INHERITED MATRIX ENTRIES:
LU FACTORIZATIONS

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ABSTRACT

For an n-by-n matrix $A = [a_{ij}]$ which has a unique unit LU factorization with $U = [u_{ij}]$, we determine combinatorial circumstances under which $u_{ij} = a_{ij}$ for a given pair $i \leq j$ or for all $i < j$ (or all $i \leq j$). Analogous results are stated for other triangular factorizations, and for the LU factorization of a principal submatrix of A. The relationship of our results to Gaussian elimination and sparse matrix analysis is noted.

1. INTRODUCTION.

An n-by-n matrix A has an LU factorization if A may be written as a product $A = LU$ in which L is a lower triangular and U is an upper triangular n-by-n matrix. If there is such a factorization in which L is nonsingular, then there is one in which all diagonal entries of L are equal to 1; we call such a factorization in which L has unit diagonal a unit LU factorization. Our interest here is in a family of questions of the following type.

Under what circumstances does $u_{ij} = a_{ij}$ for a given pair $i \leq j$? (1.1)

Under what circumstances does $u_{ij} = a_{ij}$ for all pairs $i < j$ (or all $i \leq j$)? (1.2)

Here $A = [a_{ij}]$ is an n-by-n matrix with unit LU factorization $A = LU$ and $U = [u_{ij}]$. We refer to the equalities in (1.1) and (1.2) as local and global inheritance, respectively.

In order to ask our questions, we must assume that a unit LU factorization exists. To avoid possible ambiguities we shall also assume that it is unique, and, fortunately, this circumstance may be easily characterized. For index sets $\alpha, \beta \subseteq \{1,2,\ldots,n\}$, we denote the submatrix of the n-by-n matrix A lying in the rows indicated by α and columns indicated by β as $A[\alpha|\beta]$. In case $\beta = \alpha$, the submatrix is principal and we abbreviate $A[\alpha|\alpha]$ to $A[\alpha]$. We shall often be interested in the determinant of a leading principal submatrix of A and so adopt the notation $d_k(A) \equiv \det A[\{1,2,\ldots,k\}]$. Our characterization slightly strengthens [9, Th. 4]. Note that this result is well known when A is nonsingular (see, for example, [8, Cor. 3.5.5]).

THEOREM 1.1. The n-by-n matrix A has a unique unit LU factorization iff

$$d_k(A) \neq 0, \quad k = 1, 2, \ldots, n - 1. \tag{1.3}$$

Proof: Suppose that all the proper leading principal minors of A are nonzero, that is condition (1.3) is met. Then by [8, Cor. 3.5.5] and the partitioning in [9] the required unit LU factorization exists and is unique. The converse is similar to that of [9], the only difference being that we take L (rather than U) as the normalized matrix. ∎

In view of Th. 1.1 we shall generally assume that A satisfies condition (1.3) and, in this event, we let $U = U(A) = [u_{ij}]$ be the upper triangular factor in the unique LU factorization of $A = [a_{ij}]$.

In the spirit of sparse matrix analysis, we are not interested in circumstances such as (1.1) and (1.2) that involve accidental numeric cancellation. We approach these questions from a combinatorial point of view, based upon the zero pattern of A rather than the values of the nonzero entries. For this purpose, recall that a directed graph D consists of a set of nodes and some directed edges; a subgraph is based upon the same set of nodes and a subset of the edges of D. See [1] for other graph-theoretic terms that we use.

With a given n-by-n matrix $A = [a_{ij}]$ we associate a directed graph D(A) on nodes 1, 2, ..., n by including the edge (i, j) if and only if $a_{ij} \neq 0$. This then precisely describes the zero pattern of A. We say that an n-by-n matrix A is <u>consistent</u> with a given directed graph D if D(A) is a subgraph of D, and let $\mathcal{A}$ denote the set of all n-by-n matrices A that satisfy (1.3) and are consistent with D. The precise combinatorial phrasings of questions (1.1) and (1.2) which we address are then as follows.

For which directed graphs D does $A \in \mathcal{A}$ imply that $u_{ij} = a_{ij}$ for a given pair $i \leq j$? (1.1')

For which directed graphs D does $A \in \mathcal{A}$ imply that $u_{ij} = a_{ij}$ for all pairs $i < j$ (or all $i \leq j$)? (1.2')

There are several familiar examples in which the phenomena requested by (1.2) occur. Perhaps the simplest is the case in which A itself is upper triangular. In this event $A = LU$ with $L = I$ and $U = A$, so that the upper triangular factor agrees with A above (and on) the diagonal. Another example is the following tridiagonal matrix A which factors as $A = LU$ with $L = U^T$:

$$A = \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & & \\ & & & & -1 \\ & & & -1 & 2 \end{bmatrix}, \quad U = \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & & & \\ & & & & -1 \\ & & & & 1 \end{bmatrix}.$$

Again, the upper triangular factor agrees with A above the diagonal, even though A is irreducible in this case. A very simple circumstance for the local question (1.1) is the case $i = 1$; it is well known and easy to check that the first row of A becomes the first row of U for any matrix A with unit LU factorization. It is the combinatorial basis for this sort of simplicity and sparsity preservation upon which we focus. If circumstances are such that the upper triangular factor agrees with A above the diagonal when the lower triangular factor has 1's on the diagonal, half of the assumed factorization may be written down immediately.

