tree has either no successor, viz., it is a **leaf** and consists of one element only, or has exactly two successors, $u$ and $w$, such that $u \cup w = v$ and $u \cap w = \phi$.

We shall establish the relations between positive definite nonnegative matrices whose eigenvectors form a Soules basis and two other well-known classes of matrices, namely the MMA–matrices and the strictly ultrametric matrices. To do so we define for a Soules matrix $R \in \mathbb{R}^{\mathrm{n,n}}$ the set

$$\mathcal{M}_R := \left\{ A \in \mathbb{R}^{\mathrm{n,n}} \mid \mathrm{A} = \mathrm{Rdiag}(\lambda_1, \ldots, \lambda_{\mathrm{n}})\mathrm{R}^{\mathrm{T}},\ \lambda_1 \geq \ldots \geq \lambda_{\mathrm{n}} \geq 0 \right\}.$$

We set

$$\mathcal{M} := \bigcup_R \mathcal{M}_R,$$

where the union is taken over all $n \times n$ Soules matrices $R$. By $\mathcal{M}_R^o$ we shall denote the *nonsingular* matrices in $\mathcal{M}_R$. Similarly, we define $\mathcal{M}^o$ to be the set of all nonsingular matrices in $\mathcal{M}$. We shall further denote by $\mathcal{M}_R^i$ and $\mathcal{M}^i$ the *nonsingular and irreducible* matrices in $\mathcal{M}_R$ and $\mathcal{M}$, respectively.

Recall now, e.g., Berman and Plemmons, [1], that an $n \times n$ matrix $C$ is called an M–matrix if $C = kI - G$, where $G$ is an $n \times n$ nonnegative matrix and $k \geq \rho(G)$, the *spectral radius* of $G$. When $k > \rho(G)$, $C$ is necessarily nonsingular. If a matrix $A \in \mathrm{I\!R}^{n,n}$ satisfies that $A^k$ is an irreducible M–matrix for all integers $k \geq 1$ then Friedland, Hershkowitz, and Schneider [4] called the matrix $A$ an MMA–matrix. Note that by their very definition, MMA–matrices are irreducible.

For $A \in \mathrm{I\!R}^{n,n}$ nonsingular with $A^{-1}$ an MMA–matrix, Fiedler [3] called $A$ an *$M^{-1}MA$–matrix.* However, in the following we will call such a matrix an inverse MMA–matrix. MMA–matrices as well as inverse MMA–matrices were considered in a number of papers, e.g., [9] and references cited therein. In [3], Fiedler has, quite independently of the Soules paper, studied the set of all symmetric MMA–matrices. He has shown that any symmetric MMA–matrix has an orthonormal set of eigenvectors which, in our present terminology, forms a Soules basis. Here we shall show, using Fiedler's result, that the set of matrices $\mathcal{M}^i$ and the set of all symmetric inverse MMA–matrices coincide. This then furnishes a new approach how to construct inverse MMA–matrices, since, as mentioned above, we show how to construct all Soules matrices.

Interestingly, we shall show that matrices in $\mathcal{M}^o$ are closely related to another class of inverse M–matrices which has been studied lately:

**DEFINITION 1.2** (Martínez, Michon, and San Martín [5]) A matrix $B = (b_{i,j}) \in \mathrm{I\!R}^{n,n}$ is called *strictly ultrametric* if*:*

**(i)** $B$ is symmetric*.*

**(ii)** $b_{i,j} \geq \min\{b_{i,k}, b_{k,j}\}$ for all $i, j, k \in \langle n \rangle$*.*

**(iii)** $b_{i,i} > \max\{b_{i,k} | k \in \langle n \rangle / \{i\}\}$*,* for all $i \in \langle n \rangle$*,*

where $\langle n \rangle := \{1, \ldots, n\}$. Martínez, Michon, and San Martín show that any strictly ultrametric matrix is an inverse of a symmetric diagonally dominant

M–matrix. Further properties and characterizations of the strictly ultrametric matrices have been considered by Nabben and Varga in [7]. Generalizations to nonsymmetric matrices have been found by Nabben and Varga in [8] and by McDonald, Neumann, Schneider, and Tsatsomeros in [6].

Let $A \in \mathcal{M}^i$ so that, by the foregoing, $A$ is an inverse MMA–matrix, and let $x = (x_1, \ldots, x_n)^T$ be a Perron vector of $A$. We shall show that with $D = \text{diag}(1/x_1, \ldots, 1/x_n)$, the matrix $DAD$ is a strictly ultrametric matrix and conversely, if $A$ is an irreducible strictly ultrametric matrix, then there exists a positive diagonal matrix $F$ such that the matrix $FAF$ is an inverse MMA–matrix, or equivalently, that the matrix $FAF$ has a Soules matrix of eigenvectors.

Finally, suppose that $R$ is a Soules matrix which corresponds to a binary tree (as described above) in which every subset (viz., every vertex of the tree) $\mathcal{N}_{i,j}$, $j = 1, \ldots, i$ of $\mathcal{N}_i$, $i = 1, \ldots, n$, consists of consecutive integers. We shall show that the QR–factorization of any $A \in \mathcal{M}^o_R$ consists of an orthogonal factor $Q = (q_{i,j})$ with $q_{i,j} > 0$ for $n \geq i \geq j \geq 1$ and $q_{i,j} < 0$ for $1 \leq i < j \leq n$ and a nonnegative triangular factor which is itself an inverse of an M–matrix. Similarly, we shall show that if $A \in \mathcal{M}^o_R$, then $A^{-1}$ has a QR–factorization with the orthogonal factor $Q = (q_{i,j})$ with $q_{i,j} > 0$ for $n \geq j \geq i \geq 1$ and $q_{i,j} < 0$ for $n \geq i > j \geq 1$ and with the triangular factor which is an M–matrix.

For $n$ numbers $d_1, \ldots, d_n$, we shall use $\Delta(d_1, \ldots, d_n)$ to denote the diagonal matrix whose diagonal entries from first to last are $d_1, \ldots, d_n$. Moreover, for $x \in \mathbb{R}^n$ we write $x \gg 0$ if all entries of $x$ are positive.

