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Twisted factorization of a banded matrix

Christof Vömel · Jason Slemons

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Abstract The twisted factorization of a tridiagonal matrix T plays an important role in inverse iteration as featured in the MRRR algorithm. The twisted structure simplifies the computation of the eigenvector approximation and can also improve the accuracy.

A tridiagonal twisted factorization is given by $T = M_k \Delta_k N_k$ where Δ_k is diagonal, M_k, N_k have unit diagonals, and the k-th column of M_k and the k-th row of N_k correspond to the k-th column and row of the identity, that is $M_k e_k = e_k,\ e_k^t N_k = e_k^t$.

This paper gives a constructive proof for the existence of the twisted factorizations of a general *banded* matrix A. We show that for a given twist index k, there actually are *two* such factorizations.

We also investigate the implications on inverse iteration and discuss the role of pivoting.

Keywords Banded matrix · Block-tridiagonal matrix · Double factorization · Twisted factorization · Forward factorization · Backward factorization

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C. Vömel (✉)
Institute of Computational Science, ETH Zürich, Universitätsstraße 6, CAB, 8092 Zürich, Switzerland
e-mail: cvoemel@inf.ethz.ch

J. Slemons
Department of Applied Mathematics, University of Washington, Seattle, WA 98195, USA
e-mail: slemons@amath.washington.edu

1 Introduction

Let $A \in \mathcal{R}^{n\times n}$ denote a banded matrix with semi-bandwidth $b > 0$, for example a tridiagonal ($b := 1$) or a pentadiagonal ($b := 2$). We do not require A to be symmetric, but we do assume for now that it has the same number of upper and lower off-diagonal bands.

We further assume existence of the double factorization

$$A = L_+ D_+ U_+ = U_- D_- L_-, \tag{1.1}$$

with L_+, L_- and U_+, U_- respectively being lower and upper triangular with unit diagonal, and with D_+ and D_- containing the pivots of the 'forward' and 'backward' factorizations. If one excludes the case where A is actually block-diagonal, existence of (1.1) implies that except for the last (first) one, all pivots in D_+ (D_-) have to be nonzero.

We are interested in the construction of a twisted factorization

$$A = M_k \Delta_k N_k, \tag{1.2}$$

where Δ_k is diagonal, and the k-th column of M_k and the k-th row of N_k correspond to the k-th column and row of the identity, that is

$$\begin{aligned} M_k e_k &= e_k, \\ e_k^t N_k &= e_k^t. \end{aligned} \tag{1.3}$$

So far, a twisted factorization of this kind has mainly been considered for tridiagonal matrices, see for example [7, 12, 16, 20] and also [12, Sect. 4] for historic references.

We derive in this paper a generalization of that construction. One important applications lies in the computation of eigenvectors. Indeed, the symmetric tridiagonal twisted factorization is at the core of the MRRR algorithm [1–4, 12, 13] because it allows us to compute a good approximation to the eigenvector of a relatively isolated eigenvalue.

Consider now inverse iteration to compute an approximate right eigenvector of a symmetric tridiagonal matrix as described by Wilkinson [17, Chaps. 5.53, 5.54]. Without knowledge of a good right-hand side, that is the starting vector for the iteration, one is presented with the difficult task of finding one that is 'rich' in the eigenvector of interest. However, as discussed in [12], if $\gamma_k := e_k^t \Delta_k e_k$, then from (1.2) and (1.3), one has for the special right-hand side $\gamma_k e_k$ that

$$Az = \gamma_k e_k \quad \Longleftrightarrow \quad N_k z = e_k. \tag{1.4}$$

For the tridiagonal case,

$$N_k = \begin{pmatrix} 1 & U_+(1,2) & & & & & & & \\ & 1 & U_+(2,3) & & & & & & \\ & & \ddots & \ddots & & & & & \\ & & & 1 & U_+(k-1,k) & & & & \\ & & & & 1 & & & & \\ & & & & L_-(k+1,k) & 1 & & & \\ & & & & & L_-(k+2,k+1) & 1 & & \\ & & & & & & \ddots & \ddots & \\ & & & & & & & L_-(n,n-1) & 1 \end{pmatrix},$$

so that the solution z of (1.4) satisfies $z(k)=1$. Its other entries can be computed using only multiplications, starting from index k upwards and downwards, see also [12, Corollary 5]. Moreover, it is possible to choose k so that it corresponds to an entry of large magnitude in the normalized eigenvector of interest. This ensures both stability and rapid convergence of inverse iteration.

To deal with matrices of a semi-bandwidth greater than one, Parlett and Dhillon considered in [12, Sect. 7] a block extension of (1.1) and (1.2). They show that by allowing blocks on the diagonal of D_+ and D_-, a suitable twisted block factorization can be defined but then they require a singular value decomposition to proceed.

Parlett communicated to us privately that until recently, he believed that the block extension was the only way to obtain a generalized twisted factorization of matrices of semi-bandwidth greater than one because his derivation of (1.2) involved deep properties of the tridiagonal form.

