# Crout versions of ILU for general sparse matrices *

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**Abstract**

This paper presents an efficient implementation of incomplete LU (ILU) factorizations that are derived from the Crout version of Gaussian elimination (GE). At step $k$ of the elimination, the $k$-th row of $U$ and the $k$-th column of $L$ are computed using previously computed rows of $U$ and columns of $L$. The data structure and implementation borrow from already known techniques used in developing both sparse direct solution codes and incomplete Cholesky factorizations. It is shown that this version of ILU has many practical advantages. In particular, its data structure allows efficient implementation of more rigorous and effective dropping strategies. Numerical tests show that the method is far more efficient than standard threshold-based ILU factorizations computed row-wise or column-wise.

**Key words**: Incomplete LU factorization, ILU, Sparse Gaussian Elimination, Crout factorization, Preconditioning, ILU with threshold, ILUT, Iterative methods, Sparse linear systems.

**AMS subject classifications**: 65F10, 65N06.

## 1 Introduction

The rich variety of existing Gaussian elimination algorithms has often been exploited, for example, to extract the most efficient variant for a given computer architecture. It was noted in [11] that these variants can be unraveled from the orderings of the three main loops in Gaussian elimination. A short overview here serves the purpose of introducing notation. Gaussian elimination is often presented in the following form:

1. for $k = 1 : n-1$
2. for $i = k+1 : n$
3. for $j = k+1 : n$
4. $a_{ij} = a_{ij} - a_{ik} * a_{kj}$

where some calculations (e.g., pivots) have been omitted for simplicity. This form will be referred to as the $KIJ$ version, due to the ordering of the three loops. Swapping the first and second loops results in the $IKJ$ version:

1. for $i = 2 : n$
2. for $k = 1 : i-1$
3. for $j = k+1 : n$

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4. $a_{ij} = a_{ij} - a_{ik} * a_{kj}$

which is often referred to as the "delayed-update" version, and sometimes the Tinney-Walker algorithm (see, e.g., [6]). There is also a column variant, which is the $JKI$ version of GE.

Bordering methods can be viewed as modifications of the delayed-update methods. The loop starting in Line 3 of the above $IKJ$ version is shortened into "for $j = k + 1 : i - 1$" which computes the $k$-th row of $L$. A similar loop is then added to compute the $k$-th *column* of $U$. In theory, these different implementations of Gaussian elimination all yield the same (complete) factorization in exact arithmetic. However, their computational patterns rely on different matrix kernels and this gave rise to specialized techniques for different computer architectures. In the context of incomplete factorizations, these variants result in important practical differences.

Incomplete LU factorizations can be derived from any of these variants, see, e.g., [14, 2, 1] although the $IKJ$ version has often been preferred because it greatly simplifies the data structure required by the implementation. In fact, a key factor in selecting one of the options is the convenience of the data structure that is used. For example, the $KIJ$ algorithm requires rank-one updates and this causes up to $n - k$ rows and columns to be altered at step $k$. Since the matrices are stored in sparse mode, this is in not efficient for handling the fill-ins introduced during the factorization [6]. However, other methods were developed as well. For example, a technique based on bordering was advocated in [5].

This papers considers incomplete LU factorizations based on yet another version of Gaussian elimination known as the Crout variant, which which can seen as a combination of the $IKJ$ algorithm shown above to compute the $U$ part and a transposed version to compute the $L$ part. The $k$-th step will therefore compute the pieces $U(k, k : n)$ and $L(k : n, k)$ of the factorization. This version of Gaussian elimination was used in the Yale Sparse Matrix Package (YSMP) [7] to develop sparse Cholesky factorizations. More recently, the Crout version was also used to develop an efficient incomplete Cholesky factorization in [10]. The current paper extends this method to nonsymmetric matrices and explores effective dropping strategies that are enabled by the Crout variant.

## 2 The Crout LU and ILU

The main disadvantage of the standard delayed-update $IKJ$ factorization is that it requires access to the entries in the current row of $L$ by topological order [8]. One topological order, which is perhaps most appropriate for threshold-based incomplete factorizations, is increasing order by column number (since the nonzero pattern of the factorization is not known beforehand). The entries in this order must be found via searches, which are further complicated by the fact that the current row is dynamically being modified by the fill-in process. In SPARSKIT [12], a simple linear search is used, which is suitable in the case of small amounts of fill-in. When a high number of fill-ins are required, which is the case for more difficult problems, the cost of searching for the leftmost pivot may make the factorization ineffective. An alternative is to maintain the current row in a binary tree and to utilize binary searches. This strategy was mentioned in [14] and was recently implemented by Bollhoefer in ILUT and ILUTP [4]. This code will be used for comparisons later in this paper.

In this paper we will make the case that among the various Gaussian elimination algorithms, the Crout formulation provides perhaps the most practically useful option when developing incomplete LU factorizations. It was observed in [10] that the Crout-based incomplete factorization is effective in the symmetric positive definite case, as it bypasses the need for the costly searches mentioned above. As will be

seen, this can be easily generalized to the nonsymmetric case. Moreover, this version has one other compelling advantage, namely that it leads to an efficient implementation of inverse-based dropping strategies [3]. These strategies have been shown to be effective in [3] and this will be verified in the numerical experiments section of this paper.

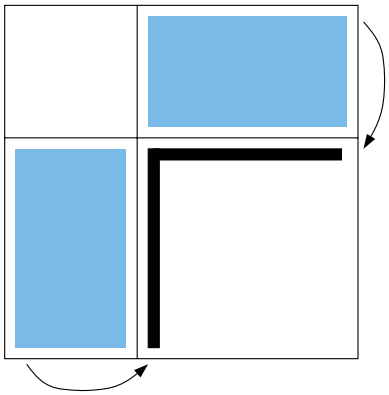

Figure 1: The computational pattern for the Crout factorization. The dark area shows the parts of the factors being computed at the $k$-th step. The shaded areas show the parts of the factors being accessed at the $k$-th step.

## 2.1 The Crout formulation

The Crout formulation can be viewed as yet another "delayed-update" form of GE. At step $k$ the entries $a_{k+1:n,k}$ (in the unit lower triangular factor, $L$) and $a_{k,k:n}$ (in the upper triangular factor, $U$) are computed and the rank-one update which characterizes the $KIJ$ version is postponed. At the $k$-th step, all the updates of the previous steps are applied to the entries $a_{k+1:n,k}$ and $a_{k,k:n}$. Thus it is natural to store $L$ by columns and $U$ by rows, and to have $A$ stored such that its lower triangular part is stored by columns and its upper triangular part is stored by rows. The computational pattern for the factorization is shown in Figure 1.

