LU decomposition of totally nonnegative matrices

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Abstract

A uniqueness theorem for an LU decomposition of a totally nonnegative matrix is obtained.

Keywords: Totally nonnegative matrices, LU decomposition
2000 MSC: 15B48

0. Introduction

An $m \times n$ matrix M with entries from $\mathbb{R}$ is said to be *totally nonnegative* if each of its minors is nonnegative. Further, such a matrix is *totally positive* if each of its minors is strictly positive. (Warning: in some texts, the terms totally positive and strictly totally positive are used for our terms totally nonnegative and totally positive, respectively.)

Totally nonnegative matrices arise in many areas of mathematics and there has been considerable interest lately in the study of these matrices. For background information and historical references, there is the newly published book by Pinkus, [17] and also two good survey articles [2] and [7].

In this paper, we are interested in the LU decomposition theory of totally nonnegative matrices. Cryer, [6, Theorem 1.1], has proved that any totally nonnegative matrix A has a decomposition $A = LU$ with L totally nonnegative lower triangular and U totally nonnegative upper triangular. If, in addition, A is square and nonsingular then this decomposition is essentially unique, see, for example, [17, pages 50-55], especially Theorem 2.10 and Proposition 2.11. However, in the singular case such decompositions need not be unique, as is pointed out in [5, Page 91].

The aim in this paper is to refine the methods of Cryer, [5, 6], and Gasca and Peña, [9], to produce an LU decomposition for which there is a uniqueness result.

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[1]Supported in part by the National Science Foundation (USA).

A short word concerning the genesis of this result may be interesting to readers. In a series of recent papers, [10, 11, 13], a very close connection has emerged between the theory of totally nonnegative matrices and the theory of the torus invariant prime ideals of the algebra of quantum matrices. This opens up the possibility of using results and methods from one of these areas to produce results in the other. The existence of the results of this paper was suggested by the tensor product decomposition theorem for torus invariant prime ideals in quantum matrices obtained in an earlier paper of the present authors, [12, Theorem 3.5].

Conventions. If a matrix is denoted by a given capital Roman letter, its entries will be denoted by the corresponding lower case letter, with subscripts. E.g., the entries of a matrix named L will be denoted l_{ij}.

When writing sets of row or column indices, we assume that the indices have been listed in strictly ascending order.

Recall the standard partial order on index sets of the same cardinality, say $I := \{i_1, \dots, i_s\}$ and $I' := \{i'_1, \dots, i'_s\}$, where $i_1 < i_2 < \cdots < i_s$ and $i'_1 < i'_2 < \cdots < i'_s$ according to our convention above. Then: $I \leq I'$ if and only if $i_k \leq i'_k$ for each $k = 1, \dots, s$.

If A is a matrix and I, J are subsets of row indices and column indices for A then $A(I, J)$ denotes the submatrix of A obtained by using the rows indexed by I and columns indexed by J. If $|I| = |J|$, the minor determined by $A(I, J)$, that is, $\mathrm{Det}(A(I, J))$, is denoted by $[I|J]_A$, or simply by $[I|J]$ if there is no danger of confusion. By convention, $[\varnothing|\varnothing]_A := 1$ for any matrix A.

1. *LU* decomposition with specified echelon forms

We begin by giving an LU decomposition for certain rectangular matrices, in which the matrices L (respectively, U) have specified lower (respectively, upper) echelon forms. The specification of the matrices for which this decomposition holds, and the decomposition itself, hold over arbitrary fields, and we keep that generality for this section. In Section 2, we shall prove that all totally nonnegative real matrices satisfy the required hypotheses, and that for such matrices, the resulting factors L and U are also totally nonnegative (see Theorem 2.10).

1.1. Echelon forms. We say that a matrix $U = (u_{ij})$ is in *upper echelon form* (or *row echelon form*) if the following hold:

1. If the ith row of U is nonzero and u_{ij} is the leftmost nonzero entry in this row, then $u_{kl} = 0$ whenever both $k > i$ and $l \leq j$;
2. If the ith row of U is zero then all the rows below it are zero.

If, in addition to (1) and (2), there are no zero rows then we say that U is in *strictly upper echelon form.*

Similar definitions are made for lower triangular matrices. Namely, a matrix $L = (l_{ij})$ is in *lower echelon form* provided the transpose of L is in upper echelon form, that is:

1. If the jth column of L is nonzero and l_{ij} is the uppermost nonzero entry in this column, then $l_{kl} = 0$ whenever $k \leq i$ and $l > j$;
2. If the jth column of L is zero then all the columns to the right of it are zero.

If, in addition to (1) and (2), there are no zero columns then we say that L is in *strictly lower echelon form*.

In order to obtain the desired uniqueness results, we need to be more precise concerning the echelon shapes of matrices as above. Let $\boldsymbol{r} := \{r_1, r_2, \dots, r_t\}$ and $\boldsymbol{c} := \{c_1, c_2, \dots, c_t\}$, where $1 \le r_1 < r_2 < \cdots < r_t \le m$ and $1 \le c_1 < \cdots < c_t \le n$.

1. We say that an $m \times t$ matrix $L = (l_{ij})$ is in the class $\mathcal{L}_{\boldsymbol{r}}$ provided that for all $j = 1, \dots, t$, we have $l_{r_j j} \ne 0$ and $l_{ij} = 0$ for all $i < r_j$. Further, $L \in \mathcal{L}^*_{\boldsymbol{r}}$ if also $l_{r_j j} = 1$ for all j. Note that all the matrices in $\mathcal{L}_{\boldsymbol{r}}$ are in strictly lower echelon form.
2. Similarly, we say that a $t \times n$ matrix $U = (u_{ij})$ is in the class $\mathcal{U}_{\boldsymbol{c}}$ provided that for all $i = 1, \dots, t$, we have $u_{ic_i} \ne 0$ and $u_{ij} = 0$ for all $j < c_i$. All such matrices are in strictly upper echelon form.