To his and our surprise, Xu and Qiao [18], while developing a factorization method for computing the Takagi vectors of a complex symmetric tridiagonal matrix, and without taking much notice, found a non-blocked expression for one twisted factorization of a symmetric pentadiagonal matrix of the form (1.2), with Δ being diagonal and the triangular factor satisfying constraint (1.3).

This prompted us to systematically investigate the subject of twisted factorizations for general banded matrices. The rest of this paper is organized as follows. Section 2.1 gives a constructive proof for the existence of the banded twisted factorization. It is also shown that there are *two* different factorizations that satisfy (1.3). In Sect. 2.2, we discuss the connection of twisted factorizations to the triangular factors of the symmetrically permuted band matrix. Sections 2.3 and 2.4 exhibit connections to A^{-1} and eigenvector computations. Section 3 proves existence of the twisted factorization of a general matrix with variable band structure and discusses the implications of this representation for eigenvector computations, and Sect. 4 discusses the pivoting issue. Section 5 summarizes and concludes.

2 The banded twisted factorization

2.1 2-level construction of a banded twisted factorization

In this section, we show how to obtain a non-blocked twisted factorization (1.2) of a banded matrix. To make the presentation easier, we demonstrate the construction by the example of a pentadiagonal matrix A. However, the procedure is completely general. To begin, we consider a partitioning

$$A = \left[\begin{array}{ccccc|cc|cccccc}
* & * & * & & & & & & & & & & \\
* & * & * & * & & & & & & & & & \\
* & * & * & * & * & & & & & & & & \\
 & * & * & * & * & * & & & & & & & \\
 & & * & * & * & * & * & & & & & & \\
\hline
 & & & * & * & * & * & * & & & & & \\
 & & & & * & * & * & * & * & & & & \\
\hline
 & & & & & * & * & * & * & * & & & \\
 & & & & & & * & * & * & * & * & & \\
 & & & & & & & * & * & * & * & * & \\
 & & & & & & & & * & * & * & * & * \\
 & & & & & & & & & * & * & * & * \\
 & & & & & & & & & & * & * & *
\end{array}\right]. \tag{2.1}$$

One of the indices corresponding to the 2×2 middle diagonal block of (2.1) will be the location of the twist. In general, A can be written as block-tridiagonal

$$A = \begin{bmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22} & A_{23} \\ & A_{32} & A_{33} \end{bmatrix} \begin{matrix} \}p \\ \}b \\ \}q \end{matrix}. \tag{2.2}$$

A_{11} and A_{33} are banded, here: pentadiagonal, matrices, of dimensions p and q respectively. $A_{12}, A_{21}, A_{23}, A_{32}$ are of rectangular shapes (either tall and skinny, or short and fat), and A_{22} is a dense matrix of dimension of the semi-bandwidth b, in this case two.

Now consider the forward factorization

$$A_{11} = L_+ D_+ U_+ \tag{2.3}$$

and the backward factorization

$$A_{33} = U_- D_- L_-. \tag{2.4}$$

For clarity, we here omit block indices, i.e. $L_+ D_+ U_+ := L_+(1,1) D_+(1,1) U_+(1,1)$ etc. Suppose that A_{11} and A_{33} are nonsingular, then

$$\begin{bmatrix} L_+ & & \\ A_{21} U_+^{-1} D_+^{-1} & I & A_{23} L_-^{-1} D_-^{-1} \\ & & U_- \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & A'_{22} & \\ & & D_- \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1} L_+^{-1} A_{12} & \\ & I & \\ & D_-^{-1} U_-^{-1} A_{32} & L_- \end{bmatrix} \tag{2.5}$$

is a block-twisted factorization of (2.2), where the Schur complement A'_{22} of A_{11} and A_{33} is

$$
\begin{aligned}
A'_{22} &= A_{22} - A_{21}A_{11}^{-1}A_{12} - A_{23}A_{33}^{-1}A_{32} && (2.6)\\
&= A_{22} - A_{21}U_+^{-1}D_+^{-1}L_+^{-1}A_{12} - A_{23}L_-^{-1}D_-^{-1}U_-^{-1}A_{32}. && (2.7)
\end{aligned}
$$

Consider the double factorization

$$A'_{22} = L_{2+}D_{2+}U_{2+} = U_{2-}D_{2-}L_{2-}. \tag{2.8}$$

Since A_{22} is a dense matrix, the triangular factors $L_{2+}, U_{2+}, U_{2-}, L_{2-}$ will generally be dense as well. The lower triangular matrices L_{2+}, L_{2-} and the upper triangular matrices U_{2+}, U_{2-} all have unit diagonals. Thus, independent of the dimension of A_{22}—that is the semi-bandwidth of A—the last column of L_{2+} and the first column of U_{2-} will be columns of the identity. Likewise, the last row of U_{2+} and the first row of L_{2-} will be rows of the identity.

