SYM-ILDL: Incomplete LDL<sup>T</sup> Factorization of Symmetric Indefinite and Skew-Symmetric Matrices

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SYM-ILDL is a numerical software package that computes incomplete LDL<sup>T</sup> (or ‘ILDL’) factorizations of symmetric indefinite and skew-symmetric matrices. The core of the algorithm is a Crout variant of incomplete LU (ILU), originally introduced and implemented for symmetric matrices by [Li and Saad, *Crout versions of ILU factorization with pivoting for sparse symmetric matrices*, Transactions on Numerical Analysis 20, pp. 75–85, 2005]. Our code is economical in terms of storage and it deals with skew-symmetric matrices as well, in addition to symmetric ones. The package is written in C++ and it is templated, open source, and includes a MATLAB<sup>TM</sup> interface. The code includes built-in RCM and AMD reordering, two equilibration strategies, threshold Bunch-Kaufman pivoting and rook pivoting, among other features. We also include an efficient MINRES implementation, applied with a specialized symmetric positive definite preconditioning technique based on the ILDL factorization.

1. INTRODUCTION

For the numerical solution of symmetric and skew-symmetric linear systems of the form

\[ Ax = b, \]

stable (skew-)symmetry-preserving decompositions of \( A \) often have the form

\[ PAP^T = LDL^T, \]

where \( L \) is a (possibly dense) lower triangular matrix and \( D \) is a block-diagonal matrix with 1-by-1 and 2-by-2 blocks [Bunch 1982, Bunch and Kaufman 1977]. The matrix \( P \) is a permutation matrix, satisfying \( PP^T = I \), and the right-hand side vector \( b \) is permuted accordingly: in practice we solve \( (PAP^T)(Px) = Pb \).

In the context of incomplete LDL<sup>T</sup> (ILDL) decompositions of sparse and large matrices for preconditioned iterative solvers, various element-dropping strategies are commonly used to impose sparsity of the factor, \( L \). Fill-reducing reordering strategies are also used to encourage the sparsity of \( L \), and various scaling methods are applied to improve conditioning. For a symmetric linear system, several methods have been developed. Recently proposed approaches perturb or partition \( A \) so that incomplete Cholesky may be used [Lin and Moré 1999, Orban 2014, Scott and Tuma 2014a]. While [Lin and Moré 1999] is designed for positive definite matrices, the recent papers of Orban [2014] and Scott and Tuma [2014a] are applicable to a large set of 2 × 2 block structured indefinite systems.

We present SYM-ILDL — a software package based on a left-looking Crout version of LU, which is stabilized by pivoting strategies such as Bunch-Kaufman and rook pivoting. The algorithmic principles underlying our software are based on (and extend) an incomplete LDL<sup>T</sup> factorization approach proposed by [Li and Saad 2005], which itself extends work by [Li et al. 2003] and [Jones and Plassmann 1995]. We offer the following new contributions:

— A Crout-based incomplete LDL<sup>T</sup> factorization for skew-symmetric matrices is introduced in this paper for the first time. It features a similar mechanism to the one for symmetric indefinite matrices, but there are notable differences. Most importantly, for skew-symmetric matrices the diagonal elements of \( D \) are zero and the pivots are always 2 × 2 blocks.

— We offer an integrated preconditioned MINRES solver, specialized to our ILDL code. The main challenge here is to design a positive definite preconditioner, even though ILDL produces an indefinite (or skew-symmetric) factorization. To that end, for the symmetric case we implement the technique presented in [Gill et al. 1992]. For the skew-symmetric case we introduce a positive definite preconditioner based on exploiting the simple 2 × 2 structure of the pivots.
The code is written in C++, and is templated and easily extensible. As such, it can be easily modified to work in other fields of numbers, such as C. SYM-ILDL is self-contained and it includes implementations of reordering methods (AMD and RCM), equilibration methods (in the max-norm, 1-norm, and 2-norm), and pivoting methods (Bunch-Kaufman and rook pivoting). To facilitate ease of use, a MATLAB™ interface is provided.

Incomplete factorizations of symmetric indefinite matrices have received much attention recently and a few numerical packages have been developed in the past few years. Scott and Tuma [2014a] have developed a numerical software package based on signed incomplete Cholesky factorization preconditioners due to Lin and Moré [1999]. For saddle-point systems, Scott and Tuma [2014a] have extended their limited memory incomplete Cholesky algorithm to a signed incomplete Cholesky factorization. Their approach builds on the ideas of Tismenetsky [1991] and Kaporin [1998]. In the case of breakdown (a zero pivot), a global shift is applied (see also Lin and Moré [1999]).

Scott and Tuma [2014a] Section 6.4] have made comparisons with our code, and have found that in general, the two codes are comparable in performance for several of the test problems, whereas for some of the problems each code outperforms the other. Given the comprehensive nature of the comparisons in Scott and Tuma [2014a], we do not provide further comparisons between the two packages in this paper.

Orban [2014] has developed LDL, a generalization of the limited-memory Cholesky factorization of Lin and Moré [1999] to the symmetric indefinite case with special interest in symmetric quasi-definite matrices. The code generates a factorization of the form LDLᵀ with D diagonal. We are currently engaged, jointly with Orban, in a comparison of our code to LDL.

The remainder of this paper is structured as follows. In Section 2 we outline a Crout-based factorization for symmetric and skew-symmetric matrices, symmetry-preserving pivoting strategies, equilibration approaches and reordering strategies. In Section 3 we discuss how to modify the output of SYM-ILDL to produce a positive definite preconditioner for MINRES. In Section 4 we discuss the implementation of SYM-ILDL, and how the pivoting strategies of Section 2 may be efficiently implemented within SYM-ILDL’s data structures. Finally, we show the performance of SYM-ILDL on some general (skew-)symmetric matrices and some saddle-point matrices in Section 5.