# 2 The Structure of Soules matrices

We start this section with the following characterization of a Soules matrix:

**OBSERVATION 2.1** *Let $R = (r_{i,j}) \in \mathbb{R}^{n,n}$ be a matrix with columns $r_1, \ldots, r_n$ where $r_1$ is positive. Then the following are equivalent:*

(i) *$R = (r_{i,j})$ is a Soules matrix.*

(ii) *For $l = 1, \ldots, n$,*

$$\sum_{i=1}^{\ell} r_i r_i^T \;\geq\; 0 \tag{2.1}$$

*and*

$$\sum_{i=1}^{n} r_i r_i^T \;=\; I. \tag{2.2}$$

<u>**Proof**</u>: (i)⇒(ii). For $1 \leq l \leq n$ let $D_\ell$ be the $n \times n$ diagonal matrix given by:

$$D_\ell \;=\; \mathrm{diag}(\underbrace{1, \ldots, 1}_{\ell \text{ times}}, 0, \ldots, 0).$$

As for $l = 1, \ldots, n$, $RD_lR^T \geq 0$ by (i), and

$$RD_\ell R^T \;=\; \sum_{i=1}^{\ell} r_i r_i^T, \tag{2.3}$$

we have (2.1).

(ii)⇒(i). Observe that any nonnegative diagonal matrix $\Lambda = \Delta(\lambda_1, \ldots, \lambda_n)$ with **nonincreasing diagonal entries** can be rewritten as

$$\Lambda \;=\; (\lambda_1 - \lambda_2)D_1 + \ldots + (\lambda_{n-1} - \lambda_n)D_{n-1} + \lambda_n D_n,$$

where the coefficients of the $D_1, \ldots, D_n$ are nonnegative. Using the identity given in (2.3) and the assumption made in (2.1), it follows at once that $R\Lambda R^T \geq 0$ so that $R$ is a Soules matrix. □

It follows immediately from the above observation and its proof that $A = R\Lambda R^T \in \mathcal{M}$ is irreducible if and only if $\lambda_1 > \lambda_2$ and that in this case $A$ is, necessarily, positive.

In the following we show precisely how to construct, from a given positive vector $x$, all possible Soules bases. This we do beginning with a simple, but essential, observation characterizing when the sum of two rank one matrices that are mutually orthogonal is a nonnegative matrix.

We start with a positive vector $w \in \mathrm{I\!R}^n$ from which we construct a second vector $\tilde{w}$ such that $ww^T + \tilde{w}\tilde{w}^T \geq 0$. But first, let $0 \neq w \in \mathrm{I\!R}^n$ with $\|w\|_2 = 1$

and partition $w$ into $\binom{u}{v}$, where $0 \neq u \in \mathrm{IR}^{\mathrm{p}}$ and $0 \neq v \in \mathrm{IR}^{\mathrm{n-p}}$. Then it is straightforward to ascertain that the vector

$$\tilde{w} \;=\; \begin{pmatrix} (\|v\|_2 \,/\, \|u\|_2)u \\ \\ -(\|u\|_2 \,/\, \|v\|_2)v \end{pmatrix} \tag{2.4}$$

satisfies $\|\tilde{w}\|_2 = 1$ and $\tilde{w}^T w = 0$. Now suppose that, in addition, $w \gg 0$. Then it holds that

$$ww^T + \tilde{w}\tilde{w}^T \;=\; \begin{pmatrix} uu^T/\,\|u\|_2 & 0 \\ \\ 0 & vv^T/\,\|v\|_2 \end{pmatrix} \;\geq\; 0. \tag{2.5}$$

The converse of this observation is also true, namely, that if $w \gg 0$ is in $\mathrm{IR}^{\mathrm{n}}$ and if $\tilde{w} \in \mathrm{IR}^{\mathrm{n}}$ is a vector such $\tilde{w}^T w = 0$ and such that the matrix $ww^T + \tilde{w}\tilde{w}^T \geq 0$, then $\tilde{w}$ must be of the form specified by (2.4). This is implicit in the proof of our Theorem 2.2. Returning to $w \gg 0$ from which we constructed $\tilde{w}$ according to (2.4), we can enlarge the orthogonal basis by further re–partitioning the vectors $(\|v\|_2 \,/\, \|u\|_2)u$ and $(\|u\|_2 \,/\, \|v\|_2)v$ to obtain a bigger set $w_1, w_2, \ldots, w_k$, $k \leq n$, of $n$–vectors which are mutually orthogonal and such that $w_1 w_1^T + w_2 w_2^T + \ldots + w_k w_k^T$ is a nonnegative matrix. This will be the basis of our construction below.

Obviously such a construction will lead after $n-1$ steps to a matrix $R$ with columns $(w_1, \ldots, w_n)$, which, by Observation 2.1, is a Soules matrix. The coming theorem will show that our approach accounts for all Soules bases.

To achieve our above stated goal we need to introduce some further notations. Let $x \gg 0$ be in $\mathrm{IR}^{\mathrm{n}}$ and consider a sequence of partitions of $\langle n \rangle$ of the form

$$\mathcal{N}_1, \ldots, \mathcal{N}_i, \quad i = 1, \ldots, n,$$

where

$$\mathcal{N}_1 \;=\; \{\mathcal{N}_{1,1}\}, \ldots, \mathcal{N}_i \;=\; \{\mathcal{N}_{i,1}, \ldots, \mathcal{N}_{i,i}\}, \quad i = 1, \ldots, n,$$

in which $\mathcal{N}_{i+1}$ is constructed from $\mathcal{N}_i$ by splitting one of the sets $\mathcal{N}_{i,j}$ into two subsets as follows: there exist $k(i)$ such that

$$\begin{cases} \mathcal{N}_{i+1,j} \;=\; \mathcal{N}_{i,j}, & 1 \le j < k(i), \\ \mathcal{N}_{i+1,j} \;=\; \mathcal{N}_{i,j-1}, & k(i)+1 < j < i+1, \\ \mathcal{N}_{i+1,k(i)} \cup \mathcal{N}_{i+1,k(i)+1} \;=\; \mathcal{N}_{i,k(i)}. & \end{cases} \tag{2.6}$$