As a consequence, we can obtain the following two different twisted factorizations of the banded matrix (2.2). The first one,

$$A = \begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & L_{2+} & A_{23}L_-^{-1}D_-^{-1} \\ & & U_- \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & D_{2+} & \\ & & D_- \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & \\ & U_{2+} & \\ & D_-^{-1}U_-^{-1}A_{32} & L_- \end{bmatrix} \tag{2.9}$$

corresponds to a twist in the *lower right* corner of the $(2,2)$ block of A, denote its index by $k_+ = p + b = n - q$. The second one

$$\begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & U_{2-} & A_{23}L_-^{-1}D_-^{-1} \\ & & U_- \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & D_{2-} & \\ & & D_- \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & \\ & L_{2-} & \\ & D_-^{-1}U_-^{-1}A_{32} & L_- \end{bmatrix} \tag{2.10}$$

corresponds to a twist in the *upper left* corner of the $(2,2)$ block of A, denote the index by $k_- = p + 1 = n - (q + b) + 1$. Summarizing, we have shown the following Theorem 2.1.

Theorem 2.1 *Let $A \in \mathcal{R}^{n\times n}$ denote a banded matrix with semi-bandwidth $b > 0$ and partitioned as in* (2.2)*. Provided that the factorizations* (2.3), (2.4), *and* (2.8) *exist, both* (2.9) *and* (2.10) *constitute non-blocked twisted factorizations of A.*

Note that the banded structure of A is preserved in the off-diagonal blocks of (2.9) and (2.10). For example, in (2.9), $A_{21}U_+^{-1}D_+^{-1}$ and $D_-^{-1}U_-^{-1}A_{32}$ are right upper triangular and $D_+^{-1}L_+^{-1}A_{12}$ and $A_{23}L_-^{-1}D_-^{-1}$ are left lower triangular matrices. For illustration purposes, we show the first factor of (2.9) with the twist in bold,

$$\begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & L_{2+} & A_{23}L_-^{-1}D_-^{-1} \\ & & U_- \end{bmatrix}$$

$$= \left[\begin{array}{ccccc|cc|cccccc}
1 & & & & & & & & & & & & \\
* & 1 & & & & & & & & & & & \\
* & * & 1 & & & & & & & & & & \\
 & * & * & 1 & & & & & & & & & \\
 & & * & * & 1 & & & & & & & & \\
\hline
 & & & * & * & 1 & & * & & & & & \\
 & & & & * & * & \mathbf{1} & * & * & & & & \\
\hline
 & & & & & & & 1 & * & * & & & \\
 & & & & & & & & 1 & * & * & & \\
 & & & & & & & & & 1 & * & * & \\
 & & & & & & & & & & 1 & * & * \\
 & & & & & & & & & & & 1 & * \\
 & & & & & & & & & & & & 1
\end{array}\right]. \tag{2.11}$$

Let us briefly compare to the symmetric tridiagonal case investigated by Parlett and Dhillon [12] where the dimension of A_{22} is one. There is only a single twisted factorization per index k, and the Schur complement is a scalar γ_k. One of the referees mentioned that in [1, Sect. 3.6], Dhillon had suggested a way to extend twisted factorization to more general than tridiagonal matrices, something we had not been aware of.

Our contribution in this section is a systematic derivation of such factorizations from block elimination, as well as showing the existence of actually *two* such factorizations, (2.9) and (2.10).

2.2 Connection to triangular factorization of symmetric permutations of A

In [1, Sect. 3.6], Dhillon commented that a twisted factor may be considered as a symmetrically permuted triangular matrices as well as triangular factor of a symmetric permutation of A.

We here explore this observation more systematically by the example of the pentadiagonal matrix (2.1), using the notation in (2.2). This leads us to an alternative derivation of (2.9) and (2.10). We consider the following two symmetric permutations:

- P_1 reverses the order of the leading $1 : p + b$ rows and columns of A but does not change the order of anything beyond. Call the resulting matrix $A^{(1)} := P_1 A P_1^t$.
- P_2 reverses the order of the trailing $p + 1 : n$ rows and columns of A but does not change the order of anything before. Call the resulting matrix $A^{(2)} := P_2 A P_2^t$.

We first investigate $A^{(1)}$ where for clarity, we have numbered the diagonal entries according to their original position on the diagonal of A:

$$A^{(1)} = \left[\begin{array}{ccccc|cc|cccccc}
7 & * & * & & & & & * & * & & & & \\
* & 6 & * & * & & & & * & & & & & \\
* & * & 5 & * & * & & & & & & & & \\
 & * & * & 4 & * & * & & & & & & & \\
 & & * & * & 3 & * & * & & & & & & \\
\hline
 & & & * & * & 2 & * & & & & & & \\
 & & & & * & * & 1 & & & & & & \\
\hline
* & * & & & & & & 8 & * & * & & & \\
* & & & & & & & * & 9 & * & * & & \\
 & & & & & & & * & * & 10 & * & * & \\
 & & & & & & & & * & * & 11 & * & * \\
 & & & & & & & & & * & * & 12 & * \\
 & & & & & & & & & & * & * & 13
\end{array}\right]. \tag{2.12}$$