1.2. Some classes of matrices

Let $\boldsymbol{r} := \{r_1, \dots, r_t\}$ and $\boldsymbol{c} := \{c_1, \dots, c_t\}$ be subsets of $\{1, \dots, m\}$ and $\{1, \dots, n\}$, respectively. An $m \times n$ matrix A is said to be in the class $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$ provided that

1. $\mathrm{Rank}(A) = t$;
2. For each s with $s \le t$, the minor $[r_1, r_2, \dots, r_s | c_1, c_2, \dots, c_s]_A$ is nonzero;
3. $[I|J]_A = 0$ whenever $|I| = |J| = s \le t$ and either $I \not\ge \{r_1, \dots, r_s\}$ or $J \not\ge \{c_1, \dots, c_s\}$.

Remark 1.3. It is easy to check that a matrix belongs to at most one class $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$. However, in general, a matrix need not belong to any such class – consider, for example, the matrix $A := \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$.

Suppose that $L \in \mathcal{L}_{\boldsymbol{r}}$ where $\boldsymbol{r} := \{r_1, \dots, r_t\}$. Note that

$$[r_1, \dots, r_s | 1, \dots, s]_L = l_{r_1 1} \cdots l_{r_s s} \ne 0,$$

for each $s \le t$. In particular, $[r_1, \dots, r_t | 1, \dots, t]_L \ne 0$, so that $\mathrm{Rank}(L) = t$.

Suppose that $\{i_1, \dots, i_s\} \not\ge \{r_1, \dots, r_s\}$. Then $i_k < r_k$ for some k. Thus, any submatrix of the form $L(\{i_1, \dots, i_s\}, J)$ is a lower triangular matrix with a zero in the kth position on the diagonal; and so $[i_1, \dots, i_s | J]_L = 0$. Since all s-element index sets $J \subseteq \{1, \dots, t\}$ satisfy $J \ge \{1, \dots, s\}$, we thus see that $L \in \mathcal{M}_{\boldsymbol{r},[1,t]}$, where $[1, t] := \{1, \dots, t\}$.

Similarly, any $U \in \mathcal{U}_{\boldsymbol{c}}$ belongs to $\mathcal{M}_{[1,t],\boldsymbol{c}}$, where $t = |\boldsymbol{c}|$.

Lemma 1.4. *Suppose that L is an $m \times t$ matrix in the class $\mathcal{L}_{\boldsymbol{r}}$ and that U is a $t \times n$ matrix in the class $\mathcal{U}_{\boldsymbol{c}}$.*

(i) *Let $s \le t$ and let I (respectively, J) be an s-element subset of $\{1, \dots, m\}$ (respectively, $\{1, \dots, t\}$). Then $[r_1, \dots, r_s | J]_L \ne 0$ if and only if $J = \{1, \dots, s\}$, and $[I|J]_L = 0$ if $I \not\ge \{r_1, \dots, r_s\}$.*

(ii) *Let $s \le t$ and let I (respectively, J) be an s-element subset of $\{1, \dots, t\}$ (respectively, $\{1, \dots, n\}$). Then $[I | c_1, \dots, c_s]_U \ne 0$ if and only if $I = \{1, \dots, s\}$, and $[I|J]_U = 0$ if $J \not\ge \{c_1, \dots, c_s\}$.*

(iii) *$A := LU$ is an $m \times n$ matrix in the class $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$.*

Proof. (i) We already have $[r_1,\ldots,r_s|1,\ldots,s]_L \neq 0$, and $[I|J]_L = 0$ for $I \not\geq \{r_1,\ldots,r_s\}$, by Remark 1.3. If $J = \{j_1,\ldots,j_s\}$ and $J \neq \{1,\ldots,s\}$, then some $j_k > k$, whence $r_{j_k} > r_k$. In this case, $L(\{r_1,\ldots,r_s\},J)$ is a lower triangular matrix whose k,k entry is zero, and so $[r_1,\ldots,r_s|J]_L = 0$.

(ii) This is proved symmetrically.

(iii) First, $\text{Rank}(A) \leq t$, as A is the product of an $m \times t$ matrix and a $t \times n$ matrix. However, by the Cauchy-Binet identity (Lemma 4.3),

$$[r_1,\ldots,r_t|c_1,\ldots,c_t]_A \quad = \quad [r_1,\ldots,r_t|1,\ldots,t]_L[1,\ldots,t|c_1,\ldots,c_t]_U \neq 0,$$

so $\text{Rank}(A) = t$.

For any $s \leq t$, by the Cauchy-Binet identity together with (i),

$$\begin{aligned}[r_1,\ldots,r_s|c_1,\ldots,c_s]_A &= \sum_K [r_1,\ldots,r_s|K]_L[K|c_1,\ldots,c_s]_U \\ &= [r_1,\ldots,r_s|1,\ldots,s]_L[1,\ldots,s|c_1,\ldots,c_s]_U \neq 0.\end{aligned}$$

Now, suppose that we have a row index set $I \not\geq \{r_1,\ldots,r_s\}$. For any s-element subset K of $\{1,\ldots,t\}$, we have $[I|K]_L = 0$ by (i), and therefore, for any s-element subset J of $\{1,\ldots,n\}$, Lemma 4.3 implies that $[I|J]_A = \sum_K [I|K]_L[K|J]_U = 0$. Similarly, $[I|J]_A = 0$ for any I, J with $|I| = |J| = s \leq t$ and $J \not\geq \{c_1,\ldots,c_s\}$. Therefore $A \in \mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$. □

The following theorem gives an explicit LU decomposition for matrices in the classes $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$. Uniqueness of these decompositions will be proved once existence has been established.

