Spec. Matrices 2019; 7:20–26 DE GRUYTER

Research Article **Open Access**

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Bidiagonalization of $(k, k+1)$-tridiagonal matrices

https://doi.org/10.1515/spma-2019-0002
Received April 2, 2018; accepted September 28, 2018

Abstract: In this paper, we present the bidiagonalization of n-by-n $(k, k+1)$-tridiagonal matrices when $n \le 2k$. Moreover, we show that the determinant of an n-by-n $(k, k+1)$-tridiagonal matrix is the product of the diagonal elements and the eigenvalues of the matrix are the diagonal elements. This paper is related to the fast block diagonalization algorithm using the permutation matrix from [T. Sogabe and M. El-Mikkawy, Appl. Math. Comput., 218, (2011), 2740-2743] and [A. Ohashi, T. Sogabe, and T. S. Usuda, Int. J. Pure and App. Math., 106, (2016), 513-523].

Keywords: $(k, k+1)$-tridiagonal matrix, bidiagonalization, eigenvalues

MSC: Primary 65F15; Secondary 65F30

1 Introduction

We consider an n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ defined by

$$T_n^{(k,k+1)} := \begin{array}{c} \\ 1 \\ 2 \\ \vdots \\ \vdots \\ k+2 \\ \vdots \\ n \end{array} \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & \cdots & k+1 & \cdots & \cdots & n \end{array} \\ \begin{pmatrix} d_1 & & & a_1 & & & \\ & d_2 & & & \ddots & & \\ & & \ddots & & & \ddots & \\ & & & d_{n-k} & & & a_{n-k} \\ b_1 & & & & \ddots & & \\ & \ddots & & & & \ddots & \\ & & b_{n-k-1} & & & & d_n \end{pmatrix} \end{array}. \tag{1}$$

The numbers of elements d_i, a_i and b_i are n, $n-k$ and $n-k-1$, respectively. The matrix $T_n^{(k,k+1)}$ can also be described as follows:

$$T_n^{(k,k+1)} = \sum_{i=1}^{n} d_i \boldsymbol{e}_i \boldsymbol{e}_i^{\mathrm{T}} + \sum_{i=1}^{n-k} a_i \boldsymbol{e}_i \boldsymbol{e}_{k+i}^{\mathrm{T}} + \sum_{i=1}^{n-k-1} b_i \boldsymbol{e}_{i+k+1} \boldsymbol{e}_i^{\mathrm{T}}, \tag{2}$$

where $\boldsymbol{e}_i$ denotes the i-th canonical n dimensional basis vector and $\boldsymbol{e}_i^{\mathrm{T}}$ denotes the transpose of $\boldsymbol{e}_i$.

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$(k, k+1)$-tridiagonal matrices arise in applications such as the discrete hungry Lotka-Volterra system and linear systems (see, e.g., [3, 4]). These matrices are related to k-Hessenberg matrices $H_n(k)$ [2], in that $T_n^{(k,k+1)}$ with $k = 1$ corresponds to $H_n(k)$ with $k = 2$, and can be regarded as a variant of k-tridiagonal matrices (see, e.g., [1, 7]). Moreover, a $(k, k+1)$-tridiagonal matrix is a special case of a (k, k')-pentadiagonal matrix (see, e.g., [6]). In fact, if $k' = k+1$, and the k-th superdiagonal and k'-th subdiagonal are all zero, then a (k, k')-pentadiagonal matrix is a $(k, k+1)$-tridiagonal matrix. For k-tridiagonal matrices and (k, k')-pentadiagonal matrices, the fast block diagonalization algorithm using a permutation matrix is discussed in [6, 7]. However, the $(k, k+1)$-tridiagonal matrices are irreducible in the sense that the block size of the matrix produced by the block diagonalization algorithm in [6] is one.

In this paper, we consider another type of diagonalization, that is, bidiagonalization using a permutation matrix. The bidiagonalization of $T_n^{(k,k+1)}$ is the process of finding a lower bidiagonal matrix T' and a permutation matrix P such that

$$T' = P^{\mathrm{T}} T_n^{(k,k+1)} P, \tag{3}$$

where P is the n-by-n permutation matrix defined as

$$P := \sum_{i=1}^{n} \boldsymbol{e}_{\sigma(i)} \boldsymbol{e}_i^{\mathrm{T}}, \tag{4}$$

and σ is a permutation in the symmetric group of order n. Moreover, we give an explicit representation of the bidiagonal matrix T' and the permutation matrix P. We consider only bidiagonalizations of the form $P^{\mathrm{T}} T_n^{(k,k+1)} P$, and in particular do not consider bidiagonalizations of the form $P^{\mathrm{T}} T_n^{(k,k+1)} Q$ for different permutation matrices P and Q. One reason is that, as we will see in Corollary 4, the eigenvalues of an n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ are the diagonal elements $d_1, d_2, \dots, d_n$.