If the backward factorization

$$A^{(1)} = U_-^{(1)} D_-^{(1)} L_-^{(1)} \tag{2.13}$$

exists, then no fill-in occurs in the unit triangular factors $U_-^{(1)}$ and $L_-^{(1)}$, and

$$A = P_1^t A^{(1)} P_1 = \left(P_1^t U_-^{(1)} P_1\right) \left(P_1^t D_-^{(1)} P_1\right) \left(P_1^t L_-^{(1)} P_1\right). \tag{2.14}$$

The re-permuted triangular factor $P_1^t U_-^{(1)} P_1$ has the structure

$$P_1^t U_-^{(1)} P_1 = \left[\begin{array}{ccccc|cc|cccccc}
1 & & & & & & & & & & & & \\
* & 1 & & & & & & & & & & & \\
* & * & 1 & & & & & & & & & & \\
 & * & * & 1 & & & & & & & & & \\
 & & * & * & 1 & & & & & & & & \\
\hline
 & & & * & * & 1 & & * & & & & & \\
 & & & & * & * & 1 & * & * & & & & \\
\hline
 & & & & & & & 1 & * & * & & & \\
 & & & & & & & & 1 & * & * & & \\
 & & & & & & & & & 1 & * & * & \\
 & & & & & & & & & & 1 & * & * \\
 & & & & & & & & & & & 1 & * \\
 & & & & & & & & & & & & 1
\end{array}\right]. \tag{2.15}$$

This is exactly (2.11), and (2.14) thus turns out to be (2.9).

We then investigate $A^{(2)}$ where again, the diagonal entries are numbered according to their original position on the diagonal of A:

$$A^{(2)} = \left[\begin{array}{ccccc|cc|cccccc}
1 & \ast & \ast & & & & & & & & & & \\
\ast & 2 & \ast & \ast & & & & & & & & & \\
\ast & \ast & 3 & \ast & \ast & & & & & & & & \\
 & \ast & \ast & 4 & \ast & & & & & & & & \ast \\
 & & \ast & \ast & 5 & & & & & & & \ast & \ast \\
\hline
 & & & & & 13 & \ast & \ast & & & & & \\
 & & & & & \ast & 12 & \ast & \ast & & & & \\
\hline
 & & & & & \ast & \ast & 11 & \ast & \ast & & & \\
 & & & & & & \ast & \ast & 10 & \ast & \ast & & \\
 & & & & & & & \ast & \ast & 9 & \ast & \ast & \\
 & & & & & & & & \ast & \ast & 8 & \ast & \ast \\
 & & & & \ast & & & & & \ast & \ast & 7 & \ast \\
 & & & \ast & \ast & & & & & & \ast & \ast & 6
\end{array}\right]. \tag{2.16}$$

If the forward factorization

$$A^{(2)} = L_+^{(2)} D_+^{(2)} U_+^{(2)} \tag{2.17}$$

exists, then no fill-in occurs in the unit triangular factors $L_+^{(2)}$ and $U_+^{(2)}$, and

$$A = P_2^t A^{(2)} P_2 = \left(P_2^t L_+^{(2)} P_2\right)\left(P_2^t D_+^{(2)} P_2\right)\left(P_2^t U_+^{(2)} P_2\right). \tag{2.18}$$

The re-permuted triangular factor $P_2^t L_+^{(2)} P_2$ has the structure

$$P_2^t L_+^{(2)} P_2 = \left[\begin{array}{ccccc|cc|cccccc}
1 & & & & & & & & & & & & \\
\ast & 1 & & & & & & & & & & & \\
\ast & \ast & 1 & & & & & & & & & & \\
 & \ast & \ast & 1 & & & & & & & & & \\
 & & \ast & \ast & 1 & & & & & & & & \\
\hline
 & & & \ast & \ast & 1 & \ast & \ast & & & & & \\
 & & & & \ast & & 1 & \ast & \ast & & & & \\
\hline
 & & & & & & & 1 & \ast & \ast & & & \\
 & & & & & & & & 1 & \ast & \ast & & \\
 & & & & & & & & & 1 & \ast & \ast & \\
 & & & & & & & & & & 1 & \ast & \ast \\
 & & & & & & & & & & & 1 & \ast \\
 & & & & & & & & & & & & 1
\end{array}\right]. \tag{2.19}$$

By comparison of the entries, (2.18) thus turns out to be (2.10).

2.3 Connection to A^{-1}

It has been noted already in [11, Sect. 3] that block twisted factorizations of block tridiagonal matrices permit an elegant connection between blocks of the inverse and the twisted factors. Thus, it is not very surprising that [12, Sect. 7] uses the block twisted factorization (2.5) of the block-partitioned matrix A from (2.2) to prove block-extensions of results on the tridiagonal twisted factorization from [12].

Theorem 2.2 *Let A be as in* (2.2).

- *If $D_+(2,2) := A_{22} - A_{21}A_{11}^{-1}A_{12}$ denotes the second block pivot from its forward block factorization, and $D_-(2,2) := A_{22} - A_{23}A_{33}^{-1}A_{32}$ denotes the second block pivot from its backward block factorization, then*

$$A'_{22} = D_+(2,2) + D_-(2,2) - A_{22}. \tag{2.20}$$

- *If A is nonsingular, then*

$$\left[A'_{22}\right]^{-1} = (A^{-1})_{22}. \tag{2.21}$$

If the block double factorization of A exists, then

$$\text{blockdiag}(A) + \left[\text{blockdiag}(A^{-1})\right]^{-1} = \text{blockdiag}(D_+(:,:)) + \text{blockdiag}(D_-(:,:)). \tag{2.22}$$

It is interesting to compare this to the non-blocked factorizations of a band matrix as those in (2.9) and (2.10).