Theorem 1.5. *Let A be an $m \times n$ matrix which belongs to the class $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$ where $\boldsymbol{r} := \{r_1,\ldots,r_t\}$ and $\mathbf{c} := \{c_1,\ldots,c_t\}$.*

Set $L := (l_{ij})$ and $U := (u_{ij})$ to be the $m \times t$ and $t \times n$ matrices, respectively, with entries as follows: $l_{ij} := 0$ for $i < r_j$ and

$$l_{ij} := [r_1,r_2,\ldots,r_{j-1},i|c_1,c_2,\ldots,c_j]_A[r_1,r_2,\ldots,r_j|c_1,c_2,\ldots,c_j]_A^{-1}$$

for $i \geq r_j$, while $u_{ij} := 0$ for $j < c_i$ and

$$u_{ij} := [r_1,r_2,\ldots,r_i|c_1,c_2,\ldots,c_{i-1},j]_A[r_1,r_2,\ldots,r_{i-1}|c_1,c_2,\ldots,c_{i-1}]_A^{-1}$$

for $j \geq c_i$.

Then L belongs to the class $\mathcal{L}^*_{\boldsymbol{r}}$, while U belongs to the class $\mathcal{U}_{\boldsymbol{c}}$, and $A = LU$.

Proof. It is obvious from the definitions that $L \in \mathcal{L}^*_{\boldsymbol{r}}$ and $U \in \mathcal{U}_{\boldsymbol{c}}$; so we need to prove that $A = LU$. The proof is by induction on $\min\{m,n\}$ with the cases where $m = 1$ or $n = 1$ being trivial. In this proof, any minor $[I|J]$ without a subscript is a minor of A; that is, $[I|J] = [I|J]_A$. Minors of other matrices are given subscripts.

Assume that $m,n \geq 2$, and suppose first that $a_{11} = 0$. Then either $r_1 > 1$ or $c_1 > 1$. It follows that either the first row or first column of A is zero, because $A \in \mathcal{M}_{\mathbf{r},\mathbf{c}}$. Suppose that the first row of A is zero, in which case $r_1 > 1$. Let $\widetilde{A}$ be the $(m-1) \times n$ matrix obtained from A by deleting the first row. Then $\widetilde{A} \in \mathcal{M}_{\boldsymbol{r}',\boldsymbol{c}}$ where $\boldsymbol{r}' := \{r_1-1,\ldots,r_t-1\}$.

By using the inductive hypothesis, there are matrices $\widetilde{L}$, $\widetilde{U}$, with entries as specified above, such that $\widetilde{A} = \widetilde{L}\widetilde{U}$. Note that $\widetilde{U} = U$.

Now,

$$A = \left(\begin{array}{ccc} 0 & \cdots & 0 \\ \hline & & \\ & \widetilde{A} & \\ & & \end{array}\right) = \left(\begin{array}{ccc} 0 & \cdots & 0 \\ \hline & & \\ & \widetilde{L} & \\ & & \end{array}\right) \widetilde{U}$$

and it is easy to check that $\left(\begin{array}{ccc} 0 & \cdots & 0 \\ \hline & & \\ & \widetilde{L} & \\ & & \end{array}\right) = L.$

The case where the first column of A is zero is dealt with in a similar way.

Next, assume that $a_{11} \neq 0$ and note that $r_1 = c_1 = 1$ in this case. Then, by elementary row operations using a_{11} as the pivot, we see that $A = \widetilde{L}\widetilde{A}$, where

$$\widetilde{L} = \left(\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline a_{21}a_{11}^{-1} & & & \\ \vdots & & I & \\ a_{m1}a_{11}^{-1} & & & \end{array}\right), \qquad \widetilde{A} = \left(\begin{array}{c|ccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline 0 & & & \\ \vdots & & D & \\ 0 & & & \end{array}\right),$$

and $D = (d_{ij})$ is the $(m-1) \times (n-1)$ matrix with entries

$$d_{ij} := a_{i+1,j+1} - a_{i+1,1}a_{11}^{-1}a_{1,j+1} = [1, i+1|1, j+1][1|1]^{-1}.$$

Also, set $B := \big([1, i+1|1, j+1]\big)$, so that $D = [1|1]^{-1}B$.

Let $\{i_1, \ldots, i_s\}$ and $\{j_1, \ldots, j_s\}$ be subsets of $\{1, \ldots, t-1\}$. Then

$$[i_1, \ldots, i_s|j_1, \ldots, j_s]_B = [1, i_1+1, \ldots, i_s+1|1, j_1+1, \ldots, j_s+1][1|1]^{s-1},$$

by Sylvester's identity (Lemma 4.5). It follows that

$$\begin{aligned} [i_1, \ldots, i_s|j_1, \ldots, j_s]_D &= [i_1, \ldots, i_s|j_1, \ldots, j_s]_B[1|1]^{-s} \\ &= [1, i_1+1, \ldots, i_s+1|1, j_1+1, \ldots, j_s+1][1|1]^{-1}. \end{aligned} \tag{*}$$

From this, it follows that D belongs to the class $\mathcal{M}_{\boldsymbol{r}',\boldsymbol{c}'}$ where $\boldsymbol{r}' := \{r_2 - 1, \ldots, r_t - 1\}$ and $\boldsymbol{c}' := \{c_2 - 1, \ldots, c_t - 1\}$.