We now give a necessary condition for bidiagonalization of n-by-n $(k, k+1)$-tridiagonal matrices $T_n^{(k,k+1)}$ when the elements d_i, a_i, b_i are all nonzero. Then, the number of nonzero elements of $T_n^{(k,k+1)}$ is $3n - 2k - 1$. Thus, we have the necessary condition given in the following remark.

Remark 1. *Suppose that the elements d_i, a_i, b_i of an n-by-n $(k, k+1)$-tridiagonal matrices $T_n^{(k,k+1)}$ are all nonzero. Then $n \le 2k$ is a necessary condition for bidiagonalization of $T_n^{(k,k+1)}$ using a permutation matrix.*

Proof. The number of elements of d_i, a_i, b_i of $T_n^{(k,k+1)}$ is $3n - 2k - 1$. The position of nonzero elements of the bidiagonal matrix T' must be on the diagonal or on the subdiagonal. The number of nonzero elements of $T_n^{(k,k+1)}$ is equal to the number of nonzero elements of T' because we consider the bidiagonalization by a permutation matrix. Thus, we have $3n - 2k - 1 \le n + n - 1$, that is $n \le 2k$. □

Therefore, we consider only the case $n \le 2k$.

2 Main Result

We present the bidiagonalization of the n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ when $n \le 2k$ and an explicit representation of the permutation matrix as a theorem. In addition, we give the determinant and eigenvalues of the n-by-n $(k, k+1)$-tridiagonal matrix when $n \le 2k$ as corollaries of the theorem.

Theorem 2. *Let $T_n^{(k,k+1)}$ be the n-by-n $(k, k+1)$-tridiagonal matrix in Eq.(1) with $n \le 2k$. Then there is a bidiagonalization T' of $T_n^{(k,k+1)}$ of the form*

$$\begin{aligned} T' = P^{\mathrm{T}} T_n^{(k,k+1)} P = &\sum_{i=1}^{n-k} (d_i \boldsymbol{e}_{2i} \boldsymbol{e}_{2i}^{\mathrm{T}} + d_{k+i} \boldsymbol{e}_{2i-1} \boldsymbol{e}_{2i-1}^{\mathrm{T}}) + \sum_{i=n-k+1}^{k} d_i \boldsymbol{e}_{n-k+i} \boldsymbol{e}_{n-k+i}^{\mathrm{T}} \\ &+ \sum_{i=1}^{n-k} a_i \boldsymbol{e}_{2i} \boldsymbol{e}_{2i-1}^{\mathrm{T}} + \sum_{i=1}^{n-k-1} b_i \boldsymbol{e}_{2i+1} \boldsymbol{e}_{2i}^{\mathrm{T}}, \end{aligned} \tag{5}$$

where P is the permutation matrix

$$P = \sum_{j=1}^{n-k} (\boldsymbol{e}_{k+j}\boldsymbol{e}_{2j-1}^{\mathrm{T}} + \boldsymbol{e}_j\boldsymbol{e}_{2j}^{\mathrm{T}}) + \sum_{j=n-k+1}^{k} \boldsymbol{e}_j\boldsymbol{e}_{n-k+j}^{\mathrm{T}}. \tag{6}$$

Proof. For an n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$, we define

$$D_n := \sum_{i=1}^{n} d_i\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}}, \quad A_n := \sum_{i=1}^{n-k} a_i\boldsymbol{e}_i\boldsymbol{e}_{k+i}^{\mathrm{T}}, \quad B_n := \sum_{i=1}^{n-k-1} b_i\boldsymbol{e}_{i+k+1}\boldsymbol{e}_i^{\mathrm{T}}, \tag{7}$$

and compute each of $P^{\mathrm{T}}D_nP$, $P^{\mathrm{T}}A_nP$, $P^{\mathrm{T}}B_nP$ to obtain $P^{\mathrm{T}}T_n^{(k,k+1)}P$.