Theorem 2.3 *Let $A \in \mathcal{R}^{n\times n}$ as in* (2.2), *with $n = p + b + q$,* $\dim(A_{11}) = p$, $\dim(A_{22}) = b$, $\dim(A_{33}) = q$. *As in* (2.8), *let the double factorization*

$$A'_{22} = L_{2+}D_{2+}U_{2+} = U_{2-}D_{2-}L_{2-}. \tag{2.23}$$

Then by (2.10)

$$\mu_{p+1}^{-1} := e_{p+1}^t A^{-1} e_{p+1} = e_1^t\, D_{2-}^{-1}\, e_1, \tag{2.24}$$

and by (2.9)

$$\nu_{p+b}^{-1} := e_{p+b}^t A^{-1} e_{p+b} = e_b^t\, D_{2+}^{-1}\, e_b. \tag{2.25}$$

The respective last pivots of the back- and forward factorizations in D_{2+} and D_{2-} are thus reciprocals of the diagonal elements of A^{-1}. (The other entries of D_{2+} and D_{2-} are not as directly related to the diagonal of A^{-1}.)

In the tridiagonal case [12, Corollary 7], one could explicitly construct a product representation of the scalar γ_k at the twist index in terms of the pivots from the double factorization. Since μ_{p+1} and ν_{p+b} do not arise directly but come from a second-level triangular factorization of the Schur complement, such a product representation is no longer possible for general banded matrices. However, the twisted factorizations can still be used advantageously for eigenvector computations as we will discuss in Sect. 2.4.

2.4 Connection to eigenvectors

The twisted factorizations (2.9) and (2.10) enable us to stably and efficiently compute eigenvector approximations where the right-hand side is a row or column of the identity.

For example, let k denote a twist index and let $A = M_k \Delta_k N_k$ as in (2.9). Further, let ν_k denote the last entry of D_{2+}. Then the approximate right eigenvector z_r

$$Az_r = \nu_k e_k \quad \Longleftrightarrow \quad \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & \\ & U_{2+} & \\ & D_-^{-1}U_-^{-1}A_{32} & L_- \end{bmatrix} z_r = e_k. \tag{2.26}$$

Since the last row of U_{2+} is a row of the identity, the k-th row of the matrix on the right-hand side of '$\Leftrightarrow$' is a row of the identity too, hence $z_r(k) = 1$. Moreover, the $(1:2, 1:2)$ block-submatrix is right upper triangular, so that components $z_r(1:k-1)$ can be computed using backward substitution. The semi-bandwidth of A determines the complexity of this computation. In the tridiagonal case, $z_r(1:k-1)$ can be obtained using simply multiplications, in the more general case it is a difference of b terms. Once $z_r(k-b+1:k)$ have been obtained, one can compute $z_r(k+1:n)$ via forward substitution.

For an approximate left eigenvector z_l^*, using analogous notation, one finds

$$z_l^* A = \nu_k e_k^* \quad \Longleftrightarrow \quad z_l^* \begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & L_{2+} & A_{23}L_-^{-1}D_-^{-1} \\ & & U_- \end{bmatrix} = e_k^*. \tag{2.27}$$

Thus again $z_l(k) = 1$. One can compute $z_l(1:k-1)$ using backward substitution. At last, $z_l(k+1:n)$ follows from $z_l(k-b+1:k)$ via forward substitution.

If A is normal, its unitary eigen-decomposition $A = V\Lambda V^*$ allows us to easily connect its inverse (Sect. 2.3) with the pivots at the twist index: let λ_j denote the simple eigenvalue of A closest to zero, then with $k := p + b$ in (2.25)

$$\frac{1}{\nu_k} = e_k^* V \Lambda^{-1} V^* e_k = \frac{|v_j(k)|^2}{\lambda_j} + \sum_{i \neq j} \frac{|v_i(k)|^2}{\lambda_i}. \tag{2.28}$$

As a consequence, one has for shifted $A - \sigma I$ the following

Theorem 2.4 [12, Lemma 13] *Let $A - \sigma I$ be a normal, invertible matrix, and let (2.9) exist. Suppose that σ is closer to the simple eigenvalue λ_j than to any other eigenvalue of A. Then if $v_j(k) \neq 0$, one has for z_r from (2.26) that*

$$\frac{|\nu_k|}{\|z_r\|_2} = \frac{|\lambda_j - \sigma|}{|v_j(k)|}\left[1 + \left(|v_j(k)|^{-2} - 1\right)\mathcal{A}\right]^{-1/2} \leq \frac{|\lambda_j - \sigma|}{|v_j(k)|}. \tag{2.29}$$

Here $\mathcal{A}$ is a weighted arithmetic mean of $\{|\frac{\lambda_j - \sigma}{\lambda_i - \sigma}|^2,\ i \neq j\}$, $0 \leq |\mathcal{A}| < \frac{|\lambda_j - \sigma|^2}{\mathrm{gap}^2(\sigma)}$, where $\mathrm{gap}(\sigma) = \min_{i \neq j} |\lambda_i - \sigma|$.