ALGORITHM **2.1** *Crout LU Factorization*

1. *For* $k = 1 : n$ *Do :*
2. *For* $i = 1 : k-1$ *and if* $a_{ki} \neq 0$ *Do :*
3. $a_{k,k:n} = a_{k,k:n} - a_{ki} * a_{i,k:n}$
4. *EndDo*
5. *For* $i = 1 : k-1$ *and if* $a_{ik} \neq 0$ *Do :*
6. $a_{k+1:n.k} = a_{k+1:n,k} - a_{ik} * a_{k+1:n,i}$
7. *EndDo*
8. $a_{ik} = a_{ik}/a_{kk}$ *for* $i = k+1, ..., n$
9. *EndDo*

The $k$-th step of the algorithm generates the $k$-th row of $U$ and the $k$-th column of $L$. This step is schematically represented in Figure 2. Notice now that the updates to the $k$-th row of $U$ (resp. the $k$-th column of $L$) can be made in any order. There is also a certain symmetry in the data structure representing $L$ and $U$ since the $U$ matrix is accessed by rows and the $L$ matrix by columns. By adapting Algorithm 2.1 for

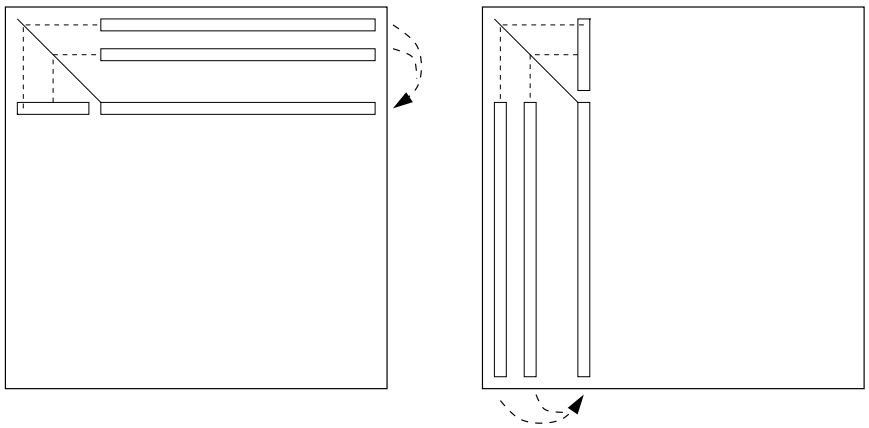

Figure 2: Construction of the $k$-th row of $U$ (left side) and the $k$-column of $L$ (right side).

sparse computations and by adding a dropping strategy, the following Crout version of ILU (termed ILUC) is obtained.

ALGORITHM **2.2** *ILUC - Crout version of ILUC*

1. *For* $k = 1 : n$ *Do :*
2. *Initialize row* $z$*:* $z_{1:k-1} = 0, \quad z_{k:n} = a_{k,k:n}$
3. *For* $\{i \mid 1 \leq i \leq k-1$ *and* $l_{ki} \neq 0\}$ *Do :*
4. $z_{k:n} = z_{k:n} - l_{ki} * u_{i,k:n}$
5. *EndDo*
6. *Initialize column* $w$*:* $w_{1:k} = 0, \quad w_{k+1:n} = a_{k+1:n,k}$
7. *For* $\{i \mid 1 \leq i \leq k-1$ *and* $u_{ik} \neq 0\}$ *Do :*
8. $w_{k+1:n} = w_{k+1:n} - u_{ik} * l_{k+1:n,i}$
9. *EndDo*
10. *Apply a dropping rule to row* $z$
11. *Apply a dropping rule to column* $w$
12. $u_{k,:} = z$
13. $l_{:,k} = w/u_{kk}, \quad l_{kk} = 1$
14. *Enddo*

The operations in Lines 4 and 8 are sparse vector updates and must be done in sparse mode.

## 2.2 Implementation

There are two potential sources of difficulty in the sparse implementation of the algorithm just described.

1. Consider Lines 4 and 8. Only the section $(k : n)$ of the $i$-th row of $U$ is required, and similarly, only the section $(k + 1 : n)$ of the $i$-th column of $L$ is needed. Accessing entire rows of $U$ or columns of $L$ and then extracting only the desired part is an expensive option.

2. Consider Lines 3 and 7. The nonzeros in row $k$ of $L$ must be accessed easily, but $L$ is stored by columns. Similarly, the nonzeros in column $k$ of $U$ must be accessed easily, but $U$ is stored by rows.

A solution to these difficulties was presented for the symmetric case in [7] and later in [10]. Here we extend this technique to nonsymmetric problems. The extension is straightforward, except that we can no longer use the optimizations available when $L$ and $U$ have the same nonzero pattern.

To address the first difficulty, consider the factor $U$ and assume its nonzeros in each row are stored in order by column number. Then, a pointer for row $j$, with $j < k$, can be used to signal the starting point of row $j$ needed to update the current row $k$. The pointers for each row are stored in a pointer array called $Ufirst$. This pointer array is updated after each elimination step by incrementing each pointer to point to the next nonzero in the row, if necessary. A pointer for row $k$ is also added after the $k$-th step. There is a similar pointer array for the $L$ factor called $Lfirst$.

To address the second difficulty, consider again the factor $U$, and the need to traverse column $k$ of $U$, although $U$ is stored by rows. An implied linked list for the nonzeros in column $k$ of $U$ is used, called $Ulist$. $Ulist(k)$ contains the first nonzero in column $k$ of $U$, and $Ulist(Ulist(k))$ contains the next nonzero, etc. At the end of step $k$, $Ulist$ is updated so that it becomes the linked list for column $k+1$. Ulist is updated when Ufirst is updated: when $Ufirst(i)$ is incremented to point to a nonzero with column index $c$, then $i$ is added to the linked list for column $c$. For the $L$ factor, there is a linked list called Llist.

In summary, we use four length $n$ arrays: $Ufirst$, $Ulist$, $Lfirst$, and $Llist$, which we call a *bi-index* structure. Figure 3 illustrates the relationship between the arrays in the bi-index structure.

a. $Ufirst(i)$ points to the first entry with column index greater than or equal to $k$ in row $i$ of $U$, where $i = 1, ..., k-1$;

b. $Ulist(k)$ points to a linked list of rows that will update row $k$;

c. $Lfirst(i)$ points to the first entry with row index greater than or equal to $k$ in column $i$ of $L$, where $i = 1, ..., k-1$;

d. $Llist(k)$ points to a linked list of columns that will update column $k$.

In [10] the entire diagonal of the $LDL^T$ factorization is updated at the end of each elimination step. In contrast, Eisenstat et. al [7] only update the $k$-th entry of $D$ at the $k$-th step. In the symmetric case, there is no additional cost incurred in updating all $D$. In the nonsymmetric case, this update, which can be written as

$$u_{i,i} := u_{i,i} - l_{i,k}u_{k,i}, \quad i = k+1, \ldots, n. \tag{1}$$

may increase the computational cost slightly because $l_{:,k}$ and $u_{k,:}$ do not in general have the same pattern. However, the option of having the entire updated diagonal at each step may be attractive when developing other possible variants of the algorithm and will be considered in our future work.

# 3 Dropping Strategies

Any dropping rule can be applied in Lines 10 and 11 of Algorithm 2.2. In this section, we consider a number of different options which were implemented and tested. The most straightforward of these options is a threshold-based technique that is similar to the one used in ILUT. A very important consideration with ILUC is that its data structure allows options that were not practically feasible with standard $IKJ$ implementations of ILU or their column-based equivalent. In particular, note that at step $k$ the first $k$ columns (resp. rows) of $L$ (resp. U) are available. In particular, this enables us to obtain dropping techniques that utilize estimates of the inverse factors which were shown to be quite successful in [3]. These two techniques are considered in turn. Several other strategies were also tested but lead to mixed results.