The equalities of (1.1) and (1.2) may occur for non-combinatorial reasons. For example, if

$$A = \begin{bmatrix} 1 & 1 & 1 & 2 \\ 1 & 2 & 1 & 1 \\ 2 & 6 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \quad \text{then} \quad U = \begin{bmatrix} 1 & 1 & 1 & 2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

and $a_{34} = u_{34} = 0$ (see [1], ex. 4.1). The inheritance of this zero entry is due to the numerical values of the entries, not to the structure of $D(A)$. To exclude such instances of "accidental cancellation", we give the following definition. Given a matrix A with digraph $D(A)$, we say that two values f and g computable from the entries of A are <u>equal generically</u> (written $f = g$ (generically)) if $f(\hat{A}) = g(\hat{A})$ for all $\hat{A}$ such that $D(\hat{A}) = D(A)$.

We first answer question (1.1') with a simple graph-theoretic condition in section 2, and then use this answer to address question (1.2') in section 3. In section 4 we indicate the analogous solutions for the dual problems regarding $L = [\ell_{ij}]$ when U is normalized. Also in section 4 we consider the situation in which both $u_{ij} = a_{ij}$ for $i \leq j$, and $\ell_{ij} = a_{ij}$ for $i \geq j$. Some analogs for UL factorizations are stated in section 5. The occurrence of $U(A)_{ij} = U(A[\beta])_{ij}$ and the relationship with known results about Gaussian elimination are discussed in sections 6 and 7.

2. LOCAL INHERITANCE

In this section we address the local questions and begin with a sufficient condition for (1.1).

THEOREM 2.1. Let A be an n-by-n matrix with $d_k(A) \neq 0$, $k = 1, 2, \ldots, n-1$. If there is no path from i to $j \geq i$ through $\{1,2,\ldots,i-1\}$ in $D(A)$, then $u_{ij} = a_{ij}$ in the unit LU factorization of A.

Proof: By [6, p. 26],

$$u_{ij} = \frac{\det A[\{1,\ldots,i-1,i\}|\{1,\ldots,i-1,j\}]}{d_{i-1}(A)} \quad \text{for} \quad j \geq i. \tag{2.1}$$

Expanding about the ith row,

$$\det A[\{1,\ldots,i-1,i|1,\ldots,i-1,j\}] = a_{ij}\, d_{i-1}(A), \tag{2.2}$$

as there are no paths from i to j through $\{1,\ldots,i-1\}$. Equations (2.1) and (2.2) imply that $u_{ij} = a_{ij}$. ■

The above path condition and an analogous one play an important part in our work, so we introduce some related terminology. For $1 \leq i, j \leq n$, A is <u>(i,j) lower restricted</u> if there is no path (of length ≥ 2) in $D(A)$ from i to j such that all intermediate nodes on this path are $< \min\{i,j\}$. Note that A is always $(1,j)$ and $(i,1)$ lower restricted. Letting $i, j \in \{1,2,\ldots,n\}$ and $S \subseteq \{1,2,\ldots,n\}$, <u>$j$ is reachable from i through S</u> (see [1]) if there is a (simple) path in D (of length ≥ 2) from i to j such that all intermediate nodes on this path are in S. Thus for $1 \leq i, j \leq n$, A is (i,j) lower restricted iff j is not reachable from i through

$S = \{1,2,\ldots,\min\{i,j\}\}$. In the case that $i < j$ and A is (i,j) lower restricted, then $a_{ij} = 0$ implies that the submatrix $A[\{1,2,\ldots,i,j\}]$ is reducible, whereas for $a_{ij} \neq 0$ this submatrix may be irreducible. If A is (i,i) lower restricted, then $A[\{1,2,\ldots,i\}]$ is always reducible.

Provided A satisfies (1.3), Th. 2.1 can be restated as follows. If A is (i,j) lower restricted, then $u_{ij} = a_{ij}$ for given $i \leq j$ in the unit LU factorization of A. For example, if there is a positive integer p such that $a_{ij} = 0$ for all $j \geq p + i$, then A is (i,j) lower restricted for all $j \geq p + i - 1$. Thus $u_{ij} = a_{ij}$ for all pairs (i,j) with $j \geq p + i - 1$; and in particular $u_{ij} = a_{ij} = 0$ for all such pairs with $j \geq p + i$. Note that this situation includes matrices of bandwidth $p-1$ and lower Hessenberg matrices $(p = 2)$.

We use the idea of a reachable node to determine necessary and sufficient conditions to answer (1.1').

