A NECESSARY AND SUFFICIENT SYMBOLIC CONDITION FOR THE EXISTENCE OF INCOMPLETE CHOLESKY FACTORIZATION*

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Abstract. This paper presents a sufficient condition on sparsity patterns for the existence of the incomplete Cholesky factorization. Given the sparsity pattern $P(A)$ of a matrix A, and a target sparsity pattern P satisfying the condition, incomplete Cholesky factorization successfully completes for all symmetric positive definite matrices with the same pattern $P(A)$. It is also shown that this condition is necessary in the sense that for a given $P(A)$ and target pattern P, if P does not satisfy the condition then there is at least one symmetric positive definite matrix B whose Cholesky factor has the same sparsity pattern as the Cholesky factor of A, for which incomplete Cholesky factorization fails because of a nonpositive pivot.

1. Introduction. Incomplete Cholesky factorization (IC) is a widely known and effective method of accelerating the convergence of conjugate gradient (CG) iterative methods for solving symmetric positive definite linear systems. A major weakness of IC is that it may break down due to nonpositive pivots. Methods of overcoming this problem can be divided into two classes: numerical and structural strategies. A numerical strategy uses numerical values generated during the factorization process to modify the factorization, as in the work by [Jennings and Malik, 1977, Manteuffel, 1979, Munksgaard, 1980, Wittum and Liebau, 1989]. A structural strategy, as in the work by [Coleman, 1988], selects the sparsity pattern to insure the completion of the IC process. In this paper, we do not give any specific algorithm for modifying the sparsity pattern to assure the existence of IC. Instead, we prove a sufficient and necessary condition on the sparsity pattern of the incomplete Cholesky factor for the existence of IC on the symmetric positive definite matrices with a given sparsity. The condition is more general than that in [Coleman, 1988], and includes Coleman's sparsity pattern condition as a special case.

Structural strategies are especially important for applications where a sequence of linear systems must be solved, each coefficient matrix with the same non-zero pattern. This occurs when solving linear programming problems using interior point methods, or when solving discretized nonlinear partial differential equations with a fixed mesh. Although the values can change from one step to another, the sparsity pattern is fixed. Using a target IC sparsity pattern that satisfies our sufficient condition, the preconditioner can be set up on each step using a static data structure and with assurance that the preconditioner will exist. Some specific algorithms that modify a sparsity pattern to satisfy the sufficient condition have been proposed and tested in [Wang et al., 1994b, Wang, 1993].

2. Definitions and Notation. Before the main results are presented, some definitions and notation that are used are given. Unless otherwise specified, we assume that matrices are

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real and symmetric positive definite. The examples will only display the upper triangular part of matrices, with the understanding that the lower triangular parts are specified by symmetry.

Capital letters denote matrices, and the elements of a matrix will be denoted as the corresponding lower case letter with two subscripts indicating the row and column indices. For example, a_{ij} denotes the element of matrix A in the ith row and jth column.

Let $P_n = \{(i,j)|1 \leq i \leq j \leq n\}$ be the set of all possible non-zero positions in an $n \times n$ upper triangular matrix. The sparsity pattern $P(A)$ of a symmetric matrix A is defined as $P(A) = \{(i,j)|a_{ij} = a_{ji} \neq 0, \;\; 1 \leq i \leq j \leq n\}$. Note that $P(A)$ only considers the positions of the non-zero elements of A in upper triangular part and $P(A) \subseteq P_n$. Let U be the upper triangular Cholesky factor of A formed assuming no cancellation[1], so that $A = U^T U$. Since it is clear from context when we are discussing a triangular or symmetric matrix, we exploit a convenient abuse of notation and let $P(U)$ denote the sparsity pattern of U and $P(U) \subseteq P_n$.

The incomplete Cholesky factorization of a matrix A using sparsity pattern P refers to a Cholesky factorization where all entries occurring outside of the specified sparsity pattern are immediately discarded, and no other numerical modification is made to the matrix. Given a matrix A and a sparsity pattern $P \subseteq P_n$ of the target factor U, it is assumed that $P \subseteq P(U)$ without loss of generality because a position $(i,j) \notin P(U)$ will not affect the final factor. In order for the IC factorization to complete all diagonal positions (i,i) must be in P, a requirement we now impose on all the sparsity patterns P dealt with in this paper. The IC algorithm can be described as follows:

Algorithm [R]=IC[A,P]

begin
for $k = 1, 2, \ldots, n,$
  if $a_{kk} > 0$ **then**
(1) $r_{kk} = \sqrt{a_{kk}}$
   for $j = k+1, \; k+2, \; \ldots, \; n$
(2) $r_{kj} = \begin{cases} 0 & (k,j) \notin P \\ a_{kj}/r_{kk} & (k,j) \in P \end{cases}$
   endfor
   for $i = k+1, \; k+2, \; \ldots, \; n$
    for $j = i, \; i+1, \; \ldots, \; n$
(3) $a_{ij} = a_{ij} - a_{ki}a_{kj} \quad (i,j) \in P, \;\; (k,j) \in P \text{ and } (k,i) \in P$
    endfor
   endfor
  else
(6) *Stop (incomplete factorization fails)*
  endif
endfor
end

Although the algorithm is most commonly stated (and implemented) by initially copying A to R and then referring to R alone, the form shown above is valid for target sparsity patterns $P \nsubseteq P(A)$, and simplifies the proof of Theorem 1. In practice, the updates to A would not be performed since generally A needs to be retained for the iterative method that is preconditioned by R.