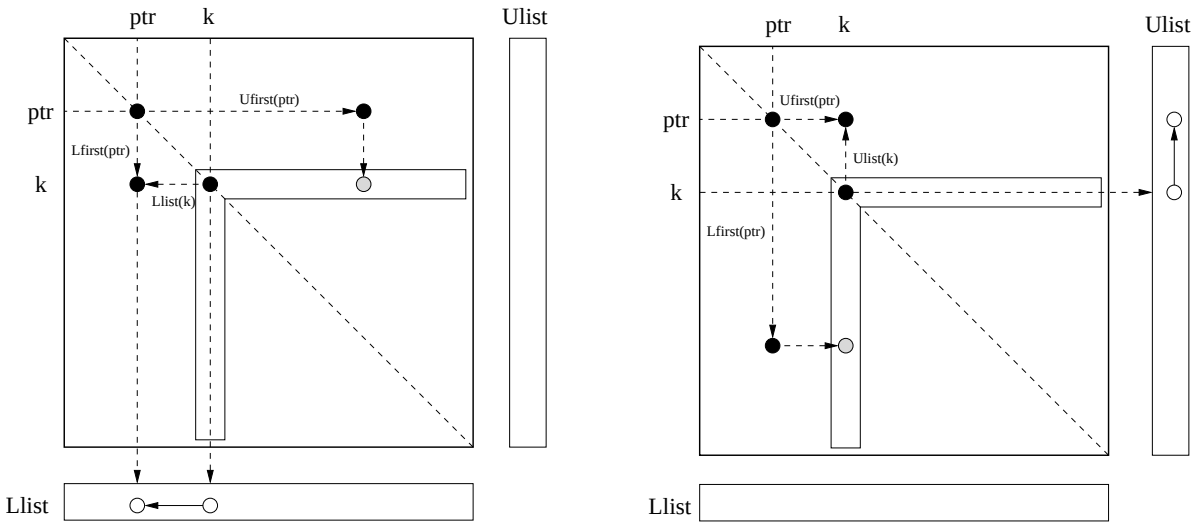


Figure 3: Procedure for updating row $k$ of $U$ and column $k$ of $L$.

### 3.1 Standard dual criterion dropping strategy

The dual dropping strategy, similar to the one in ILUT [13, 14], consists of the following two steps.

1. Any element of $L$ or $U$ whose magnitude is less than a tolerance $\tau$ (relative to the norm of the $k$-th column of $L$ or the $k$-th row of $U$ respectively) is dropped.

2. Then, only the "Lfil" largest elements in magnitude in the $k$-th column of $L$ are kept. Similarly the "Lfil" largest elements in the $k$-th row of $U$ in addition to the diagonal element are kept. This controls the total storage that can be used by the preconditioner.

The above strategy is referred to as the "standard strategy" in the experiments. It is often observed that it is more effective to use a drop tolerance only, rather than to force a limited fill-in. This means that better results are often achieved by taking a large value of "Lfil" and varying the parameter $\tau$ to achieve a given amount of fill-in.

### 3.2 Dropping based on condition number estimators

In order to reduce the impact of dropping an element on the subsequent steps of Gaussian elimination, it is useful to devise dropping strategies which estimate the norms of the rows of $L^{-1}$ and the columns of $U^{-1}$. Such techniques were proved to be quite effective in the ILU context by Bollhoefer [3]. The guiding criterion is to drop an entry $l_{jk}$ at step $k$ when it satisfies

$$|l_{jk}| \ \|e_k^{\mathrm{T}} L^{-1}\| \leq \epsilon$$

where $e_k$ denotes the $k$-th unit vector, and $\epsilon$ is the ILU drop tolerance. A similar criterion is used for the $U$ part: drop $u_{kj}$ when $|u_{kj}|\|U^{-1}e_k\| \leq \epsilon$. In the sequel we only discuss the strategy for the $L$ part. The justification for this criterion given in [3] was based on exploiting the connection with the approximate inverse. Here we use a similar, although somewhat simpler, argument.

It is well-known that for ILU preconditioners, the error made in the inverses of the factors is more important to control than the errors in the factors themselves, because when $A = LU$, and

$$\tilde{L}^{-1} = L^{-1} + X \qquad \tilde{U}^{-1} = U^{-1} + Y,$$

then the preconditioned matrix is given by

$$\tilde{L}^{-1} A \tilde{U}^{-1} = (L^{-1} + X)A(U^{-1} + Y) = I + AY + XA + XY.$$

This means that if the errors $X$ and $Y$ in the inverses of $L$ and $U$ are small, then the preconditioned matrix will be guaranteed to be close to the identity matrix. In contrast, small errors in the factors themselves may yield arbitrarily large errors in the preconditioned matrix.

Let $L_k$ denote the matrix composed of the first $k$ rows of $L$ and the last $n-k$ rows of the identity matrix. Consider a term $l_{jk}$ with $j > k$ that is dropped at step $k$. Then, the resulting perturbed matrix $\tilde{L}_k$ differs from $L_k$ by $l_{jk} e_j e_k^T$. Noticing that $L_k e_j = e_j$ we have

$$\tilde{L}_k = L_k - l_{jk} e_j e_k^T = L_k (I - l_{jk} e_j e_k^T)$$

from which we can obtain the following relation between the inverses:

$$\tilde{L}_k^{-1} = (I - l_{jk} e_j e_k^T)^{-1} L_k^{-1} = L_k^{-1} + l_{jk} e_j e_k^T L_k^{-1}.$$

Therefore, the inverse of $L_k$ will be perturbed by $l_{jk}$ times the $k$-th row of $L_k^{-1}$. This perturbation will affect the $j$-th row of $L_k^{-1}$. Hence, using the infinity norm for example, it is important to limit the norm of this perturbing row which is $\|l_{jk} e_j e_k^T L_k^{-1}\|_\infty = |l_{jk}| \; \|e_k^T L_k^{-1}\|_\infty$.