By induction, there are $(m-1) \times (t-1)$ and $(t-1) \times (n-1)$ matrices $\approx\!\!\!\!L = (\approx\!\!\!\!l_{ij})$ and $\approx\!\!\!\!U = (\approx\!\!\!\!u_{ij})$ such that $D = \approx\!\!\!\!L\approx\!\!\!\!U$, with $\approx\!\!\!\!l_{ij} = 0 = l_{i+1,j+1}$ for $i < r_{j+1} - 1$ and

$$\begin{aligned} \approx\!\!\!\!l_{ij} &= [r_2{-}1, \ldots, r_j{-}1, i|c_2{-}1, \ldots, c_{j+1}{-}1]_D[r_2{-}1, \ldots, r_{j+1}{-}1|c_2{-}1, \ldots, c_{j+1}{-}1]_D^{-1} \\ &= [1, r_2, \ldots, r_j, i{+}1|1, c_2, \ldots, c_{j+1}][1|1]^{-1}[1, r_2, \ldots, r_{j+1}|1, c_2, \ldots, c_{j+1}]^{-1}[1|1] \\ &= l_{i+1,j+1} \end{aligned}$$

for $i \geq r_{j+1} - 1$; while $\approx\!\!\!\!u_{ij} = 0 = u_{i+1,j+1}$ for $j < c_{i+1} - 1$ and

$$\begin{aligned} \approx\!\!\!\!u_{ij} &= [r_2{-}1, \ldots, r_{i+1}{-}1|c_2{-}1, \ldots, c_i{-}1, j]_D[r_2{-}1, \ldots, r_i{-}1|c_2{-}1, \ldots, c_i{-}1]_D^{-1} \\ &= [1, r_2, \ldots, r_{i+1}|1, c_2, \ldots, c_i, j{+}1][1|1]^{-1}[1, r_2, \ldots, r_i|1, c_2, \ldots, c_i]^{-1}[1|1] \\ &= u_{i+1,j+1} \end{aligned}$$

for $j \geq c_{i+1} - 1$, by using $(*)$ above.

Now, observe that

$$A = \widetilde{L}\widetilde{A} = \left(\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline a_{21}a_{11}^{-1} & & & \\ \vdots & & I & \\ a_{m1}a_{11}^{-1} & & & \end{array}\right) \left(\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline 0 & & & \\ \vdots & & \approx\atop{L} & \\ 0 & & & \end{array}\right) \left(\begin{array}{c|ccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline 0 & & & \\ \vdots & & \approx\atop{U} & \\ 0 & & & \end{array}\right).$$

From our calculations of the entries of $\overset{\approx}{L}$ and $\overset{\approx}{U}$ above, we see that

$$L = \left(\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline a_{21}a_{11}^{-1} & & & \\ \vdots & & \overset{\approx}{L} & \\ a_{m1}a_{11}^{-1} & & & \end{array}\right) \qquad \text{and} \qquad U = \left(\begin{array}{c|ccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline 0 & & & \\ \vdots & & \overset{\approx}{U} & \\ 0 & & & \end{array}\right),$$

and therefore $A = LU$. This completes the inductive step. □

Theorem 1.6. *Suppose that A is in the class $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$ where $\boldsymbol{r} := \{r_1, r_2, \ldots, r_t\}$ and $\boldsymbol{c} := \{c_1, c_2, \ldots, c_t\}$. There are unique matrices $L \in \mathcal{L}_{\boldsymbol{r}}^*$ and $U \in \mathcal{U}_{\boldsymbol{c}}$ such that $A = LU$, namely those given in Theorem* 1.5.

Proof. We show that if $A = (a_{ij})$ is in the class $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$ and $A = LU$ with $L = (l_{ij}) \in \mathcal{L}_{\boldsymbol{r}}^*$ and $U = (u_{ij}) \in \mathcal{U}_{\boldsymbol{c}}$, then the entries of L and U can be uniquely specified from this information. The result then follows.

Note that the equations

$$a_{r_1 j} = (LU)_{r_1 j} = \sum_{k=1}^{t} l_{r_1 k} u_{kj} = l_{r_1 1} u_{1j} = u_{1j}$$

specify the first row of U. Similarly,

$$a_{ic_1} = (LU)_{ic_1} = \sum_{k=1}^{t} l_{ik} u_{kc_1} = l_{i1} u_{1c_1}$$

for all i, which specifies the first column of L, as $u_{1c_1} \neq 0$.

Assume as an inductive hypothesis that the first s rows of U and the first s columns of L have been specified. Then

$$\begin{aligned} a_{r_{s+1} j} = (LU)_{r_{s+1} j} &= \sum_{k=1}^{t} l_{r_{s+1} k} u_{kj} = \sum_{k=1}^{s} l_{r_{s+1} k} u_{kj} + l_{r_{s+1} s+1} u_{s+1,j} \\ &= \sum_{k=1}^{s} l_{r_{s+1} k} u_{kj} + u_{s+1,j} \end{aligned}$$

for all j, which specifies the $(s+1)$-st row of U because the terms in the last summation are already known by induction.

Finally,

$$a_{ic_{s+1}} = (LU)_{ic_{s+1}} = \sum_{k=1}^{t} l_{ik}u_{k,c_{s+1}} = \sum_{k=1}^{s} l_{ik}u_{k,c_{s+1}} + l_{i,s+1}u_{s+1,c_{s+1}}$$

for all i, which specifies the $(s+1)$-st column of L because the terms in the summation on the right are already known by induction and $u_{s+1,c_{s+1}} \neq 0$.