Next, we define a new property on sparsity patterns. This property uses an auxiliary

[1] This assumption is made throughout the paper when referring to the Cholesky factorization of a matrix

sparsity pattern Q, and when Q is the sparsity pattern, $P(U)$, of the complete Cholesky factorization the property gives our sufficient condition for existence of the IC factorization.

DEFINITION 2.1. *Let $Q \subseteq P_n$ and $P \subseteq P_n$ be given sparsity patterns. P is said to have* **property $\mathbf{C}_+$** *on Q, if the following condition is satisfied: for any position $(j,k) \in P \cap Q$, if (i,j) and (i,k), $1 \leq i < j$, are both in Q, then they both are in P or neither is in P. If the condition is not satisfied then P is said to violate property C_+ on Q.*

DEFINITION 2.2. *Let $Q \subseteq P_n$ and $P \subseteq P_n$ be given sparsity patterns and let $C_+(Q)$ denote the set of all patterns in P_n that have property C_+ on Q. $P \in C_+(Q)$ and $P \notin C_+(Q)$ will denote P having property C_+ on Q and violating it, respectively.*

From the matrix sparsity point of view, $P \in C_+(Q)$ means that for any $(j,k) \in P \cap Q$, columns j and k of any matrix with sparsity pattern P have the same structure in rows $i < j < k$ where (i,j) and (i,k) are in Q. Because property C_+ requires either both elements to be present or both elements to be absent, it can also be viewed as an "not exclusive or" condition, modulo the sparsity pattern Q. The structure of rows $1 \leq i < j$ where at least one of (i,j) and (i,k) is not in Q, is unrestricted.

EXAMPLE 1. *Let A be a 3×3 full matrix. All sparsity patterns $P \subseteq P_3$ are in $C_+(P_3)$ except the following two patterns: $P = \{(1,1),(2,2),(3,3),(1,2),(2,3)\}$ and $P = \{(1,1),(2,2),(3,3),(1,3),(2,3)\}$.*
The example follows by considering the following cases. If $(2,3) \in P$ then among the 4 possible combinations of $(1,2)$, $(1,3)$ in or not in P, only the listed patterns violate property $C_+(P_3)$. If $(2,3) \notin P$, then any combination of $(1,2)$ and $(1,3)$ in or not in P will satisfy property $C_+(P_3)$.

EXAMPLE 2. *If A is the matrix arising from a five-point difference operator on a regular two-dimensional mesh using the red-black ordering, then $P(A) \in C_+(P(U))$.*
A simple way of generating a pattern for IC is to start with U and consider subsets of $P(U)$. The next example shows that a simple selection strategy is consistent with property C_+.

EXAMPLE 3. *Let A be a matrix with Cholesky factor U. If V is a submatrix of U that consists of all the diagonal elements and any subset of the set of rows of U, then $P(V) \in C_+(P(U))$.*
To see this fact, note first that $(j,k) \in P(V)$ implies $(j,k) \in P(U)$. Now consider any pair of positions (i,j) and (i,k) in $P(U)$. If row i of U is a row included in V, then both (i,j) and (i,k) are in $P(V)$ by construction of V. Otherwise, by construction, the complete row i of U is not in V and both (i,j) and (i,k) are not in $P(V)$. No other possibilities exists so by the definition, we have $P(V) \in C_+(P(U))$. For a given matrix A, there is a combinatorially large number of submatrices V satisfying the construction conditions in Example 3, but for each $P(V) \in C_+(P(U))$. In addition, the density of target sparsity patterns can vary from as sparse as a diagonal matrix to the pattern of the complete Cholesky factor U.

EXAMPLE 4. *Suppose the graph of A is chordal and the factorization of A is performed using the perfect elimination ordering that guarantees no fill-in, then $P(A) = P(U)$ and $P(A) \in C_+(P(U))$, i.e., this is a special case of Example 3.*
Example 4 indicates the relationship of Coleman's preconditioner and property C_+. Coleman identifies submatrices of A which are chordal and permutes A so that these chordal blocks form a block diagonal submatrix of A. The block diagonal matrix is used as a preconditioner by performing Cholesky factorization on each diagonal block using the appropriate perfect elimination ordering. Example 4 shows that such a preconditioner satisfies proper C_+.

EXAMPLE 5. *Let* $A = \begin{bmatrix} \times & \times & \times & \times & \\ & \times & & \times & \\ & & \times & & \\ & & & \times & \times \\ & & & & \times \end{bmatrix}$, *so that* $U = \begin{bmatrix} \times & \times & \times & \times & \\ & \times & \times & \times & \\ & & \times & \times & \\ & & & \times & \times \\ & & & & \times \end{bmatrix}$ *is the symbolic Cholesky factor of* A, *and* $P(U) = P(A) \cup \{(2,3),(3,4)\}$. *Then* $P(A) \in C_+(P(U))$.