2. LDL AND ILDL FACTORIZATION

SYM-ILDL uses a Crout variant of LU factorization. To maintain stability, SYM-ILDL allows the user to choose one of two pivoting symmetry-preserving strategies: Bunch-Kaufman partial pivoting [Bunch and Kaufman 1977] (Bunch in the skew-symmetric case [Bunch 1982]) and rook pivoting. The details of the factorization and pivoting procedures, as well as simplifications for the skew-symmetric case, are provided in the following sections. See also Duff [2009] for more details on the use of direct solvers for solving skew-symmetric matrices.

2.1. Crout-based factorizations

The Crout order is an attractive way for computing an ILDL factorization of symmetric or skew-symmetric matrices, because it naturally preserves structural symmetry, especially when dropping rules for the incomplete factorization are applied. As opposed to the IKJ-based approach [Li and Saad 2005], Crout relies on computing and applying dropping rules to a column of L and a row of U simultaneously. The Crout procedure for a symmetric matrix is outlined in Algorithm 2 using a delayed update procedure for the factors which is laid out in Algorithm 1 (As discussed in the sequel, the procedure in Algorithm 1 may be called multiple times when various pivoting procedures are employed.)
ALGORITHM 1: Factors update procedure

Input: A symmetric matrix A, partial factors L and D, matrix size n, current column index k
Output: Updated factors L and D

1. $L_{k,n,k} \leftarrow A_{k,n,k}$
2. $i \leftarrow 1$
3. while $i < k$ do
   4. $s_i \leftarrow$ size of the diagonal block with $D_{i,i}$ as its top left corner
   5. $L_{k,n,k} \leftarrow L_{k,n,k} - L_{k,n,i:i+s_i-1}D^{-1}_{i:i+s_i-1,i:i+s_i-1}L_{k,i:i+s_i-1}^T$
   6. $i \leftarrow i + s_i$
4. end

ALGORITHM 2: Crout factorization, LDL^T

Input: A symmetric matrix A
Output: Matrices $P$, $L$, and $D$, such that $PAP \approx LDL^T$

1. $k \leftarrow 1$
2. $L \leftarrow 0$
3. $D \leftarrow 0$
4. while $k < n$ do
   5. Call Algorithm 1 to update $L$ and $D$
   6. Find a pivoting matrix in $A_{k,n,k}$ and permute $A$ accordingly
   7. $s \leftarrow$ size of the pivoting matrix
   8. $D_{k,k+s-1,k:k+s-1} \leftarrow L_{k,k+s-1,k:k+s-1}$
   9. $L_{k+k+s-1,k:k+s-1} \leftarrow L_{k+k+s-1,k:k+s-1}D^{-1}_{k,k+s-1,k:k+s-1}$
   10. Apply dropping rules to $L_{k+k+s-1,k:k+s-1}$
   11. $k \leftarrow k + s$
5. end

For computing the ILDL factorization, we apply dropping rules; see line 10 of Algorithm 2. These are the standard rules: we drop all entries below a pre-specified tolerance (referred to as drop_tol throughout the paper), multiplied by the norm of a column of $L$, keeping up to a pre-specified maximum number of the largest nonzero entries in every column. We use here the term fill_factor to signify the maximum allowed ratio between the number of nonzeros in any column of $L$ and the average number of nonzeros per column of $A$.

In Algorithm 2, the $s \times s$ pivot is typically $1 \times 1$ or $2 \times 2$, as per the strategy devised by Bunch and Kaufman [1977], which we briefly describe next.

2.2. Symmetric partial pivoting

Pivoting in the symmetric or skew-symmetric setting is challenging, since we seek to preserve the (skew-)symmetry and it is not sufficient to use $1 \times 1$ pivots to maintain stability. Much work has been done in this front; see, for example, [Duff et al. 1989; Duff et al. 1991; Hogg and Scott 2014] and the references therein.

Bunch and Kaufman [1977] proposed a partial pivoting strategy for symmetric matrices, which relies on finding $1 \times 1$ and $2 \times 2$ pivots. The cost of finding a pivot is $O(n)$, as it only involves searching up to two columns. We provide this procedure in Algorithm 3.

The constant $\alpha = (1 + \sqrt{17})/8$ in line 1 of the algorithm controls the growth factor, and $a_{ij}$ is the $ij$-th entry of the matrix $A$ after computing all the delayed updates in Algorithm 1 on column $i$. Although the partial pivoting strategy is backward stable [Higham 2002], the possibly large elements in the unit lower triangular matrix $L$ may cause numerical difficulty. Rook pivoting provides an alternative that in practice proves to be more stable, at a modest additional cost. This procedure is presented in Algorithm 4. The algorithm searches the
ALGORITHM 3: Bunch-Kaufman LDL\top using partial pivoting strategy

1 \( \alpha \leftarrow (1 + \sqrt{17})/8 \) (\( \approx 0.64 \))
2 \( \omega_1 \leftarrow \) maximum magnitude of any subdiagonal entry in column 1
3 if \( |a_{11}| \geq \alpha \omega_1 \) then
4 Use \( a_{11} \) as a \( 1 \times 1 \) pivot (\( s = 1 \))
5 else
6 \( r \leftarrow \) row index of first (subdiagonal) entry of maximum magnitude in column \( r \)
7 \( \omega_r \leftarrow \) maximum magnitude of any off-diagonal entry in column \( r \)
8 if \( |a_{11}| \omega_r \geq \alpha \omega_r^2 \) then
9 Use \( a_{11} \) as a \( 1 \times 1 \) pivot (\( s = 1 \))
10 else if \( |a_{11}| \geq \alpha \omega_r \) then
11 Use \( a_{rr} \) as a \( 1 \times 1 \) pivot (\( s = 1 \), swap rows and columns 1, \( r \))
12 else
13 Use \( \begin{pmatrix} a_{11} & a_{r1} \\ a_{r1} & a_{rr} \end{pmatrix} \) as a \( 2 \times 2 \) pivot (\( s = 2 \), swap rows and columns 2, \( r \))
14 end
15 end
16 end

pivots of the matrix in spiral order until it finds an element that is largest in absolute value in both its row and its column, or terminates if it finds a relatively large diagonal element. Although theoretically rook pivoting could traverse many columns, we have found that it is fast in practice, and we use it as the default pivoting scheme of SYM-ILDL.

