STABLE FACTORIZATIONS OF SYMMETRIC TRIDIAGONAL AND TRIADIC MATRICES

HAW-REN FANG   AND DIANNE P. O'LEARY*

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Abstract. We call a matrix triadic if it has no more than two nonzero off-diagonal elements in any column. A symmetric tridiagonal matrix is a special case. In this paper we consider LXL^T factorizations of symmetric triadic matrices, where L is unit lower triangular and X is diagonal, block diagonal with 1×1 and 2×2 blocks, or the identity with L lower triangular. We prove that with diagonal pivoting, the LXL^T factorization of a symmetric triadic matrix is sparse, study some pivoting algorithms, discuss their growth factor and performance, analyze their stability, and develop perturbation bounds. These factorizations are useful in computing inertia, in solving linear systems of equations, and in determining modified Newton search directions.

1. Introduction. A symmetric matrix $A \in R^{n \times n}$ can be factored in the form LXL^T in several ways:

1. LL^T *factorization* with L lower triangular and X the identity.
2. LDL^T *factorization* with L unit lower triangular and X diagonal.
3. LBL^T *factorization* with L unit lower triangular and X block diagonal with block order 1 or 2.

These LXL^T factorizations can be used to solve linear systems [1, 3, 4, 5], to determine a downhill search direction in modified Newton methods [9, 10], and to compute the inertia of a matrix [4].

Since not all symmetric matrices have LDL^T factorizations (e.g., $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$), we allow diagonal pivoting and factor PAP^T, where P is a permutation matrix. With diagonal pivoting, we can ensure the existence of an LBL^T factorization of any symmetric matrix and the existence of an LDL^T factorization if A is positive semidefinite or diagonally dominant. Diagonal pivoting is also used to improve numerical stability of the LBL^T factorization when A is indefinite [1, 3, 4, 5]. Interchanging rows and columns can ruin the sparsity of LXL^T factorizations of band matrices, so for tridiagonal matrices, attempts have been made to develop stable algorithms that do not require interchanges[3, 13].

In this paper, we study the sparsity and stability of LXL^T factorizations for a class of symmetric matrices called triadic. A matrix A is *triadic* if the number of non-zero off-diagonal elements in each column is bounded by 2. Tridiagonal matrices are a special case of these, but other matrices, such as block diagonal matrices with full 3×3 blocks, and matrices that are tridiagonal except for entries in each corner are also triadic. These latter matrices arise in solution of differential equations with periodic boundary conditions.

In Section 2 we show that LXL^T factorizations of a symmetric triadic matrix using diagonal pivoting remain sparse. Section 3 reviews various diagonal pivoting strategies for symmetric matrices, and they are applied to triadic matrices in Section 4. In Section 5 the perturbation analysis of these factorizations is discussed. Section 6 gives conclusions. A rounding error analysis for these factorizations is given in [7],

which also includes analysis when A is rank-deficient.

One application of LXL^T factorizations of triadic matrices is in modified Cholesky algorithms to safeguard the Newton method. Modified Cholesky algorithms replace the Hessian matrix A by $A + E$, for a suitable chosen error matrix E, in order to ensure that we are factoring a positive definite matrix and therefore computing a downhill search direction. In a subsequent paper, we will discuss the usefulness of triadic matrices in such algorithms [8].

2. Diagonal pivoting in LXL^T factorization preserves triadic structure. In this section, we show that diagonal pivoting preserves sparsity in the LXL^T factorizations of symmetric triadic matrices. This is a consequence of the property that for any permutation matrix P, PAP^T is symmetric triadic if and only if A is symmetric triadic.

First we consider the sparsity of LDL^T (and thus LL^T) factorizations. The following lemma on the structure of the Schur complements leads to the desired result. We define e_k to be the column vector that is zero except for a 1 in its kth position.

LEMMA 2.1.

Let $A = \begin{bmatrix} a_{11} & c_1^T \\ c_1 & A_{22} \end{bmatrix}$ be a symmetric triadic matrix with $a_{11} \neq 0$. Then the Schur complement $\bar{A} = A_{22} - c_1 c_1^T / a_{11}$ is symmetric triadic.

Proof. Since A is triadic, c_1 has at most two non-zero elements. We denote them by $c_{i1} = \xi$ and $c_{j1} = \eta$. The matrix A_{22} is also triadic and its ith row and jth rows have at most one off-diagonal element each. Moreover,

$$c_1 c_1^T = \xi^2 e_i e_i^T + \xi\eta(e_i e_j^T + e_j e_i^T) + \eta^2 e_j e_j^T$$

has at most four non-zero elements. Two of these are on the diagonal, and the others are in positions (i,j) and (j,i). Thus the sum of A_{22} and $-c_1 c_1^T / a_{11}$ is triadic. ☐

THEOREM 2.2. *In the LDL^T factorization of a symmetric triadic matrix, L is triadic.*

Proof. The proof is by finite induction. At the kth step, assume that the remaining $(n-k+1) \times (n-k+1)$ matrix $\bar{A}$ is symmetric triadic. Then the next column of L is computed as c_1/a_{11} where

$$\bar{A} = \begin{bmatrix} a_{11} & c_1^T \\ c_1 & A_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ c_1/a_{11} & I \end{bmatrix} \begin{bmatrix} a_{11} & 0 \\ 0 & \tilde{A} \end{bmatrix} \begin{bmatrix} 1 & c_1^T/a_{11} \\ 0 & I \end{bmatrix}$$

and $\tilde{A} = A_{22} - c_1 c_1^T / a_{11}$ is the Schur complement of A. Notice that c_1 has at most two elements. By Lemma 2.1, the matrix $\tilde{A}$, which becomes $\bar{A}$ for the next iteration, is triadic, so we can continue the induction. ☐

Now we establish the same result for the LBL^T factorization. The algorithm for LBL^T factorization is the same as LDL^T factorization with diagonal pivoting, except when all diagonal elements of the Schur complement are zeros. In such a case, we diagonally pivot some non-zero off-diagonal element in the lower triangular part to be at the second row and first column in the Schur complement and pivot with respect to the 2×2 block. This decomposition can be used to control element growth for numerical stability, even if we find a nonzero diagonal element [1, 3, 4, 5].

LEMMA 2.3. Let $A = \begin{bmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix}$ be a symmetric triadic matrix, where $A_{11} = \begin{bmatrix} \sigma_1 & a \\ a & \sigma_2 \end{bmatrix}$, $a \neq 0$, and $\det(A_{11}) \neq 0$. Then the Schur complement $\bar{A} = A_{22} - A_{21} A_{11}^{-1} A_{21}^T$ with respect to the 2×2 pivot A_{11} is symmetric triadic.

Proof. Since $\det(A_{11}) \neq 0$, $A_{11}^{-1} = \frac{1}{\det(A_{11})} \begin{bmatrix} \sigma_2 & -a \\ -a & \sigma_1 \end{bmatrix}$. Since A has at most two non-zero off-diagonal elements in each column and A_{11} already has one non-zero off-diagonal element in each column, A_{21} has at most one non-zero element in each column, so we denote it as $A_{21} = \begin{bmatrix} \xi e_i & \eta e_j \end{bmatrix}$. Then

$$
\begin{aligned}
A_{21} A_{11}^{-1} A_{21}^T &= \frac{1}{\det(A_{11})} \begin{bmatrix} \xi e_i & \eta e_j \end{bmatrix} \begin{bmatrix} \sigma_2 & -a \\ -a & \sigma_1 \end{bmatrix} \begin{bmatrix} \xi e_i^T \\ \eta e_j^T \end{bmatrix} \\
&= \frac{1}{\det(A_{11})} (\sigma_2 \xi^2 e_i e_i^T - a\xi\eta e_j e_i^T + \sigma_1 \eta^2 e_j e_j^T - a\xi\eta e_i e_j^T).
\end{aligned}
$$

Thus the only two off-diagonal elements of this matrix are in positions (i, j) and (j, i). Since A is triadic, A_{22} has at most one non-zero element in each of ith and jth rows, so the sum of A_{22} and $A_{21} A_{11}^{-1} A_{21}^T$ is triadic. ∎

THEOREM 2.4. *In the LBL^T factorization of a symmetric triadic matrix, L is triadic.*

Proof. Again the proof is by finite induction. At the kth step, assume that the remaining matrix $\bar{A}$ is triadic. If the next pivot is 1×1, then Lemma 2.1 and the argument in the proof of Theorem 2.2 shows that the the next column of L is triadic, as is the new remaining matrix. If the next pivot is 2×2, then the factorization produces

$$
\bar{A} = \begin{bmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} I_2 & 0 \\ A_{21} A_{11}^{-1} & I_{k-2} \end{bmatrix} \begin{bmatrix} A_{11} & 0 \\ 0 & \tilde{A} \end{bmatrix} \begin{bmatrix} I_2 & A_{11}^{-T} A_{21}^T \\ 0 & I_{k-2} \end{bmatrix},
$$

The off-diagonal part of the two new columns of L are

$$
\begin{aligned}
A_{21} A_{11}^{-1} &= \frac{1}{\det(A_{11})} \begin{bmatrix} \xi e_i & \eta e_j \end{bmatrix} \begin{bmatrix} \sigma_2 & -a \\ -a & \sigma_1 \end{bmatrix} \\
&= \frac{1}{\det(A_{11})} \begin{bmatrix} \sigma_2 \xi e_i - a\eta e_j & -a\xi e_i + \sigma_1 \eta e_j \end{bmatrix},
\end{aligned}
$$

also triadic, and Lemma 2.3 shows that $\tilde{A}$ is triadic, so the induction can be continued. ∎

Combining these two theorems with the fact that the triadic property of a matrix is preserved under symmetric permutation, we see that sparsity is preserved in all of these factorizations if diagonal pivoting is used.