Theorem 1 below shows that $P(A) \in C_+(P(U))$ implies that IC(0), incomplete Cholesky factorization with zero levels of fill-in, exists regardless of the numerical values in the positive definite matrix of Example 5. When IC(0) fails to accelerate convergence sufficiently, a standard technique for generating a pattern with better convergence accleration is to augment $P(A)$ and move towards $P(U)$. Suppose $P' = P(A) \cup \{(2,3)\}$ in Example 5. Then $P' \in C_+(P(U))$ and IC will also exist for this pattern. However, if we let $Q = P(A) \cup \{(3,4)\}$ then $Q \notin C_+(P(U))$ because $(3,4)$ is in Q, both $(2,3)$ and $(2,4)$ are in $P(U)$, but only one of $(2,4)$ and $(2,3)$ is in Q. In this case the IC factorization may or may not exist, but in Section 4 we will show there exists some matrix B whose full Cholesky factor has the same sparsity pattern as that of A, and for which IC with the augmented pattern Q will fail to exist.

These examples indicate how property C_+ can be satisfied and violated in some common circumstances. The next Section shows that property C_+ is sufficient for completion of IC factorization.

3. Sufficiency of Property C_+. The first theorem shows that property C_+ guarantees the existence of the IC factorization.

THEOREM 1. *Let matrix* $A \in \Re^{n\times n}$ *be symmetric positive definite and have Cholesky factor* U. *Suppose that position set* $P \in C_+(P(U))$. *The incomplete Cholesky factorization of* A *using position set* P *completes successfully.*

Proof: Since any $(i,j) \notin P(U)$ will not affect the computation of the incomplete Cholesky factorization, we assume that $P \subseteq P(U)$ in the proof without loss of generality.

Let $C_i = \{j|(j,i) \in P\}$ be the set of row indices of elements of P in column i for each $1 \le i \le n$. Construct a set S_i in the following way: Initialize $S_i = C_i$, and then repeat the augmentation of $S_i \leftarrow S_i \bigcup_{j\in S_i} C_j$ until S_i does not grow (which occurs in $n-1$ or fewer steps). This construction assures that for any $j \in S_i$, $C_j \subset S_i$. The principal submatrix of A defined by S_i consists of the components of A with row and column indices both in S_i.

We prove the theorem by showing that if $P \in C_+(P(U))$, then the computation of the incomplete Cholesky factorization of A on each principal submatrix defined by S_i, $1 \le i \le n$ is equivalent to the computation of complete Cholesky factorization on the submatrix. Therefore the diagonal elements of the matrix at each step of the incomplete Cholesky factor will always be positive. This implies that the IC factorization will not break down due to nonpositive pivots.

We first show that for any i and any $\{j,k\} \subseteq S_i$, if $(j,k) \in P(U)$ then $(j,k) \in P$. Assume that $(j,k) \notin P$. Then there is $(j,l) \in P$ with $l \in S_i$, or otherwise j would not be in S_i. Now consider the position $(\min\{l,k\}, \max\{l,k\})$. Since both (j,l) and (j,k) are in $P(U)$, it follows that $(\min\{l,k\}, \max\{l,k\})$, the position that will be affected (updated or filled) by the element (j,k) and (j,l), must be in $P(U)$. If $(\min\{l,k\}, \max\{l,k\})$ in P, this contradicts $P \in C_+(P(U))$ because (j,l) is in P but (j,k) is not in P. If $(\min\{l,k\}, \max\{l,k\}) \notin P$ then we have a position $(\min\{l,k\}, \max\{l,k\})$ which has the same status as (j,k): $\{l,k\} \subseteq S_i$, $(\min\{l,k\}, \max\{l,k\}) \in P(U)$, but $(\min\{l,k\}, \max\{l,k\}) \notin P$. Note that $\min\{l,k\} > j$ and $\max\{l,k\} \ge k$. By replacing (j,k) with $(\min\{l,k\}, \max\{l,k\})$ and applying this argument recursively, eventually we reach a row number $m \in S_i$ that has only one off-diagonal index in S_i. This last element must be in P, or m would not be in S_i, proving the assertion by contradiction and $(j,k) \in P$ follows.

On the other hand, any position (j,k) with $\{j,k\} \not\subseteq S_i$ will not affect the values of the elements on the submatrix defined by S_i in the incomplete factorization. To see this, let's examine how a element in such a principal submatrix changes its value during the IC factorization. Let $\{s,t\} \subseteq S_i$. Now a_{st} will be updated by

$$a_{st} = a_{st} - a_{ks}a_{kt}/a_{kk}$$

only when there exists a k such that both (k,s) and (k,t) are in P. If $k \notin S_i$ then it can be shown that either $(k,s) \notin P(U)$ or $(k,s) \notin P$: consider $(k,s) \in P(U)$, otherwise it does not affect the computation. If $(k,s) \in P$ then k will be in S_i by construction of S_i, contradicting the assumption that $k \notin S_i$. Hence $(k,s) \notin P$. Therefore, (k,s) is either not in P or not in $P(U)$. The same argument can also be applied to (k,t). Therefore, the value of elements in the principal submatrix defined by S_i are not affected by elements outside this submatrix.