ALGORITHM 4: LDL\top using rook pivoting strategy

1 \( \alpha \leftarrow (1 + \sqrt{17})/8 \) (\( \approx 0.64 \))
2 \( \omega_1 \leftarrow \) maximum magnitude of any subdiagonal entry in column 1
3 if \( |a_{11}| \geq \alpha \omega_1 \) then
4 Use \( a_{11} \) as a \( 1 \times 1 \) pivot (\( s = 1 \))
5 else
6 \( i \leftarrow 1 \)
7 while a pivot is not yet chosen do
8 \( r \leftarrow \) row index of first (subdiagonal) entry of maximum magnitude in column \( i \)
9 \( \omega_r \leftarrow \) maximum magnitude of any off-diagonal entry in column \( r \)
10 if \( |a_{rr}| \geq \alpha \omega_r \) then
11 Use \( a_{rr} \) as a \( 1 \times 1 \) pivot (\( s = 1 \), swap rows and columns 1 and \( r \))
12 else if \( \omega_i = \omega_r \) then
13 Use \( \begin{pmatrix} a_{ii} & a_{ri} \\ a_{ri} & a_{rr} \end{pmatrix} \) as a \( 2 \times 2 \) pivot (\( s = 2 \), swap rows and columns 1 and \( i \), and 2 and \( r \))
14 else
15 \( i \leftarrow r \)
16 \( \omega_i \leftarrow \omega_r \)
17 end
18 end
19 end

2.3. Equilibration and reordering strategies

In many cases of practical interest, the input matrix is ill-conditioned. For these cases, equilibration schemes have been shown to be effective in lowering the condition number of the matrix. Symmetric equilibration schemes rescale entries of the matrix by computing a diagonal matrix \( D \) such that \( DAD \) has equal row norms and column norms.
SYM-ILDL offers two equilibration schemes: Bunch’s equilibration in the max norm [Bunch 1971] and Ruiz’s iterative equilibration in any $L_p$-norm [Ruiz 2001].

Bunch’s equilibration allows the user to scale the max norm of every row and column to 1 before factorization. Let $T$ be the lower triangular part of $A$ in absolute value (diagonal included), that is, $T_{ij} = |A_{ij}|$, $1 \leq j \leq i \leq n$. Then Bunch’s algorithm runs in $O(nnz(A))$ time, and is based on the following greedy procedure:

For $1 \leq i \leq n$, set

$$D_{ii} := \left( \max \left\{ \sqrt{T_{ii}}, \max_{1 \leq j \leq i-1} D_{jj} T_{ij} \right\} \right)^{-1}.$$

Ruiz’s equilibration allows the user to scale every row and column of the matrix to 1 in any $L_p$ norm, provided that $p \geq 1$ and the matrix has support [Ruiz 2001]. For the max norm, Ruiz’s algorithm scales each column’s norm to within $\varepsilon$ of 1 in $O(nnz(A) \log \frac{1}{\varepsilon})$ time for any given tolerance $\varepsilon$.

Let $r(A,i)$ and $c(A,i)$ denote the $i$-th row and column of $A$ respectively, and let $D(i,\alpha)$ to be the diagonal matrix with $D_{jj} = 1$ for all $j \neq i$ and $D_{ii} = \alpha$. Using this notation, our variant of Ruiz’s algorithm is shown in Algorithm 5.

**Algorithm 5: Equilibrating general matrices in the max-norm**

**Input:** A general matrix $A$

**Output:** Diagonal matrices $R$ and $C$ such that $RAC$ has max-norm 1 in every row and column

1. $R \leftarrow I$
2. $C \leftarrow I$
3. $\tilde{A} \leftarrow A$
4. while $R$ and $C$ have not yet converged do
5.   for $i := 1$ to $n$ do
6.     $\alpha_r \leftarrow \sqrt{\|r(\tilde{A},i)\|_\infty}$
7.     $\alpha_c \leftarrow \sqrt{\|c(\tilde{A},i)\|_\infty}$
8.     $R \leftarrow R \cdot D(i,\alpha_r)$
9.     $C \leftarrow C \cdot D(i,\alpha_c)$
10. $\tilde{A} \leftarrow D(i,\alpha_r) \tilde{A} D(i,\alpha_c)$
11. end
12. end

Our presentation differs from Ruiz’s original algorithm in that it operates one row and column at a time as opposed to operating on the entire matrix in each iteration. We implemented the algorithm this way as it naturally adapts to our storage structures; our code is more easily amenable to single column operations rather than matrix-vector products. However, a proof of correctness similar to that of of Ruiz’s algorithm applies, with the same guarantee for the running time.

Ruiz’s strategy seems to perform well in terms of preserving diagonal dominance when no reordering strategy is used. In fact, we have observed that for certain skew-symmetric systems, Ruiz’s equilibration leads to convergence of the iterative solver, while Bunch’s approach does not. On the other hand, Bunch’s equilibration strategy is faster, being a one-pass procedure. In our experiments we use Bunch as the default.