THEOREM 2.2. Let D be a directed graph on n nodes and let i, j be a given pair, $i \leq j \leq n$. Then for all $A \in \mathcal{A}$, $u_{ij} = a_{ij}$ in the unit LU factorization of A iff

(i) j is not reachable from i through $\{1,2,\ldots,i-1\}$,

or

(ii) if j is reachable from i through nodes $p_1, p_2, \ldots, p_t \in \{1,2,\ldots,i-1\}$, then $\det A[\{1,2,\ldots,i-1\} - \{p_1,p_2,\ldots,p_t\}] = 0$ for all $A \in \mathcal{A}$.

Proof: Expanding the numerator of (2.1) about the ith row (cf. (2.2)),

$$\det A[\{1,\ldots,i-1,i|1,\ldots,i-1,j\}] = a_{ij}\, d_{i-1}(A) + \sum \pm\, a_{ip_1} a_{p_1p_2} \cdots a_{p_tj} \det A[\{1,2,\ldots,i-1\}-\{p_1,p_2,\ldots,p_t\}], \quad (2.3)$$

where the summation is over all simple paths from i to j through $p_1, p_2, \ldots, p_t \in \{1,\ldots,i-1\}$, $t \geq 1$, and the $\pm$ sign depends on i, j, t (see [1]). If $u_{ij} = a_{ij}$ for all $A \in \mathcal{A}$, then each term in this summation must be zero, so either there is no such path (condition (i)) or the complementary principal minor must be zero (condition (ii)). Conversely, if (i) is true then Th. 2.1 gives $u_{ij} = a_{ij}$, while if (ii) is true equations (2.1) and (2.3) give this equality. ■

The following observation now follows from the inheritance in U of a subset of a row of entries of A (cf. [5, Lemma 2]).

COROLLARY 2.3. Let D be a directed graph on n nodes with a self loop at each node. Given $i \in \{1,2,\ldots,n-1\}$, if $u_{ij} = 0$ for all $j > i$ in the unit LU factorization of all $A \in \mathcal{A}$ having $a_{kk} \neq 0$ for $k = 1,2,\ldots,n-1$, then D is not strongly connected (that is, all such $A \in \mathcal{A}$ are reducible).

Proof: Since $u_{ij} = 0$ for all such $A \in \mathcal{A}$, a_{ij} must equal zero and so D cannot have an edge (i,j) for all $j > i$. Since, for all such A, $a_{kk} \neq 0$ for $k = 1,2,\ldots,n-1$, condition (ii) of Th. 2.2 is vacuous. By condition (i), all such A are (i,j) lower restricted for all $j > i$. Thus there is no path from i to j in D, so the result follows. ■

Note that this corollary is in general false without the condition that $a_{kk} \neq 0$ for $k = 1, 2, \ldots, n-1$. Consider the following example (cf. the transpose of the example in [3, pg. 944]). Let $D = D(A)$ where

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & 0 & a_{23} & 0 \\ a_{31} & 0 & a_{33} & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}.$$

It can be shown that for arbitrary a_{ij} (subject to (1.3)), $u_{34} = 0$ (generically) in the unit LU factorization of A; thus $u_{34} = a_{34} = 0$ (generically), but A is irreducible. Here the inheritance of the $(3,4)$ entry is a consequence of condition (ii) of Th. 2.2. Although node 4 is reachable from node 3 via node 1, the complementary determinant $\det A[2] = a_{22} = 0$. It is the combinatorial structure of A, not accidental cancellation, that insures this inheritance.

When A is a nonsingular M-matrix [2, Ch. 6] then all principal minors of A are positive, so A has a unique unit LU factorization (with L and U also M-matrices) and condition (ii) of Th. 2.2 is vacuous. Thus, if A is a nonsingular M-matrix and is (i,j) lower restricted, then $u_{ij} = a_{ij}$ for given $i \leq j$ in the unit LU factorization of A. In fact this last statement also holds for a singular, irreducible M-matrix A as every principal submatrix of a matrix in this set (other than A itself) is a nonsingular M-matrix [2, Th. 6.4.16]. If A is a singular, reducible M-matrix, then it need not have an LU factorization. However, if in this case we impose our usual hypothesis (1.3), then $A[1,2,\ldots,n-1]$ is a nonsingular M-matrix, and the same statement holds.

If A is any M-matrix that has a unique unit LU factorization, then the sign pattern of A insures that $u_{ij} \leq a_{ij}$ for all $i \leq j$. Moreover, if $u_{ij} < a_{ij}$, then the (i,j) entry of A monotonically decreases to u_{ij} during the Gaussian elimination process. Thus, in the case of an M-matrix, it is not possible that $u_{ij} = a_{ij}$ because of accidental cancellation; such equality can occur only for combinatorial reasons, giving the following.

COROLLARY 2.4. Let A be an n-by-n M-matrix satisfying (1.3), and let i, j be a given pair with $i \leq j \leq n$. Then $u_{ij} = a_{ij}$ in the unit LU factorization of A iff A is (i,j) lower restricted. ■

3. GLOBAL INHERITANCE

We now address questions (1.2), (1.2') and first answer the more general graph question (1.2') for all $i < j$. In contrast to the result for local inheritance, it turns out that the complementary minor condition (Th. 2.2 (ii)) disappears from the characterization of global inheritance.