Therefore, for any $1 \le i \le n$, the computation of the diagonal element a_{ii} of the incomplete Cholesky factorization of A is equivalent to computing the last diagonal element of a complete Cholesky factorization of the principal submatrix defined by S_i. Because any principal submatrix of a symmetric positive definite matrix is symmetric positive definite, Cholesky factorization of the principal submatrix of A defined by S_i can be completed, and hence all the diagonal elements will remain positive in the incomplete Cholesky factorization of A with pattern P. $\square$

This establishes a sufficient condition on the target factor for the existence of an incomplete Cholesky factorization. In order to illustrate Theorem 1 and its proof, consider a particular matrix that has the sparsity patterns given in Example 5, for which $P(A) \in C_+(P(U))$. The steps of the incomplete Cholesky factorization algorithm with sparsity pattern $P = P(A)$ shown earlier, with A^i defined as the updated matrix A after step i of IC factorization, are:

$$A^0 = A \quad = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 5 & & 4 & \\ & & 8 & & \\ & & & 9 & 1 \\ & & & & 10 \end{bmatrix}, \quad A^1 = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 4 & & 2 & \\ & & 4 & & \\ & & & 5 & 1 \\ & & & & 10 \end{bmatrix},$$

$$A^2 \quad = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 4 & & 2 & \\ & & 4 & & \\ & & & 4 & 1 \\ & & & & 10 \end{bmatrix}, \quad A^3 = A^2, \quad A^4 = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 4 & & 2 & \\ & & 4 & & \\ & & & 4 & 1 \\ & & & & 39/4 \end{bmatrix}$$

The IC factor R can then be obtained by setting $r_{ii} = \sqrt{a_{ii}}$, and $r_{ij} = a_{ij}/r_{ii}$ if $(i,j) \in P$, giving

$$R = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 2 & & 1 & \\ & & 2 & & \\ & & & 2 & 1/2 \\ & & & & \sqrt{39}/2 \end{bmatrix}.$$

From the definition of S_i given in the proof of the theorem, $S_1 = \{1\}$, $S_2 = \{1,2\}$, $S_3 = \{1,3\}$, $S_4 = \{1,2,4\}$, $S_5 = \{1,2,4,5\}$, Let B_i be the principal submatrix of A defined by S_i. If we consider the computation of IC of A above and extract the principal submatrix defined by S_i after each step, we see exactly the computation of complete Cholesky factorization on the submatrix. For example, complete Cholesky factorization for $i = 3$ gives,

$$B_3^0 = B_3 = \begin{pmatrix} 1 & -2 \\ & 8 \end{pmatrix}, \quad B_3^1 = \begin{pmatrix} 1 & -2 \\ & 4 \end{pmatrix},$$

and for $i = 5$,

$$\begin{aligned} B_5^0 &= B_5 = \begin{pmatrix} 1 & 1 & 2 & \\ & 5 & 4 & \\ & & 9 & 1 \\ & & & 10 \end{pmatrix} \quad B_5^1 = \begin{pmatrix} 1 & 1 & 2 & \\ & 4 & 2 & \\ & & 5 & 1 \\ & & & 10 \end{pmatrix} \\ B_5^2 &= \begin{pmatrix} 1 & 1 & 2 & \\ & 4 & 2 & \\ & & 4 & 1 \\ & & & 10 \end{pmatrix} \quad B_5^3 = \begin{pmatrix} 1 & 1 & 2 & \\ & 4 & 2 & \\ & & 4 & 1 \\ & & & 39/4 \end{pmatrix} \end{aligned}$$

The proof of Theorem 1 relied on noting that these computations are exactly the same as those of IC of A on the principal submatrix defined by S_3 and S_5, respectively.

On the other hand, from Example 5, $P = P(A) \cup \{(3,4)\} \notin C_+(P(U))$. Using this target sparsity pattern causes IC to break down because of a zero pivot in step 3:

$$\begin{aligned} A^0 = A &= \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 5 & & 4 & \\ & & 8 & & \\ & & & 9 & 1 \\ & & & & 10 \end{bmatrix}, \quad A^1 = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 4 & & 2 & \\ & & 4 & 4 & \\ & & & 5 & 1 \\ & & & & 10 \end{bmatrix}, \\ A^2 &= \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 4 & & 2 & \\ & & 4 & 4 & \\ & & & 4 & 1 \\ & & & & 10 \end{bmatrix}, \quad A^3 = \begin{bmatrix} 1 & 1 & -2 & 2 & \\ & 4 & & 2 & \\ & & 4 & 4 & \\ & & & 0 & 1 \\ & & & & 10 \end{bmatrix}. \end{aligned}$$

4. Necessity of Property C_+. $P \in C_+(P(U))$ is not a *necessary* condition for IC completion on a particular symmetric positive definite matrix; examples are readily constructed to show this. However, property C_+ is a necessary condition in the sense that incomplete Cholesky factorization with a given target sparsity P will exist for *all* symmetric positive definite matrices A with the same pattern $P(U)$ only if $P \in C_+(P(U))$.