After equilibration, we carry out a reordering strategy. The user is given the option of choosing from Approximate Minimum Degree (AMD) [Amestoy et al. 1996] and Reverse Cuthill-McKee (RCM) [George and Liu 1981]. We have found AMD to be generally more effective for our test cases, and it is set as the default in the code.
2.4. LDL and ILDL factorizations for skew-symmetric matrices

The skew-symmetric case is different than the symmetric indefinite case in the sense that here, we must always use $2 \times 2$ pivots, because diagonal elements of skew-symmetric matrices are zero. This significantly simplifies the Bunch-Kaufman procedure: we have only one case rather than four. Algorithm 6 illustrates the simplification for rook pivoting. Furthermore, as opposed to a typical $2 \times 2$ symmetric matrix, which is defined by three parameters, the analogous skew-symmetric matrix is defined by one parameter only. As a result, at the $k$th step, the computation of the multiplier and the subsequent update of pair of columns associated with the pivoting operation can be expressed as follows:

$$
A_{k+2:n,k+1}^{-1}A_{k+1:n,k+1}^{-1} = A_{k+2:n,k+1}^{-1} \begin{pmatrix} 0 & -a_{k+1,k} \\ a_{k+1,k} & 0 \end{pmatrix}^{-1} = \frac{1}{a_{k+1,k}} A_{k+2:n,k+1}^{-1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},
$$

which can be trivially computed by swapping columns $k$ and $k + 1$ and scaling.

**Algorithm 6:** LDL$^T$ using rook pivoting strategy for skew-symmetric matrices

```
1 $\omega_1 \leftarrow$ maximum magnitude of any subdiagonal entry in column 1
2 $i \leftarrow 1$
3 while a pivot is not yet chosen do
4     $r \leftarrow$ row index of first (subdiagonal) entry of maximum magnitude in column $i$
5     $\omega_r \leftarrow$ maximum magnitude of any off-diagonal entry in column $r$
6     if $\omega_1 = \omega_r$ then
7         $U$
8     else
9         $s$
10    end
11    $e \begin{pmatrix} 0 & -a_{ri} \\ a_{ri} & 0 \end{pmatrix}$ as a $2 \times 2$ pivot (swap rows and columns 1 and $i$, and 2 and $r$)
12 end
13 $i \leftarrow r$
14 $\omega_1 \leftarrow \omega_r$
```

The ILDL factorization for skew-symmetric matrices can thus be carried out similarly to the manner in which it is developed for symmetric indefinite matrices, but the eventual algorithm gives rise to the above described simplifications. Skew-symmetric matrices are often ill-conditioned, and we have experimentally found that computing a numerical solution effectively for those systems is challenging. More details are provided in Section 5.

3. A SPECIALIZED PRECONDITIONER FOR MINRES

Our goal is to use a symmetric solver with our ILDL factorization, given that LDL$^T$ is indefinite (for symmetric indefinite $A$) or skew-symmetric (for skew-symmetric $A$). The main difficulty lies in the fact that preconditioners for short recurrence solvers typically must be symmetric positive definite.

We describe below techniques for generating MINRES preconditioned iterations, using positive definite versions of the incomplete factorization. For the symmetric indefinite case, we apply the method presented in [Gill et al. 1992]. Given $M = LDL^T$, let us focus our attention on the various options for the blocks of $D$. Our ultimate goal is to modify $D$ and $L$ such that $D$ is diagonal with only 1 or $-1$ as its diagonal entries. If a block of the matrix $D$...
from the original LDL factorization was $2 \times 2$, then the corresponding modified (diagonal) block would become

$$
\begin{pmatrix}
\pm 1 & 0 \\
0 & \mp 1
\end{pmatrix}.
$$

For a diagonal entry of $D$ that appears as a $1 \times 1$ block, say, $d_{i,i}$, we rescale the $i$th row of $L$: $L(i,:) \rightarrow L(i,:)\sqrt{|d_{i,i}|}$. We can then set the new value of $d_{i,i}$ as $\pm 1$. In practice there is no need to perform a multiplication of a row of $L$ by $\sqrt{|d_{i,i}|}$; instead, this scalar is stored separately and its multiplicative effect is computed as an $O(1)$ operation for every matrix vector product.

Now, consider a $2 \times 2$ block of $D$, say $D_j$. For this case, we compute the eigendecomposition

$$
D_j = Q_j \Lambda_j Q_j^T,
$$

and similarly to the case of a $1 \times 1$ block, we implicitly rescale two rows of $L$ by $Q_j \sqrt{\Lambda_j}$. This means that $L$ is no longer triangular; it is in fact lower Hessenberg, since some values above the main diagonal may become nonzero. But the solve is just as straightforward, since the decomposition is explicitly given.

In the skew-symmetric case, we may use a specialized version of MINRES [Greif and Varah 2009]. We only have $2 \times 2$ blocks, and for those, we know that

$$
\begin{pmatrix}
0 & a_{j,j} \\
-a_{j,j} & 0
\end{pmatrix} =
\begin{pmatrix}
\sqrt{|a_{j,j}|} & 0 \\
0 & \sqrt{|a_{j,j}|}
\end{pmatrix}
\begin{pmatrix}
0 & \pm 1 \\
\mp 1 & 0
\end{pmatrix}
\begin{pmatrix}
\sqrt{|a_{j,j}|} & 0 \\
0 & \sqrt{|a_{j,j}|}
\end{pmatrix}.
$$

Therefore, we do not need an eigendecomposition (as in the symmetric case), and instead we just scale the two affected rows of $L$ by $\sqrt{|a_{j,j}|} I_2$.