THEOREM 3.1. Let D be a directed graph on n nodes. Then, for all $A \in \mathcal{A}$ and for all pairs i, j with $i < j \leq n$, $u_{ij} = a_{ij}$ in the unit LU factorization of A iff j is not reachable from i through $\{1,2,\ldots,i-1\}$.

Proof: Assume that for all $i < j$, j is not reachable from i through $\{1,2,\ldots,i-1\}$; that is, there is no path from i to j through nodes $< i$. By condition (i) of Th. 2.2 this implies that $u_{ij} = a_{ij}$ for all $i < j$.

For the converse, assume that $u_{ij} = a_{ij}$ for all pairs $i < j$ and all $A \in \mathcal{A}$. Using Th. 2.2, if condition (i) is true for all such pairs and all $A \in \mathcal{A}$, then our theorem is proved. Otherwise let $A \in \mathcal{A}$ and let i be the smallest node for which there is a path in $D(A)$ from i to $j > i$ through nodes $p_1, p_2, \ldots, p_t \in \{1,2,\ldots,i-1\}$ such that $\det A[\alpha] = 0$, where $\alpha \equiv \{1,2,\ldots,i-1\} - \{p_1,p_2,\ldots,p_t\}$. Then there exists a node $m \in \alpha$ such that

(a) $a_{mm} = 0$, since $\det A[\alpha] = 0$ for all A consistent with D; and

(b) m lies on a cycle $m \to q_1 \to \cdots \to q_r \to m$ in $D(A[1,2,\ldots,m])$ (since $d_m(A) \neq 0$) with some q_s, $1 \leq s \leq r$, not in α (since if each node with no 1-cycle lies on a cycle entirely in α, then there is a nonzero term in $\det A[\alpha]$).

Thus $q_s \in \{p_1,p_2,\ldots,p_t\}$, so there exists a path $m \to q_1 \to \cdots \to q_s = p_v \to \cdots \to p_w$ where $p_v, \ldots, p_w \in \{p_1,p_2,\ldots,p_t,j\}$ and $p_w = \min\{j,$ first node > m on the path from i to $j\}$. All intermediate nodes on the path from m to p_w are $< m$, and, by the choice of i, all principal minors of $A[1,2,\ldots,m-1]$ are nonzero. Thus by Th. 2.2 $u_{mp_w} \neq a_{mp_w}$, which contradicts our assumption. ■

Matrices with digraphs satisfying the condition of Th. 3.1 are, in the terminology of section 2, (i,j) lower restricted for all pairs $i < j$; we call such matrices <u>forward lower restricted</u>. With this terminology and the result of Th. 3.1, question (1.2) may now be answered succinctly as follows.

COROLLARY 3.2. Let A be an n-by-n matrix satisfying (1.3). If A is forward lower restricted, then $u_{ij} = a_{ij}$ for all $i < j$ in the unit LU factorization of A. Conversely, if $u_{ij} = a_{ij}$ (generically) for all $i < j$, then A is forward lower restricted. ■

For example, a lower Hessenberg matrix is forward lower restricted, and thus satisfies the condition of the corollary; see the example after Th. 2.1. If A is an M-matrix, then Cor. 2.4 shows that the conditions of Cor 3.2 are necessary and sufficient without generic equality.

We now restrict A to be combinatorially symmetric and reconsider our global inheritance question (1.2) in this special case. When the undirected graph of A is a forest, we define A to be <u>invariantly ordered</u> if it has at most one nonzero entry in each column below the diagonal; for example, any tridiagonal matrix is invariantly ordered. This definition leads to the following characterization.

THEOREM 3.3. Let A be an n-by-n combinatorially symmetric matrix satisfying (1.3). If the undirected graph of A is a forest and A is invariantly ordered, then $u_{ij} = a_{ij}$ for all $i < j$ in the unit LU factorization of A. Conversely, if $u_{ij} = a_{ij}$ (generically) for all $i < j$, then A is invariantly ordered.

Proof: Assume that A is combinatorially symmetric and invariantly ordered. Then there exists at most one edge out of each node to a higher numbered node, so there can be no path $p \to q \to r$ where $r > p > q$. Thus A is forward lower restricted, and so, by Cor. 3.2, U has the desired inherited entries. For the converse, assume that $u_{ij} = a_{ij}$ (generically) for all $i < j$ in the unit LU factorization of A; then (by Cor. 3.2) A is forward lower restricted. Since A is also assumed to be combinatorially symmetric, the graph of A can have no p-cycle for $p \geq 3$, implying that the graph of A is a forest. Moreover, A must be invariantly ordered, else there would exist a node k with two higher numbered nodes i, j $(k < i < j)$ connected to it, giving (by Th. 3.1) $u_{ij} \neq a_{ij}$, which is a contradiction. ∎

We now consider the more restrictive version of our question (1.2), in which we characterize inheritance of all entries for $i \leq j$. Note that for the tridiagonal matrix given in the introduction, $u_{ij} = a_{ij}$ for all $i < j$ but not for all $i = j$. By analogy with Cor. 3.2 we have the following result.