LEMMA 4.1. *A symmetric positive definite matrix $A \in \mathbb{R}^{n \times n}$ can be created with any given sparsity pattern P and any given symmetric positive definite principal submatrix S such that the sparsity pattern of S is consistent with P.*

For example, given the sparsity pattern

$$P = \begin{pmatrix} \times & \times & \times & & \\ & \times & & \times & \\ & & \times & & \\ & & & \times & \times \\ & & & & \times \end{pmatrix}$$

and given the positive definite principal submatrix $A(2:4,2:4) = \begin{pmatrix} 1 & & 1 \\ & 1 & \\ & & 2 \end{pmatrix}$, Lemma 4.1 says that the unspecified entries $\times$ in

$$
A = \begin{pmatrix} \times & \times & \times & & \\ & 1 & & 1 & \\ & & 1 & & \\ & & & 2 & \times \\ & & & & \times \end{pmatrix} \tag{1}
$$

can be defined so that A is positive definite.

Proof: The proof is by construction. Assume that $S \in \mathbb{R}^{k\times k}$. Let P' be the symmetrically permuted pattern of P so that the principal submatrix S of A becomes the leading submatrix. Generate A' as the symmetric positive definite matrix with sparsity pattern P' in the following way: Let the leading principle $k \times k$ submatrix of A' be S. The expansion starts from row and column $k+1$. At each step i, $k+1 \le i \le n$, compute the Cholesky factorization of the leading submatrix of size $i-1$ of A', and denote the lower triangular factor as L_{i-1}. Let v be a vector of length $i-1$ with sparsity pattern consistent with that of the off–diagonal part of column i of A'. Set the ith diagonal element to be $a_{ii} = v^T A_{i-1}^{-1} v + \delta = v^T L_{i-1}^{-T} L_{i-1}^{-1} v + \delta$, where $\delta > 0$ is arbitrary, and define the off–diagonal part of column i to equal v (of course, the off–diagonal part of row i must also be set to v^T to retain symmetry.) Continue this process until an $n \times n$ symmetric positive definite matrix is generated. Then apply the symmetric inverse permutation to A', completing the creation of matrix A. □

To illustrate the process in Lemma 1, we construct the unspecified entries in Equation (1). First, permute the first row and column of sparsity pattern P to the be the last so that the principal submatrix defined by indices $\{2,3,4\}$ in the matrix A will be the leading principal submatrix. The permuted pattern P' becomes

$$
P' = \begin{pmatrix} \times & & \times & & \times \\ & \times & & & \times \\ & & \times & \times & \\ & & & \times & \\ & & & & \times \end{pmatrix}
$$

Denote A'_i as the leading submatrix of A' of size i. The expansion starts with $i = 3$. $A'_3 = S = \begin{pmatrix} 1 & & 1 \\ & 1 & \\ & & 2 \end{pmatrix}$. Let $v = (0 \;\; 0 \;\; 1)^T$, and $\delta = 1$. Then $a'_{44} = v^T L_{i-1}^{-T} L_{i-1}^{-1} v + \delta = 2$, giving $A'_4 = \begin{pmatrix} 1 & & 1 & \\ & 1 & & \\ & & 2 & 1 \\ & & & 2 \end{pmatrix}$. Next, let $v = (1 \;\; 1 \;\; 0 \;\; 0)^T$ and $\delta = 1$, giving $a'_{55} = 5$ and so $A'_5 = \begin{pmatrix} 1 & & 1 & & 1 \\ & 1 & & & 1 \\ & & 2 & 1 & \\ & & & 2 & \\ & & & & 5 \end{pmatrix}$. Finally, apply the inverse permutation to get $A = \begin{pmatrix} 5 & 1 & 1 & & \\ & 1 & & 1 & \\ & & 1 & & \\ & & & 2 & 1 \\ & & & & 2 \end{pmatrix}$.

Lemma 4.2. *Let $A \in \mathbb{R}^{3\times 3}$ be symmetric positive definite. Let U be the upper triangular Cholesky factor of A. If $P \subset P(U)$ does not have property C_+ on $P(U)$, then there is a* *symmetric positive definite matrix $B \in \mathbb{R}^{3\times 3}$ such that the Cholesky factor of B has the same structure as U and incomplete Cholesky factorization of B using P fails because of a nonpositive pivot.*

Proof: The only possible pattern $P(U)$ with subsets $P \subseteq P(U)$ not in $C_+(P(U))$ is $P(U) = P_3$. Furthermore, if $(2,3) \notin P$ then $P \in C_+(P(U))$. So assume that $(2,3) \in P$. Then $P \notin C_+(P(U))$ implies

$$P = \{(1,1),(2,2),(3,3),(1,2),(2,3)\} \quad \text{or}$$

$$P = \{(1,1),(2,2),(3,3),(1,3),(2,3)\},$$

as in Example 1. Note that in both cases the incompleteness affects the pattern in the first row. The trailing principal submatrix of order 2 is dense in both. Therefore, the strategy of the proof is to make the trailing principal submatrix of order 2 positive definite after one step of complete Cholesky is performed and not positive definite after one step of incomplete Cholesky.