Figure 1 shows the clustering effect that the proposed preconditioning approach has. We generate a symmetric random $300 \times 300$ matrix, say $A$, and compute the eigenvalues of $(LDL^T)^{-1} A$, where $L$ and $D$ are the matrices generated in the above described preconditioning procedure. Our fill factor is 2.0 and the drop tolerance was $10^{-4}$. We note that the eigenvalue distribution in the figure is typical for other cases that were tested.

![Eigenvalues of a preconditioned symmetric random 300 x 300 matrix. The horizontal blue lines mark 1 and -1.](image)
4. IMPLEMENTATION
4.1. Matrix storage in SYM-ILDL
Since we are dealing with symmetric or skew-symmetric matrices, one of our goals is to avoid duplicating data. At the same time, it is necessary for SYM-ILDL to have fast column access as well as fast row access. In terms of storage, we deal with these requirements by generating a format similar to standard compressed sparse column form, along with compressed sparse row form without the nonzero floating point matrix values. Matrices are stored in a list-of-arrays format. Each column is represented internally as two arrays, storing both its nonzero values \( \text{col\_val} \) and row indices (\( \text{col\_list} \)). One advantage of this format is that swapping columns and deallocating their memory is much easier. Additionally, a row-major data structure (\( \text{row\_list} \)) is used to maintain fast access across the nonzeros of each row (see Figure 2). This is obtained by representing each row internally as a single array, storing the column indices of each row in an array (the nonzero values are already stored in the column-major representation).

![Graphical representation of the data structures of SYM-ILDL.](image)

Our format is a modest improvement over storing the full matrix in standard CSC, as used in [Li and Saad 2005]. Assuming that the row and column indices are stored in 32-bit integers and the nonzero values are stored in 64-bit doubles, this gives us an overall 33% saving in storage if we were to store the factorization in-place. This is an easy modification of Algorithm 3. In the default implementation, we find it more useful to store an equilibrated and permuted copy of the original matrix, so that we may use it for MINRES after the preconditioner is computed. An in-place version that returns only the preconditioner is included as part of our package.

4.2. Data structures for matrix access
In ILUC [Li and Saad 2005], a bi-index data structure was developed to address two implementation difficulties in sparse matrix operations, following earlier work by Eisenstat et al. [1981] in the context of the Yale Sparse Matrix Package (YSMP), and Jones and Plassmann [1995]. Our implementation uses a similar bi-index data structure, which we describe below. Internally, the column and row indices in the matrix are stored in unsorted order. This avoids the cost of sorting whenever we need to pivot. Due to the unsortedness, accessing specific elements of the matrix is difficult and requires a slow linear search. Luckily, because Algorithm 3 accesses elements in a predictable fashion, we can speed up access to subcolumns.
required during the factorization to $O(1)$ amortized time. The strategy we use to speed up matrix access is similar to that of [Jones and Plassmann 1995]. To ensure fast access to the submatrix $L_{k+1:n,i,k}$ and the row $L_k$: during factorization, we use one additional length $n$ array: $\text{col\_first}$. The $i$-th element of $\text{col\_first}$ array effectively holds a pointer to the start of the submatrix $L_{k+1:n,i}$ in $\text{col\_list}$ and speeds up Algorithm 1, allowing us access to the submatrix in $O(1)$ time. To get fast access to the list of columns that contribute to the update of the $(k+1)$-st column, we use the row structure $\text{row\_list}$ discussed in section 4.1. Overall, this reduces the access time of the submatrix $L_{k+1:n,1:k}$ and row $L_k$ down to a cost proportional to the number of nonzeros in these submatrices.

To ensure that $\text{col\_first}(i)$ points to the start of the subcolumn $L_{k+1:n,i}$ on step $k$, we advance the pointer for $\text{col\_first}(i)$ (if needed) at the end of processing the $k$-th column. Since the column indices in $\text{col\_list}$ are unsorted, this step requires a linear search to find the smallest element in $\text{col\_list}$. Once this element is found, we swap it to the correct spot so that the column indices for $L_{k+1:n,i}$ are in a contiguous segment of memory.

Similarly, we will also need to access the subrows $A_{1:k,1}$ and $A_{1:k}$ during the pivoting stage (lines 11 to 15 in Algorithm 3 and Algorithm 4). This is sped up by an analogous $\text{row\_first}(i)$ structure that points to the end of the subrow $A_{1:k}$ ($A_{1:k}$ is the memory region that encompasses everything from the start of memory for that row to $\text{row\_first}(i)$). At the end of step $k$, we also advance the pointers for $\text{row\_first}$ if needed.

A summary of data structures can be found in Table I.

<table>
<thead>
<tr>
<th>Variable name</th>
<th>Data structure type</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>col_first</td>
<td>$n$ length array</td>
<td>Speeds up access to $L_{k+1:n,i}$, i.e., $\text{row_list}$</td>
</tr>
<tr>
<td>row_first</td>
<td>$n$ length array</td>
<td>Speeds up access to $A_{1:k}$, i.e., $\text{col_list}$</td>
</tr>
<tr>
<td>row_list</td>
<td>$n$ linked lists (row-major)</td>
<td>Stores indices of $A$ across the rows</td>
</tr>
<tr>
<td>col_list</td>
<td>$n$ linked lists (col-major)</td>
<td>Stores indices of $A$ across the columns</td>
</tr>
<tr>
<td>col_val</td>
<td>$n$ linked lists (col-major)</td>
<td>Stores nonzero coefficients of $A$</td>
</tr>
</tbody>
</table>

5. NUMERICAL EXPERIMENTS

For testing our code, we use the University of Florida (UF) collection [Davis and Hu 2011], as well as our own matrices. The UF collection provides a variety of symmetric matrices, which we specify in Tables II and IV. We have used some of the same matrices that have been used in the papers [Li and Saad 2005; Li et al. 2003; Scott and Tuma 2014a].