COROLLARY 3.4. Let A be an n-by-n matrix satisfying (1.3). If A is (i,j) lower restricted for all pairs $i \leq j$, then $u_{ij} = a_{ij}$ for all $i \leq j$ in the unit LU factorization of A. Conversely, if $u_{ij} = a_{ij}$ (generically) for all $i \leq j$, then A is (i,j) lower restricted for all pairs $i \leq j$. ∎

Matrices which satisfy these conditions can have no p-cycle for $p \geq 2$, and thus must be reducible; in fact they must be essentially triangular (although not all essentially triangular matrices satisfy these conditions). In addition, if A is (i,j) lower restricted for all pairs $i \leq j$, then $\det A = \prod_{i=1}^{n} a_{ii}$. Some examples of matrices satisfying these conditions are given below, where the entries a_{ij} are arbitrary (subject to (1.3)).

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} \\ 0 & a_{42} & 0 & a_{44} \end{bmatrix}, \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & 0 \\ 0 & 0 & a_{43} & a_{44} \end{bmatrix}, \begin{bmatrix} a_{11} & 0 & a_{13} & 0 \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & 0 \\ a_{41} & 0 & a_{43} & a_{44} \end{bmatrix}.$$

4. INHERITANCE IN THE RIGHT UNIT LU FACTORIZATION

Results in the previous two sections characterize inheritance in the upper triangular factor when the main diagonal entries of the lower triangular factor are all unity. There are obviously analogous characterizations for inheritance in the lower triangular factor when the diagonal entries of the upper triangular factor are all unity. We call this the right unit LU factorization of a matrix A. By taking transposes, $A^T = U^T L^T$ and it is easy to see that Th. 2.1 and 2.2 with $\{1,2,\ldots,i-1\}$ replaced by $\{1,2,\ldots,j-1\}$ in each case give conditions for $\ell_{ij} = a_{ij}$ for particular i, $j \le i$ in the right unit LU factorization of matrix A. Thus we have the result that if A satisfying (1.3) is (i,j) lower restricted, then $\ell_{ij} = a_{ij}$ for a given pair $i \ge j$ in the right unit LU factorization of A.

To characterize global inheritance in this factorization, we introduce another definition. If a matrix A is (i,j) lower restricted for all pairs $i > j$, then we call A backward lower restricted. If this condition is true for a matrix A satisfying (1.3), then $\ell_{ij} = a_{ij}$ for all $i > j$ in its right unit LU factorization. The converse holds if the equality is generic (cf. Cor. 3.2). Assuming, in addition to the principal minor condition, that A is combinatorially symmetric, if A is invariantly ordered then $\ell_{ij} = a_{ij}$. The converse holds if the equality is generic (cf. Th. 3.3). This follows because if A is combinatorially symmetric with a forest graph, then A is invariantly ordered iff A^T is. Thus, for the class of matrices specified above, inheritance in one unit LU factorization implies inheritance in the other unit LU factorization. Tridiagonal matrices are in this class (see the example in the introduction).

In the following result we characterize the simultaneous inheritance of entries (including those on the diagonal) in both LU factorizations.

THEOREM 4.1. Let A be an n-by-n matrix satisfying (1.3). If for each $p \in \{1,2,\ldots,n-1\}$ either $a_{pq} = 0$ or else $a_{qp} = 0$ for all q with $n \geq q > p$, then $u_{ij} = a_{ij}$ for all $i \leq j$ in the unit LU factorization and $\ell_{ij} = a_{ij}$ for all $i \geq j$ in the right unit LU factorization. The converse holds if the equalities are generic.

Proof: Let $U = [u_{ij}]$ and $L = [\ell_{ij}]$, respectively, denote the upper and lower factors in the unit LU and right unit LU factorizations. Let $1 \leq p \leq n-1$ and assume first that either $a_{pq} = 0$ or else that $a_{qp} = 0$ for all $q > p$. Thus, in the digraph of A there cannot exist a path of the form $q_1 \to p \to q_2$ for any $q_1, q_2 > p$. That is, A is (i,j) lower restricted for all pairs (i,j), and therefore $u_{ij} = a_{ij}$ and $\ell_{ij} = a_{ij}$ for all $i \leq j$ and $i \geq j$ respectively.

To prove the converse, assume that $u_{ij} = a_{ij}$ (generically) and $\ell_{ij} = a_{ij}$ (generically) for $i \leq j$ and $i \geq j$, respectively. Let $1 \leq p \leq n-1$ and $p < r \leq n$, and suppose that $a_{pr} \neq 0$. If $a_{qp} \neq 0$ for any $q > p$, then $a_{qp}a_{pr} \neq 0$ implies either that $u_{qr} \neq a_{qr}$ (when $q \leq r$) or $\ell_{qr} \neq a_{qr}$ (when $q \geq r$). In either case the assumption is contradicted and thus $a_{qp} = 0$ for all $q > p$. Similarly, it can be shown that $a_{rp} \neq 0$ for $r > p$ implies that a_{pq} must equal zero for all $q > p$. ∎

We call a matrix which satisfies the zero/nonzero pattern of Th. 4.1 a <u>sawtooth</u> matrix, and note that it can be displayed as

$$A = \left[\begin{array}{c|c|c} a_{11} & \multicolumn{2}{c}{A_{12}} \\ \hline A_{21} & a_{22} & A_{23} \\ \cline{2-3} & A_{32} & a_{33} \\ & & \ddots \end{array}\right],$$

where a_{ii} are arbitrary and one of $A_{i\ i+1}$, $A_{i+1\ i}$ is 0 while the other is arbitrary. Note that the first two examples at the end of section 3 are sawtooth matrices, but the third example is not.