This finishes the inductive step and so the result is proved. $\square$

2. Modified Neville elimination

We now restrict attention to real matrices and focus on total nonnegativity. Our aim is to show that any $m \times n$ totally nonnegative matrix A lies in one of the classes $\mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$, and that the matrices L and U in the decomposition $A = LU$ of Theorem 1.5 are totally nonnegative. While it is possible to prove directly that these matrices are totally nonnegative, it is technically much less complicated to obtain that result via a modification of the Neville elimination process of Gasca and Peña, [9].

The following is an elementary, but crucial, fact about totally nonnegative matrices.

Lemma 2.1. *Suppose that $A = (a_{ij})$ is a totally nonnegative $m \times n$ matrix, and that $i < k \leq m$ and $j < l \leq n$. If $a_{ij} = 0$ then either $a_{il} = 0$ or $a_{kj} = 0$. As a consequence, if some entry in the jth column, but below the ij entry, is nonzero then all elements in the ith row, but to the right of the ij entry, are also zero.*

Proof. Note that $0 \leq [ik|jl] = a_{ij}a_{kl} - a_{il}a_{kj} = -a_{il}a_{kj}$; so that $a_{il}a_{kj} \leq 0$. As $a_{il}, a_{kj} \geq 0$ this gives the desired conclusion. $\square$

First, we give an informal description of the elimination process that we will use. We start with a totally nonnegative matrix. The aim is to use a version of the Neville elimination procedure to produce a final matrix in echelon form with no zero rows. If a zero row appears at any stage in the process then we delete it (rather than moving it to the bottom as in ordinary Neville elimination). Otherwise, we proceed as with Neville elimination: if we are clearing the lower entries in a given column and want to perform a row operation to replace the last nonzero entry in a column by zero, then we perform a row operation by subtracting a suitable multiple of the row immediately above this last position. Note that the entry immediately above this last position will be nonzero: this is guaranteed by the above lemma. In the end we produce an upper triangular matrix U in echelon form which contains no zero rows. Keeping track of the operations performed produces a lower triangular matrix L such that $A = LU$. We also show that each of L and U is totally nonnegative.

2.2. Invariants of the elimination algorithm

The modified Neville algorithm starts with $L := I$ and $U := A$, a totally nonnegative matrix, and uses two moves: (i) either delete a row of zeros of U and the corresponding column in L, or (ii) perform a Neville elimination move.

The first aim is to show that at all times during the modified Neville algorithm we retain the totally nonnegative condition for L and U and the fact that $A = LU$. There are two moves to consider. The first deletes a row of U and the corresponding column of L. Note that if we delete a row or column from a totally nonnegative matrix then the new matrix is also totally nonnegative.

Lemma 2.3. *Let B be an $m \times p$ matrix and let C be a $p \times n$ matrix. Suppose that row i of C is zero. Set B' to be the $m \times (p-1)$ matrix obtained by deleting the ith column of B and set C' to be the $(p-1) \times n$ matrix obtained by deleting the ith row of C. Then $B'C' = BC$.*

Proof. Obvious. □

Lemma 2.4. (i) *Suppose that $\boldsymbol{r} := \{r_1, r_2, \ldots, r_t\}$ and that $L \in \mathcal{L}_{\mathbf{r}}$. Let L' be the matrix obtained by deleting column i from L. Then $L' \in \mathcal{L}_{\boldsymbol{r}'}$ where*

$$\boldsymbol{r}' := \{r_1, r_2, \ldots, r_{i-1}, r_{i+1}, \ldots, r_t\}.$$

(ii) *Suppose that $\mathbf{c} := \{c_1, c_2, \ldots, c_t\}$ and that $U \in \mathcal{U}_{\mathbf{c}}$. Let U' be the matrix obtained by deleting row i from U. Then $U' \in \mathcal{U}_{\mathbf{c}'}$ where $\mathbf{c}' := \{c_1, c_2, \ldots, c_{i-1}, c_{i+1}, \ldots, c_t\}$.*

Proof. Obvious. □

The next results consider the effect of performing a Neville elimination move; that is, the row operation of subtracting a suitable multiple of row s from row $s+1$ on the minors of a matrix of the form

$$\left(\begin{array}{ccc|cccc}
\star & \cdots & \star & \star & \cdots & \cdots & \star \\
\vdots & & \vdots & \vdots & & & \vdots \\
\star & \cdots & \star & \star & \cdots & \cdots & \star \\
\hline
0 & \cdots & 0 & a_{st} & a_{s,t+1} & \cdots & a_{sn} \\
0 & \cdots & 0 & a_{s+1,t} & a_{s+1,t+1} & \cdots & a_{s+1,n} \\
0 & \cdots & 0 & 0 & \star & \cdots & \star \\
\vdots & & \vdots & \vdots & & & \vdots \\
0 & \cdots & 0 & 0 & \star & \cdots & \star
\end{array}\right)$$

when a_{st} and $a_{s+1,t}$ are nonzero, in order to clear the entry in position $(s+1, t)$. Note that the resulting matrix has the form

$$\left(\begin{array}{ccc|cccc}
\star & \cdots & \star & \star & \cdots & \cdots & \star \\
\vdots & & \vdots & \vdots & & & \vdots \\
\star & \cdots & \star & \star & \cdots & \cdots & \star \\
\hline
0 & \cdots & 0 & a_{st} & a_{s,t+1} & \cdots & a_{sn} \\
0 & \cdots & 0 & 0 & b_{s+1,t+1} & \cdots & b_{s+1,n} \\
0 & \cdots & 0 & 0 & \star & \cdots & \star \\
\vdots & & \vdots & \vdots & & & \vdots \\
0 & \cdots & 0 & 0 & \star & \cdots & \star
\end{array}\right)$$