Case 1: $P = \{(1,1),(2,2),(3,3),(1,2),(2,3)\}$ and $P(U) = P_3$. Define B as follows: Let the leading 2×2 full matrix of B be any symmetric positive definite matrix and b_{23} be any non-zero number. Two elements in the third column are yet to be determined. If we apply two steps of IC with the pattern P the value of the third pivot can be determined and set to 0. This yields the value of $b_{33} = b_{11}b_{23}^2/(b_{11}b_{22} - b_{12}^2) > 0$. Satisfying this condition means that the trailing principal submatrix of order 2 is not positive definite after one step of IC. Note that b_{13} does not appear in the value for b_{33} due to P. Therefore, we must set b_{13} to guarantee that if complete Cholesky is performed it will succeed. This can be done by taking it to be a solution of the inequality $b_{13}(2b_{12}b_{23} - b_{22}b_{13}) > 0$. It follows that

$$\begin{cases} 0 < b_{13} < 2b_{12}b_{23}/b_{22} & \text{if} \quad b_{12}b_{23} > 0 \\ 2b_{12}b_{23}/b_{22} < b_{13} < 0 & \text{if} \quad b_{12}b_{23} < 0 \end{cases}$$

Applying complete Cholesky and incomplete Cholesky factorization on B shows that B is positive definite and IC breaks down with the third pivot nonpositive.

Case 2: $P = \{(1,1),(2,2),(3,3),(1,3),(2,3)\}$ and $P(U) = P_3$. Let the 2×2 trailing submatrix of B be any symmetric positive definite matrix. We can set the values in the first row of the matrix to achieve the same two conditions as in Case 1. Let b_{13} be any non-zero number. Determining the final pivot of IC and setting it to 0 yields $b_{11} = b_{22}b_{13}^2/(b_{22}b_{33} - b_{23}^2) > 0$. The completion of the Cholesky factorization can be guaranteed by setting the remaining element b_{12}. Let b_{12} be a solution of the inequalities:

$$\begin{cases} b_{12}^2 < b_{11}b_{22} \\ b_{33} - b_{13}^2/b_{11} - (b_{23} - \frac{b_{12}b_{13}}{b_{11}})^2/(b_{22} - \frac{b_{12}^2}{b_{11}}) > 0. \end{cases}$$

Solving the inequalities gives

$$\begin{cases} 0 < b_{12} < \min\{2b_{13}b_{23}/b_{33},\ \sqrt{b_{11}b_{22}}\} & \text{if} \quad b_{13}b_{23} > 0 \\ \max\{2b_{13}b_{23}/b_{33},\ -\sqrt{b_{11}b_{22}}\} < b_{12} < 0 & \text{if} \quad b_{13}b_{23} < 0. \end{cases}$$

Applying Cholesky and incomplete Cholesky factorization on B again shows that B is positive definite but IC breaks down when using pattern P. □

Examples of the two cases of Lemma 4.2 are easily generated. Let $\begin{pmatrix} 1 & 1 \\ & 2 \end{pmatrix}$ be the leading principal submatrix of a symmetric positive definite matrix A. Define B to have the same leading principle submatrix, $b_{23} = 1$, and $b_{33} = b_{11}b_{23}^2/(b_{11}b_{22} - b_{12}^2) = 1 \times 1^2/(1 \times 2 - 1^2) = 1$. Since $b_{12}b_{23} > 0$, b_{13} is required to satisfy the condition $0 < b_{13} < 2b_{12}b_{23}/b_{22} = 1$. Define $b_{13} = 1/2$, giving $B = \begin{pmatrix} 1 & 1 & 1/2 \\ & 2 & 1 \\ & & 1 \end{pmatrix}$. B is symmetric positive but IC with the pattern of Case 1 breaks down.

Similarly, let $\begin{pmatrix} 1 & 1 \\ & 2 \end{pmatrix}$ be the trailing submatrix of a symmetric positive definite A. Define B to have the same trailing submatrix, $b_{13} = 1$, and $b_{11} = b_{22}b_{13}^2/(b_{22}b_{33} - b_{23}^2) = 1 \times 1^2/(1 \times 2 - 1^2) = 1$. Since $b_{13}b_{23} > 0$, b_{12} needs to be a solution to the inequalities $0 < b_{12} < \min\{2b_{13}b_{23}/b_{33}, \sqrt{b_{11}b_{22}}\} = 1$. Let $b_{12} = 1/2$. We then have $B = \begin{pmatrix} 1 & 1/2 & 1 \\ & 1 & 1 \\ & & 2 \end{pmatrix}$. B is symmetric positive but IC with the pattern in Case 2 breaks down.