5. UL FACTORIZATIONS

Whereas we have concentrated thus far on LU factorizations, we now state results for the analagous problems for UL factorizations of A. Again we consider the two normalizations; when all diagonal entries of U [resp. L] are equal to 1, we call this a left [right] unit UL factorization. Each of these factorizations is unique (cf. Th. 1.1) iff all proper trailing principal minors are nonzero, that is, iff

$$\det A[\{n-k+1,\dots,n\}] \neq 0 \quad \text{for} \quad k = 1, 2, \dots, n-1. \tag{5.1}$$

To consider inheritance of entries, we state a definition which is the analog of (i,j) lower restricted. For $1 \leq i, j \leq n$, A is (i,j) upper restricted if there is no path (of length ≥ 2) in D(A) from i to j such that all intermediate nodes on this path are $> \max\{i,j\}$. Note that A is always (i,n) and (n,j) upper restricted. A sufficient condition for local inheritance then parallels Th. 2.1. If A satisfies (5.1) and is (i,j) upper restricted ,then $\ell_{ij} = a_{ij}$ $[u_{ij} = a_{ij}]$ for given $i \geq j$ $[i \leq j]$ in the left [right] unit UL factorization. Necessary and sufficient conditions for local inheritance can thus be given by analogy with Th. 2.2.

For global inheritance we need definitions analogous to those for lower restricted. A is backward [forward] upper restricted if A is (i,j) upper restricted for all pairs $i > j$ $[i < j]$. The result analogous to Cor. 3.2 then takes the following form.

> Given A satisfying (5.1), if A is backward [forward] upper restricted, then $\ell_{ij} = a_{ij}$ $[u_{ij} = a_{ij}]$ for all $i > j$ $[i < j]$ in the left [right] unit UL factorization of A.

The following result corresponds to Th. 3.3, and contains an analog of the condition that A is invariantly ordered.

Given a combinatorially symmetric matrix A satisfying (5.1), if the undirected graph of A is a forest and A has at most one nonzero entry in each column above the main diagonal, then $\ell_{ij} = a_{ij}$ [$u_{ij} = a_{ij}$] for all $i > j$ [$i < j$] in the left [right] unit UL factorization of A.

On requiring that all off-diagonal entries of A be inherited in L and U, we obtain the following (with the appropriate normalizations for L and U).

Given an irreducible, combinatorially symmetric matrix satisfying (1.3) and (5.1), if A is tridiagonal then $u_{ij} = a_{ij}$ for all $i < j$ in the unit LU factorization of A and $\ell_{ij} = a_{ij}$ for all $i > j$ in the left unit UL factorization of A.

The converses of the three statements above all hold if the equalities are generic.

6. SUBMATRIX INHERITANCE

Suppose that A has a unique unit LU factorization, and that some submatrix $A[\beta]$ also has such a factorization $A[\beta] = L(A[\beta])U(A[\beta])$; we now characterize when the i, j entries of $U \equiv U(A)$ and $U(A[\beta])$ are equal. For $\beta = \{1,2,\ldots,p\}$, $1 \le p \le n$, this equality obviously holds for any A satisfying (1.3), and for all $i, j \in \beta$. But for more general β this is not necessarily true, and we seek to determine combinatorial circumstances under which it does hold.

In the case that the i, j entry of A is inherited by U we have the following result. Given a directed graph D with a self loop at each node, we let $\mathcal{A}'$ denote the set of all n-by-n matrices A which have all principal minors nonzero and which are consistent with D. (Note that $\mathcal{A}' \subseteq \mathcal{A}$.)

THEOREM 6.1. Let D be a directed graph with a self loop at each node, let $\beta \subseteq \{1,2,\ldots,n\}$ and $i, j \in \beta$ with $i \le j$. If for all $A \in \mathcal{A}'$, $u_{ij} = a_{ij}$ in the unit LU factorization of A, then it is also the case that $U(A[\beta])_{ij} = a_{ij}$ in the corresponding factorization of $A[\beta]$.

Proof: As all $A \in \mathcal{A}'$ have nonzero principal minors, we can apply Th. 2.2 with condition (ii) vacuous. Thus $u_{ij} = a_{ij}$ for all $A \in \mathcal{A}'$ implies that j is not reachable from i through $\{1,2,\ldots,i-1\}$ in $D(A)$. But if this condition holds on $D(A)$ it necessarily holds (with respect to $\beta \cap \{1,2,\ldots,i-1\}$) on the subgraph of $D(A)$ induced by any set β containing i and j. Thus, using Th. 2.2 again, the i, j entry is also inherited by $U(A[\beta])$, and so $U(A[\beta])_{ij} = u_{ij} = a_{ij}$. ■

If the conditions of this theorem are relaxed to allow some $a_{ii} = 0$, then the result is not necessarily true. It is also easy to give an example that shows the converse of the theorem need not be true.