We also test with simple discrete differential operators arising from two model problems. One is a model convection-diffusion equation, which is a discrete version of

$$ -\Delta u + (\sigma, \tau, \mu) \nabla u = f, \quad (1) $$

with Dirichlet boundary conditions on the unit square, discretized using a uniform mesh of size $h$. We define the mesh Reynolds numbers $\beta = \sigma h/2, \gamma = \tau h/2, \delta = \mu h/2$. We use the skew-symmetric part of this matrix (that is, given $A$, form $\frac{A-A^T}{2}$) for our skew-symmetric experiments. Our second set are test matrices associated with the discrete Helmholtz equation,

$$ -\Delta u + \alpha u = f, \quad (2) $$
subject to Dirichlet boundary conditions. Here we choose $\alpha$ so that a symmetric indefinite matrix is generated; see Table III.

All experiments were run on a single threaded, 2.8 GHZ AMD dual core machine, with 128 GB RAM. Timings are averaged across ten runs of each test case. In the experiments below, we follow the conventions of [Li and Saad 2005; Li et al. 2003] and define the fill of a factorization as $\text{nnz}(L + D + L^T)/\text{nnz}(A)$.

5.1. Results for symmetric matrices

In Table II we show the results of experiments with a set of matrices from [Davis and Hu 2011]. The matrix dimensions go up to approximately four million, with number of nonzeros going up to approximately 100 million. We show timings for constructing the ILDL factorization and an iterative solution, applying the preconditioned MINRES approach described in Section 3. We apply Bunch’s equilibration and AMD reordering before generating the incomplete LDL factorization and running preconditioned MINRES. For the incomplete factorization, we apply rook pivoting. We observe a good convergence behavior for most of the matrices that were tested. We observe that for the matrices in this set, the computational time is $O(n \cdot \text{nnz}(A))$, as expected.

<table>
<thead>
<tr>
<th>matrix</th>
<th>n</th>
<th>nnz(A)</th>
<th>fill</th>
<th>time (s)</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>aug3dcpu</td>
<td>35543</td>
<td>128115</td>
<td>1.8</td>
<td>0.08</td>
<td>28</td>
</tr>
<tr>
<td>bloweya</td>
<td>30004</td>
<td>150009</td>
<td>1.1</td>
<td>0.05</td>
<td>18</td>
</tr>
<tr>
<td>bratu3d</td>
<td>27792</td>
<td>173796</td>
<td>3.7</td>
<td>0.35</td>
<td>80</td>
</tr>
<tr>
<td>tuma1</td>
<td>22967</td>
<td>87760</td>
<td>2.6</td>
<td>0.09</td>
<td>201</td>
</tr>
<tr>
<td>tuma2</td>
<td>12992</td>
<td>49365</td>
<td>2.6</td>
<td>0.05</td>
<td>149</td>
</tr>
<tr>
<td>boyd1</td>
<td>93279</td>
<td>1211231</td>
<td>0.9</td>
<td>0.09</td>
<td>3</td>
</tr>
<tr>
<td>brainpc2</td>
<td>27607</td>
<td>179395</td>
<td>1.1</td>
<td>0.48</td>
<td>48</td>
</tr>
<tr>
<td>marino001</td>
<td>38434</td>
<td>204912</td>
<td>3.4</td>
<td>0.44</td>
<td>146</td>
</tr>
<tr>
<td>qpdband</td>
<td>20000</td>
<td>45000</td>
<td>1.1</td>
<td>0.01</td>
<td>3</td>
</tr>
<tr>
<td>G3-circuit</td>
<td>1585478</td>
<td>7660826</td>
<td>5.0</td>
<td>9.5</td>
<td>100</td>
</tr>
<tr>
<td>Hook-1498</td>
<td>59374451</td>
<td>64531701</td>
<td>3.9</td>
<td>240.1</td>
<td>242</td>
</tr>
<tr>
<td>StocF-1465</td>
<td>1465137</td>
<td>21005398</td>
<td>1.8</td>
<td>18.9</td>
<td>379</td>
</tr>
<tr>
<td>Geo_1438</td>
<td>60236322</td>
<td>8580313</td>
<td>5.0</td>
<td>428.6</td>
<td>26</td>
</tr>
<tr>
<td>Serena</td>
<td>64131971</td>
<td>48538952</td>
<td>4.8</td>
<td>386.3</td>
<td>22</td>
</tr>
<tr>
<td>nlpkkt80</td>
<td>28192672</td>
<td>14883536</td>
<td>6.2</td>
<td>2179</td>
<td>998</td>
</tr>
<tr>
<td>nlpkkt120</td>
<td>95117792</td>
<td>96845792</td>
<td>6.2</td>
<td>788.5</td>
<td>907</td>
</tr>
</tbody>
</table>

The experiments were run with $\text{fill-factor} = 2.0$ for the smaller matrices and $\text{fill-factor} = 4.0$ for matrices larger than one million in dimension. The tolerance was $\text{drop_tol} = 10^{-4}$, and we used rook pivoting to maintain stability. The iteration was terminated when the norm of the relative residual went below $10^{-6}$.

In Table III we present results for the Helmholtz model problem. We compare SYM-ILDL to MATLAB’s ILUTP. For ILUTP we used a drop tolerance of $10^{-3}$ in all test cases. For ILDL, the $\text{fill-factor}$ was set to $\infty$ (since ILUTP does not limit its intermediate memory by a fill factor) while the $\text{drop_tol}$ parameter was then chosen to get roughly the same fill as that of ILUTP. In the context of the ILUTP preconditioner, the fill is defined as $\text{nnz}(L + U)/\text{nnz}(A)$.