The vector $P^{\mathrm{T}}\boldsymbol{e}_i$ can be written

$$\begin{aligned} P^{\mathrm{T}}\boldsymbol{e}_i &= \left(\sum_{j=1}^{n-k} \boldsymbol{e}_{2j-1}\boldsymbol{e}_{k+j}^{\mathrm{T}} + \sum_{j=1}^{n-k} \boldsymbol{e}_{2j}\boldsymbol{e}_j^{\mathrm{T}} + \sum_{j=n-k+1}^{k} \boldsymbol{e}_{n-k+j}\boldsymbol{e}_j^{\mathrm{T}} \right) \boldsymbol{e}_i, \\ &= \sum_{j=1}^{n-k} \boldsymbol{e}_{2j-1}\delta_{k+j,i} + \sum_{j=1}^{n-k} \boldsymbol{e}_{2j}\delta_{j,i} + \sum_{j=n-k+1}^{k} \boldsymbol{e}_{n-k+j}\delta_{j,i}, \\ &= \begin{cases} \boldsymbol{e}_{2i} & 1 \le i \le n-k \\ \boldsymbol{e}_{n-k+i} & n-k+1 \le i \le k \\ \boldsymbol{e}_{2(i-k)-1} & k+1 \le i \le n \end{cases}, \end{aligned} \tag{8}$$

where $\delta_{i,j}$ is the Kronecker delta, that is, $\delta_{i,i} = 1$ and $\delta_{i,j} = 0$ for $i \ne j$. Note that $n-k \le k < k+j$ for $j > 0$ because $n \le 2k$. By transposing Eq.(8), we also obtain $\boldsymbol{e}_i^{\mathrm{T}}P$.

We compute $P^{\mathrm{T}}D_nP$ as follows:

$$\begin{aligned} P^{\mathrm{T}}D_nP &= P^{\mathrm{T}} \left(\sum_{i=1}^{n-k} d_i\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}} + \sum_{i=n-k+1}^{k} d_i\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}} + \sum_{i=k+1}^{n} d_i\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}} \right) P, \\ &= \sum_{i=1}^{n-k} d_iP^{\mathrm{T}}\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}}P + \sum_{i=n-k+1}^{k} d_iP^{\mathrm{T}}\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}}P + \sum_{i=k+1}^{n} d_iP^{\mathrm{T}}\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}}P, \\ &= \sum_{i=1}^{n-k} d_i\boldsymbol{e}_{2i}\boldsymbol{e}_{2i}^{\mathrm{T}} + \sum_{i=n-k+1}^{k} d_i\boldsymbol{e}_{n-k+i}\boldsymbol{e}_{n-k+i}^{\mathrm{T}} + \sum_{i=k+1}^{n} d_i\boldsymbol{e}_{2(i-k)-1}\boldsymbol{e}_{2(i-k)-1}^{\mathrm{T}}, \\ &= \sum_{i=1}^{n-k} \left(d_i\boldsymbol{e}_{2i}\boldsymbol{e}_{2i}^{\mathrm{T}} + d_{i+k}\boldsymbol{e}_{2i-1}\boldsymbol{e}_{2i-1}^{\mathrm{T}} \right) + \sum_{i=n-k+1}^{k} d_i\boldsymbol{e}_{n-k+i}\boldsymbol{e}_{n-k+i}^{\mathrm{T}}. \end{aligned} \tag{9}$$

Next, we compute $P^{\mathrm{T}}A_nP$ as follows:

$$P^{\mathrm{T}}A_nP = \sum_{i=1}^{n-k} a_iP^{\mathrm{T}}\boldsymbol{e}_i\boldsymbol{e}_{k+i}^{\mathrm{T}}P = \sum_{i=1}^{n-k} a_i\boldsymbol{e}_{2i}\boldsymbol{e}_{2i-1}^{\mathrm{T}}. \tag{10}$$

Finally, we compute $P^{\mathrm{T}}B_nP$ as follows:

$$P^{\mathrm{T}}B_nP = \sum_{i=1}^{n-k-1} b_iP^{\mathrm{T}}\boldsymbol{e}_{i+k+1}\boldsymbol{e}_i^{\mathrm{T}}P = \sum_{i=1}^{n-k-1} b_i\boldsymbol{e}_{2i+1}\boldsymbol{e}_{2i}^{\mathrm{T}}. \tag{11}$$

Therefore, we have a bidiagonalization of the form (5). This completes the proof of Theorem 2. □

Note that the case $n = 2k$ is essential for bidiagonalization using a permutation matrix. Because, as we will see in the appendix, the permutation matrix when $n = 2k$ is uniquely derived as

$$P = \sum_{j=1}^{n-k} (\boldsymbol{e}_{k+j}\boldsymbol{e}_{2j-1}^{\mathrm{T}} + \boldsymbol{e}_j\boldsymbol{e}_{2j}^{\mathrm{T}}). \tag{12}$$

In addition, the permutation matrix when $n < 2k$ can be obtained from the permutation matrix when $n = 2k$. Moreover, bidiagonalization is not uniquely determined when $n < 2k$. For the case $n < 2k$, the matrix (5) is the block diagonal matrix that has one bidiagonal block and some 1-by-1 blocks (for example, see Example 6). Therefore, choosing an appropriate permutation matrix P' to exchange blocks, we can obtain another bidiagonalization of the form $T'' = (PP')^{\mathrm{T}} T_n^{(k,k+1)}(PP')$. However, this is not essential for bidiagonalization because such a permutation matrix P' only exchanges blocks.