However, the matrix $L^{-1}$ is not available and it is not feasible to compute it. Instead, in [3] standard techniques used for estimating condition numbers [9] are adapted for estimating the norm of the $k$-th row of $L^{-1}$ (resp. $k$-th column of $U^{-1}$). In this paper we only use the simplest of these techniques. The idea is to construct a vector $b$ with entries $+1$ or $-1$, by following a greedy strategy to try to make $L^{-1}b$ large at each step. Since the first $k$ columns of $L$ are available, this is easy to achieve. The problem to estimate $\|e_k^T L^{-1}\|_\infty$ can be reduced to that of dynamically constructing a right-hand side $b$ to the linear system $Lx = b$ so that the $k$-th component of the solution is the largest possible. Thus, if $b$ is the current right-hand side at step $k$, we write,

$$\|e_k^{\mathrm{T}} L^{-1}\|_\infty \approx \frac{\|e_k^{\mathrm{T}} L^{-1} b\|_\infty}{\|b\|_\infty},$$

where $\|e_k^{\mathrm{T}} L^{-1}\|$ was estimated as the $k$-th component of the solution $x$ of the system $Lx = b$. The implementation given next uses the simplest criterion which amounts to selecting $b_k = \pm 1$ at each step $k$, in such a way as to maximize the norm of the $k$-th component of $L^{-1}b$. The notation for the algorithm is as follows. At the $k$ step we have available the first $k-1$ columns of $L$. The $k$-th component of the solution $x$ is

$$\xi_k = b_k - e_k^T L_{k-1} x_{k-1}$$

This makes the choice clear: if $\xi_k$ is to be large in modulus, then its sign should be of the opposite sign as as $e_k^T L_{k-1} x_{k-1}$. Once $b_k$ is selected, $x_k$ is then known and all the $e_j^T L_k x_k$ are updated. These scalars are called $\nu_j$ below. Details may be found in [9].

ALGORITHM **3.1** *Estimating the norms* $\|e_k^T L^{-1}\|_\infty$

1. *Set* $\xi_1 = 1$, $\nu_i = 0, i = 1, \ldots, n$
2. *For* $k = 2, \ldots, n$ *do*
3. $\quad \xi_+ = 1 - \nu_k$ ; $\xi_- = -1 - \nu_k$ ;
4. $\quad$ *if* $|\xi_+| > |\xi_-|$ *then* $\xi_k = \xi_+$ *else* $\xi_k = \xi_-$
5. $\quad$ *For* $j = k+1 : n$ *and for* $l_{jk} \neq 0$ *Do*
6. $\quad\quad \nu_j = \nu_j + \xi_k l_{jk}$
7. $\quad$ *EndDo*
8. *EndDo*

The paper [3] also presents an improved variant of this algorithm which is also derived from a dense version described in [9]. In this variant, the $\xi_k$'s are selected to encourage growth not only in the solution $x_k$ but also in the $\nu_i$'s. Calling $p_j$ the vector with components $\nu_i$ at step $j$, this is achieved by using as a criterion for selecting $\xi_k$, the weight

$$|\xi_k| + \|p_k\|_1 \tag{2}$$

which depends on the choice made for $\xi_k$. Note that $\|p_k\|_1 = \|p_{k-1} + \xi_k l_{:,k}\|_1$ so, we need to compute the weight (2) for both of the choices in Line 3 and select the choice that gives the largest weight.

# 4 Diagonal compensation strategies

It is sometimes helpful to modify the diagonal entries in the ILU factorization to compensate for the elements being dropped during factorization. In the simplest row-oriented ILU techniques, the sum of all elements being dropped in computing a given row of the $L, U$ pair, is added to the diagonal entry. This makes the product $LU$ and $A$ have the same row-sum, and as a result the preconditioned matrix will have one eigenvalue equal to one with associated eigenvector the vector of all ones.

In the context of ILUC, we can also enforce a similar condition. In fact it is possible, as well as natural, to enforce both a row-sum and a column-sum condition. Consider the equation which defines the $k$-th column of $L$ for the equivalent $A = LDU$ factorization,

$$\tilde{l}_{k+1:n,k} = a_{k+1:n,k} - \sum_{j=1}^{k-1} u_{j,k} d_{j,j} l_{k+1:n,j}. \tag{3}$$

After this column is calculated it undergoes dropping and then scaling,

$$\hat{l}_{k+1:n,k} := \tilde{l}_{k+1:n,k} + s_{k+1:n,k}, \qquad l_{k+1:n,k} := \hat{l}_{k+1:n,k}/d_k.$$

As a result we have

$$a_{k+1:n,k} = \sum_{j=1}^{k} u_{j,k} d_{j,j} l_{k+1:n,j} + s_{k+1:n,k}.$$

Therefore, it may be possible to enforce a column-sum condition on the strict lower part of $A$, and in a similar fashion, a row-sum condition on the strict upper part of $A$. We can do better with a little additional work. The above relation can be extended to the entire column

$$a_{:,k} = \sum_{j=1}^{k} u_{j,k} d_{j,j} l_{:,j} + s_{:,k}.$$

While $s_{k+1:n}$ is available at step $k$, the elements $s_{1:k}$ represent terms dropped from the $U$-part in earlier steps. It is possible to keep a running sum of these elements for each column as the algorithm proceeds. If $e$ is a vector of all ones, then

$$e^T a_{:,k} = e^T \sum_{j=1}^{k} u_{j,k} d_{j,j} l_{:,j} + e^T s_{1:k,k} + e^T s_{k+1:n,k}.$$

The term $e^T s_{k+1:n,k}$ is the sum of elements dropped while computing $l_{:,k}$ and is therefore easily available. The second term, $e^T s_{1:k,k}$, is the sum of elements dropped in previous steps in the $U$ part of the matrix. Note that $e^T s_{1:k,k} = e^T s_{1:k-1,k}$, since no elements are dropped from the diagonal. This second sum is available provided we maintain and update a row-vector which runs all the column-sums of the terms dropped for each column. Thus, once the row $U_{k,:}$ is determined, this row, call it $r_{sum}$ will be updated by adding to it all elements dropped while building $U_{k,:}$. Similarly, a column, say $t_{sum}$, is maintained which adds up all the terms dropped when computing the successive columns of $L$.

# 5 Experimental results

The performance of ILUC was compared to standard ILUT [13] in both row-wise (r-ILUT) and column-wise (c-ILUT) forms. The codes were written in C, and the experiments were conducted on a 866 MHz Pentium III computer with 1 GB of main memory. The codes were compiled with -O3 for optimization.

The test matrices can be described using a measure of structural symmetry called the relative symmetry match (RSM) [12]. This measures the total number of matches between $a_{ij} \neq 0$ and $a_{ji} \neq 0$ divided by the total number of nonzero elements (RSM = 1 for matrices with symmetric patterns). All 10 test matrices are nonsymmetric and of those, five have a nonsymmetric pattern. Some generic information about the test matrices is shown in Table 1. The BARTHT1A matrix was supplied by T. Barth of NASA Ames. The SHERMAN2 matrix is from the Boeing-Harwell collection and is available from the Matrix Market.[1] The matrices CAVA0000 and CAVA0100[2] resulted from the simulation of a driven cavity problem. The domain of interest is 2-dimensional and the discretization uses quadrilateral elements with bi-quadratic functions for velocities and linear (discontinuous) functions for pressures. Using 40 elements in each direction yields a matrix of size $n = 17,922$ and $nnz = 567,467$ nonzero elements. These linear systems are indefinite and can be difficult to solve. The Reynolds number was used as a continuation parameter; the test matrices have Reynolds numbers 0 and 100. The other matrices are available from the University of Florida sparse matrix collection.[3] In the table, $n$ is the dimension of the matrix and $nnz$ represents the total number of nonzero elements.

Artificial right-hand sides were generated, and GMRES(60) was used to solve the systems using a random initial guess. The iterations were stopped when the residual norm was reduced by 8 orders of magnitude or when the maximum iteration count of 300 was reached.