For $\mathcal{N} \subset \langle n \rangle$, define the vector

$$x_{\mathcal{N}} \;=\; \begin{cases} x_i, & i \in \mathcal{N}, \\ 0, & i \notin \mathcal{N}. \end{cases} \tag{2.7}$$

**THEOREM 2.2** *Let $x \gg 0$ in $\mathbb{R}^n$ and suppose that $\{r_1, \ldots, r_n\}$ be a Soules basis with $r_1 = x$. Let*

$$E_i \;=\; \sum_{j=1}^{i} r_i r_i^T, \quad i = 1, \ldots, n. \tag{2.8}$$

*Then there exists a sequence $\{\mathcal{N}_1, \ldots, \mathcal{N}_n\}$ of partitions of $\langle n \rangle$, with $\mathcal{N}_i = \{\mathcal{N}_{i,1}, \ldots, \mathcal{N}_{i,i}\}$, $i = 1, \ldots, n$, such that for $2 \le i \le n-1$, $i-1$ of the $\mathcal{N}_{i,j}$'s coincide with $i-1$ of the $\mathcal{N}_{i+1,j}$'s and $\mathcal{N}_{i+1}$ is constructed from $\mathcal{N}_i$ by splitting up exactly one of the sets in $\mathcal{N}_i$ into two nonempty subsets (as described in (2.6)) with the following property:*

$$E_i \;=\; \sum_{j=1}^{i} E_{i,j}, \quad i = 1, \ldots, n, \tag{2.9}$$

*where*

$$E_{i,j} \;=\; \frac{x^{(i,j)} x^{(i,j)T}}{\|x^{(i,j)}\|_2^2} \tag{2.10}$$

*with $x^{(i,j)} = x_{\mathcal{N}_{i,j}}$, $j = 1, \ldots, i$. That is, $E_i$ is the direct sum of $i$ matrices of rank 1. In addition, $r_i$ is (up to a factor $\pm 1$) given by*

$$r_i \;=\; \frac{1}{\sqrt{\|x^{(i,t)}\|_2^2 + \|x^{(i,s)}\|_2^2}} \left\{ \frac{\left\|x^{(i,t)}\right\|_2^2}{\|x^{(i,s)}\|_2^2} x^{(i,s)} - \frac{\left\|x^{(i,s)}\right\|_2^2}{\|x^{(i,t)}\|_2^2} x^{(i,t)} \right\}, \quad i \ge 2, \tag{2.11}$$

*where $s$ and $t$ are those indices in $\{1,\ldots,i\}$ for which sets $\mathcal{N}_{i,t}$ and $\mathcal{N}_{i,s}$ do not coincide with one of the sets $\mathcal{N}_{i-1,j}$, $j = 1,\ldots,i-1$.*

*Conversely, if $r_1 = x \gg 0$ is given, then for each sequence $\{\mathcal{N}_1,\ldots,\mathcal{N}_n\}$ of partitions of $\langle n\rangle$ satisfying* (2.6) *the vectors $r_1,\ldots,r_n$ yields, by* (2.11)*, a Soules basis.*

**Proof**: The claim obviously holds for $i = n$ which is the case when $\mathcal{N}_{n,i} = \{i\}$, $i = 1,\ldots,n$. Proceeding by induction we assume that (2.9) and (2.10) hold for some $i \geq 2$. Then $\mathcal{N}_{i,j}$, $j = 1,\ldots,i$, are the sets which describe $x^{(i,j)}$ according to (2.10). As

$$E_{i-1} \; = \; E_i - r_i r_i^T \; \geq \; 0 \tag{2.12}$$

and

$$(E_i)_{t,s} \; = \; 0 \text{ for } t \in \mathcal{N}_{i,\nu}, \; s \in \mathcal{N}_{i,\mu}, \; \mu \neq \nu, \tag{2.13}$$

we have from (2.12) that

$$t \in \mathcal{N}_{i,\nu}, \; s \in \mathcal{N}_{i,\mu}, \text{ and } \mu \neq \nu \; \Rightarrow \; (r_i)_t (r_i)_s \; \leq \; 0. \tag{2.14}$$

Since $r_i^T x = 0$, there must be some $t$ for which $(r_i)_t > 0$. Suppose that $t \in \mathcal{N}_{i,i}$. But then, by (2.14), any index $t$ for which $(r_i)_t > 0$ must be in $\mathcal{N}_{i,i}$. Similarly, there must be an index $s$ for which $(r_i)_s < 0$ and so, again by (2.14), all indices $s$ for which $(r_i)_s < 0$ have to belong to the same set $\mathcal{N}_{i,\nu}$, so let us suppose that they lie in $\mathcal{N}_{i,i-1}$. Furthermore, we know that all entries of $r_i$ outside $\mathcal{N}_{i,i} \cup \mathcal{N}_{i,i-1}$ are zero. On defining

$$\mathcal{N}_{i-1,j} \; := \; \mathcal{N}_{i,j}, \; j = 1,\ldots,i-2, \text{ and } \mathcal{N}_{i-1,i-1} \; := \; \mathcal{N}_{i,i} \cup \mathcal{N}_{i,i-1}$$

we have that

$$E_{i-1} \; = \; \sum_{j=1}^{i-1} E_{i-1,j},$$

where $E_{i-1,j} = E_{i,j}$, $1 \leq j \leq i-2$, and the sum is a direct one. As $\mathrm{rank}(E_{i-1}) = i-1$, the rank of $E_{i-1,i-1}$ must be (also) 1. Next, from the sign pattern of $r_i$ and the representation (2.10) we see that

$$r_i \; = \; \alpha_i x^{(i,i+1)} + \beta_i x^{(i,i)}.$$

But then, as $r_i^T x = 0$, we get from Observation 2.1 that $r_i$ must have the form given in (2.11). The fact that $E_i x = x$ now yields (2.10).