From Theorem 2, we have the following corollary giving the determinant and eigenvalues of an n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ when $n \le 2k$.

Corollary 3. *The determinant of the n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ in Eq.(1) with $n \le 2k$ is the product of the elements on the main diagonal, that is,* $\det(T_n^{(k,k+1)}) = d_1 d_2 \cdots d_n$.

Corollary 4. *The eigenvalues λ of the n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ in Eq.(1) with $n \le 2k$ are the elements on the main diagonal, that is, $\lambda = d_1, d_2, \ldots, d_n$.*

Corollary 4 relates to the result of Theorem 1 in [5]. If diagonal elements $d_1, d_2, \ldots, d_n$ of $T_n^{(k,k+1)}$ are all zero and a_i, b_i are all positive real numbers, then the $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ coincides with the double band matrix A with $b = k + 1$ in [5]. When $n \le 2k$, the eigenvalues of the matrix are $d_1 = d_2 = \cdots = d_n = 0$ from Corollary 4, and moreover the matrix has the zero eigenvalue of multiplicity n from Theorem 1 in [5].

3 Examples

In this section, we present two examples based on the result in the previous section.

Example 5 ($n = 10$, $k = 5$). *Let $T_{10}^{(5,6)}$ be the following $(5,6)$-tridiagonal matrix:*

$$T_{10}^{(5,6)} = \begin{pmatrix} d_1 & 0 & 0 & 0 & 0 & a_1 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 & 0 & a_2 & 0 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 & 0 & 0 & a_3 & 0 & 0 \\ 0 & 0 & 0 & d_4 & 0 & 0 & 0 & 0 & a_4 & 0 \\ 0 & 0 & 0 & 0 & d_5 & 0 & 0 & 0 & 0 & a_5 \\ 0 & 0 & 0 & 0 & 0 & d_6 & 0 & 0 & 0 & 0 \\ b_1 & 0 & 0 & 0 & 0 & 0 & d_7 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 & 0 & 0 & d_8 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 & 0 & 0 & d_9 & 0 \\ 0 & 0 & 0 & b_4 & 0 & 0 & 0 & 0 & 0 & d_{10} \end{pmatrix}. \tag{13}$$

Applying Theorem 2, we have the permutation matrix

$$P = [\boldsymbol{e}_6, \boldsymbol{e}_1, \boldsymbol{e}_7, \boldsymbol{e}_2, \boldsymbol{e}_8, \boldsymbol{e}_3, \boldsymbol{e}_9, \boldsymbol{e}_4, \boldsymbol{e}_{10}, \boldsymbol{e}_5], \tag{14}$$

and the bidiagonal matrix T' is

$$P^{\mathrm{T}} T_{10}^{(5,6)} P = \begin{pmatrix} d_6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_1 & d_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_1 & d_7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_2 & d_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_2 & d_8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a_3 & d_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_3 & d_9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a_4 & d_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_4 & d_{10} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_5 & d_5 \end{pmatrix}. \tag{15}$$

This example corresponds to the case $n = 2k$. The total number of values a_i and b_i is $9 = n - 1$. We can see that some a_i or b_i appears in each position of the subdiagonal.

Example 6 ($n = 10, k = 6$)**.** *Let $T_{10}^{(6,7)}$ be the following* $(6, 7)$*-tridiagonal matrix:*

$$T_{10}^{(6,7)} = \begin{pmatrix} d_1 & 0 & 0 & 0 & 0 & 0 & a_1 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 & 0 & 0 & a_2 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 & 0 & 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & d_4 & 0 & 0 & 0 & 0 & 0 & a_4 \\ 0 & 0 & 0 & 0 & d_5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d_6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & d_7 & 0 & 0 & 0 \\ b_1 & 0 & 0 & 0 & 0 & 0 & 0 & d_8 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 & 0 & 0 & 0 & d_9 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 & 0 & 0 & 0 & d_{10} \end{pmatrix}. \tag{16}$$