Lemma 2.5. *Suppose that $A = (a_{ij})$ with $a_{st} \neq 0$ and $a_{ij} = 0$ whenever $i \geq s$ and $j < t$. Suppose that $a_{s+1,t} \neq 0$ while $a_{s+w,t} = 0$ for all $w > 1$. Set $B = (b_{ij})$ where $b_{ij} = a_{ij}$ for $i \neq s+1$ while $b_{s+1,j} = a_{s+1,j} - a_{s+1,t}a_{st}^{-1}a_{sj}$ for all j. In particular, $b_{s+1,j} = 0$ for $j \leq t$ while $b_{s+1,j} = [s, s+1|tj]_A a_{st}^{-1}$ for $j > t$.*

Then

$$[I|J]_B = \begin{cases} [I|J]_A & \text{when } s \in I \text{ or } s+1 \notin I \\ [I|J]_A - a_{s+1,t}a_{st}^{-1}[I\backslash\{s+1\} \sqcup \{s\}|J]_A & \text{when } s \notin I \text{ and } s+1 \in I\,. \end{cases}$$

Proof. Obvious from the definition of B. □

We refer to the change from A to B described in this lemma as a *Neville elimination move*. The next result shows that the totally nonnegative condition is preserved under a Neville elimination move. This result may be well-known, but we have been unable to find a clear statement in the literature.

Proposition 2.6. *In the above setting, if A is totally nonnegative then so is B.*

Proof. It follows from the fact that A is totally nonnegative and the definition of B that each $b_{ij} \geq 0$. Also, for any size minor, $[I|J]_B = [I|J]_A \geq 0$ whenever $s \in I$ or $s+1 \notin I$.

Suppose that $l \geq 2$ and that all minors of B of size less than $l \times l$ are ≥ 0. Let $[I|J]_B$ be an $l \times l$ minor. By the above remarks, we may assume that $s \notin I$ and that $s+1 \in I$. Consider the following cases:

1. $s+1$ is the least entry in I;
2. $s+1 \in I$, and there exists $i \in I$ with $i < s$.

In case (1), consider first the case where there is a $j \in J$ with $j \leq t$. Then the jth column of $B(I, J)$ is zero; so $[I|J]_B = 0$. Otherwise, note that

$$a_{st}[I|J]_B = [I \sqcup \{s\}|J \sqcup \{t\}]_B = [I \sqcup \{s\}|J \sqcup \{t\}]_A \geq 0.$$

As $a_{st} > 0$ it follows that $[I|J]_B \geq 0$.

Next, consider case (2). If $[I\backslash\{s+1\} \sqcup \{s\}|J]_A = 0$ then $[I|J]_B = [I|J]_A \geq 0$, by the previous lemma; so we may assume that

$$[I\backslash\{s+1\} \sqcup \{s\}|J]_B = [I\backslash\{s+1\} \sqcup \{s\}|J]_A \neq 0.$$

Suppose that $[I\backslash\{i, s+1\} \sqcup \{s\}|Y]_B = 0$ for all subsets Y of J with $|Y| = l-1$. Then $[I\backslash\{s+1\} \sqcup \{s\}|J]_B = 0$, by Lemma 4.2. Thus, we may assume that there exists a subset Y of J with $|Y| = l-1$ and $[I\backslash\{i, s+1\} \sqcup \{s\}|Y]_B > 0$. Suppose that $J = Y \sqcup \{k\}$. Choose $j \in Y$.

Apply the Laplace relation of Lemma 4.1(a) with $J_1 = \{j\}$ and $J_2 = \{j, k\}$ while $I = \{i, s, s+1\}$ to obtain

$$[i|j]_B[s, s+1|jk]_B - [s|j]_B[i, s+1|jk]_B + [s+1|j]_B[is|jk]_B = 0.$$

It follows that

$$[s|j]_B[i, s+1|jk]_B = [i|j]_B[s, s+1|jk]_B + [s+1|j]_B[is|jk]_B\,.$$

By using Muir's law of extensible minors (Lemma 4.4), we may introduce the $l-2$ row indices from $I\backslash\{i,s+1\}$ and the $l-2$ column indices from $Y\backslash\{j\}$ to obtain

$$[I\backslash\{i,s+1\}\sqcup\{s\}|Y]_B[I|J]_B = \\ [I\backslash\{s+1\}|Y]_B[I\backslash\{i\}\sqcup\{s\}|J]_B + [I\backslash\{i\}|Y]_B[I\backslash\{s+1\}\sqcup\{s\}|J]_B\,.$$

Now, $[I\backslash\{i,s+1\}\sqcup\{s\}|Y]_B > 0$, by assumption, and each of the four minors on the right side of this equation is ≥ 0 (the two of size $l-1$ by the inductive hypothesis and the two of size l because s is in the row set of the minor). It follows that $[I|J]_B \geq 0$, as required □

Remark 2.7. Let $E(s+1,s)$ be the matrix with 1 in the $(s+1,s)$ position and zero elsewhere. Note that, with the above notation,

$$B = (I - a_{s+1,t}a_{st}^{-1}E(s+1,s))A \qquad \text{and} \qquad A = (I + a_{s+1,t}a_{st}^{-1}E(s+1,s))B.$$

Note also that $I + a_{s+1,t}a_{st}^{-1}E(s+1,s)$ is totally nonnegative.