Table 2 compares the timings to build the preconditioners ("Pr-sec.") and the iteration timings ("Its sec.") for ILUC, r-ILUT and c-ILUT on the matrices from the set that have symmetric patterns. "Lfil" is the dropping parameter described in Section 3.1. We selected "Lfil" by basing it on the ratio $\gamma = \frac{nnz}{2n}$, which is an average number of nonzeros in each row or column of the upper or lower triangular part of the matrix. "Its" denotes the number of iterations to convergence. The symbol "-" in the table indicates

[1] `http://math.nist.gov/MatrixMarket/`
[2] Matrices available from the authors.
[3] `http://www.cise.ufl.edu/ davis/sparse/`

| Matrix | RSM | $n$ | $nnz$ |
|---|---|---|---|
| BARTHT1A | 1.0000 | 14075 | 481125 |
| RAEFSKY1 | 1.0000 | 3242 | 294276 |
| RAEFSKY2 | 1.0000 | 3242 | 294276 |
| RAEFSKY3 | 1.0000 | 21200 | 1488768 |
| VENKAT25 | 1.0000 | 62424 | 1717792 |
| UTM.3060 | 0.5591 | 3060 | 42211 |
| UTM.5940 | 0.5624 | 5940 | 83842 |
| SHERMAN2 | 0.6862 | 1080 | 23094 |
| CAVA0000 | 0.9773 | 17922 | 567467 |
| CAVA0100 | 0.9773 | 17922 | 567467 |

Table 1: Information on the 10 matrices used for tests

that convergence was not obtained in 300 iterations. "Pr-Mem." denotes the number of memory locations required by the preconditioners and "Ratio" denotes the fill-factor, i.e., the value of $nnz(L+U)/nnz(A)$.

There are two main observations that can be made in Table 2. First, the setup timings for ILUC are significantly smaller than those for r-ILUT and c-ILUT. The difference can be seen to be larger when a larger amount of fill-in is allowed. Second, ILUC may be more robust than r-ILUT and c-ILUT or may require fewer iterations to converge (see BARTHT1A and VENKAT25). For most other problems however, the iterations counts for ILUC and the other variants are similar. In general, the overall solution time is reduced by using ILUC.

Figure 4 shows the timings required for computing three preconditioners as a function of "Lfil" for the matrix RAEFSKY3. The drop tolerance was $\tau = 0.001$. The figure also shows the timings for an $IKJ$ version of ILUT (i.e., r-ILUT) when searching for the leftmost pivot is accomplished using binary search trees. This version of ILUT, which is referred to as b-ILUT [4], was coded in FORTRAN. The figure shows that ILUC is faster than all the other variants, and that the ILUC setup time increases more slowly with increasing amounts of fill-in.

Table 3 shows results which are analogous to those of Table 2 for the 5 matrices in the test set that have nonsymmetric patterns. The superiority of ILUC is not as compelling as in Table 2 which involved only matrices with symmetric patterns. The time to compute the preconditioner is still generally smaller than with the other versions. Sometimes, ILUC did help GMRES achieve convergence as shown in the case of the matrix UTM.5940. In other cases, it caused GMRES to fail to converge or to converge slowly, while r-ILUT and/or c-ILUT yielded good convergence. This is illustrated by the results with SHERMAN2 and CAVA0100.

The next tests compare the two dropping strategies described in Section 3, namely the standard threshold-based technique (termed "standard") with the technique based on norm estimates of the inverse triangular factors (termed "inverse-based"). For these tests we added four symmetric-pattern test matrices to study the effect of nonsymmetry. These matrices arise from two-dimensional finite element convection-diffusion problems. They were obtained using linear triangular elements and have 205761 equations and 1436480 nonzeros. The four matrices correspond to different sizes of the convection term, leading to increasing degrees of nonsymmetry; see Table 4.

Table 5 shows the results for those matrices in the set which have a symmetric patterns and Table 6 shows the results for the matrices with nonsymmetric patterns. In order to obtain a better comparison of the effect of the dropping strategy, we set Lfil to infinity for these tests. This means that the total number

| Matrix | Lfil | Pr-alg. | Pr-sec. | Its sec. | Its | Pr-Mem. | Ratio |
|---|---|---|---|---|---|---|---|
| BARTHT1A $\gamma \approx 17.1$ | $2.0\gamma \approx 34$ | ILUC | 0.920 | - | - | 815037 | 1.694 |
| | | r-ILUT | 1.990 | - | - | 923060 | 1.919 |
| | | c-ILUT | 2.210 | - | - | 937685 | 1.949 |
| | $2.5\gamma \approx 42$ | ILUC | 1.160 | 7.550 | 78 | 986395 | 2.050 |
| | | r-ILUT | 2.340 | - | - | 1113073 | 2.313 |
| | | c-ILUT | 2.870 | - | - | 1147112 | 2.384 |
| | $3.0\gamma \approx 51$ | ILUC | 1.450 | 5.900 | 55 | 1166370 | 2.424 |
| | | r-ILUT | 2.870 | - | - | 1319407 | 2.742 |
| | | c-ILUT | 3.690 | - | - | 1378620 | 2.865 |
| RAEFSKY1 $\gamma \approx 45.4$ | $1.0\gamma \approx 45$ | ILUC | 0.460 | 0.700 | 22 | 289594 | 0.984 |
| | | r-ILUT | 1.520 | 0.570 | 18 | 288136 | 0.979 |
| | | c-ILUT | 1.620 | 0.530 | 18 | 288168 | 0.979 |
| | $1.5\gamma \approx 68$ | ILUC | 0.790 | 0.760 | 20 | 427595 | 1.453 |
| | | r-ILUT | 2.810 | 0.610 | 16 | 430724 | 1.464 |
| | | c-ILUT | 3.010 | 0.580 | 16 | 430937 | 1.464 |
| | $2.0\gamma \approx 90$ | ILUC | 1.250 | 0.790 | 18 | 557364 | 1.894 |
| | | r-ILUT | 4.980 | 0.680 | 15 | 562961 | 1.913 |
| | | c-ILUT | 5.150 | 0.620 | 15 | 563896 | 1.916 |
| RAEFSKY2 $\gamma \approx 45.4$ | $1.0\gamma \approx 45$ | ILUC | 0.460 | 0.860 | 27 | 291078 | 0.989 |
| | | r-ILUT | 1.950 | 0.730 | 23 | 288367 | 0.980 |
| | | c-ILUT | 1.910 | 0.750 | 25 | 288345 | 0.980 |
| | $1.5\gamma \approx 68$ | ILUC | 0.790 | 0.800 | 21 | 431255 | 1.465 |
| | | r-ILUT | 3.760 | 0.680 | 18 | 431369 | 1.466 |
| | | c-ILUT | 3.710 | 0.730 | 20 | 431394 | 1.466 |
| | $2.0\gamma \approx 90$ | ILUC | 1.240 | 0.800 | 18 | 560577 | 1.905 |
| | | r-ILUT | 5.910 | 0.730 | 16 | 565818 | 1.923 |
| | | c-ILUT | 5.910 | 0.670 | 16 | 566890 | 1.926 |
| RAEFSKY3 $\gamma \approx 35.1$ | $1.0\gamma \approx 35$ | ILUCT | 1.520 | 2.080 | 13 | 1197935 | 0.805 |
| | | r-ILUT | 5.320 | 2.950 | 17 | 1467232 | 0.986 |
| | | c-ILUT | 4.920 | 1.790 | 11 | 1467145 | 0.985 |
| | $1.5\gamma \approx 52$ | ILUC | 2.290 | 2.180 | 12 | 1647174 | 1.106 |
| | | r-ILUT | 8.460 | 2.720 | 14 | 1965430 | 1.320 |
| | | c-ILUT | 7.470 | 1.840 | 10 | 1966184 | 1.321 |
| | $2.0\gamma \approx 70$ | ILUC | 3.350 | 2.000 | 10 | 2076087 | 1.395 |
| | | r-ILUT | 12.450 | 2.650 | 12 | 2406591 | 1.616 |
| | | c-ILUT | 11.120 | 2.010 | 10 | 2406519 | 1.616 |
| VENKAT25 $\gamma \approx 13.8$ | $1.0\gamma \approx 13$ | ILUC | 1.580 | 59.530 | 160 | 1668586 | 0.971 |
| | | r-ILUT | 3.720 | 91.780 | 241 | 1680052 | 0.978 |
| | | c-ILUT | 9.760 | - | - | 1681197 | 0.979 |
| | $1.5\gamma \approx 20$ | ILUC | 2.680 | 29.610 | 73 | 2537005 | 1.477 |
| | | r-ILUT | 7.180 | 41.500 | 102 | 2545032 | 1.482 |
| | | c-ILUT | 17.160 | 50.220 | 126 | 2547584 | 1.483 |
| | $2.0\gamma \approx 27$ | ILUC | 4.210 | 20.480 | 48 | 3405086 | 1.982 |
| | | r-ILUT | 10.740 | 30.230 | 69 | 3399380 | 1.979 |
| | | c-ILUT | 23.260 | 27.240 | 63 | 3407450 | 1.984 |