Since ILUTP produces an $L$ and a $U$, GMRES was used as the iterative solver instead of MINRES for both ILDL and ILUTP. In the case of ILDL, $LD$ and $L^T$ were used as the two preconditioners. Note that during the computation of the preconditioner, the in-place version of ILDL uses only about 2/3 of the memory used by ILUTP. During the GMRES solve, the ILDL preconditioner only uses about 1/2 the memory used by ILUTP.

We observe that the performance of ILDL on the Helmholtz model problem is dependent on the value of $\alpha$ chosen, but that if ILDL is given the same memory resources as ILUTP, it
outperforms it. For $\alpha = 0.3$, the ILDL approach leads to lower iteration counts even when approximately 1/2 of the memory is allocated (i.e., when the same fill is allowed), whereas for $\alpha = 0.7$, ILUTP outperforms ILDL when the fill is roughly the same. If we allow ILDL to have memory usage as large as ILUTP (i.e., up to twice the fill), we see that ILDL clearly has lower iteration counts for GMRES.

Table III. Comparison of MATLAB’s ILUTP and SYM-ILDL for Helmholtz matrices

<table>
<thead>
<tr>
<th>matrix</th>
<th>$n$</th>
<th>nnz($A$)</th>
<th>ILU fill</th>
<th>ILU GMRES iters</th>
<th>ILDL fill</th>
<th>ILDL GMRES iters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha = 0.3$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>helmholtz280</td>
<td>6400</td>
<td>31680</td>
<td>8.0</td>
<td>14</td>
<td>7.9</td>
<td>12</td>
</tr>
<tr>
<td>helmholtz120</td>
<td>14400</td>
<td>71520</td>
<td>10.8</td>
<td>17</td>
<td>10.9</td>
<td>6</td>
</tr>
<tr>
<td>helmholtz160</td>
<td>25600</td>
<td>127360</td>
<td>13.3</td>
<td>20</td>
<td>12.1</td>
<td>10</td>
</tr>
<tr>
<td>helmholtz200</td>
<td>40000</td>
<td>199200</td>
<td>16.6</td>
<td>39</td>
<td>13.4</td>
<td>15</td>
</tr>
<tr>
<td>$\alpha = 0.7$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>helmholtz280</td>
<td>6400</td>
<td>31680</td>
<td>9.8</td>
<td>11</td>
<td>9.9</td>
<td>28</td>
</tr>
<tr>
<td>helmholtz120</td>
<td>14400</td>
<td>71520</td>
<td>13.4</td>
<td>10</td>
<td>13.3</td>
<td>144</td>
</tr>
<tr>
<td>helmholtz160</td>
<td>25600</td>
<td>127360</td>
<td>19.9</td>
<td>18</td>
<td>19.4</td>
<td>84</td>
</tr>
<tr>
<td>helmholtz200</td>
<td>40000</td>
<td>199200</td>
<td>22.8</td>
<td>28</td>
<td>25.4</td>
<td>144</td>
</tr>
<tr>
<td>$\alpha = 0.7$, Equal memory for ILDL and ILUTP</td>
<td>6400</td>
<td>31680</td>
<td>9.8</td>
<td>11</td>
<td>13.6</td>
<td>6</td>
</tr>
<tr>
<td>helmholtz120</td>
<td>14400</td>
<td>71520</td>
<td>13.4</td>
<td>10</td>
<td>22.8</td>
<td>6</td>
</tr>
<tr>
<td>helmholtz160</td>
<td>25600</td>
<td>127360</td>
<td>19.9</td>
<td>18</td>
<td>29.9</td>
<td>9</td>
</tr>
<tr>
<td>helmholtz200</td>
<td>40000</td>
<td>199200</td>
<td>22.8</td>
<td>28</td>
<td>35.5</td>
<td>16</td>
</tr>
</tbody>
</table>

The parameter $\alpha$ in Equation 2 is indicated above. GMRES was terminated when the relative residual decreased below $10^{-6}$.

In Table IV, we compare our code to the code of Li et al. [2003], which was provided to us by Saad. We will refer to this code as LSC-ILDL. We use the same basic algorithms, but our approach saves on memory thanks to exploiting symmetry. One bottleneck for the code of Li et al. [2003] is input reading. On the other hand, that code is faster than our code for the factorization, as the entire input matrix is stored. Altogether, we observe SYM-ILDL has a slight edge in terms of overall computational time.

Table IV. Time comparisons between the code from Li et al. [2003] and ours

<table>
<thead>
<tr>
<th>Matrix name</th>
<th>$n$</th>
<th>nnz($A$)</th>
<th>fill</th>
<th>LSC-ILDL</th>
<th>SYM-ILDL</th>
</tr>
</thead>
<tbody>
<tr>
<td>tumu1</td>
<td>22967</td>
<td>87760</td>
<td>1.81</td>
<td>0.06</td>
<td>0.04</td>
</tr>
<tr>
<td>bratu3d</td>
<td>27792</td>
<td>173796</td>
<td>2.07</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>stokes128</td>
<td>49666</td>
<td>558594</td>
<td>1.50</td>
<td>0.36</td>
<td>0.18</td>
</tr>
<tr>
<td>d_pretok</td>
<td>182730</td>
<td>1641672</td>
<td>1.73</td>
<td>1.20</td>
<td>1.07</td>
</tr>
<tr>
<td>turon_m</td>
<td>189924</td>
<td>1690876</td>
<td>1.76</td>
<td>1.25</td>
<td>1.17</td>
</tr>
<tr>
<td>darcy003</td>
<td>389874</td>
<td>2101242</td>
<td>2.04</td>
<td>1.79</td>
<td>1.51</td>
</tr>
<tr>
<td>c_big</td>
<td>345241</td>
<td>2341011</td>
<td>1.25</td>
<td>1.63</td>
<td>1.45</td>
</tr>
<tr>
<td>maxwell7</td>
<td>532265</td>
<td>5062950</td>
<td>1.26</td>
<td>4.39</td>
<td>3.72</td>
</tr>
</tbody>
</table>

All matrices were run with $fill\_factor = 1.0$, $drop\_tol = 10^{-4}$, and used Bunch-Kaufman partial pivoting to maintain stability. The two right-most columns report computational times in seconds.