2.8. The Modified Neville Algorithm

Let A be an $m \times n$ totally nonnegative matrix of rank t. The following algorithm outputs an LU decomposition of A, which, as we shall see, coincides with the one given in Theorem 1.5.

Input Set $L := I$, the identity $m \times m$ matrix, and $U := A$. Note that $A = LU$.

Algorithm

Step 1 If U is in strictly upper echelon form then stop and output L and U. Otherwise, if there is a row of U consisting entirely of zeros, go to Step 2 and if not, then go to Step 3.

Step 2 Suppose that L is of size $m \times w$ and U of size $w \times n$, and that some row of U is zero. Choose i as large as possible so that the ith row of U is zero. Delete row i from U and column i from L to obtain new matrices L of size $m \times (w-1)$ and U of size $(w-1) \times n$. Note that we still have $A = LU$, by Lemma 2.3, and that L and U are still totally nonnegative. Go to Step 1.

Step 3 Suppose that all rows of U are nonzero, but U is not in upper echelon form. By Lemma 2.1, the leftmost nonzero column of U must have a nonzero entry in its uppermost position. Set $U = (u_{ij})$.

If the first column of U has two or more nonzero entries then set $t = 1$. Otherwise, set $t > 1$ so that the submatrix of U consisting of the first $t-1$ columns is in upper echelon form, but that consisting of the first t columns is not. Then, in view of Lemma 2.1, there is a largest integer s such that $u_{st}, u_{s+1,t} \neq 0$; moreover, $u_{ij} = 0$ for $i \geq s$ and $j < t$. Perform a Neville elimination move on U as in Lemma 2.5; that is, replace U by $(I - u_{s+1,t}u_{st}^{-1}E(s+1,s))U$; so that in the new U we have $u_{s+1,t} = 0$. At the same time, replace L by $L(I + u_{s+1,t}u_{st}^{-1}E(s+1,s))$. Note that we still have $A = LU$, and that U is totally nonnegative by Proposition 2.6, while L is the product of two totally nonnegative matrices and so is still totally nonnegative.

Go to Step 1.

Theorem 2.9. *The above algorithm outputs an $m \times t$ totally nonnegative matrix $L \in \mathcal{L}^*_{\boldsymbol{r}}$, for some $\boldsymbol{r} = \{r_1, r_2, \ldots, r_t\}$, and a $t \times n$ totally nonnegative matrix $U \in \mathcal{U}_{\boldsymbol{c}}$, for some $\boldsymbol{c} = \{c_1, c_2, \ldots, c_t\}$, such that $A = LU$.*

Proof. The algorithm outputs totally nonnegative matrices L and U, in strictly lower and upper echelon forms, respectively, such that $A = LU$. Also, note that the leading entry in each column of L is 1. Suppose that $L \in \mathcal{L}^*_{\boldsymbol{r}}$ and $U \in \mathcal{U}_{\boldsymbol{c}}$ with $\boldsymbol{r} = \{r_1, r_2, \ldots, r_w\}$ and $\boldsymbol{c} = \{c_1, c_2, \ldots, c_w\}$, As L is an $m \times w$ matrix and U is a $w \times n$ matrix, we have $t = \mathrm{Rank}(A) \leq w$. Moreover,

$$[r_1, r_2, \ldots, r_w | c_1, c_2, \ldots, c_w]_A = [r_1, r_2, \ldots, r_w | 1, \ldots, w]_L [1, \ldots, w | c_1, c_2, \ldots, c_w]_U \neq 0,$$

by using the Cauchy-Binet identity; so $t \geq w$. Hence, $w = t$, as required. □

The above theorem, combined with the results of Section 1, yields the main result of the paper:

Theorem 2.10. *Let A be an $m \times n$ totally nonnegative matrix. Then there is a unique pair $\boldsymbol{r}$, $\boldsymbol{c}$ such that $A \in \mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$. Further, there is then a unique pair $L \in \mathcal{L}^*_{\boldsymbol{r}}$, $U \in \mathcal{U}_{\boldsymbol{c}}$ such that $A = LU$. The matrices L and U are totally nonnegative. They are given explicitly in Theorem* 1.5.

Proof. By Theorem 2.9, there exist $\boldsymbol{r}$, $\boldsymbol{c}$ and totally nonnegative matrices $L \in \mathcal{L}^*_{\boldsymbol{r}}$, $U \in \mathcal{U}_{\boldsymbol{c}}$ such that $A = LU$, and $A \in \mathcal{M}_{\boldsymbol{r},\boldsymbol{c}}$ by Lemma 1.4. As noted in Remark 1.3, $\boldsymbol{r}$ and $\boldsymbol{c}$ are uniquely determined by A. The uniqueness of L and U then follows from Theorem 1.6. □

Theorem 1.5 and the total nonnegativity of the factors L and U are known for the case where A is a totally nonnegative nonsingular square matrix; see, for example, [17, Theorem 2.10 and Proposition 2.11]. However, we have not been able to locate a prior source for the result just proved. LU decompositions of non-square totally nonnegative matrices have also been obtained in [15, Theorem 3.1].

3. Examples

Example 3.1. We first illustrate the modified Neville algorithm at work on the example considered by Cryer, [5, Page 91]. The matrix in question is

$$A := \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix}$$

Cryer exhibits two distinct LU factorisations of A into totally nonnegative factors:

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

It is easy to check that A is totally nonnegative of rank one, and that A belongs to the class $\mathcal{M}_{\{2\},\{1\}}$. We start the algorithm with the pair $\{I, A\}$:

$$
\begin{aligned}
A = IA \quad &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}
\end{aligned}
$$

and one can easily check that

$$
A = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}
$$

is (essentially) the unique decomposition of A as a product of a 3×1 matrix and a 1×3 matrix.