THEOREM 2. *Let $A \in \mathbb{R}^{n \times n}$ be symmetric positive definite, U be the upper triangular Cholesky factor of A, and $P(U)$ be the sparsity pattern of U. If $P \subseteq P_n$ does not have the property C_+ on $P(U)$, then there is a symmetric positive definite matrix $B \in \mathbb{R}^{n \times n}$ such that the complete Cholesky factor of B has the same non-zero structure as U, and incomplete Cholesky factorization of B using P will fail due to a nonpositive pivot.*

Proof: The theorem is proven by induction on the size of the problem, n. Note that all sparsity patterns for 2×2 matrices necessarily have property C_+ on $P(U)$. Lemma 4.2 shows that the theorem is true for problems of size less or equal to 3, establishing the induction basis. We assume that for all the problems of size less or equal to $n-1$ the theorem is true and show below that it is true for matrices of order n.

Let P^l be the "leading" subset of P defined by $P^l = \{(i,j)|(i,j) \in P, 1 \leq i < j < n\}$ and let P^t be the "trailing" subset of P defined by $P^t = \{(i,j)|(i,j) \in P, 1 < i < j \leq n\}$. Similarly, denote $P(U)^l = \{(i,j)|(i,j) \in P(U), i < j < n\}$, $P(U)^t = \{(i,j)|(i,j) \in P(U), 1 < i < j\}$. P is in at least one of the following three cases:

Case 1: P^l does not have property C_+ on $P(U)^l$.

Case 2: P^t does not have property C_+ on $P(U)^t$.

Case 3: P^l has property C_+ on $P(U)^l$ and P^t has property C_+ on $P(U)^t$ but P does not have property C_+ on $P(U)$.

In Case 1 the induction hypothesis implies that there is a symmetric positive definite matrix S of size $n-1$ whose complete Cholesky factor has the same sparsity as $P(U)^l$, and for which incomplete Cholesky factorization breaks down when applied to S using P^l. Let the matrix B be constructed so that its leading principal submatrix of order $n-1$ is equal to S and then use the result of Lemma 4.1 to construct its last row and column. Then incomplete Cholesky factorization on the constructed symmetric positive definite matrix B breaks down during the first $n-1$ steps of computation.

In Case 2, create a matrix B in the following way: Since P^t does not have property C_+ on $P(U)^t$, by the induction hypothesis there is a symmetric positive definite matrix S of order $n-1$ such that its complete Cholesky factor has the same structure of $P(U)^t$ and the incomplete Cholesky factorization of S using P^t break down. From Lemma 4.1 we can create a symmetric positive definite matrix $C \in \mathbb{R}^{n \times n}$ such that it has the same non-zero structure as A on the first row and column and its trailing principal submatrix is equal to S. Define the vector v of length n as:

$$v_i = \begin{cases} 0, & i = 1 \\ 0, & (1,i) \in P, \\ c_{1i}/\sqrt{c_{11}}, & (1,j) \notin P, \end{cases}$$

and let $B = C + vv^T$. B is symmetric and positive definite because C is symmetric positive definite and vv^T is nonnegative definite. Furthermore, the non-zero structure of the complete Cholesky factor of B is the same as $P(U)$. After applying one step of incomplete Cholesky factorization to B, the reduced matrix of order $n-1$ is equal to S. By the definition of C, incomplete Cholesky factorization will break down.

In Case 3, P^l and P^t have property C_+ on $P(U)^l$ and $P(U)^t$, respectively but, P violates property C_+ on $P(U)$. Therefore, there must be a $(i,n) \in P$ such that both $(1,i)$ and $(1,n)$ are in $P(U)$ but only one of them is in P. After applying one step of incomplete Cholesky factorization on B, consider incomplete Cholesky factorization of the reduced matrix of order $n-1$ with sparsity pattern P^t. Since P^t has property C_+ on $P(U)^t$, we cannot use Case 2 above to show that IC can fail for some set of values assigned to the non-zero positions. However, we now show that the non-zero values can be set so that the reduced matrix of order $n-1$ has a principal submatrix which is not positive definite. Define the symmetric positive definite matrix B as follows: let B's 3×3 principal submatrix given by indices $\{1,i,n\}$ be equal to the matrix shown in Lemma 4.2 corresponding to the one of the two possible sparsity patterns that applies. Use Lemma 4.1 to expand the matrix to have the same sparsity pattern as A. As shown in the proof of Theorem 1 the computation of the IC factorization of the reduced matrix on the elements corresponding to index set S^t_{n-1} of P^t is equivalent to the computation of the complete Cholesky factorization on the principal submatrix defined by the index set S^t_{n-1}. Because B was constructed using the techniques in the proof of Lemma 4.2, the principal submatrix defined by $\{i,n\} \subseteq S^t_{n-1}$ is not positive definite after one step of IC. Therefore, the complete Cholesky factorization of the principal submatrix defined by S^t_{n-1} breaks down and the incomplete Cholesky factorization on the reduced matrix must also fail.