Table 2: Performance of ILUC, r-ILUT and c-ILUT on symmetric pattern matrices, $\tau = 0.001$

| Matrix | Lfil | Pr-alg. | Pr-sec. | Its sec. | Its | Pr-Mem. | Ratio |
|---|---|---|---|---|---|---|---|
| UTM.3060 $\gamma \approx 6.9$ | $2.5\gamma \approx 17$ | ILUC | 0.080 | 1.860 | 156 | 91568 | 2.169 |
| | | r-ILUT | 0.150 | - | - | 94910 | 2.248 |
| | | c-ILUT | 0.130 | 0.840 | 75 | 91739 | 2.173 |
| | $3.0\gamma \approx 20$ | ILUC | 0.110 | 0.780 | 58 | 106731 | 2.529 |
| | | r-ILUT | 0.180 | - | - | 110196 | 2.611 |
| | | c-ILUT | 0.150 | 0.600 | 51 | 105762 | 2.506 |
| | $3.5\gamma \approx 24$ | ILUC | 0.130 | 0.800 | 56 | 126396 | 2.994 |
| | | r-ILUT | 0.210 | - | - | 130066 | 3.081 |
| | | c-ILUT | 0.180 | 0.580 | 47 | 124268 | 2.944 |
| UTM.5940 $\gamma \approx 7.1$ | $4.0\gamma \approx 28$ | ILUC | 0.320 | 5.470 | 180 | 289406 | 3.452 |
| | | r-ILUT | 0.600 | - | - | 294066 | 3.507 |
| | | c-ILUT | 0.550 | - | - | 283592 | 3.382 |
| | $4.5\gamma \approx 31$ | ILUC | 0.350 | 3.780 | 119 | 318232 | 3.796 |
| | | r-ILUT | 0.650 | - | - | 322226 | 3.843 |
| | | c-ILUT | 0.620 | - | - | 311632 | 3.717 |
| | $5.0\gamma \approx 35$ | ILUC | 0.410 | 3.950 | 118 | 356279 | 4.249 |
| | | r-ILUT | 0.730 | - | - | 360560 | 4.300 |
| | | c-ILUT | 0.690 | - | - | 346272 | 4.130 |
| SHERMAN2 $\gamma \approx 10.7$ | $1.0\gamma \approx 10$ | ILUC | 0.010 | - | - | 11727 | 0.508 |
| | | r-ILUT | 0.030 | - | - | 16855 | 0.730 |
| | | c-ILUT | 0.010 | 0.190 | 51 | 20345 | 0.881 |
| | $1.5\gamma \approx 16$ | ILUC | 0.010 | 1.130 | 294 | 13539 | 0.586 |
| | | r-ILUT | 0.020 | - | - | 23587 | 1.021 |
| | | c-ILUT | 0.010 | 0.040 | 13 | 26674 | 1.155 |
| | $2.0\gamma \approx 21$ | ILUC | 0.020 | 1.120 | 293 | 14045 | 0.608 |
| | | r-ILUT | 0.020 | 0.060 | 18 | 26466 | 1.146 |
| | | c-ILUT | 0.010 | 0.020 | 9 | 28100 | 1.217 |
| CAVA0000 $\gamma \approx 15.8$ | $2.0\gamma \approx 31$ | ILUC | 1.330 | 5.820 | 48 | 1103714 | 1.945 |
| | | r-ILUT | 3.050 | 5.150 | 45 | 1084765 | 1.912 |
| | | c-ILUT | 3.290 | 4.840 | 42 | 1116973 | 1.968 |
| | $2.5\gamma \approx 39$ | ILUC | 1.780 | 42.710 | 300 | 1382548 | 2.436 |
| | | r-ILUT | 3.830 | 5.620 | 43 | 1357450 | 2.392 |
| | | c-ILUT | 4.390 | 7.710 | 58 | 1398952 | 2.465 |
| | $3.0\gamma \approx 47$ | ILUC | 2.180 | 6.930 | 47 | 1660151 | 2.926 |
| | | r-ILUT | 4.570 | 4.880 | 36 | 1630057 | 2.873 |
| | | c-ILUT | 4.980 | 4.720 | 36 | 1675004 | 2.952 |
| CAVA0100 $\gamma \approx 15.8$ | $2.0\gamma \approx 31$ | ILUC | 1.310 | 6.540 | 53 | 1085455 | 1.913 |
| | | r-ILUT | 3.090 | 5.130 | 43 | 1094607 | 1.929 |
| | | c-ILUT | 3.250 | 5.170 | 45 | 1083709 | 1.910 |
| | $2.5\gamma \approx 39$ | ILUC | 1.710 | 43.460 | 300 | 1359356 | 2.395 |
| | | r-ILUT | 3.850 | 5.340 | 42 | 1367359 | 2.410 |
| | | c-ILUT | 4.130 | 5.360 | 43 | 1356124 | 2.390 |
| | $3.0\gamma \approx 47$ | ILUC | 2.160 | 28.830 | 179 | 1631668 | 2.875 |
| | | r-ILUT | 4.620 | 4.290 | 32 | 1638681 | 2.888 |
| | | c-ILUT | 5.020 | 4.690 | 35 | 1627911 | 2.869 |