Example 3.2. A more complicated example. The algorithm reveals the class of A.

$$
\begin{aligned}
A = IA = &\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 2 & 4 & 2 \\ 0 & 1 & 2 & 3 \\ 0 & 3 & 6 & 11 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 3 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 2 & 4 & 2 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 0 & 2 \end{pmatrix} \\
= &\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1/2 & 1 & 0 \\ 0 & 3/2 & 3 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 2 & 4 & 2 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 1 & 1/2 & 1 & 0 \\ 3 & 3/2 & 3 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 2 \end{pmatrix} \\
= &\begin{pmatrix} 1 & 0 & 0 \\ 2 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 3 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 4 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
= &\begin{pmatrix} 1 & 0 \\ 2 & 0 \\ 1 & 1 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 2 \end{pmatrix}.
\end{aligned}
$$

It follows that A is in $\mathcal{M}_{\{1,3\},\{2,4\}}$.

4. Appendix: Matrix identities, etc.

For any index sets I and J, set $\ell(I,J) := |\{(i,j) \in I \times J \mid i > j\}|$.

Lemma 4.1. (Laplace relations; see, for example, [14, p14], [18, eqn. (3.3.4), p26]) *Let A be an $m \times n$ matrix, $I \subseteq \{1,\ldots,m\}$, and $J \subseteq \{1,\ldots,n\}$.*

(a) *If $J_1, J_2 \subseteq \{1, \ldots, n\}$ with $|J_1| + |J_2| = |I|$, then*

$$\sum_{\substack{I_1 \sqcup I_2 = I \\ |I_\nu| = |J_\nu|}} (-1)^{\ell(I_1;I_2)} [I_1|J_1]_A [I_2|J_2]_A = \begin{cases} (-1)^{\ell(J_1;J_2)} [I|J_1 \sqcup J_2]_A & (J_1 \cap J_2 = \varnothing) \\ 0 & (J_1 \cap J_2 \neq \varnothing). \end{cases}$$

(b) *If $I_1, I_2 \subseteq \{1, \ldots, n\}$ with $|I_1| + |I_2| = |J|$, then*

$$\sum_{\substack{J_1 \sqcup J_2 = J \\ |J_\nu| = |I_\nu|}} (-1)^{\ell(J_1;J_2)} [I_1|J_1]_A [I_2|J_2]_A = \begin{cases} (-1)^{\ell(I_1;I_2)} [I_1 \sqcup I_2|J]_A & (I_1 \cap I_2 = \varnothing) \\ 0 & (I_1 \cap I_2 \neq \varnothing). \end{cases}$$

Lemma 4.2. *Let A be an $m \times n$ matrix, $I \subseteq \{1, \ldots, m\}$, and $J \subseteq \{1, \ldots, n\}$, with $|I| = |J|$.*

(a) *Fix $J_1 \subseteq J$. If $[I_1|J_1]_A = 0$ for all $I_1 \subseteq I$ with $|I_1| = |J_1|$, then $[I|J]_A = 0$.*
(b) *Fix $I_1 \subseteq I$. If $[I_1|J_1]_A = 0$ for all $J_1 \subseteq J$ with $|J_1| = |I_1|$, then $[I|J]_A = 0$.*

Proof. By symmetry, we need only prove (a). Set $J_2 = J \backslash J_1$. There is a Laplace relation of the form

$$[I|J]_A = \sum_{I_1 \sqcup I_2 = I} \pm [I_1|J_1]_A [I_2|J_2]_A \,.$$

As all $[I_1|J_1]_A = 0$, by assumption, it follows that $[I|J]_A = 0$. □

Lemma 4.3. (Cauchy-Binet Identity; see, for example, [1, eqn. (6), p86], [14, p14]) *Let A be an $m \times t$ matrix and B a $t \times n$ matrix, and let $I \subseteq \{1, \ldots, m\}$ and $J \subseteq \{1, \ldots, n\}$ be k-element sets with $k \leq t$. Then*

$$[I|J]_{AB} = \sum_K [I|K]_A [K|J]_B$$

where K ranges over all k-element subsets of $\{1, \ldots, t\}$.

Lemma 4.4. (Muir's Law of Extensible Minors; see, for example, [16, p179, §187], [4, p205]) *Let F be a field and suppose that*

$$\sum_{s=1}^{d} c_s [I_s|J_s][K_s|L_s] = 0$$

is a homogeneous determinantal identity for matrices over F. Suppose that P is a set of row indices disjoint from each of the sets I_s and Q is a set of column indices disjoint from each of the sets J_s, with $|P| = |Q|$. Then

$$\sum_{s=1}^{d} c_s [I_s \sqcup P|J_s \sqcup Q][K_s \sqcup P|L_s \sqcup Q] = 0$$

is also a determinantal identity for matrices over F.

Lemma 4.5. (Sylvester's Identity; see, for example, [8, p32], [3, eqn. (8), p772]) *Let $A = (a_{ij})$ be an $n \times n$ matrix and let $m < n$. Set $B = (b_{ij})$ to be the $(n-m) \times (n-m)$ matrix where $b_{ij} := [1, \ldots, m, m+i|1, \ldots, m, m+j]$. Then,*

$$\det(B) = [1, \ldots, n|1, \ldots, n]_A [1, \ldots, m|1, \ldots, m]_A^{n-m-1} \,.$$

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