The converse follows immediately from the construction mentioned just prior to Theorem 2.2. $\square$

Note that, by the above theorem, the vectors $r_{i+1}$ have nonzero entries only at positions which belongs to $\mathcal{N}_{i,k(i)} = \mathcal{N}_{i+1,k(i)} \cup \mathcal{N}_{i+1,k(i)+1}$, $i = 1, \ldots, n-1$.

It is readily seen that for $i = 1, \ldots, n$, the matrix $E_i$ given in (2.9) has the following block diagonal form:

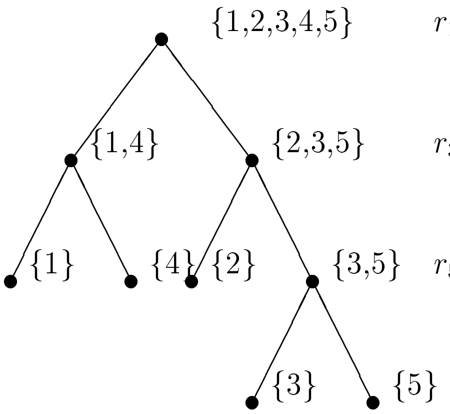
$$E_i = \sum_{j=1}^{i} r_i r_i^T = \begin{pmatrix} \frac{x^{(i,1)}x^{(i,1)T}}{\|x^{(i,1)}\|_2^2} & 0 & \ldots & 0 \\ & \frac{x^{(i,2)}x^{(i,2)T}}{\|x^{(i,2)}\|_2^2} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \ldots & \ldots & \frac{x^{(i,i)}x^{(i,i)T}}{\|x^{(i,i)}\|_2^2} \end{pmatrix}, \tag{2.15}$$

Thus we have exhibited that each Soules basis can, essentially, be associated with a rooted binary tree $\mathcal{F}$ on the nonempty subsets of $\langle n \rangle$. Each vertex $v$ of the tree has either no successor, viz., it is a **leaf** and consists of one element only, or has exactly two successors, $u$ and $w$, such that $u \cup w = v$ and $u \cap w = \phi$. Moreover, each interior vertex (including the root) of the tree is associated with one $r_i, (i \geq 2)$, where the numbering of the $r_i$ must be consistent with the tree. The vector $r_i$ has nonzero entries only at that positions which belong to the subset of $\{1, \ldots, n\}$ associated with the same vertex. The vectors $r_i$ are given by (2.11) and have the form

$$r_i = \alpha_i x^{(i,k(i))} + \beta_i x^{(i,k(i)+1)}, \tag{2.16}$$

where $\alpha_i, \beta_i \in \mathbb{R}$.

As an illustration consider Fig. 1. There we consider one possible structure of a $5 \times 5$ Soules matrix. The vector $r_1$ is positive. We then start at the root with the associated set $\mathcal{N}_1 = \{1, 2, 3, 4, 5\}$ and the vector $r_2$ of the form $r_2 = (*, *, *, *, *)$. Here, $*$ means a nonzero entry. Then $\mathcal{N}_1$ is split into $\mathcal{N}_{2,1} = \{1, 4\}$ and $\mathcal{N}_{2,2} = \{2, 3, 5\}$ which gives $\mathcal{N}_2 = \{\{1, 4\}, \{2, 3, 5\}\}$. The associated vectors have the form $r_3 = (*, 0, 0, *, 0)$ and $r_4 = (0, *, *, 0, *)$. Next the sets $\mathcal{N}_{2,1}$ and $\mathcal{N}_{2,2}$ are split as indicated in Fig. 1, which give $\mathcal{N}_3 = \{\{1\}, \{4\}, \{2, 3, 5\}\}$ and $\mathcal{N}_4 = \{\{1\}, \{4\}, \{2\}, \{3, 5\}\}$. We continue until each vertex is associated with one element only. Note that $r_5$ is associated with that vertex which is associated with the set {3,5}. Thus, $r_5$ has the form $r_5 = (0, 0, *, 0, *)$.




$r_1 := (*, *, *, *, *)^T$; $r_2 := (*, *, *, *, *)^T$

$r_3 := (*, 0, 0, *, 0)^T$; $r_4 := (0, *, *, 0, *)^T$

$r_5 := (0, 0, *, 0, *)^T$;

FIG. 1

We come now to the relation between matrices in $\mathcal{M}^o$ on the one hand and M–matrices and inverse MMA–matrices on the other hand.

**LEMMA 2.3** *Let $R$ be a Soules matrix and let $B \in \mathcal{M}^o_R$. If $f$ is a positive nonincreasing function on $(0, \infty)$, then $f(B)$ is a nonsingular M–matrix.*

**Proof**: We know that $f(B) = Rf(\Lambda_B)R^T$, where, because $\lambda_1 \geq \ldots \geq \lambda_n$ and the nonincreasingness of $f$, the diagonal entries $f(\lambda_i)$, $i = 1 \ldots, n$, of $f(\Lambda_B)$ satisfy that

$$0 \ < \ f(\lambda_1) \ \leq \ \ldots \ \leq \ f(\lambda_n).$$

Let $s > f(\lambda_n)$. Then, for $i = 1, \ldots, n$, we can write that

$$f(\lambda_i) \ = \ s - (s - f(\lambda_i)) \, .$$

Put $\mu_i = s - f(\lambda_i)$, $i = 1, \ldots, n$, so that $\mu_1 \geq \ldots \geq \mu_n > 0$. Then

$$f(B) \ = \ R\Delta(s - \mu_1, \ldots, s - \mu_n)R^T \ =: \ sI - C,$$

where $C = R\Delta(\mu_1, \ldots, \mu_n)R^T$. Finally, observe that $C$ is nonnegative by virtue of $R$ being a Soules–matrix. As $s > \rho(C) = \mu_1$, $f(B)$ is a nonsingular

M–matrix. $\square$

An immediate corollary to the above lemma is the following:

**COROLLARY 2.4** *Let $B = R\Lambda_B R^T$ be an $n \times n$ positive positive definite matrix with $R$ being a Soules–matrix. Then for any $p \in [1, \infty)$, $B^{-p}$ is an M–matrix. In particular $B^{-1}$ is an M–matrix.*

**Proof**: Choose $f(x) = 1/x^p$ in Lemma 2.3. $\square$

We remark that since by the above corollary $B^{-k}$ is an M–matrix for all integers $k \geq 1$, it follows that if $B$ is irreducible, then $B$ is an inverse MMA–matrix or $B^{-1}$ is an MMA–matrix. As mentioned in the introduction Fiedler, [3], has shown that any symmetric MMA–matrix, and therefore any symmetric inverse MMA–matrix, has an orthonormal set of eigenvectors which, in our present terminology, forms a Soules basis. Thus, the set $\mathcal{M}^i$ and the set of all $n \times n$ symmetric inverse MMA–matrices are the same, namely,

$$\mathcal{M}^i \;=\; \mathcal{M}^{-1}\mathcal{MA}, \tag{2.17}$$

where $\mathcal{M}^{-1}\mathcal{MA}$ denotes the set of all $n \times n$ symmetric inverse MMA–matrices.

# 3 Inverse MMA–matrices and strictly ultrametric matrices

In this section we shall investigate the relationship between the class of inverse MMA–matrices and the class of strictly ultrametric matrices introduced in Definition 1.2. By definition MMA–matrices and inverse MMA–matrices are irreducible, while strictly ultrametric matrices can be reducible. However, a reducible strictly ultrametric matrix is just a direct sum of irreducible ones, since strictly ultrametric matrices are symmetric. Therefore we shall only consider irreducible matrices in the following. The reader is reminded again that the set $\mathcal{M}^i$ and the set of symmetric inverse MMA–matrices coincide.

**THEOREM 3.1** *Let $A$ be a symmetric inverse MMA–matrix and let $x$ be the Perron vector of $A$. Then for $D = \mathrm{diag}(x_1^{-1}, \ldots, x_n^{-1})$, $DAD$ is a strictly ultrametric matrix.*

**Proof**: ¿From the remark following Corollary 2.4, there exists a Soules matrix $R$ with $A = R\Lambda R^T$ where $\Lambda = \Delta(\lambda_1, \ldots, \lambda_n)$ with $\lambda_1 > \lambda_2 \geq \lambda_3 \ldots \lambda_n > 0$.

Let $r_1 = x, \ldots, r_n$ be the columns of $R$ and observe first that $A$ can be represented as follows:

$$A \;=\; \sum_{i=1}^{n} \lambda_i r_i r_i^T \;=\; \sum_{i=1}^{n-1} (\lambda_i - \lambda_{i+1}) \sum_{j=1}^{i} r_j r_j^T + \lambda_n \underbrace{\sum_{i=1}^{n} r_j r_j^T}_{I}. \tag{3.1}$$

In this way we see, using (ii) of Observation 2.1, that $A$ can be written as a linear combination, with nonnegative weights, of the nonnegative matrices $E_i$. Specifically,

$$A \;=\; \sum_{i=1}^{n-1} (\lambda_i - \lambda_{i+1}) E_i + \lambda_n I. \tag{3.2}$$

Hence

$$DAD \;=\; \sum_{i=1}^{n-1} (\lambda_i - \lambda_{i+1}) DE_iD + \lambda_n D^2. \tag{3.3}$$

We then see from Theorem 2.2, from (2.7), and from the explicit representation given in (2.15), that $DE_1D$ is a matrix of all ones and that for $2 \leq i \leq n$, $DE_iD$ is a completely reducible matrix whose diagonal blocks are each a multiple, possibly different from diagonal block to diagonal block, of the all ones matrix. Thus, each matrix $DE_iD$ satisfy (i) and (ii) of Definition 1.2 while in (iii) of Definition 1.2 a weak inequality is fulfilled. Since $(DE_iD)_{s,t} = 0 \Rightarrow (DE_{i+1}D)_{s,t} = 0$, $i = 1, \ldots, n-1$ and since the $x^{(i,j)}$ of each $E_i$ are given by partitions of $\langle n \rangle$ which satisfy (2.6), the sum of the $(\lambda_i - \lambda_{i+1})DE_iD$ plus $\lambda_n D^2$ is a strictly ultrametric matrix. $\square$

Recall now that according to the result of Martínez, Michon, and San Martín [5] quoted following Definition 1.2, if $A$ is strictly ultrametric, then $A^{-1}$ is a strictly diagonally dominant matrix, so that the vector

$$p \;:=\; A^{-1}e \;\gg 0. \tag{3.4}$$

**THEOREM 3.2** *Let $A \in R^{n,n}$ be an irreducible strictly ultrametric matrix and let $p = (p_1, \ldots, p_n)^T$ be the vector given in (3.4). Let $F = \operatorname{diag}\left(p_1^{1/2}, \ldots, p_n^{1/2}\right)$. Then $FAF$ is an inverse MMA–matrix.*

**Proof**: Let $y = (p_1^{1/2}, \ldots, p_n^{1/2})^T$. Then $Ap = AF^2e = e$ and $y = Fe$ imply that

$$FAFy = y. \tag{3.5}$$

Now, according to Nabben and Varga [7, Theorem 2.2], A can be written as

$$A = \sum_{i=1}^{2n-1} \tau_i u_i u_i^T \tag{3.6}$$

where the $u_i$, $i = 1, \ldots, 2n-1$, have entries in $\{0, 1\}$. Next, identify the vectors $u_i$ with the sets $U_i$ given by

$$U_i = \{j \in \langle n \rangle \mid (u_i)_j = 1\}$$

and order these sets so that

$$i \geq j \Rightarrow U_i \cap U_j = \phi \text{ or } U_i \subseteq U_j.$$

This is always possible because, as shown by Nabben and Varga, the nonzero entries of $u_i$ correspond to vertices of a rooted tree. Let $P_i$ be the projection matrix on the coordinate subspace determined by $U_i$, viz., $P_i e = u_i$. Also let $y^{(i)} = P_i y = F u_i$. Then

$$FAF = \sum_{i=1}^{2n-1} \tau_i F u_i u_i^T F = \sum_{i=1}^{2n-1} \tau_i y^{(i)} y^{(i)T}. \tag{3.7}$$