THEOREM 2.5. *If we factor a symmetric triadic matrix using any LXL^T factorization with diagonal pivoting, then L is triadic.*

Although the columns of L are sparse, the number of non-zero elements in each row of L is bounded only by n; if A is tridiagonal, for example, and

$$
\tilde{Z} = \begin{bmatrix} 0 & & & 1 \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{bmatrix}
$$

is the circular shift-down matrix, then the last row of L in the factorization $\tilde{Z} A \tilde{Z}^T = LDL^T$ is generally full.

3. Diagonal pivoting strategies for symmetric indefinite matrices. If the symmetric matrix $A \in R^{n \times n}$ is positive semidefinite [6][14, Section 9.5] or diagonally dominant [14, Section 10] (i.e., $|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|$ for $i = 1, \ldots, n$), then the largest magnitude element will appear on the diagonal. Each Schur complement inherits the property of positive semidefiniteness or diagonal dominance. Therefore, in either case, the elements of L in the LDL^T factorization are bounded in magnitude by 1. It has been shown that the growth factor for D is $\rho(A) = 1$ if A is symmetric positive semi-definite, and $\rho(A) \leq 2$ if A is diagonally dominant, where $\rho(A)$ is the ratio of the largest element in the Schur complements to the largest element in A.

We would like to compute factorizations of symmetric indefinite matrices that also give bounds on the elements of L and B. In order to do this, it is necessary to pivot. There are three kinds of pivoting strategies in the literature: Bunch-Parlett [5] (complete pivoting); bounded Bunch-Parlett and fast Bunch-Kaufman [1] (rook pivoting); and Bunch-Kaufman [4] (partial pivoting). For full matrices, complete pivoting requires $O(n^3)$ comparisons, partial pivoting requires $O(n^2)$, and the cost of rook pivoting varies between $O(n^2)$ and $O(n^3)$. Therefore, it is important to uncover the advantages of the more expensive strategies. We consider each strategy in turn, applying each to the current Schur complement matrix A, noting that each depends on a preset constant $0 < \alpha < 1$.

3.1. Complete pivoting. Bunch and Parlett [5] devised the pivoting strategy presented in Algorithm 1.

Algorithm 1 Bunch-Parlett pivot selection

Let a_{kk} be the largest magnitude diagonal element.
Let a_{ij} $(i < j)$ be the largest magnitude off-diagonal element.
if $|a_{kk}| \geq \alpha |a_{ij}|$ **then**
  Use a_{kk} as a 1×1 pivot.
else
  Use $\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}$ as a 2×2 block pivot.
end if

The process continues until $a_{kk} = a_{pq} = 0$ or the factorization completes. The resulting pivot satisfies the following *strong condition*:

1. If a 1×1 pivot a_{kk} is chosen, then $|a_{kk}| \geq \alpha |a_{pk}|$ for $p \neq k$.

2. If a 2×2 block pivot $\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}$ is chosen, then each of the 1×1 pivots a_{ii} and a_{jj} satisfy $|a_{ii}| < \alpha |a_{ij}|$ and $|a_{jj}| < \alpha |a_{ij}|$, and a_{ij} is the element of maximum magnitude in both column i and column j.

For any algorithm satisfying the strong condition, the elements in L are bounded and the element growth in B during the factorization is well controlled as we will show in Subsection 3.5.

3.2. Rook pivoting. The cost for finding a pivot satisfying the strong condition can be reduced by the iterative process in Algorithm 2.

If the initial pivot index $i = 1$, this is called *bounded Bunch-Kaufman* pivot selection, while if a_{ii} is the maximal magnitude diagonal element, it is called *fast Bunch-Parlett* pivot selection [1]. Note that for fast Bunch-Parlett selection, we do not need to test whether a_{jj} is a 1×1 pivot, because the initial maximum magnitude

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Algorithm 2 Pivot selection by rook pivoting, given an initial pivot index i

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Find the index $j \neq i$ such that $|a_{ji}| = \max_{p \neq i} |a_{pi}|$.
if $|a_{ii}| \geq \alpha|a_{ji}|$ **then**
  Use a_{ii} as a 1×1 pivot.
else
  Find the index $k \neq j$ such that $|a_{kj}| = \max_{p \neq j} |a_{pj}|$.
  repeat
    if $|a_{jj}| \geq \alpha|a_{kj}|$ **then**
      Use a_{jj} as a 1×1 pivot.
    else if $|a_{ij}| = |a_{kj}|$ **then**
      Use $\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}$ as a 2×2 pivot.
    else
      Set $i := j$ and $j := k$.
      Find index $k \neq j$ such that $|a_{kj}| = \max_{p \neq j} |a_{pj}|$.
    end if
  until a pivot is chosen.
end if

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diagonal element a_{ii} failed to be a pivot at the beginning, $|a_{jj}|$ is at most $|a_{ii}|$, and $|a_{ij}|$ is increasing in the loop.

   3.3. Partial pivoting. Bunch and Kaufman [4] devised the efficient pivoting strategy shown in Algorithm 3.

Algorithm 3 Bunch-Kaufman pivot selection, given an initial pivot index i

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Find the index $j \neq i$ such that $|a_{ji}| = \max_{p \neq i} |a_{pi}| =: \lambda$.
if $|a_{ii}| \geq \alpha\lambda$, **then**
  Use a_{ii} as a 1×1 pivot.
else
  Compute $\sigma := \max_{p \neq j} |a_{pj}| \geq \lambda$.
  if $|a_{ii}|\sigma \geq \alpha\lambda^2$ **then**
    Use a_{ii} as a 1×1 pivot.
  else if $|a_{jj}| \geq \alpha\sigma$ **then**
    Use a_{jj} as a 1×1 pivot.
  else
    Use $\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}$ as a 2×2 pivot.
  end if
end if

   Bunch-Kaufman pivoting does not guarantee the strong condition, but satisfies the following *weak condition*:
   1. If a 1×1 pivot a_{kk} is chosen, then
      - $|a_{kk}| \max_{p \neq q}\{|a_{pq}| : (a_{qk} \neq 0 \text{ or } q = k)\} \geq \alpha \max_{p \neq k} |a_{pk}|^2$.
   2. If a 2×2 block pivot $\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}$ is chosen, then
      - $|a_{ii}| < \alpha\lambda$,
      - $|a_{ii}|\sigma < \alpha\lambda^2$,

- $|a_{jj}| < \alpha\sigma$,

where $\lambda = \max_{k \neq i} |a_{ki}|$ and $\sigma = \max_{k \neq j} |a_{kj}|$.

We compare the weak condition with the strong condition. For 1×1 pivots, $\max\{|a_{pq}| : p \neq q \text{ and } (a_{qk} \neq 0 \text{ or } q = k)\} \geq \max_{p \neq k} |a_{pk}|$ so the strong condition guarantees the weak condition. For 2×2 block pivots, the weak condition meets the strong condition if $\sigma = \lambda$. We conclude that the strong condition implies the weak condition.

The natural choice of the initial pivot index i in Algorithm 3 is $i = 1$, which achieves the least cost to satisfy the weak condition[4].