We now give a characterization of inheritance of all entries in a certain submatrix.

THEOREM 6.2. Let D be a directed graph with a self loop at each node and let $A \in \mathcal{A}'$. Then for given $i, j \in \beta \subseteq \{1,2,\ldots,n\}$ with $i \leq j$, $u_{ij} = U(A[\beta])_{ij}$ for all $A \in \mathcal{A}'$ (in the unit LU factorizations of A and $A[\beta]$) iff for all $A \in \mathcal{A}'$ every path from i to j through $\gamma = \{1,2,\ldots,i-1\}$ passes through nodes only in β.

Proof: Let $v_{ij} = U(A[\beta])_{ij}$. Then (cf. (2.1))

$$v_{ij} = \frac{\det A[(\gamma\cap\beta)\cup\{i\}\,|\,(\gamma\cap\beta)\cup\{j\}]}{\det A[\gamma\cap\beta]}. \tag{6.1}$$

This numerator can be expanded about the ith row (cf. (2.3)), giving

$$\begin{aligned}\det A[(\gamma\cap\beta)\cup\{i\}\,|\,(\gamma\cap\beta)\cup\{j\}] &= a_{ij} \det A[\gamma\cap\beta] \\ &\quad + \sum \pm\, a_{iq_1} a_{q_1q_2} \cdots a_{q_sj} \det A[(\gamma\cap\beta) - \{q_1,q_2,\ldots,q_s\}]\end{aligned} \tag{6.2}$$

where the summation is now over all paths from i to j through nodes $q_1, q_2, \ldots, q_s \in \gamma \cap \beta$, $s \geq 1$.

Assume first that $u_{ij} = v_{ij}$ for all $A \in \mathcal{A}'$. Then the terms involved in the summations of (2.3) and (6.2) must be equal for all such A. If for some A there is a path from i to j in γ which includes a node not in β, then this path product multiplied by its complementary determinant will occur in u_{ij} (from (2.3)) but not in v_{ij} (from (6.2)). As A has all principal minors nonzero, in particular this complementary determinant is nonzero, so we have a contradiction.

For the converse, assume that for all $A \in \mathcal{A}'$ every path from i to j passes through nodes only in β. Then the summations in (2.3) and (6.2) are over an identical set of paths from i to j. Thus $u_{ij} = v_{ij}$ for all $A \in \mathcal{A}'$ iff we have for all such matrices

$$\frac{\det A[\gamma-\{p_1,p_2,\ldots,p_t\}]}{\det A[\gamma]} = \frac{\det A[(\gamma\cap\beta)-\{p_1,p_2,\ldots,p_t\}]}{\det A[\gamma\cap\beta]}, \tag{6.3}$$

for all $\{p_1,p_2,\ldots,p_t\} \subseteq \beta$ such that there exists a path in γ from i to j through p_1, p_2, ..., p_t in $D(A)$. Now, as each A is assumed to have nonzero principal minors, all submatrices in (6.3) are nonsingular, so that Schur complements exist, and we can use ideas developed in [1]. Let ϵ be the set of nodes in β which are on no path from i to j. For any given path as above, let δ denote the set of all nodes in β such that $q_k \in \delta$, $k = 1, 2, \ldots, u$, iff there is a path from i to j through q_1, q_2, ..., q_u and $\{p_1,p_2,\ldots,p_t\} \cap \{q_1,q_2,\ldots,q_u\} \neq \emptyset$. Note that $\{p_1,p_2,\ldots,p_t\} \subseteq \delta$. The nodes can be ordered so that A is given in partitioned form as

$$A[\gamma\cap\beta] = \begin{bmatrix} A[\epsilon] & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \text{ where } A_{22} = \begin{bmatrix} A[\delta] & A_{23} \\ A_{32} & A[(\gamma\cap\beta)-\epsilon-\delta] \end{bmatrix}.$$

On taking the Schur complement of $A[\epsilon]$ in $A[\gamma\cap\beta]$:

$$\det A[\gamma\cap\beta] = \det A[\epsilon] \det(A_{22} - A_{21}\, A[\epsilon]^{-1}\, A_{12}).$$

But $A_{21}\, A[\epsilon]^{-1}\, A_{12}$ must be zero for every matrix A satisfying our assumptions, as otherwise there would exist a path from i to j through β including nodes of ϵ, which contradicts the definition of ϵ. Consequently,

$\det A[\gamma\cap\beta] = \det A[\epsilon] \det A_{22}$. Similarly taking the Schur complement of $A[\delta]$ in A_{22} gives

$$\det A[\gamma\cap\beta] = \det A[\epsilon] \det A[\delta] \det A[(\gamma\cap\beta)-\epsilon-\delta].$$

But $\{p_1,p_2,\ldots,p_t\} \subseteq \delta$, so the right side of (6.3) reduces to

$$\frac{\det A[\delta - \{p_1,p_2,\ldots,p_t\}]}{\det A[\delta]} . \tag{6.4}$$

Using the same reasoning on the left side of (6.3), it is also equal to (6.4) and the result follows. ■

Note that if there is no path from i to j in γ (that is, j is not reachable from i through $\{1,2,\ldots,i-1\}$), then the conclusion of the above theorem is that $u_{ij} = U(A[\beta])_{ij} = a_{ij}$ for all $A \in \mathcal{A}'$, giving inheritance of this entry. Obvious analogous results hold for the other three unit factorizations described in sections 4 and 5.