We claim that for $i = 1 \ldots, 2n-1$, $y^{(i)}$ is an eigenvector of $\sum_{j=i+1}^{2n-1} \tau_j y^{(j)} y^{(j)T}$. To see this we use (3.5) and (3.7) as follows:

$$\begin{aligned} P_i y = y^{(i)} &= P_i FAFy \\ &= \sum_{j=1}^{2n-1} \tau_j P_i y^{(j)} y^{(j)T} y \\ &= \sum_{j=1}^{i} \tau_j P_i y^{(j)} y^{(j)T} y + \sum_{j=i+1}^{2n-1} \tau_j P_i y^{(j)} y^{(j)T} y. \end{aligned}$$

The first sum is a multiple of $y^{(i)}$ as each term in it is either 0 (if $U_i \cap U_j = \phi$) or a multiple of $y^{(i)}$ (if $U_i \subseteq U_j$). The second sum coincides with $\sum_{j=i+1}^{2n-1}(\tau_j y^{(j)} y^{(j)^T}) y^{(i)}$ because

$$\tau_j y^{(j)} y^{(j)T} y^{(i)} \;=\; \tau_j P_i y^{(j)} y^{(j)T} y,$$

namely, if $U_j \cap U_i = \phi$ both terms vanish, while if $U_i \subseteq U_j$, then $P_i y^{(j)} = y^{(j)}$ and $y^{(j)T} y^{(i)} = y^{(j)T} y$. Thus

$$\left(\sum_{j=i+1}^{2n-1} \tau_j y^{(j)} y^{(j)T}\right) y^{(i)} \;=\; c_i y^{(i)} \tag{3.8}$$

for some nonnegative $c_i$ which proves our present claim.

Suppose now that $B$ is a second strictly ultrametric matrix such that

$$B \;=\; \sum_{i=1}^{2n-1} \sigma_i u_i u_i^T,$$

where the $u_i$ are given by (3.6), and such that $FBFy = y$. We then have that

$$FBF \;=\; \sum_{i=1}^{2n-1} \sigma_i y^{(i)} y^{(i)T}$$

and

$$\left(\sum_{j=i+1}^{2n-1} \sigma_j y^{(j)} y^{(j)T}\right) y^{(i)} \;=\; d_i y^{(i)} \tag{3.9}$$

for some nonnegative $d_i$. But then

$$\begin{aligned}(FAF)(FBF) \;&=\; \left(\sum_{i=1}^{2n-1} \tau_i y^{(i)} y^{(i)T}\right)\left(\sum_{j=1}^{2n-1} \sigma_j y^{(j)} y^{(j)T}\right) \\ &=\; \sum_{i,j=1}^{2n-1} \tau_i \sigma_j y^{(i)} y^{(i)T} y^{(j)} y^{(j)T}\end{aligned}$$

By splitting the summation $\sum_{i,j=1}^{2n-1}$ into $\sum_{i=j=1}^{2n-1}$ plus $\sum_{j=1}^{2n-1}\sum_{i<j}^{2n-1}$ plus $\sum_{j=1}^{2n-1}\sum_{i>j}^{2n-1}$ and using (3.8) and (3.9) we see that

$$(FAF)(FBF) \;=\; \sum_{j=1}^{2n-1} \gamma_i y^{(j)} y^{(j)T} \;=\; F \sum_{j=1}^{2n-1} \gamma_i u^{(j)} u^{(j)T} F.$$

for some $\gamma_i$. According to Nabben and Varga [7, Theorem 2.2] again, the matrix $\sum_{j=1}^{2n-1} \gamma_i u^{(j)} u^{(j)T}$ is a strictly ultrametric matrix. Hence, on choosing $B = A$, we see that for $m \geq 1$ $(FAF)^m = FU_mF$ for strictly ultrametric matrices $U_m$. Hence, $FAF$ is an inverse MMA matrix. $\square$

We **remark** that the Theorems 3.1 and 3.2 describe nonlinear mappings $\Phi$ and $\Psi$ where $\Phi$ maps the symmetric inverse MMA–matrices into the strictly ultrametric matrices, $\Phi$ is unique if we use the normalized Perron vector, and $\Psi$ maps the strictly ultrametric matrices into the symmetric inverse MMA–matrices. The mappings $\Phi$ and $\Psi$ are up to a normalization inverse mappings. More precisely if we introduce for strictly ultrametric matrices $A$ the mapping $\tilde{\Psi}(A) = \Psi(A)||A^{-1}e||_2^{-1}$ then $\tilde{\Psi}\Phi = id$ and $\Phi\tilde{\Psi} = id$. We refrain from giving the straightforward proof.

Theorems 3.1 and 3.2 show that for any $n \geq 1$ and **up to conjugation via positive diagonal matrices**, the class of all nonnegative positive definite matrices with a Soules matrix of eigenvectors coincides with the class of all strictly ultrametric matrices. However, in what follows we show that as classes of matrices they do not coincide. As a first example let $x = (1, 2, 3, 4, 5)^T$. Then a Soules matrix constructed from $x$ using the original Soules construction (see [10, Display (7)]), which corresponds to the sequence of partitioning (2.6) of $\langle n \rangle$ in which $\mathcal{N}_i = \{\langle n-i+1 \rangle, \{n-i+2\}, \ldots, \{n\}\}$, is given by

$$R = \begin{pmatrix} 0.1348 & 0.1231 & 0.1952 & 0.3586 & 0.8944 \\ 0.2697 & 0.2462 & 0.3904 & 0.7171 & -0.4472 \\ 0.4045 & 0.3693 & 0.5855 & -0.5976 & 0 \\ 0.5394 & 0.4924 & -0.6831 & 0 & 0 \\ 0.6742 & -0.7385 & 0 & 0 & 0 \end{pmatrix}.$$

On choosing $\Lambda = \Delta(.9\ .6\ .58\ .2\ .05)$ we obtain

$$A \;=\; R\Lambda R^T \;=\; \begin{pmatrix} 0.1133 & 0.1265 & 0.09979 & 0.02448 & 0.02727 \\ 0.1265 & 0.3031 & 0.1996 & 0.04897 & 0.05455 \\ 0.09979 & 0.1996 & 0.4994 & 0.07345 & 0.08182 \\ 0.02448 & 0.04897 & 0.07345 & 0.6779 & 0.1091 \\ 0.02727 & 0.05455 & 0.08182 & 0.1091 & 0.7364 \end{pmatrix},$$

and find that $A^{-1}e$ is not positive. Hence $A$ can not be a strictly ultrametric matrix.