Ashcraft, Grimes and Lewis [1] argued that a bounded L can improve stability. We can improve the probability that the Bunch-Kaufman algorithm has a bounded L by choosing the largest magnitude diagonal entry as the search starting point at each pivot step [4]. The additional number of comparisons is $\frac{n^2}{2} + O(n)$, so the total comparison count remains $O(n^2)$. By making this change, we usually find a 1×1 pivot at the very first test at each step of pivot selection. The strong condition usually holds, but it is not guaranteed as shown in the following example [12].

$$A = \begin{bmatrix} \epsilon^2 & \epsilon & \epsilon \\ \epsilon & 0 & 1 \\ \epsilon & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & & \\ \frac{1}{\epsilon} & 1 & \\ \frac{1}{\epsilon} & 0 & 1 \end{bmatrix} \begin{bmatrix} \epsilon^2 & & \\ & -1 & \\ & & -1 \end{bmatrix} \begin{bmatrix} 1 & \frac{1}{\epsilon} & \frac{1}{\epsilon} \\ & 1 & 0 \\ & & 1 \end{bmatrix} = LBL^T,$$

where L is unbounded as $\epsilon \to 0$.

3.4. The weak condition controls the growth factor for B. In summary, the Bunch-Parlett, fast Bunch-Parlett, and bounded Bunch-Kaufman pivoting strategies satisfy the strong condition, whereas the Bunch-Kaufman pivoting strategy and that of Ashcroft *et al.* satisfy the weak condition. The weak condition controls element growth in B during the factorization, as shown by an argument similar to those in [1, 4, 5, 12] [14, chapter 11]. The *growth factor* in factoring $A \in R^{n \times n}$ is defined by

$$(3.1) \qquad \rho(A) = \frac{\max_{i,j,k} |a_{ij}^{(k)}|}{\max_{i,j} |a_{ij}|} \equiv \frac{\max_k \|A^{(k)}\|_M}{\|A\|_M},$$

where a_{ij} and $a_{ij}^{(k)}$ are the (i,j) entries of A and $A^{(k)}$, respectively and $\|\cdot\|_M$ is the maximum magnitude element in the given matrix.

When a 1×1 pivot is chosen, we have

$$(3.2) \qquad \frac{\max_{p \neq k} |a_{pk}|^2}{|a_{kk}|} \leq \frac{1}{\alpha} \max\{|a_{pq}| : p \neq q \text{ and } (a_{qk} \neq 0 \text{ or } q = k)\}$$

$$\leq \frac{1}{\alpha} \max_{p \neq q} |a_{pq}|.$$

Therefore, the element growth is bounded by $1 + \frac{1}{\alpha}$.

If a 2×2 block pivot is chosen, the weak condition guarantees $|a_{ii}a_{jj}| < \alpha^2 \lambda^2$. Then

$$(3.3) \qquad |\det(\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix})| = |a_{ij}^2 - a_{ii}a_{jj}| > (1 - \alpha^2)\lambda^2.$$

Since $0 < \alpha < 1$,

$$|\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix}^{-1}| < \frac{1}{(1 - \alpha^2)\lambda^2} \begin{bmatrix} |a_{jj}| & \lambda \\ \lambda & |a_{ii}| \end{bmatrix}.$$

Therefore, the increase of each element in magnitude for the 2×2 block decomposition is bounded by

$$\frac{1}{(1-\alpha^2)\lambda^2} \begin{bmatrix} \lambda & \sigma \end{bmatrix} \begin{bmatrix} |a_{jj}| & \lambda \\ \lambda & |a_{ii}| \end{bmatrix} \begin{bmatrix} \lambda \\ \sigma \end{bmatrix} = \frac{1}{(1-\alpha^2)\lambda^2}(\lambda^2(|a_{jj}|+\sigma)+(\lambda^2+\sigma|a_{ii}|)\sigma)$$

$$< \frac{1}{(1-\alpha^2)\lambda^2}(\lambda^2(\alpha\sigma+\sigma)+(\lambda^2+\alpha\lambda^2)\sigma)$$

(3.4)
$$= \frac{2(1+\alpha)\sigma}{1-\alpha^2} = \frac{2\sigma}{1-\alpha},$$

and the element growth for the 2×2 block decomposition is bounded by $1+\frac{2}{1-\alpha}$.

Therefore, element growth in B is bounded by

$$g = \max\{1+\frac{1}{\alpha}, \sqrt{1+\frac{2}{1-\alpha}}\}.$$

The minimum of g is $\frac{1+\sqrt{17}}{2} \approx 2.56$, which is attained when $\alpha = \frac{1+\sqrt{17}}{8} \approx 0.64$.

Thus

(3.5)
$$\frac{\max_k \|A^{(k)}\|_M}{\|A\|_M} = \rho(A) \le g^{n-1}.$$

The attainability of the last inequality is a research problem [14, Problem 11.10].

With complete pivoting (the Bunch-Parlett pivoting strategy), we can bound the growth factor of $A \in R^{n \times n}$ as

$$\rho(A) \le 3nf(n), \text{ where } f(n) = (\prod_{k=2}^{n} k^{1/(k-1)})^{1/2} \le 1.8n^{(\ln n)/4}$$

with the pivoting argument $\alpha = \frac{1+\sqrt{17}}{8}$. This was shown by Bunch [2] with an analysis similar to Wilkinson's for Gaussian elimination with complete pivoting [15].

We note that the bounds on element increases in (3.2) and (3.4) are in terms of off-diagonal elements. Therefore, the growth factor $\bar{\rho}(A)$ for off-diagonal elements is bounded by g^{n-2}, i.e.,

(3.6)
$$\bar{\rho}(A) = \frac{\max_{i \neq j,k} |a_{ij}^{(k)}|}{\max_{i \neq j} |a_{ij}|} \le g^{n-2}.$$

This is attainable, for example, with $\alpha = \frac{1+\sqrt{17}}{8}$ and

$$A = \begin{bmatrix} -\alpha & 1 & 1 & \cdots & 1 \\ 1 & -\alpha g - \frac{1}{\alpha} & 1 & \cdots & 1 \\ 1 & 1 & -\alpha g^2 - \frac{g}{\alpha} & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 1 \\ 1 & 1 & \cdots & 1 & -\alpha g^{n-1} - \frac{g^{n-2}}{\alpha} \end{bmatrix}.$$

The weak condition is stronger than necessary to bound the growth factor; we need only

$$|a_{kk}| \max_{p \neq q} |a_{pq}| \ge \alpha \max_{p \neq k} |a_{pk}|^2$$

for 1×1 pivots, but our version of the weak condition is useful for the triadic case considered in Subsection 4.2.

In practice, the average growth factors for both tridiagonal and full matrices are far from this bound. Figure 3.1 shows the maximum growth factor of $20,000$ random symmetric $n \times n$ matrices for each $n = 1, \ldots, 100$ with $\alpha = \frac{1+\sqrt{17}}{8} \approx 0.64$. In our experiments, all matrix elements are drawn independently from a uniform distribution on $[-1, 1]$; results for a normal distribution are similar. Although $\alpha \approx 0.64$ minimizes the a priori bound on the growth factor, our experiments show that the best α to minimize the average growth factor with Bunch-Kauffman pivoting is usually between 0.74 and 0.78, as shown in Figure 3.2, where $20,000$ random matrices are generated for each matrix size and each α.
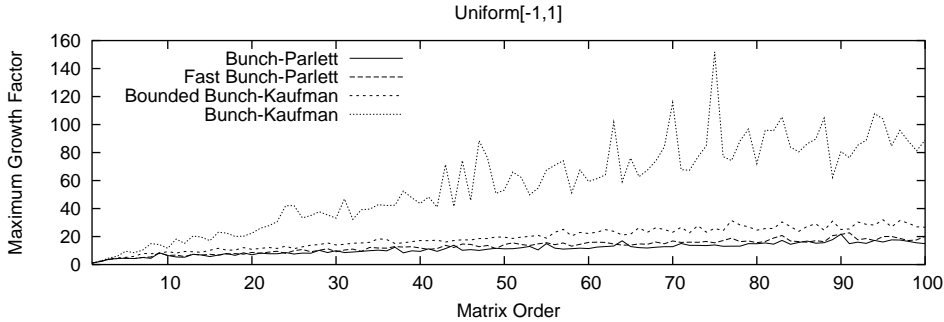
FIG. 3.1. *Experimental maximum growth factor for factoring a symmetric matrix.*
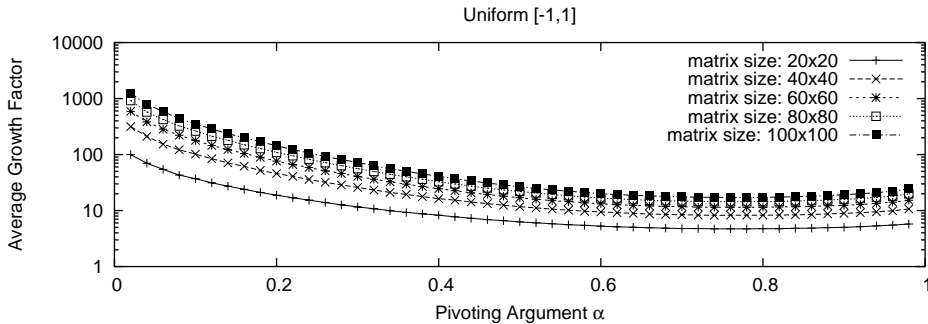
FIG. 3.2. *Experimental average growth factor for factoring a symmetric matrix, Bunch-Kaufman.*