Together, this shows that for a problem of order n, if P does not have property C_+ on $(P(U))$, then there is a symmetric positive definite matrix B such that its Cholesky factor has the same sparsity pattern as the Cholesky factor of A, but incomplete Cholesky factorization of B will fail. By induction the theorem is true. □

To illustrate the proof of Case 3 above, let

$$P(A) = \begin{pmatrix} \times & \times & \times & \times & \times \\ & \times & & \times & \times \\ & & \times & & \\ & & & \times & \times \\ & & & & \times \end{pmatrix},$$

so that $P(U) = P_5$. Let $P = P(A) - \{(1,5)\}$. Then $P^l \in C_+(P(U)^l)$ and $P^t \in C_+(P(U)^t)$, but $P \notin C_+(P(U))$. Now for $i = 4$, as indicated in the proof $(i,n) \in P$, both $(1,i)$ and $(1,n)$ are in $P(U)$, but only one of them is in P. Construct the matrix B as follows: let B's 3×3 principal submatrix given by indices $\{1,4,5\}$ be $\begin{pmatrix} 1 & 1 & 1/2 \\ & 2 & 1 \\ & & 1 \end{pmatrix}$, which is equal to the matrix shown in the example corresponding to Case 1 in Lemma 4.2. Using Lemma 4.1 we can expand the matrix B to have the same sparsity pattern as A, for example,

$$B = \begin{pmatrix} 1 & 1 & 1 & 1 & 1/2 \\ & 5 & & 2 & 2 \\ & & 7 & & \\ & & & 2 & 1 \\ & & & & 1 \end{pmatrix}.$$

Applying one step of incomplete Cholesky factorization using P on B gives

$$B^1 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1/2 \\ & 4 & & 1 & 2 \\ & & 6 & & \\ & & & 1 & 1 \\ & & & & 1 \end{pmatrix}.$$

Since $(1,5) \notin P$, no updates are performed on column 5 in computing B^1. Now consider incomplete Cholesky factorization of the reduced matrix of order $n-1$ with sparsity pattern P^t, and recall that P^t has property C_+ on $P(U)^t$. As shown in the proof of Theorem 1 performing incomplete Cholesky factorization on the reduced matrix with pattern P^t has the same effect on the elements corresponding to index set $S^t_{n-1} = \{2,4,5\}$ as the computation of complete Cholesky factorization on the principal submatrix $\begin{pmatrix} 4 & 1 & 2 \\ & 1 & 1 \\ & & 1 \end{pmatrix}$. However, the principal submatrix defined by $\{4,5\} \subseteq S^t_{n-1}$ is not positive definite. Therefore, the complete Cholesky factorization of the principal submatrix defined by S^t_{n-1} breaks down and the incomplete Cholesky factorization on the reduced matrix also fails on the next step:

$$B^2 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1/2 \\ & 4 & & 1 & 2 \\ & & 6 & & \\ & & & 3/4 & 1/2 \\ & & & & 0 \end{pmatrix}$$

5. Summary and Future Work. In this paper we define property C_+ for a target sparsity pattern for incomplete Cholesky factorization. Property C_+ is a sufficient condition on the sparsity pattern that ensures the existence of incomplete Cholesky factorization of a symmetric positive definite matrix. If property C_+ is not satisfied, then a symmetric positive definite matrix with the same non-zero structure of its Cholesky factor can be found so that when applying incomplete Cholesky factorization with the specified pattern, the factorization will break down due to a nonpositive pivot.

These results show that property C_+ is fundamental for incomplete Cholesky factorization. Every other sufficient condition on the sparsity pattern that we know of is a special case of property C_+, including the reordered chordal graph strategy in [Coleman, 1988] and the trivial cases of P containing only diagonal entries and $P = P(U)$. Theorem 2 implies that property C_+ is necessary and sufficient, if only the sparsity pattern of the matrix is considered.

The proof of these results show that property C_+ relates portions of the incomplete factorization of a matrix A to complete factorizations of particular principal submatrices. This work was originally motivated by research on the incomplete Gram-Schmidt factorization

(IGS) of a least squares problem, for which A is the coefficient matrix of the normal equations. The existence of that IGS factorization can be guaranteed [Wang et al., 1994a], and property C_+ is the condition under which IC applied to A is essentially equivalent to IGS and therefore also guaranteed to exist.

Algorithms for modifying a given sparsity pattern to assure that property C_+ holds have been proposed in [Wang, 1993]. However, the algorithms proceed simply by either always dropping positions that cause violations, or by always adding positions into P to prevent violations. A more effective strategy is likely to be based on a combination of those two approaches, allowing the amount of storage used by the preconditioner to be specified in advance.

This work is of great importance in applications where a sequence of problems are solved, each with the same sparsity pattern. This occurs in the solution of nonlinear partial differential equations, and in the iterative solution of the linear systems occurring in interior point methods for linear programming. This suggests one direction of future work: what conditions on a discretization will *a priori* assure that IC(s), incomplete Cholesky factorization with s levels of fill, will exist? Extensive research has also been carried out by other researchers to assure the existence of incomplete Cholesky factorization based on modifying the numerical values encountered, most often by augmenting pivot elements. Combining the two approaches, structural and numerical, is another promising research direction.

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