Table 3: Performance of ILUC, r-ILUT and c-ILUT on nonsymmetric pattern matrices, $\tau = 0.001$

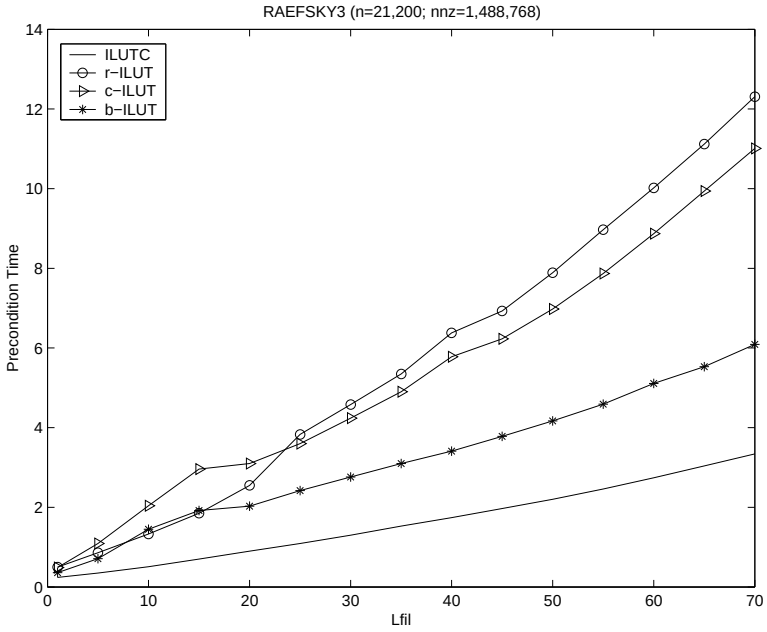


Figure 4: Precondition time vs. Lfil for ILUC, r-ILUT, c-ILUT and b-ILUT ($\tau = 0.001$)

| Matrix | $\eta$ |
|---|---|
| CONVDIFF0 | $3 \times 10^{-4}$ |
| CONVDIFF1 | $3 \times 10^{-3}$ |
| CONVDIFF2 | $3 \times 10^{-2}$ |
| CONVDIFF3 | $3 \times 10^{-1}$ |

Table 4: Four symmetric-pattern matrices from a convection-diffusion problem. The matrices have 205761 equations and 1436480 nonzeros. The value $\eta$ measures the degree of nonsymmetry, $\|A - A^T\|_F / \|A + A^T\|_F$.

| Matrix | Drop-strategy | Droptol | Pr-sec. | Its sec. | Its | Ratio |
|---|---|---|---|---|---|---|
| BARTHT1A | Inverse-based | 0.1 | 2.880 | 6.460 | 49 | 3.501 |
| | Standard | 0.01 | 2.820 | 8.480 | 60 | 3.382 |
| | Inverse-based | 0.01 | 28.560 | 5.100 | 19 | 9.660 |
| | Standard | 0.001 | 35.140 | 6.490 | 22 | 10.890 |
| RAEFSKY1 | Inverse-based | 0.01 | 0.500 | 0.560 | 18 | 0.924 |
| | Standard | 0.1 | 0.470 | 0.670 | 20 | 1.096 |
| | Inverse-based | 0.001 | 7.710 | 0.700 | 10 | 3.670 |
| | Standard | 0.01 | 6.190 | 0.820 | 12 | 3.522 |
| RAEFSKY2 | Inverse-based | 0.01 | 1.060 | 0.730 | 17 | 1.736 |
| | Standard | 0.1 | 0.630 | 0.700 | 19 | 1.325 |
| | Inverse-based | 0.001 | 13.270 | 0.810 | 9 | 5.074 |
| | Standard | 0.01 | 8.300 | 0.900 | 12 | 4.030 |
| RAEFSKY3 | Inverse-based | 0.1 | 7.070 | 13.510 | 57 | 1.391 |
| | Standard | 0.1 | - | - | - | 1.083 |
| | Inverse-based | 0.01 | 18.180 | 2.360 | 9 | 2.280 |
| | Standard | 0.01 | 14.800 | 2.190 | 8 | 2.402 |
| VENKAT25 | Inverse-based | 0.1 | 7.330 | 63.920 | 127 | 2.539 |
| | Standard | 0.1 | 2.900 | 37.000 | 91 | 1.522 |
| | Inverse-based | 0.01 | 68.450 | 24.710 | 25 | 9.300 |
| | Standard | 0.01 | 30.800 | 15.180 | 21 | 6.175 |
| CONVDIFF0 | Inverse-based | 0.01 | 5.800 | 100.550 | 95 | 3.644 |
| | Standard | 0.01 | 5.840 | 165.450 | 132 | 3.909 |
| | Inverse-based | 0.001 | 15.820 | 38.340 | 34 | 7.137 |
| | Standard | 0.001 | 21.320 | 83.010 | 46 | 9.391 |
| CONVDIFF1 | Inverse-based | 0.01 | 5.930 | 123.110 | 97 | 3.646 |
| | Standard | 0.01 | 5.950 | 153.840 | 116 | 3.910 |
| | Inverse-based | 0.001 | 15.840 | 36.860 | 33 | 7.139 |
| | Standard | 0.001 | 19.910 | 71.250 | 43 | 9.389 |
| CONVDIFF2 | Inverse-based | 0.01 | 6.170 | 52.120 | 49 | 3.665 |
| | Standard | 0.01 | 6.100 | 82.310 | 60 | 3.924 |
| | Inverse-based | 0.001 | 16.110 | 16.540 | 17 | 7.174 |
| | Standard | 0.001 | 20.900 | 32.700 | 22 | 9.323 |
| CONVDIFF3 | Inverse-based | 0.1 | 2.400 | 98.260 | 100 | 1.523 |
| | Standard | 0.1 | 2.450 | 102.970 | 101 | 1.744 |
| | Inverse-based | 0.01 | 6.340 | 12.520 | 17 | 3.848 |
| | Standard | 0.01 | 6.670 | 19.840 | 21 | 4.221 |