3.5. The strong condition bounds elements in L. The weak condition does not bound L for general matrices. For example [12][14, Section 11.1.2],

$$A = \begin{bmatrix} 0 & \epsilon & \\ \epsilon & 0 & 1 \\ & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ \frac{1}{\epsilon} & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \epsilon & \\ \epsilon & 0 & \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & \frac{1}{\epsilon} \\ & 1 & 0 \\ & & 1 \end{bmatrix} = LBL^T,$$

when the Bunch-Kaufman pivoting strategy is applied. As $\epsilon \to 0$, L is unbounded.

In contrast, the strong condition does ensure a bound on elements in L. When a 1×1 pivot is chosen, then the magnitude of elements in the pivot column of L is

bounded by $\frac{1}{\alpha}$. If a 2×2 block pivot is chosen, the strong condition implies $\lambda = \sigma$ and therefore the two columns of L corresponding to this 2×2 block pivot have elements bounded by

$$\frac{1}{(1-\alpha^2)\lambda^2} \begin{bmatrix} \lambda & \sigma \end{bmatrix} \begin{bmatrix} |a_{jj}| & \lambda \\ \lambda & |a_{ii}| \end{bmatrix} < \frac{1}{(1-\alpha^2)\lambda^2} \begin{bmatrix} \lambda & \lambda \end{bmatrix} \begin{bmatrix} \alpha\lambda & \lambda \\ \lambda & \alpha\lambda \end{bmatrix}$$
$$= \frac{1+\alpha}{1-\alpha^2} \begin{bmatrix} 1 & 1 \end{bmatrix} = \frac{1}{1-\alpha} \begin{bmatrix} 1 & 1 \end{bmatrix}.$$

Therefore, the elements in L are bounded in magnitude by

$$\gamma = \max\{\frac{1}{\alpha}, \frac{1}{1-\alpha}\}.$$

3.6. The growth factor and element bounds. We summarize the results on element growth in the following theorem, which extends some previous results to general α.

THEOREM 3.1. *For LBL^T factorization of a symmetric matrix $A \in R^{n \times n}$, if the weak condition holds, then the growth factor $\rho(A)$ defined in (3.1) is bounded by*

$$\rho(A) \le g^{n-1}$$

where

$$g = \max\{1 + \frac{1}{\alpha}, \sqrt{1 + \frac{2}{1-\alpha}}\},$$

where α is the parameter in the factorization algorithm. If the strong condition holds, then the elements in L are bounded in magnitude by

$$\gamma = \max\{\frac{1}{\alpha}, \frac{1}{1-\alpha}\}.$$

As shown above, $\alpha = \frac{1+\sqrt{17}}{8}$ minimizes the element growth g. But $\alpha = 0.5$ minimizes the bound γ on the elements of L. The consequences of each of these choices are summarized in Table 3.1.

TABLE 3.1
The element growth bound g for B and the bound γ for L (when complete or rook pivoting is used) with two optimal choices of α.

	α	γ	g
minimize g	$\frac{1+\sqrt{17}}{8} \approx 0.64$	$\frac{1+\sqrt{17}}{2} \approx 2.56$	$\frac{8}{7-\sqrt{17}} \approx 2.78$
minimize γ	$\frac{1}{2}$	3	3

4. Diagonal pivoting strategies for triadic symmetric matrices. In Section 2, we showed that sparsity is preserved in the LXL^T factorization of a symmetric triadic matrix with any diagonal pivoting strategy. In this section, we study a pivoting strategy particular to symmetric tridiagonal matrices [3] and also apply the pivoting strategies from the previous section to triadic matrices.

Algorithm 4 Bunch's pivot selection

$\alpha = \frac{\sqrt{5}-1}{2} \approx 0.62$
if $|a_{11}|\sigma \geq \alpha|a_{21}|^2$ **then**
    Use a_{kk} as a 1×1 pivot.
else
    Use $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ as a 2×2 block pivot.
end if

4.1. A pivoting strategy specific to symmetric tridiagonal matrices.
One pivoting strategy has been proposed for LBL^T factorizations of irreducible tridiagonal matrices. Consider the variant proposed by Higham [13] of the algorithm of Bunch [3] represented in Algorithm 4, with parameter $\sigma = max_{i,j}|a_{ij}|$. The algorithm's great advantage is that there are *no* interchanges of rows and columns, yet the growth factor is bounded by

$$\rho(A) = \max\{1 + \frac{1}{\alpha}, \frac{1}{1-\alpha}\},$$

whose minimum is achieved by choosing $\alpha = \frac{\sqrt{5}-1}{2}$. This method is excellent for applications relying on B, (e.g., computing inertia), but there is no element bound on L, illustrated, for example, as $\epsilon \to 0$ and

$$A = \begin{bmatrix} \epsilon^2 & \epsilon \\ \epsilon & 1 \end{bmatrix} = \begin{bmatrix} 1 & \\ 1/\epsilon & 1 \end{bmatrix} \begin{bmatrix} \epsilon^2 & \\ & 0 \end{bmatrix} \begin{bmatrix} 1 & 1/\epsilon \\ & 1 \end{bmatrix}.$$

A similar example is given in [13]. Therefore, this algorithm is not well suited to computing Newton-like directions or solving circulant systems of equations. Nevertheless, Higham showed that it is a stable method for solving linear symmetric tridiagonal systems [13].

4.2. Pivoting strategies from those for dense matrices. All the pivoting strategies from Section 3 can be applied to a symmetric triadic matrix $A \in R^{n \times n}$. The growth factor is constrained because of the triadic structure, and we obtain a sharper result for $\rho(A)$ than that of Theorem 3.1, although the bound γ on the elements of L remains the same.

THEOREM 4.1. *For LBL^T factorization of a symmetric triadic $A \in R^{n \times n}$, consider the growth factor of off-diagonal elements, defined in (3.1). If the weak condition holds,*

$$\rho(A) \leq \begin{cases} \frac{4g(g^{(n-3)/2}-1)}{g-1} + 2(g^{(n-1)/2} + g^{(n+1)/2}) + 1, & \text{if } n \text{ odd.} \\ \frac{4g(g^{(n-2)/2}-1)}{g-1} + 2g^{n/2} + 1, & \text{if } n \text{ even.} \end{cases}$$

That is, $\rho(A) = O(g^{n/2})$. If the strong condition holds,

$$\rho(A) \leq 2ng^{\lfloor \lg(n-1) \rfloor} \leq 2n(n-1)^{\lg g} = \Theta(n^{1+\lg g}),$$

where $g = \max\{\frac{1}{\alpha}, \frac{1}{1-\alpha^2}\}$.

The proof of this theorem is given in Appendix A.

If we choose $\alpha = \frac{\sqrt{5}-1}{2}$ to minimize g, then $\lg g \approx 0.694$, and therefore the bound for the strong condition is sub-quadratic. Even linear growth is rare, but it

is possible; for example, if we take the circulant matrix A with second row equal to $[1, -2, 1, 0, \ldots, 0]$, and change its (1,1) element to -1, then $\rho(A) = n/2 + O(1)$.

For the weak condition, exponential growth is achievable: let

$$(4.1) \qquad A = \begin{bmatrix} -a & -1 & & 1 & & & & & \\ -1 & -a & & & & & & & 1 \\ & & -a & -1 & & 1 & & & \\ 1 & & -1 & (g-1)a & & & & & 0 \\ & & & & -a & -1 & & \ddots & \\ & & 1 & & -1 & (g-1)a & & & 0 \\ & & & & & & \ddots & \ddots & \vdots \\ & & \ddots & & & & \ddots & \ddots & 0 \\ & 1 & & 0 & & 0 & \cdots & 0 & 1 \end{bmatrix},$$

where $|a| < \alpha$. Then when $|a| \to \alpha^-$, $\rho(A) = \Theta(g^{n/2})$ and the explicit zeros indicate where the growth is maximal. Despite these examples, in our experiments, $\rho(A)$ is almost always bounded by a constant for both the weak and the strong conditions.