By (2.26), the quotient $|\nu_k|/\|z_r\|_2$ on the left-hand side of (2.29) is exactly the scaled residual norm of z_r with respect to σ. The bound on the right-hand side of (2.29) is tightest when the twist index k corresponds to the largest entry of the eigenvector v. By (2.28), this corresponds to the ν_k smallest in magnitude.

For a non-normal matrix A, let λ denote a simple, generally complex, eigenvalue of A closest to zero and y and x its associated left and right eigenvectors. By [15, Theorem 1.8, pp. 244–245], one can find matrices X_2 and Y_2 such that the bi-orthonormality condition $(y, Y_2)^*(x, X_2) = (x, X_2)^*(y, Y_2) = I$ is fulfilled and the spectral decomposition of A can be represented in block-diagonal form

$$A = (x, X_2)\begin{pmatrix} \lambda & \\ & L_2 \end{pmatrix}\begin{pmatrix} y^* \\ Y_2^* \end{pmatrix} = \lambda x y^* + X_2 L_2 Y_2^*. \tag{2.30}$$

Again, (2.25) yields

$$\frac{1}{\nu_k} = \frac{x(k)\bar{y}(k)}{\lambda} + e_k^* X_2 L_2^{-1} Y_2^* e_k. \tag{2.31}$$

If λ is complex, then ν_k will be complex as well. Provided that λ is well separated from the spectrum of L_2 and $x(k)\bar{y}(k) \neq 0$, a small $|\nu_k|$ corresponds to a large product $|x(k)\bar{y}(k)|$.

In certain instances, one can say even more. For example, suppose that A is a balanced real unsymmetric tridiagonal matrix, that is $A = ST$ where T is real symmetric tridiagonal and S is a diagonal matrix containing only ± 1. If λ is real and simple with right eigenvector x, then $y^t = x^t S$ is its associated left eigenvector. Thus, left and right eigenvector entries agree in magnitude and a small $|\nu_k|$ corresponds to a large $|x(k)|$, just like in the normal case.

3 A remark on the twisted factorization of a square matrix with different lower and upper bandwidths, or with a general block structure

Extending the procedure from Sect. 2.1, we show the existence of twisted factorizations of a matrix

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}. \tag{3.1}$$

The difference from (2.2) are the generally non-vanishing blocks A_{31} and A_{13}. The blocks on the diagonal are assumed to have square shape. If A is a banded matrix where the lower bandwidth differs from the upper one, the dimension of A_{22} is the *minimum* of the lower and upper bandwidths. (For example, A_{22} would be 1×1 for a Hessenberg matrix.) For general dense matrices however, there is no natural block size.

If the forward factorization

$$A_{11} = L_+ D_+ U_+ \tag{3.2}$$

exists and is nonsingular, we can write A from (3.1) as

$$\begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & I & \\ A_{31}U_+^{-1}D_+^{-1} & & I \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & A'_{22} & A'_{23} \\ & A'_{32} & A'_{33} \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & D_+^{-1}L_+^{-1}A_{13} \\ & I & \\ & & I \end{bmatrix}, \tag{3.3}$$

with

$$A'_{ij} = A_{ij} - A_{i1}A_{11}^{-1}A_{1j} = A_{ij} - A_{i1}U_+^{-1}D_+^{-1}L_+^{-1}A_{1j}, \quad 2 \le i,\ j \le 3. \tag{3.4}$$

Continuing, let

$$A'_{33} = U'_- D'_- L'_- \tag{3.5}$$

be nonsingular. Using the notation $X^{-\prime} := (X')^{-1}$, we have from (3.3) that

$$A = \begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & I & A'_{23}L_-^{-\prime}D_-^{-\prime} \\ A_{31}U_+^{-1}D_+^{-1} & & U'_- \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & A''_{22} & \\ & & D'_- \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & D_+^{-1}L_+^{-1}A_{13} \\ & I & \\ & D_-^{-\prime}U_-^{-\prime}A'_{32} & L'_- \end{bmatrix}, \tag{3.6}$$

with

$$A''_{22} = A'_{22} - A'_{23}A_{33}^{-\prime}A'_{32} = A'_{22} - A'_{23}U_-^{-\prime}D_-^{-\prime}L_-^{-\prime}A'_{32}. \tag{3.7}$$

At last, let exist the double factorization

$$A''_{22} = L''_+ D''_+ U''_+ = U''_- D''_- L''_-. \tag{3.8}$$

Then, we find the following two twisted factorizations of the block matrix (3.1).