As a second example let

$$B \;=\; \begin{pmatrix} 4 & 2 & 1 & 1 \\ 2 & 3 & 1 & 1 \\ 1 & 1 & 8 & 2 \\ 1 & 1 & 2 & 6 \end{pmatrix}.$$

It is readily checked that $B$ is a strictly ultrametric matrix, but a computation shows that

$$B^{-2} \;=\; \begin{pmatrix} 0.20273 & -0.21566 & 0.00032792 & -0.0010609 \\ -0.21566 & 0.32645 & -0.011767 & -0.020755 \\ 0.00032792 & -0.011767 & 0.021932 & -0.012133 \\ -0.0010609 & -0.020755 & -0.012133 & 0.039254 \end{pmatrix}$$

which is not an M–matrix and so, by Corollary 2.4, $B$ **cannot** be a nonnegative positive definite matrix having a Soules basis of eigenvectors.

To conclude this section we consider nonsymmetric matrices. It is proved in [4] that every MMA–matrix is uniquely positive diagonally similar to a symmetric MMA–matrix. Specifically, Hershkowitz and Schneider in [2] showed that the diagonal matrix yielding the similarity is given by

$$D \;=\; \mathrm{diag}(u_1^{\frac{1}{2}} v_1^{-\frac{1}{2}}, \ldots, u_n^{\frac{1}{2}} v_n^{-\frac{1}{2}}),$$

where $u = (u_1 \ldots u_n)^T$ and $v = (v_1 \ldots v_n)^T$ are right and left Perron vectors of $A$, respectively. With this result in mind we immediately obtain:

**THEOREM 3.3** *Let $A \in \mathrm{I\!R}^{n,n}$ be an inverse MMA–matrix. Let $u = (u_1 \dots u_n)^T$ and $v = (v_1 \dots v_n)^T$ be right and left Perron vectors of $A$, respectively. Set $D_1 := \mathrm{diag}(u_1^{-1}, \dots, u_n^{-1})$ and $D_2 := \mathrm{diag}(v_1^{-1}, \dots, v_n^{-1})$. Then $D_1 A D_2$ is a strictly ultrametric matrix.*

**Proof**: Since $A$ is a inverse MMA–matrix, then, with $D = \mathrm{diag}(u_i^{\frac{1}{2}} v_i^{-\frac{1}{2}})$, the matrix

$$D^{-1}AD$$

is symmetric with right and left Perron vector $p = (p_1 \dots p_n)^T$, where $p_i = (u_i v_i)^{-1}$. Let $\tilde{D} = \mathrm{diag}(p_1^{\frac{1}{2}}, \dots, p_n^{\frac{1}{2}})$. Then using Theorem 3.1 it follows that the matrix

$$\tilde{D}D^{-1}AD\tilde{D}$$

is a strictly ultrametric and we easily see that

$$\tilde{D}D^{-1}AD\tilde{D} \;=\; D_1 A D_2.$$

$\square$

# 4 QR–Decompositions

In this section we shall show that for certain Soules matrices $R$, the matrices in $\mathcal{M}_R^o$ and their inverses possess a QR–factorization with the entries of both the orthogonal and the upper triangular factors having a definitive sign pattern.

**THEOREM 4.1** *Let $R$ be a Soules matrix with columns $r_1 = x \gg 0, r_2, \dots, r_n$ to which there corresponds a sequence of partitionings $\{\mathcal{N}_1, \dots, \mathcal{N}_n\}$ of $\langle n \rangle$ such for each $i = 1, \dots, n$, the subsets $\mathcal{N}_{i,1}, \dots, \mathcal{N}_{i,i}$ each consists of consecutive integers. Then for any $A \in \mathcal{M}_R^o$, $A$ has the QR–factorization $A = QS$ with the entries of $Q = (q_{\mu,\nu})$ satisfying that*

$$q_{\mu,\nu} \begin{cases} > \;0, & \text{if } \mu \geq \nu, \\ < \;0, & \text{if } \mu < \nu, \end{cases} \tag{4.1}$$

*and with $S$ a nonnegative, nonsingular, upper triangular matrix whose inverse is an M–matrix.*

**Proof**: Let $A = QS$ be the unique QR–factorization of $A$ with $S$ having positive diagonal entries. Since $A^2 \in \mathcal{M}_R^o$, $A^{-2}$ is a nonsingular symmetric M–matrix and so has a "reversed" Cholesky factorization $UU^T$, where $U$ is a nonsingular upper triangular M–matrix, showing that $U^{-T}U^{-1}$ is the Cholesky factorization of $A^2$. As $S = U^{-1}$, the upper triangular factor $S$ in the QR–factorization of $A$ has the desired properties.