Although $\alpha = \frac{\sqrt{5}-1}{2} \approx 0.618$ minimizes the a priori bound on the relative element increase, our experiments show that the best α to minimize the average growth factor is usually between 0.82 and 0.86 for Bunch-Kaufman pivoting, as illustrated in Figure 4.1, where $20,000$ random matrices are generated for each matrix size and α.

FIG. 4.1. *Experimental average growth factor for Bunch-Kaufman pivoting on a symmetric circulant triadic matrix or a tridiagonal matrix.*

With pivoting argument $\alpha = \frac{\sqrt{5}-1}{2}$, there are symmetric triadic matrices A having

$\rho(A) = \Theta(g^{n/2})$ and $\rho(A) = \Theta(n)$ for the weak and strong conditions, respectively. But our experiments show that, in practice, LBL^T factorizations of symmetric tridiagonal or symmetric tridiagonal matrices with corner elements added usually show only constant growth in $\rho(A)$, whenever any of the four pivoting strategies are applied. Figure 4.2 shows the maximum growth factor of $20,000$ random symmetric tridiagonal $n \times n$ matrices for each $n = 1, \ldots, 100$ and for random symmetric circulant matrices with 3 bands.
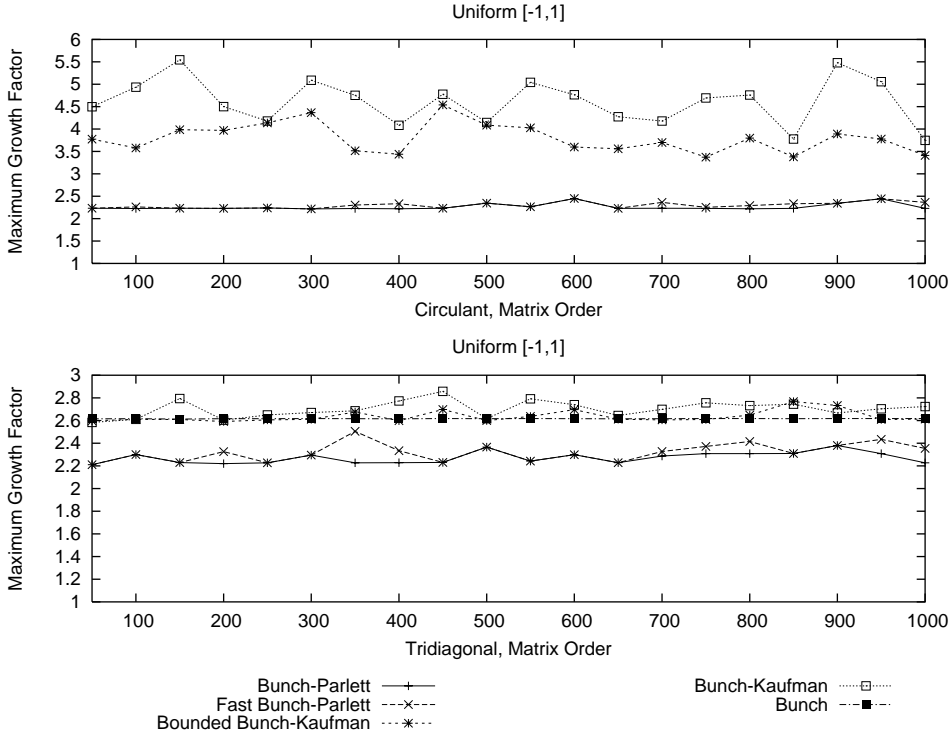

FIG. 4.2. *Experimental average growth factor for factoring a symmetric circulant triadic matrix or a tridiagonal matrix.*

4.3. Pivoting cost. When the Bunch-Parlett algorithm is applied, it is natural to search the whole matrix instead of only the lower (or upper) triangular part due to the data structure for sparse matrices. So the number of comparisons is at most $3k + O(1)$ to select a pivot in a $k \times k$ Schur complement. Therefore, the total number of comparisons is bounded by $\frac{3}{2}n^2 + O(n)$ for a symmetric triadic $A \in R^{n \times n}$, which is more expensive than the $O(n)$ cost of the factorization. The Bunch-Kaufman algorithm requires at most $5n + O(1)$ comparisons for a symmetric triadic $A \in R^{n \times n}$. For the bounded Bunch-Parlett and fast Bunch-Kaufman pivoting strategies, the worst case number of comparisons is the same as that of Bunch-Parlett pivoting. The average number of element comparisons is between that for the Bunch-Kaufman and Bunch-Parlett pivoting strategies. Figure 4.3 shows the average number of comparisons of $1,000,000$ symmetric matrices for each $n = 1, \ldots, 100$.

5. Perturbation theory. The perturbation analysis of LL^T factorization of a positive semidefinite symmetric matrix with complete pivoting is discussed in [11].
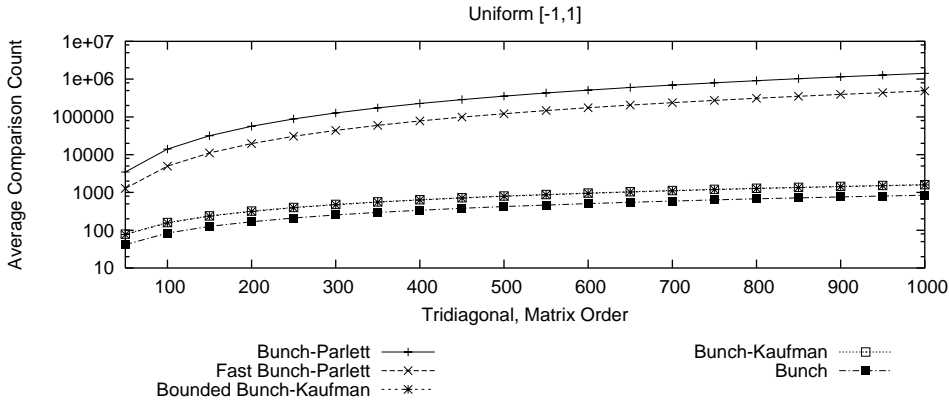
FIG. 4.3. *Experimental average number of comparisons to factor a symmetric tridiagonal matrix.*

Partition A as

$$A = \left[\begin{array}{cc} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{array} \right]$$

where $A_{11} \in \mathcal{R}^{k \times k}$, and partition L and E accordingly. Assume that both A_{11} and $A_{11} + E_{11}$ are nonsingular, and let $W = A_{11}^{-1} A_{21}^T = L_{11}^{-T} L_{21}^T$. In [11], Higham showed that with complete pivoting applied to a general positive semidefinite matrix,

$$\|W\|_{2,F} \leq \sqrt{\frac{1}{3}(n-k)(4^k - 1)}.$$

We give bounds on $\|W\|_{2,F}$ for LXL^T factorization of both full symmetric and symmetric triadic matrices.

THEOREM 5.1. *Let $S_k(A)$ be the Schur complement appearing in an LXL^T factorization of a symmetric matrix A after processing the first k columns and k rows, $k < n$. Suppose there is a symmetric perturbation in A, denoted by E. Let $\|\cdot\|$ be a p-norm or the Frobenius norm. Assume that both A_{11} and $A_{11} + E_{11}$ are nonsingular. Then*

$$S_k(A + E) - S_k(A) = E_{22} - (E_{21}W + W^T E_{21}^T) + W^T E_{11}W + O(\|E\|^2),$$

so

$$|S_k(A + E) - S_k(A)| \leq |E_{22}| + |E_{21}||W| + |W^T||E_{21}^T| + |W^T||E_{11}||W| + O(\|E\|^2)$$

and

$$\|S_k(A + E) - S_k(A)\| \leq \|E\|(1 + \|W\|^2)^2 + O(\|E\|^2),$$

where

$$\|W\| \leq \sqrt{\frac{\gamma}{\gamma + 2}(n - k)\left((1 + \gamma)^{2k} - 1\right)}$$

and γ is a bound on the absolute value of the elements of L.

If A is triadic, then this bound improves to

$$\|W\| \le 2\gamma\Phi_\gamma\sqrt{\frac{\Phi_\gamma^{2k} - 1}{\Phi_\gamma^2 - 1}},$$

where

$$\Phi_\gamma = \frac{1 + \sqrt{1 + 4/\gamma}}{2}\,\gamma.$$

The proof of the theorem is contained in the following series of lemmas. We begin by generalizing to LXL^T factorizations a result of Higham [11] for LL^T factorization.