Table 5: Performance of two dropping strategies used by ILUC on symmetric pattern matrices, Lfil = $\infty$

| Matrix | Drop-strategy | Droptol | Pr-sec. | Its sec. | Its | Ratio |
|---|---|---|---|---|---|---|
| UTM.3060 | Inverse-based | 0.6 | - | - | - | 1.224 |
| | Standard | 0.1 | 0.050 | 2.130 | 150 | 1.455 |
| | Inverse-based | 0.06 | 0.210 | 0.680 | 37 | 4.251 |
| | Standard | 0.01 | 0.180 | 0.590 | 31 | 4.178 |
| UTM.5940 | Inverse-based | 0.1 | 0.850 | 4.720 | 115 | 6.251 |
| | Standard | 0.01 | 0.500 | 2.650 | 54 | 5.217 |
| | Inverse-based | 0.01 | 5.530 | 2.290 | 31 | 15.279 |
| | Standard | 0.001 | 4.430 | 2.080 | 25 | 14.771 |
| SHERMAN2 | Inverse-based | 0.1 | 0.030 | 0.030 | 7 | 1.444 |
| | Standard | 5e-5 | 0.020 | 0.060 | 14 | 1.155 |
| | Inverse-based | 0.01 | 0.060 | 0.010 | 2 | 2.196 |
| | Standard | 5e-6 | 0.050 | 0.020 | 5 | 1.927 |
| CAVA0000 | Inverse-based | 0.0008 | 22.660 | 6.640 | 27 | 6.824 |
| | Standard | 0.01 | 38.580 | 40.390 | 128 | 6.491 |
| | Inverse-based | 0.005 | 45.580 | 7.620 | 24 | 9.539 |
| | Standard | 0.001 | 49.480 | 28.060 | 74 | 10.013 |
| CAVA0100 | Inverse-based | 0.1 | 19.910 | 24.920 | 88 | 5.500 |
| | Standard | 0.6 | 31.330 | 51.800 | 204 | 5.905 |
| | Inverse-based | 0.01 | 6.680 | 5.010 | 23 | 4.310 |
| | Standard | 0.06 | 65.230 | 14.440 | 46 | 8.832 |

Table 6: Performance of two dropping strategies used by ILUC on nonsymmetric pattern matrices, Lfil = $\infty$

of nonzeros in the rows of $U$ or columns of $L$ is limited only by the drop tolerance. In addition, an effort was made to obtain LU factors that use more or less the same amount of memory for the preconditioners being compared, as reflected by the fill ratios. This was accomplished by a trial and error process, where various drop tolerances were tested for each matrix. As can be seen, the inverse-based method seems to drop small elements more precisely than the standard technique, in the sense that elements are dropped when they are least likely to affect convergence of the iteration. The tests also show that, in most cases, fewer GMRES iterations are needed to converge with the inverse-based dropping version.

This observation is further illustrated by the plots shown in Figure 5 which compare iteration times required by GMRES to converge when the fill-in ratio is varied for the two strategies. This is done for the four matrices BARTHT1A, CONVDIFF2 (symmetric patterns) and UTM.5940 and CAVA0100 (nonsymmetric patterns). Of the four cases, only UTM.5940 showed poorer overall performance for the inverse-based dropping. For reasons which are unclear, ILUC does not perform as well, relatively speaking, for matrices with nonsymmetric patterns.

# 6 Conclusion

The new version of ILU presented in this paper has several advantages over standard ILU techniques. The most obvious of these, which provided the primary motivation for this work, is that it leads to an efficient implementation that bypasses the need for searches. These costly searches constitute the main drawback of standard delayed-update implementations. Perhaps more significant is the advantage that this new version of ILU enables efficient implementations of some variations that were not practically possible with standard ILUT. For example, the more rigorous dropping strategies based on estimating the norms of the inverse

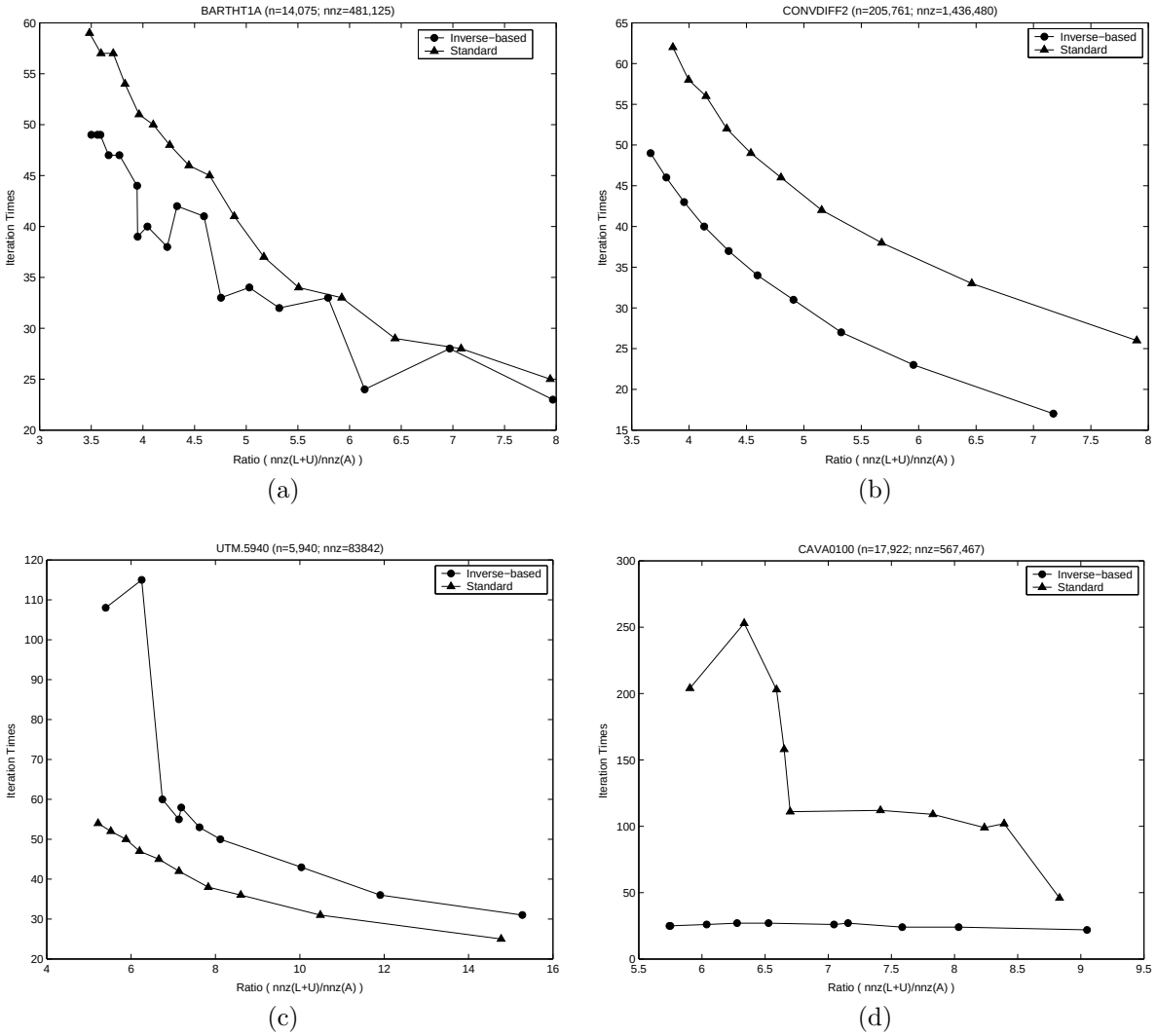


Figure 5: *Iteration times vs fill-in ratio for inverse-based dropping and standard dropping*

factors described in [3] can easily be implemented and lead to effective algorithms. In the same vein, this version of ILU also allows the implementation of potentially more effective pivoting strategies. This was not considered in this paper but will be the subject of a forthcoming study.

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