5.2. Results for skew-symmetric matrices

We now report on the performance of SYM-ILDL for skew-symmetric matrices. We have tested on the skew-symmetric part of the model convection-diffusion equation (1). We have found that for the matrices we have tested, equilibration has not been particularly effective. We speculate that this might have to do with a property related to block diagonal dominance that these matrices have for certain values of the convective coefficients. Specifically, the norm of the tridiagonal part of the matrix is significantly larger than the norm of the remaining part. Equilibration tends to adversely affect this property by scaling down entries.
near the diagonal, and as a result the performance of an iterative solver often degrades. We thus do not apply equilibration in our skew-symmetric solver.

In Table V we manipulate the drop tolerance for ILDL, to obtain a fill nearly equal to that of ILUTP. For the latter we fix the drop tolerance at 0.001. This is done for the purpose of comparing the performance of the iterative solvers, when the memory requirements of ILUTP and ILDL are similar. Note, though, that our ILDL still consumes only about \( \frac{2}{3} \) of the memory of ILUTP, due to the fact that the floating point entries of only half of the matrix are stored. We see that the iteration counts are significantly better for ILDL, especially when rook pivoting is used.

Table V. Comparison of MATLAB’s ILUTP and SYM-ILDL for a skew-symmetric matrix arising from a model convection-diffusion equation

<table>
<thead>
<tr>
<th>n</th>
<th>nnz(A)</th>
<th>method</th>
<th>drop tol</th>
<th>fill</th>
<th>GMRES(100)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(20^3 = 8000)</td>
<td>45600</td>
<td>ILDL-rook 4e-4</td>
<td>7.008</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILDL-partial 5e-4</td>
<td>6.861</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILUTP 1e-3</td>
<td>7.758</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>(30^3 = 27000)</td>
<td>156600</td>
<td>ILDL-rook 2e-4</td>
<td>10.973</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILDL-partial 3e-4</td>
<td>11.235</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILUTP 1e-3</td>
<td>11.758</td>
<td>13</td>
<td></td>
</tr>
<tr>
<td>(40^3 = 64000)</td>
<td>374400</td>
<td>ILDL-rook 9e-5</td>
<td>15.205</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILDL-partial 3e-4</td>
<td>15.686</td>
<td>18</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILUTP 1e-3</td>
<td>15.654</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>(50^3 = 125000)</td>
<td>735000</td>
<td>ILDL-rook 2e-5</td>
<td>21.560</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILDL-partial 2e-4</td>
<td>22.028</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILUTP 1e-3</td>
<td>22.691</td>
<td>31</td>
<td></td>
</tr>
<tr>
<td>(60^3 = 216000)</td>
<td>127400</td>
<td>ILDL-rook 2e-5</td>
<td>22.595</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILDL-partial 4e-4</td>
<td>22.899</td>
<td>NC</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILUTP 1e-3</td>
<td>23.483</td>
<td>70</td>
<td></td>
</tr>
<tr>
<td>(70^3 = 343000)</td>
<td>202800</td>
<td>ILDL-rook 5e-6</td>
<td>32.963</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILDL-partial – – –</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ILUTP 1e-3</td>
<td>33.861</td>
<td>61</td>
<td></td>
</tr>
</tbody>
</table>

The parameter used were \( \beta = 20, \gamma = 2, \delta = 1 \). The MATLAB ILUTP used a drop tolerance of 0.001. 'NC' stands for 'no convergence'.

In Figure 3 we show the (complex) eigenvalues of the preconditioned matrix \((LDLT)^{-1}A\), where \(A\) is the skew-symmetric part of \(A\) with convective coefficients \((\beta, \gamma, \delta) = (0.4, 0.5, 0.6)\), and \(LDLT\) is the preconditioner generated by running SYM-ILDL with a drop tolerance of \(10^{-3}\) and a fill-in parameter of 20. As seen in the figure, most of the eigenvalues are very strongly clustered around 1, which indicates that a preconditioned iterative solver is expected to rapidly converge.

6. CONCLUSION

We have presented SYM-ILDL, a C++ software package for solving and preconditioning symmetric or skew-symmetric matrices. Our algorithmic approach is based on that of Li and Saad [2005]. Our code extends the functionality of the code of Li and Saad [2005] by adding multiple pivoting, reordering, and equilibration schemes. For ease of use, the code is templated and offers a MATLAB interface. SYM-ILDL is open source, and can be found at [http://www.cs.ubc.ca/~greif/code/sym-ildl.html](http://www.cs.ubc.ca/~greif/code/sym-ildl.html). To facilitate the use of the factorization as a preconditioner for a symmetric solver, we apply a symmetric positive definite variant of the output factors of SYM-ILDL, which is similar to Gill et al. [1992] in the symmetric case. For the skew-symmetric case we derive a positive definite preconditioner which takes advantage of the simple nonzero structure of the \(2 \times 2\) pivots.

Numerical results for SYM-ILDL and comparisons with the code of Li et al. [2003] and the widely used ILUTP preconditioner (as implemented by MATLAB) indicate that for symmetric matrices, SYM-ILDL with rook pivoting is faster.
Fig. 3. Eigenvalues of a preconditioned skew-symmetric 1000 × 1000 matrix A arising from a convection-diffusion model problem.

More code optimization is possible, such as parallelization; such tasks remain as items for future work.

Acknowledgments
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References