LEMMA 5.2. *Let $S_k(A)$ be the Schur complement appearing in an LXL^T factorization of a symmetric matrix A after processing the first k columns and k rows, $k < n$. Suppose there is a symmetric perturbation in A, denoted by E. Partition A as*

$$A = \left[\begin{array}{cc} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{array}\right]$$

where $A_{11} \in \mathcal{R}^{k \times k}$, and partition E accordingly. If A_{11} and $A_{11} + E_{11}$ are nonsingular then

$$S_k(A + E) = S_k(A) + E_{22} - (E_{21}W + W^T E_{21}^T) + W^T E_{11} W + O(\|E\|^2),$$

where $W = A_{11}^{-1} A_{21}^T$.

Proof. The factorization takes the form

$$A = \left[\begin{array}{cc} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{array}\right] = \left[\begin{array}{cc} L_{11} & \\ L_{21} & I_{n-k} \end{array}\right]\left[\begin{array}{cc} X & \\ & S_k(A) \end{array}\right]\left[\begin{array}{cc} L_{11}^T & L_{21}^T \\ & I_{n-k} \end{array}\right],$$

where $L_{11} \in \mathcal{R}^{k \times k}$ is lower triangular and the symmetric matrix $X \in \mathcal{R}^{k \times k}$ is block diagonal with block order 1 or 2. The matrix X is either the identity, a diagonal matrix, or a block diagonal matrix, depending on the factorization. In any case, $A_{11} = L_{11}XL_{11}^T$ and $A_{21} = L_{21}XL_{11}^T$. Therefore, $W = A_{11}^{-1}A_{21}^T = L_{11}^{-T}L_{21}^T$. We also know that $S_k(A) = A_{22} - A_{21}A_{11}^{-1}A_{21}^T$ and since A_{11} is nonsingular, $(A_{11} + E_{11})^{-1} = (I + A_{11}^{-1}E_{11})^{-1}A_{11}^{-1} = (I - A_{11}^{-1}E_{11})A_{11}^{-1} + O(\|E_{11}\|^2)$. The result is obtained by substituting the previous two equations into $S_k(A + E) = (A_{22} + E_{22}) - (A_{21} + E_{21})(A_{11} + E_{11})^{-1}(A_{21} + E_{21})^T$ and collecting the $O(\|E\|^2)$ terms. □

Next, we bound the elements in $W = L_{11}^{-T}L_{21}^T$.

LEMMA 5.3. *If L is unit lower triangular, with off-diagonal elements bounded in absolute value by γ, then*

$$|W| = |L_{11}^{-T}L_{21}^T| \le \gamma y e^T$$

where $y_{k-j} = (1 + \gamma)^{j+1} - 1$ and e is a vector of ones.

Proof. The matrix W satisfies $L_{11}^T W = L_{21}^T$, so let's consider a single column of this relationship. Letting r be a column of W. We will compute a vector y satisfying $|r| \le y$. Note that $|r_k|/\gamma$ is bounded by 1, and $|r_{k-j}|/\gamma$ is bounded by 1 plus the sum of the later entries in r. If we let s_{k-j} be a bound on the sum of the entries $k - j, \ldots, k$, then for $j = 1, 2, \ldots, k - 1$, we have the recursions

$$y_{k-j} = \gamma(1 + s_{k-j+1}),$$
$$s_{k-j} = s_{k-j+1} + y_{k-j},$$

with $y_k = \gamma$ and $s_k = \gamma$. The solution to these recursions is

$$y_{k-j} = \gamma(1+\gamma)^j,$$
$$s_{k-j} = (1+\gamma)^{j+1} - 1.$$

Therefore, each column of W is bounded in absolute value by y and the result follows.
□

The bound on $\|W\|$ follows immediately. This takes care of the general case and leaves only the triadic bound to be demonstrated. We begin with two simple lemmas and then proceed to the main result.

LEMMA 5.4. *Let* $F_\gamma(n) = \sum_{i=1}^{\lceil n/2 \rceil} \binom{n-i}{i-1} \gamma^{n-i}$ *and* $\Phi_\gamma = \frac{1+\sqrt{1+4/\gamma}}{2}\gamma$. *Then*

$$\frac{1}{1+(1/\gamma)}\Phi_\gamma^{n-1} \le F_\gamma(n) \le \Phi_\gamma^{n-1}$$

for $n = 1, 2, \ldots$ *and* $\gamma > 0$.

Proof. We first observe that $F_\gamma(n) = \gamma(F_\gamma(n-1) + F_\gamma(n-2))$ for $n > 2$, with $F_\gamma(1) = 1$ and $F_\gamma(2) = \gamma$. Note that $\gamma + \gamma\Phi_\gamma = \Phi_\gamma^2$. The result can be obtained by mathematical induction. □

LEMMA 5.5. *Let* $C \ge 0$ *be an* $m \times n$ *matrix with* $n \ge 2$. *Then* $\|C\|_p \le \|C\hat{I}\|_p$, *where* $1 \le p \le \infty$ *or* $p = F$, *and the* $n \times (n-1)$ *matrix* $\hat{I}$ *is the identity matrix of size* $n - 1$, *with its last row repeated.*

Proof. The cases of $p = F$ (Frobenius-norm) and $p = \infty$ (∞-norm) are trivial. When $0 \le p < \infty$, $\|C\|_p = \max_{\|x\|_p=1} \|Cx\|_p = \|Cz\|_p$ and this value is achieved for some z with $\|z\|_p = 1$. Note that $z_i \ge 0$ for $i = 1, \ldots, n$, since all the elements of C are non-negative. Let $\hat{z} = [z_1, \ldots, z_{n-2}, \max(z_{n-1}, z_n)]^T$. Then $\|\hat{z}\|_p \le 1$, and

$$\|C\|_p = \|Cz\|_p \le \|C\hat{I}\hat{z}\|_p \le \|C\hat{I}(\hat{z}/\|\hat{z}\|_p)\|_p \le \max_{\|x\|_p=1} \|C\hat{I}x\|_p = \|C\hat{I}\|_p.$$

□

LEMMA 5.6. *The* LBL^T *factorization for symmetric triadic matrices has*

$$\|W\| \le 2\gamma\Phi_\gamma \sqrt{\frac{\Phi_\gamma^{2k} - 1}{\Phi_\gamma^2 - 1}} = O(\Phi_\gamma^k).$$

Proof. Recall that $W = L_{11}^{-T}L_{21}^T \in R^{k \times (n-k)}$. Since L_{11} is triadic, $|L_{11}^{-T}e| \le y$, where

$$y_{k-j} = \gamma(y_{k-j+1} + y_{k-j+2})$$

for $j = 2, \ldots, k-1$ with base case $y_k = \gamma$ and $y_{k-1} = \gamma + \gamma^2$. By Lemma 5.4,

$$y_{k-j+1} = F_\gamma(j+1) = \sum_{i=1}^{\lceil (j+1)/2 \rceil} \binom{j+1-i}{i-1} \gamma^{j+1-i}$$

for $j = 1, \ldots, k$. Therefore,

(5.1) $$\|L_{11}^{-T}e\| \le \|y\| \le \sqrt{\sum_{j=1}^{k} \Phi_\gamma^{2j}} \le \Phi_\gamma \sqrt{\frac{\Phi_\gamma^{2k} - 1}{\Phi_\gamma^2 - 1}}.$$

Because of the triadic structure, each row of L_{21}^T has at most two non-zero elements. Let $|L_{21}^T| = R_1 + R_2$, where the non-zeros in R_1 are the first non-zero elements in each row and R_2 contains of the seconds. Then

$$\|L_{11}^{-T} L_{21}^T\| \le \| \, |L_{11}^{-T}| \, |L_{21}^T| \, \| \le \| \, |L_{11}^{-T}| \, R_1\| + \| \, |L_{11}^{-T}| \, R_2\|.$$

By Lemma 5.5 and (5.1),

$$
\begin{aligned}
\| \, |L_{11}^{-T}| \, R_1\| &\le \| \, |L_{11}^{-T}| \, R_1 \hat{I}_{n-k}\| \\
&\le \| \, |L_{11}^{-T}| \, R_1 \hat{I}_{n-k} \hat{I}_{n-k-1}\| \\
&\le \cdots \le \| \, |L_{11}^{-T}| \, R_1 \hat{I}_{n-k} \hat{I}_{n-k-1} \cdots \hat{I}_2\| \\
&\le \| \, |L_{11}^{-T}| \, (\gamma e)\| \\
&\le \gamma \Phi_\gamma \sqrt{\frac{\Phi_\gamma^{2k} - 1}{\Phi_\gamma^2 - 1}}.
\end{aligned}
$$

Similarly, $\| \, |L_{11}^{-T}| \, R_2\| \le \gamma \Phi_\gamma \sqrt{\frac{\Phi_\gamma^{2k}-1}{\Phi_\gamma^2-1}}$. Therefore,

$$\|W\| = \|L_{11}^{-T} L_{21}^T\| \le 2\gamma \Phi_\gamma \sqrt{\frac{\Phi_\gamma^{2k} - 1}{\Phi_\gamma^2 - 1}}.$$

Note that this bound is halved when $n - k = 1$. $\square$

For positive semidefinite triadic matrices and complete pivoting, $\gamma = 1$ so $\Phi_\gamma^k = (\frac{(1+\sqrt{5})}{2})^k$.