7. RELATIONS WITH GAUSSIAN ELIMINATION.

The relationship between Gaussian elimination and LU factorization is well known, especially in the numerical analysis literature. There also is a relationship between Gaussian elimination and Schur complements, so our results concerning inheritance of entries in U are related to results in [1].

Consider an n-by-n matrix A which satisfies (1.3) or, equivalently, for which all Gaussian elimination pivots are nonzero. Then $u_{ij} = a_{ij}$ in the unit LU factorization of A iff this entry is inherited when Gaussian elimination is applied to A. When $a_{ij} = 0$ but $u_{ij} \neq 0$ or $\ell_{ij} \neq 0$ for some $\hat{A}$ with $D(\hat{A}) = D(A)$, then there is said to be <u>fill-in</u> at the (i, j) entry. This idea is particularly important for large, sparse matrices, where it is desirable to minimize the fill-in. This has been discussed by many authors (see, e.g. [3, 4, 7, 10, 11]). In [7] consideration is restricted to symmetric positive definite matrices using the undirected graph of A and the Cholesky factorization $A = LL^T$. Theorem 5.12 in [7], which involves only condition (i) of our Th. 2.2 (since all principal minors of a positive definite matrix are nonzero), characterizes fill-in for this class of matrices. The following generalization of that result is an immediate consequence of our Th. 2.2 and the analogous result for inheritance of the entries in L (see the first paragraph of section 4).

COROLLARY 7.1. Let A be an n-by-n matrix satisfying (1.3) and suppose $a_{ij} = 0$. Then there is fill-in at the (i, j) entry when Gaussian elimination is applied to A iff there exists a path $i \to k_1 \to k_2 \to \cdots \to k_t \to j$ in $D(A)$ with $k_p \in \{1, 2, \ldots, \min(i,j)-1\}$, $1 \leq p \leq t$, and

$$\det A[\{1, 2, \ldots, \min(i,j)-1\} - \{k_1, k_2, \ldots, k_t\}] \neq 0. \quad \blacksquare$$

Our results are more general than those contained in the literature concerning fill-in in sparse matrices since we require only that A has a unique unit LU factorization. In addition, we characterize the inheritance of both zero and nonzero entries. As shown by the example following Th. 2.2, the use of condition (ii) of that theorem to deduce that $u_{ij} = a_{ij}$ (generically) is interesting in that the (i,j) entry of U may indeed change during the process of determining the LU factorization; however, the equality is guaranteed by the combinatorial structure.

Much of the emphasis in the literature concerning fill-in in sparse matrices concerns the determination of matrices P, Q so that either PAP^T or PAQ has less fill-in than A. We have not discussed this important practical problem.

REFERENCES

[1] W.W. BARRETT, C.R. JOHNSON, D.D. OLESKY and P. VAN DEN DRIESSCHE, Inherited matrix entries: principal submatrices of the inverse. SIAD, (1987) to appear.

[2] A. BERMAN and R.J. PLEMMONS, Nonnegative Matrices in the Mathematical Sciences, Academic, 1979.

[3] R.K. BRAYTON, F.G. GUSTAVSON, and R.A. WILLOUGHBY, Some results on sparse matrices. Math. Comp. 24(1970), pp. 937-954.

[4] I.S. DUFF, Research directions in sparse matrix computations, MAA Studies in Math. Studies in Numerical Analysis, G.H. Golub, ed., 24, 1984.

[5] I.S. DUFF, A.M. ERISMAN, C.W. GEAR and J.K. REID, Some remarks on inverses of sparse matrices, Argonne Nat. Lab. Tech. Memo. 51(1985), pp. 1-10.

[6] F.R. GANTMACHER, Matrix Theory, V.I., Chelsea, 1959.

[7] J.A. GEORGE and J.W.H. LIU, Computer Solutions of Large Sparse Positive Definite Systems, Prentice-Hall, 1981.

[8] R. HORN and C.R. JOHNSON, Matrix Analysis, Cambridge University Press, 1985.

[9] C.M. LAU and T.L. MARKHAM, LU factorizations, Czech. Math. J. 29(1979), pp. 546-550.

[10] S. PISSANETSKY, Sparse Matrix Technology, Academic Press, 1984.

[11] D.J. ROSE and R.E. TARJAN, Algorithmic aspects of vertex elimination on directed graphs, SIAM J. Appl. Math. 34(1978), pp. 176-197.