Next observe that as $r_1 = x$ is an eigenvector of $A$ we have $A^{-2}x \gg 0$ and so, as $S^{-1} = A^{-2}S^T$,

$$x^T S^{-1} \; = \; x^T A^{-2} S^T \; \gg \; 0.$$

which gives that

$$x x^T S^{-1} \; \gg \; 0.$$

Thus, as $S^{-1}$ is an M–matrix and so has all its off diagonal entries nonpositive, we easily see that for any subset $\alpha$ of $\langle n \rangle$ of consecutive indices,

$$(xx^T)[\alpha]S^{-1}[\alpha] \; \geq \; \left( xx^T S^{-1} \right)[\alpha] \; \gg \; 0. \tag{4.2}$$

Now by 2.2 and (2.15), for each $i = 1, \ldots, n$, $E_i$ is a nonnegative block diagonal matrix which, up to a positive multiple scalar which can differ from block to block, is a principal submatrix of $xx^T$. Thus, by (4.2), the diagonal blocks of the block upper triangular matrix $E_i S^{-1}$ are positive and so

$$\left( E_i S^{-1} \right)_{\mu,\nu} \; \geq \; 0, \quad for \ all \ 1 \leq \nu \leq \mu \leq n. \tag{4.3}$$

Recall now that by (2.15), $A = \sum_{i=1}^n \beta_i E_i$ for some $\beta_i \geq 0$ with $\beta_1 > 0$. Then

$$Q \; = \; AS^{-1} \; = \; \sum_{i=1}^{n} \beta_i E_i S^{-1}$$

and so (4.3) now yields the upper branch of (4.1). To complete the proof we need only show that the strictly upper triangular portion of $Q$ is negative. But this follows easily from the sign pattern and upper triangularity of $S^{-1}$, the positivity of $A$, and the equality $Q = AS^{-1}$. $\square$

Next we give an example of a positive vector x and a Soules basis derived from it via sequences of partitionings of $\langle n \rangle$ which do not all consist of consecutive indices and which lead to QR–factorizations of matrices in $\mathcal{M}_R^o$

that do not possess the sign pattern of (4.1). Let $x = (1\ 1\ 1\ 1)^T$. Then with $\mathcal{N}_1 = \{1,2,3,4\}$, $\mathcal{N}_2 = \{\{1,3\},\{2,4\}\}$, $\mathcal{N}_3 = \{\{1\},\{3\},\{2,4\}\}$ and $\mathcal{N}_4 = \{\{1\},\{2\},\{3\},\{4\}\}$, the corresponding Soules basis is given by

$$R = \begin{pmatrix} 0.5 & 0.5 & 0.7071 & 0 \\ 0.5 & -0.5 & 0 & -0.7071 \\ 0.5 & 0.5 & -0.7071 & 0 \\ 0.5 & -0.5 & 0 & 0.7071 \end{pmatrix}.$$

Taking $\Lambda = \Delta(9,5,3,1)$, we obtain that

$$A := R\Lambda R^T = \begin{pmatrix} 5 & 1 & 2 & 1 \\ 1 & 4 & 1 & 3 \\ 2 & 1 & 5 & 1 \\ 1 & 3 & 1 & 4 \end{pmatrix}$$

has the QR–factorization given whose factors are:

$$Q = \begin{pmatrix} 0.89803 & -0.27667 & -0.34065 & -0.031024 \\ 0.17961 & 0.78034 & -0.10661 & -0.58945 \\ 0.35921 & 0.021282 & 0.93250 & -0.031024 \\ 0.17961 & 0.56042 & -0.055141 & 0.80661 \end{pmatrix}$$

and

$$S = \begin{pmatrix} 5.5678 & 2.5145 & 3.9513 & 2.5145 \\ 0 & 4.5472 & 0.89384 & 4.3273 \\ 0 & 0 & 3.8194 & 0.051465 \\ 0 & 0 & 0 & 1.3961 \end{pmatrix}.$$

Thus we see that the entries of $Q$ do not have the sign pattern specified by (4.1).

In our final result we determine the sign pattern of the QR–factors of the inverses of the matrices $A$ considered in the last theorem.

**THEOREM 4.2** *Let $R$ be a Soules matrix with columns $r_1 = x \gg 0, r_2, \ldots, r_n$ to which there corresponds a sequence of partitionings $\{\mathcal{N}_1, \ldots, \mathcal{N}_n\}$ of $\langle n \rangle$ such for each $i = 1, \ldots, n$, the subsets $\mathcal{N}_{i,1}, \ldots, \mathcal{N}_{i,i}$ each consists of consecutive integers. Then for any $A \in \mathcal{M}_R^o$, $A^{-1}$ has the QR–factorization $A^{-1} = QS$ with the entries of $Q = (q_{\mu,\nu})$ satisfying that*

$$q_{\mu,\nu} \begin{cases} > 0, & \text{if } \nu \geq \mu, \\ < 0, & \text{if } \mu > \nu, \end{cases} \tag{4.4}$$

*and with $S$ a nonsingular, upper triangular M–matrix.*

**Proof**: Let $Q$ and $S$ be the QR–factors of $A^{-1}$ so that $A = S^{-1}Q^T = QS^{-T}$, where the second equality follows from the symmetry of $A$. Let $P$ be the permutation matrix which sends $1, 2, \ldots, n$ to $n, n-1, \ldots, 1$. Then $B := PAP = (PQP)(PS^{-T}P) =: \tilde{Q}Z$. Now $\tilde{Z}$ is an upper triangular nonnegative matrix. Thus $\tilde{Q}Z$ is the QR–factorization of the matrix $B$. It is readily seen that if $A = R\Lambda R^T$, where $\Lambda = \Delta(\lambda_1, \ldots, \lambda_n)$ with $\lambda_1 \geq \ldots \lambda_n$, then $B = (PR)\Lambda(PR)^T$. Notice that because of the choice of $P$, $PR$ is a Soules matrix corresponding to a Soules basis determined by a sequence of partitions of $\langle n \rangle$ in which each partition again consists of sets of consecutive indices. Thus, by Theorem 4.1, the orthogonal matrix $PQP$ has negative entries in its strictly upper triangular portion and positive entries elsewhere. Thus $Q$ clearly satisfies the conditions in (4.4).

Finally, that $S$ is an M–matrix follows from the fact that, by Corollary 2.4, $A^{-2}$ is an M–matrix and so $S^TS$ is its Cholesky factorization giving that $S$ is an upper triangular nonsingular M–matrix. □

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