In the LBL^T factorization of a symmetric triadic matrix with diagonal pivoting, γ can be 2 or $\frac{8}{7-\sqrt{17}} \approx 2.78$, to minimize the element bound of matrix L or the element growth factor, respectively.

6. Concluding remarks. We have studied various pivoting strategies in computing the LXL^T factorizations of symmetric triadic matrices. We denote the strategies as **BT** (Bunch's pivoting strategy for a symmetric tridiagonal matrix), **BP** (Bunch-Parlett), **FBP** (Fast Bunch-Parlett), **BBK** (Bounded Bunch-Kaufman), and **BK** (Bunch-Kaufman). We summarize our results as follows:

1. The LL^T, LDL^T and LBL^T factors of a symmetric triadic matrix with any diagonal pivoting strategy remain sparse.

2. We have analyzed the boundedness of the factors in case the pivoting strategy satisfies either a strong or a weak condition.

3. We have presented a new choice of the α parameter that better controls the growth factor.

4. In the LBL^T factorization with various pivoting strategies, L is bounded for Bunch-Parlett, bounded Bunch-Parlett and fast Bunch-Kaufman pivoting strategies, whereas Bunch-Kaufman pivoting strategy may result in L unbounded. All the four pivoting strategies have the growth factor controlled for full symmetric matrices. The bound on the growth factor is smaller for symmetric triadic matrices.

5. For symmetric matrices, pivoting strategies **BT** and **BK** produce an L matrix with no bounds on its elements, whereas the magnitude of elements in L from pivoting strategies **BBK**, **BP** and **FBP** is bounded by a constant γ given in Table 3.1, depending on the parameter α in the algorithm.

6. For LDL^T factorization of a positive definite symmetric matrix A with complete pivoting, the magnification factor in the the error bound for the Schur complement after k steps is $\frac{1}{3}(n-k)(4^k - 1)$ if A is full [11], and $O((\frac{1+\sqrt{5}}{2})^k)$ if A triadic.

7. For two pivoting strategies D and E, we will say $D \succ E$, $D \succeq E$ and $D \simeq E$ if D is better than, slightly better than, or similar to E, respectively. Our experimental results with pivoting argument $\alpha = \frac{\sqrt{5}-1}{2} \approx 0.62$ are: For LBL^T factorizations of tridiagonal matrices, the average growth factors satisfy $\mathbf{BP} \succeq \mathbf{FBP} \succ \mathbf{BBK} \simeq \mathbf{BK} \succ \mathbf{BT}$ as shown in Figure 4.2, whereas the number of comparisons satisfies $\mathbf{BT} \succ \mathbf{BBK} \simeq \mathbf{BK} \succ \mathbf{FBP} \succ \mathbf{BP}$ as shown in Figure 4.3. Thus, the more expensive the pivoting, the smaller the growth factor.

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Appendix A: Proof of bounds for pivoting on triadics in Theorem 4.1.

THEOREM 6.1. *For LBL^T factorization of a symmetric triadic $A \in R^{n \times n}$, the growth factor of off-diagonal elements, defined in (3.6), is bounded as*

$$\bar{\rho}(A) \leq \begin{cases} 2g^{\lfloor \lg(n-1) \rfloor} \leq 2(n-1)^{\lg g}, & \text{if strong condition holds;} \\ 2g^{\lfloor (n-1)/2 \rfloor}, & \text{if weak condition holds,} \end{cases}$$

where

$$g = \max\{\frac{1}{\alpha}, \frac{1}{1-\alpha^2}\}.$$

Proof. Without loss of generality, we assume the required interchanges of rows and columns for pivoting are done prior to the factorization. Let $S_k(A)$ be the Schur complement of A after reducing k rows and k columns, and let

$$A^{(k+1)} = \begin{array}{c} \\ k \\ n-k \end{array} \begin{array}{cc} k & n-k \\ \left[\begin{array}{cc} 0 & 0 \\ 0 & S_k(A) \end{array} \right] \end{array}.$$

By Lemma 2.1 and Lemma 2.3, at most two diagonal and two off-diagonal elements are changed in the Schur complement. We denote them by $a_{ii}^{(k+1)}$, $a_{jj}^{(k+1)}$, $a_{ij}^{(k+1)}$ and $a_{ji}^{(k+1)}$. In addition to $a_{ij}^{(k+1)}$ and $a_{ji}^{(k+1)}$, $A^{(k+1)}$ has at most one non-zero off-diagonal element in each of ith and jth rows, inherited from $A^{(k-p)}$. Let $p = 1$ or $p = 2$ for the previous selection being 1×1 or 2×2, respectively.

Assume for now that

$$(6.1) \qquad\qquad a_{ij}^{(k+1-p)} = a_{ji}^{(k+1-p)} = 0$$

for each k. Later we will show that if this assumption breaks, the bounds on the off-diagonal growth factor are at most doubled.

For a 1×1 pivot, (6.1) implies that the weak condition coincides with the strong condition. Therefore,

$$(6.2) \qquad |a_{ij}^{(k+1)}| = \frac{|a_{ik}^{(k)}||a_{jk}^{(k)}|}{|a_{kk}^{(k)}|} \le \frac{1}{\alpha}\min\{|a_{ik}^{(k)}|, |a_{jk}^{(k)}|\} \le g\min\{|a_{ik}^{(k)}|, |a_{jk}^{(k)}|\}$$

For a 2×2 pivot $\left[\begin{array}{cc} a_{k-1,k-1}^{(k-1)} & a_{k-1,k}^{(k-1)} \\ a_{k,k-1}^{(k-1)} & a_{kk}^{(k-1)} \end{array} \right]$, there are at most two non-zero off-diagonal

elements under the pivot, denoted by $a_{i,k-1}^{(k-1)}$ and $a_{jk}^{(k-1)}$. If $i = j$, then the only element changed in $A^{(k+1)}$ from $A^{(k-1)}$ is $a_{ii}^{(k+1)}$. In this case, the matrix size is reduced without increasing the off-diagonal elements. In order to maximize $\bar{\rho}(A)$, we assume $i \ne j$. The weak condition ensures (3.3). Therefore,

$$|a_{ij}^{(k+1)}| \le \frac{1}{(1-\alpha^2)|a_{k,k-1}^{(k-1)}|^2} \left[\begin{array}{cc} |a_{i,k-1}^{(k-1)}| & 0 \end{array} \right] \left[\begin{array}{cc} |a_{kk}^{(k-1)}| & |a_{k-1,k}^{(k-1)}| \\ |a_{k,k-1}^{(k-1)}| & |a_{k-1,k-1}^{(k-1)}| \end{array} \right] \left[\begin{array}{c} 0 \\ |a_{jk}^{(k-1)}| \end{array} \right]$$

$$= \frac{|a_{i,k-1}^{(k-1)}||a_{jk}^{(k-1)}|}{(1-\alpha^2)|a_{k,k-1}^{(k-1)}|}$$

$$(6.3) \qquad \le \left\{ \begin{array}{ll} g\min\{|a_{i,k-1}^{(k-1)}|, |a_{jk}^{(k-1)}|\}, & \text{if strong condition holds.} \\ g|a_{jk}^{(k-1)}|, & \text{if weak condition holds.} \end{array} \right.$$

Since the Schur complement is symmetric, we consider the elements in the lower triangular. Let $G(m) = g^m \max_{i \ne j} |a_{ij}|$.