The one with a twist index k_+ in the *lower right* corner of A_{22} is

$$\begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & L''_+ & A'_{23}L_-^{-\prime}D_-^{-\prime} \\ A_{31}U_+^{-1}D_+^{-1} & & U'_- \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & D''_+ & \\ & & D'_- \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & D_+^{-1}L_+^{-1}A_{13} \\ & U''_+ & \\ & D_-^{-\prime}U_-^{-\prime}A'_{32} & L'_- \end{bmatrix}, \tag{3.9}$$

and the one with a twist index k_- in the *upper left* corner of A_{22} is

$$\begin{bmatrix} L_+ & & \\ A_{21}U_+^{-1}D_+^{-1} & U''_- & A'_{23}L_-^{-\prime}D_-^{-\prime} \\ A_{31}U_+^{-1}D_+^{-1} & & U'_- \end{bmatrix} \cdot \begin{bmatrix} D_+ & & \\ & D''_- & \\ & & D'_- \end{bmatrix} \cdot \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & D_+^{-1}L_+^{-1}A_{13} \\ & L''_- & \\ & D_-^{-\prime}U_-^{-\prime}A'_{32} & L'_- \end{bmatrix}. \tag{3.10}$$

As in Sect. 2.3, one can derive connections to A^{-1}. However, exploiting the structure of the factors to efficiently compute an eigenvector approximation as in Sect. 2.4 requires a bit more care. For the approximate right eigenvector, one has

$$Az_r = \nu_k e_k \quad \Longleftrightarrow \quad \begin{bmatrix} U_+ & D_+^{-1}L_+^{-1}A_{12} & D_+^{-1}L_+^{-1}A_{13} \\ & U''_+ & \\ & D_-^{-\prime}U_-^{-\prime}A'_{32} & L'_- \end{bmatrix} z_r = e_k. \tag{3.11}$$

In this case, one first has to compute $z_r(k-b+1:k)$ from equations $k-b+1:k$, afterwards one can obtain $z_r(k+1:n)$ from the last $n-k+1$ equations, and finally one can compute $z_r(1:k-1)$. Computing the approximate left eigenvector is similar.

The task may partially simplify if at least one of the blocks A_{31} or A_{13} vanishes. For example, $A_{31}=0$ if A is an upper Hessenberg matrix. In this case, the computation of a left eigenvector approximation reduces to the standard banded case, but the right eigenvector approximation remains as described here.

We also remark that the factorization technique could be applied recursively if A''_{22} is large enough. One can block-partition A''_{22} again as in (3.1) instead of directly performing the double factorization (3.8). If the bandwidth is large enough, this can also be done for A'_{22} as an alternative to (2.8).

At last, for readers familiar with the WZ factorization [6, 14, 19], we note that (3.9) and (3.10) differ in that they are defined for an arbitrary twist index, and that their respective first and third factors do not have the WZ 'butterfly' shapes.

4 Stability and pivoting

The discussion thus far assumed existence of the double factorization (1.1), $A=L_+D_+U_+=U_-D_-L_-$. It is of course possible to encounter zero pivots so that (1.1) does not exist.

In the tridiagonal case, this situation can be handled very elegantly. We quote from [12, Sect. 6]: '*One of the attractions of an unreduced tridiagonal matrix is that the damage done by a zero pivot is localized. Indeed, if ∞ is added to the number system then triangular factorization cannot break down and the algorithm always maps [the matrix] J into unique triplets L, D, U. [...] It is no longer true that $LDU=J$ but equality does hold for all entries except for those at or adjacent to any infinite pivot.*'

Unfortunately, this approach does not readily extend for matrices with greater bandwidth. Take for example the pentadiagonal matrix from (2.1) and assume that the (1,1) entry is zero, but that no further zero occurs in the first row and column. If (1,1) is taken as the pivot, all four entries of the leading 2×2 block of the Schur complement become $\pm\infty$. Thus, the factorization breaks down in the subsequent step where quotients of the form ∞/∞ are encountered. Pivoting is needed in general in order to achieve stability in the banded factorization, see the classical reference [10]. For background material on inverse iteration, see [9].

The effects of pivoting on banded Gaussian elimination are described for example in [8, Sect. 4.3.3] and [5, Sect. 10.2]. We here consider again the pentadiagonal example (2.1) and assume that its *lowest* subdiagonal band b, in this case the second lower one, $b=2$, contains no zeros. Since the $(b+1:n, 1:n-b)$ submatrix is nonsingular, any eigenvalue with higher algebraic multiplicity can have a geometric multiplicity of at most b. Furthermore, it can be verified that the first $n-b$ steps of the $L_+D_+U_+$ factorization with *row* interchanges, and of the $U_-D_-L_-$ with *column* interchanges, cannot break down. In

$$\left[\begin{array}{ccccc|cc|cccccc}
* & * & 3 & * & * & & & & & & & & \\
* & 2 & * & * & & & & & & & & & \\
1 & * & * & & & & & & & & & & \\
 & * & * & 4 & * & * & & & & & & & \\
 & & * & * & 5 & * & * & & & & & & \\
\hline
 & & & * & * & 6 & * & * & & & & & \\
 & & & & * & * & 7 & * & * & & & & \\
\hline
 & & & & & * & * & 8 & * & * & & & \\
 & & & & & & * & * & 9 & * & & & * \\
 & & & & & & & * & * & 10 & & * & * \\
 & & & & & & & & * & * & * & * & 11 \\
 & & & & & & & & & * & * & 12 & * \\
 & & & & & & & & & & 13 & * & *
\end{array}\right], \tag{4.1}$$