Consider the case that the strong condition holds. By (6.3) for a 2×2 pivot, an off-diagonal element of size $G(m)$ requires three $G(m-1)$ elements: $|a_{i,k-1}^{(k-1)}|, |a_{jk}^{(k-1)}|$

and $|a_{k,k-1}^{(k-1)}|$. Note that the strong condition guarantees $|a_{k,k-1}^{(k-1)}| \geq |a_{i,k-1}^{(k-1)}|$. By (6.2) for a 1×1 pivot, if $|a_{ij}^{(k+1)}| \geq G(m)$, then $|a_{ik}^{(k)}|, |a_{jk}^{(k)}| \geq G(m-1)$. In other words, for a 1×1 pivot, an off-diagonal element of size $G(m)$ requires two off-diagonal supporting elements of size $G(m-1)$. Therefore, the bound on element growth using 1×1 pivots is higher than that using 2×2 pivots. Considering a sequence of 2^{m-1} pivots of size 1×1, we see by induction that a $G(m)$ element requires 2^m $G(0)$ elements. We illustrate this in the following diagram for obtaining a $G(3)$ element with the smallest number of pivots. The last column indicates the Schur complements as the sources of the two off-diagonal elements in each row if they were not present initially. Note that $G(0)$ elements are from the original matrix A.

```
 *          G(0)                              G(0)
       *    G(0)                    G(0)
 G(0) G(0)   *                      G(1)       G(1)      A^(2), A^(1)
             *       G(0)      G(0)
                 *   G(0) G(0)
                 G(0) G(0)  *    G(1)  G(1)              A^(5), A^(4)
      G(0) G(1)  G(0) G(1)  *    G(2)  G(2)              A^(6), A^(3)
                 G(0)       G(1)  *    G(2)  G(2)  G(3)  A^(7)
 G(0)      G(1)       G(1) G(2)  *    G(3)
                           G(2) G(3)   *
```

The number of pivots is $2^{m-1} + 2^{m-2} + \cdots + 2^0 = 2^m - 1$. The last 2×2 Schur complement, with or without a row/column reduced afterward, cannot contribute to off-diagonal element growth. Therefore, the dimension of the smallest matrix that can have a $G(m)$ off-diagonal element is $(2^m - 1) + 2 = 2^m + 1$. If A has dimension less than $2^m + 1$ but larger than 2^{m-1} then the off-diagonal elements in the Schur complements are at most $G(m-1)$ in magnitude. In other words,

$$(6.4) \qquad \bar{\rho}(A) \leq g^{\lfloor \lg(n-1)\rfloor} \leq (n-1)^{\lg g}.$$

Consider the case that the weak condition holds. Recall that for a 1×1 pivot, the weak condition coincides with the strong condition, and an off-diagonal element of size $G(m)$ requires two $G(m-1)$ elements. By (6.3) for a 2×2 pivot, an off-diagonal element of size $G(m)$ requires only one $G(m-1)$ element. For maximal growth from $G(0)$ to $G(1)$ we use a 1×1 pivot. Otherwise, the bound on element growth using 2×2 pivots is at least as big as that using 1×1 pivots. The bound can increase by a factor of g for every two rows reduced during the decomposition, except from $G(0)$ to $G(1)$ (one row/column reduced). The last Schur complement cannot contribute to off-diagonal element growth. Therefore,

$$(6.5) \qquad \bar{\rho}(A) \leq g^{\lfloor (n-1)/2 \rfloor},$$

where $A \in R^{n \times n}$ is symmetric triadic.

So far we assume (6.1) holds. Now we show that if (6.1) breaks, the bounds in (6.4) and (6.5) are at most doubled. If $a_{ij}^{(k+1-p)} = a_{ji}^{(k+1-p)} \neq 0$, then there are no other off-diagonal elements in ith and jth rows and columns in $A^{(k+1)}$, where $p = 1, 2$ stands for 1×1, 2×2 pivots, respectively. As a result, $A^{(k+1)}$ is a reducible matrix. After diagonally interchanging rows and columns, $A^{(k+1)}$ consists of two diagonal blocks: $\begin{bmatrix} a_{ii}^{(k+1)} & a_{ij}^{(k+1)} \\ a_{ji}^{(k+1)} & a_{jj}^{(k+1)} \end{bmatrix}$ and the remaining matrix, in which all the elements are

taken from $A^{(k+1-p)}$. The bound on $a_{ji}^{(k+1)}$ in the 2×2 block is at most doubled, since it is a sum of two terms each of which is bounded as (6.4) or (6.5), depending on whether the condition satisfied is strong or weak. Note that no off-diagonal element growth occurs afterward in this 2×2 block, and the other block is intact. Therefore, we obtain the result by safely declaring that the bounds in (6.4) and (6.5) are at most doubled if (6.1) breaks. ☐

THEOREM 6.2. *For LBL^T factorization of a symmetric triadic $A \in R^{n \times n}$, consider the growth factor of off-diagonal elements, defined in (3.1). If the weak condition holds,*

$$\rho(A) \leq \begin{cases} \frac{4g(g^{(n-3)/2}-1)}{g-1} + 2(g^{(n-1)/2} + g^{(n+1)/2}) + 1, & \text{if } n \text{ odd.} \\ \frac{4g(g^{(n-2)/2}-1)}{g-1} + 2g^{n/2} + 1, & \text{if } n \text{ even.} \end{cases}$$

That is, $\rho(A) = O(g^{n/2})$. If the strong condition holds,

$$\rho(A) \leq 2ng^{\lfloor \lg(n-1) \rfloor} \leq 2n(n-1)^{\lg g} = \Theta(n^{1+\lg g}),$$

where $g = \max\{\frac{1}{\alpha}, \frac{1}{1-\alpha^2}\}$.

Proof. The major difference between $\rho(A)$ and $\bar{\rho}(A)$ is that the diagonal element increases can accumulate, whereas the accumulation of two off-diagonal element increases results in a reducible Schur complement so further accumulation is impossible. Therefore, the diagonal element growth factor is bounded by the sum of n elements, each of which is bounded by Theorem 4.1. So we obtain the bound on $\rho(A)$ for the strong condition. Though this approach also gives a bound for the weak condition, a tighter bound can be obtained as follows.

The proof of Theorem 6.1 shows that the off-diagonal element bound in the Schur complement depends on the number of rows/columns reduced. We follow the notation in the proof of Theorem 6.1.

If the weak condition holds, the off-diagonal elements $a_{ij}^{(k+1)}$ in $A^{(k+1)}$ (after reducing k rows/columns) are bounded as $|a_{ij}^{(k+1)}| \leq 2g^{\lfloor (k+1)/2 \rfloor} \max|a_{ij}|$ for $i \neq j$ and k from 1 to $n-2$. This is also the bound on the diagonal element increase of A_{k+1} from the previous iteration. We sum up all the relative element increases during the decomposition to obtain a bound on $\rho(A)$, where $A \in R^{n \times n}$ is symmetric triadic.

$$\rho(A) \leq \underline{1} + 2g^{\lfloor 2/2 \rfloor} + 2g^{\lfloor 3/2 \rfloor} + \cdots + 2g^{\lfloor (n-1)/2 \rfloor} + \underline{2g^{\lfloor (n-1)/2 \rfloor + 1}}$$

$$= \begin{cases} \frac{4g(g^{(n-3)/2}-1)}{g-1} + 2(g^{(n-1)/2} + g^{(n+1)/2}) + 1, & \text{if } n \text{ odd.} \\ \frac{4g(g^{(n-2)/2}-1)}{g-1} + 2g^{n/2} + 1, & \text{if } n \text{ even.} \end{cases}$$

The first underlined 1 is because each diagonal element in the initial A can be $G(0)$. The reason for the last term $\underline{2g^{\lfloor (n-1)/2 \rfloor + 1}}$ is as follows. If a 1×1 pivot is chosen in the last 2×2 Schur complement or a 2×2 pivot is chosen in the last 3×3 Schur complement, the reduction can still increase the very last diagonal element, but there is no off-diagonal element growth. If (6.1) breaks, the reduced 2×2 block can have diagonal element growth but no off-diagonal element growth. This case is also taken into account in $\underline{2g^{\lfloor (n-1)/2 \rfloor + 1}}$. In a similar vein, we can also obtain a slightly tighter bound for the strong condition, but it is also $\Theta(n^{1+\lg g})$.

$$\rho(A) \leq 1 + 2g^{\lfloor \lg 2 \rfloor} + 2g^{\lfloor \lg 3 \rfloor} + \cdots + 2g^{\lfloor \lg(n-1) \rfloor} + 2g^{\lfloor \lg(n-1) \rfloor + 1} = \Theta(n^{1+\lg g}).$$

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