we simultaneously illustrate interchanges of rows 1 & 3 and of columns 11 & 13 (the diagonal entries are labeled according to their original position on the diagonal). Both the $L_+D_+U_+$ and the $U_-D_-L_-$ factorizations will now encounter fill-in. Moreover, U_+ and L_- might double their bandwidth. However, if the pivoting is only needed up to the indices adjacent to the (2, 2) block (which are in this example elements 6 & 7), one can include pivoting into the framework of Sect. 3 and thus obtain twisted factorizations of the form (3.9) and (3.10).

Note that above, we only assumed only one of the exterior bands to be unreduced. This is relevant for matrices where the lower bandwidth differs from the upper one. In this case, if both bands contain only nonzero entries, one can choose the exterior band which is closer to the diagonal, that is the minimum of the lower and upper bandwidths.

5 Summary and conclusions

This paper gives a constructive proof for the existence of twisted factorizations of a band matrix. One of their important applications is inverse iteration and we showed how to exploit the twisted form.

We close with a question to the reader regarding choice of nomenclature: because of their 2-level construction, one may argue that ‘twisted’ is not the most descriptive adjective to describe the banded factorizations (2.9) and (2.10). This is even truer for the general factorizations (3.10) and (3.9). Maybe ‘interwoven’ should be used? Only in the simplest, tridiagonal, case, the factorization is simply twisted.

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References

1. Dhillon, I.S.: A New $O(n^2)$ Algorithm for the Symmetric Tridiagonal Eigenvalue/Eigenvector Problem. Ph.D. Thesis, University of California, Berkeley, California (1997)

2. Dhillon, I.S., Parlett, B.N.: Multiple representations to compute orthogonal eigenvectors of symmetric tridiagonal matrices. Linear Algebra Appl. **387**, 1–28 (2004)
3. Dhillon, I.S., Parlett, B.N.: Orthogonal eigenvectors and relative gaps. SIAM J. Matrix Anal. Appl. **25**(3), 858–899 (2004)
4. Dhillon, I.S., Parlett, B.N., Vömel, C.: The design and implementation of the MRRR algorithm. ACM Trans. Math. Softw. **32**(4), 533–560 (2006)
5. Duff, I.S., Erisman, A.M., Reid, J.K.: Direct Methods for Sparse Matrices. Oxford University Press, London (1986)
6. Evans, D.J.: Implicit matrix elimination (IME) schemes. Int. J. Comput. Math. **48**(3–4), 229–237 (1993)
7. Fernando, K.V.: On computing an eigenvector of a tridiagonal matrix. Part I: basic results. SIAM J. Matrix Anal. Appl. **18**(4), 1013–1034 (1997)
8. Golub, G.H., van Loan, C.: Matrix Computations, 3rd edn. John Hopkins University Press, Baltimore (1996)
9. Ipsen, I.C.F.: Computing an eigenvector with inverse iteration. SIAM Rev. **39**(2), 254–291 (1997)
10. Martin, R.S., Wilkinson, J.H.: Solution of symmetric and unsymmetric band equations and the calculation of eigenvectors of band matrices. Numer. Math. **9**(4), 279–301 (1967)
11. Meurant, G.: A review on the inverse of symmetric tridiagonal and block tridiagonal matrices. SIAM J. Matrix Anal. Appl. **13**(3), 707–728 (1992)
12. Parlett, B.N., Dhillon, I.S.: Fernando's solution to Wilkinson's problem: an application of double factorization. Linear Algebra Appl. **267**, 247–279 (1997)
13. Parlett, B.N., Dhillon, I.S.: Relatively robust representations of symmetric tridiagonals. Linear Algebra Appl. **309**(1–3), 121–151 (2000)
14. Sekhara Rao, S.C.: Existence and uniqueness of WZ factorization. Parallel Comput. **23**(8), 1129–1139 (1997)
15. Stewart, G.W.: Matrix Algorithms II: Eigensystems. SIAM, Philadelphia (2001)
16. van der Vorst, H.A.: Analysis of a parallel solution method for tridiagonal linear systems. Parallel Comput. **5**(3), 303–311 (1987)
17. Wilkinson, J.H.: The Algebraic Eigenvalue Problem. Oxford University Press, London (1965)
18. Xu, W., Qiao, S.: A Twisted Factorization Method for Symmetric SVD of a Complex Symmetric Tridiagonal Matrix. Technical Report CAS 06-01-SQ, Department of Computing and Software, McMaster University, Hamilton, Ontario, Canada (2006)
19. Yalamov, P., Evans, D.J.: The WZ matrix factorisation method. Parallel Comput. **21**(7), 1111–1120 (1995)
20. Zhang, Z.-Y., Ouyang, T.-W.: Computing eigenvectors of normal matrices with simple inverse iteration. J. Comput. Math. **21**(5), 657–670 (2003)