Applying Theorem 2, we have the permutation matrix

$$P = [\boldsymbol{e}_7, \boldsymbol{e}_1, \boldsymbol{e}_8, \boldsymbol{e}_2, \boldsymbol{e}_9, \boldsymbol{e}_3, \boldsymbol{e}_{10}, \boldsymbol{e}_4, \boldsymbol{e}_5, \boldsymbol{e}_6], \tag{17}$$

and the bidiagonal matrix T' is

$$P^{\mathrm{T}} T_{10}^{(6,7)} P = \begin{pmatrix} d_7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_1 & d_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_1 & d_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_2 & d_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_2 & d_9 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a_3 & d_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_3 & d_{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a_4 & d_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d_6 \end{pmatrix}. \tag{18}$$

This example corresponds to the case $n < 2k$. The total number of values a_i and b_i is $7 < (n - 1)$. Thus, there are two zero elements in the subdiagonal. In particular, both the $(9, 8)$ element and the $(10, 9)$ element are zero.

Acknowledgement: We thank Peter Humphries, PhD, from Edanz Group (www.edanzediting.com/ac) for editing a draft of this manuscript. We also thank the editor and the anonymous referees for the comments for the original manuscript of this paper. This work has been supported in part by JSPS KAKENHI Grant Numbers JP16H04367, JP18H05392.

Appendix A : Derivation of the bidiagonalization

In this appendix, we derive the bidiagonalization of an n-by-n $(k, k + 1)$-tridiagonal matrix $T_n^{(k,k+1)}$ when $n = 2k$. Although the general case is $n \leq 2k$ from Remark 1, we consider $n = 2k$ because the permutation matrix when $n < 2k$ can be described using the permutation matrix when $n = 2k$. Moreover, the case $n = 2k$ is essential for the bidiagonalization as described in Section 2.

We first show a relationship between the elements of the matrices X and $X' = P^{\mathrm{T}}XP$ for an n-by-n matrix X. We then derive the bidiagonalization of an n-by-n $(k, k + 1)$-tridiagonal matrix and an explicit representation of the permutation matrix P when $n = 2k$.

A.1 Preliminaries

We present a relationship between the elements of X and X' in the following lemma. Throughout the paper, $X_{i,j}$ denotes the (i,j) element of a matrix X and σ^{-1} denotes the inverse of the permutation σ.

Lemma 7. *Let X be an n-by-n matrix and P be an n-by-n permutation matrix. The (i,j) element of $X' = P^{\mathrm{T}}XP$ is the $(\sigma(i), \sigma(j))$ element of X, that is, $X'_{i,j} = X_{\sigma(i),\sigma(j)}$. Alternatively, the (i,j) element of X is the $(\sigma^{-1}(i), \sigma^{-1}(j))$ element of X', that is, $X_{i,j} = X'_{\sigma^{-1}(i),\sigma^{-1}(j)}$.*

Proof. We prove this lemma by direct calculation:

$$X' = P^{\mathrm{T}}XP = \left(\sum_{i=1}^{n} \boldsymbol{e}_i \boldsymbol{e}_{\sigma(i)}^{\mathrm{T}}\right) X \left(\sum_{j=1}^{n} \boldsymbol{e}_{\sigma(j)} \boldsymbol{e}_j^{\mathrm{T}}\right) = \sum_{i=1}^{n}\sum_{j=1}^{n} \boldsymbol{e}_{\sigma(i)}^{\mathrm{T}} X \boldsymbol{e}_{\sigma(j)} \boldsymbol{e}_i \boldsymbol{e}_j^{\mathrm{T}},$$
$$= \sum_{i=1}^{n}\sum_{j=1}^{n} X_{\sigma(i),\sigma(j)} \boldsymbol{e}_i \boldsymbol{e}_j^{\mathrm{T}}. \tag{19}$$

□

A.2 The nonzero structure of the bidiagonal matrix

We describe the nonzero structure of $T' = P^{\mathrm{T}} T_n^{(k,k+1)} P$ by considering submatrices. Using Lemma 7, we can determine the submatrices for which the lower left element is a_i or b_i as follows.

Lemma 8. *Let $T_n^{(k,k+1)}$ be the n-by-n $(k, k+1)$-tridiagonal matrix in Eq.(1) and let P be the n-by-n permutation matrix in Eq.(4). If $n = 2k$ and P bidiagonalizes $T_n^{(k,k+1)}$, then the matrix $T' = P^{\mathrm{T}} T_n^{(k,k+1)} P$ has the following 2-by-2 submatrices whose lower left element is a_i:*

$$\begin{pmatrix} T'_{\sigma^{-1}(i)-1,\sigma^{-1}(i)-1} & 0 \\ T'_{\sigma^{-1}(i),\sigma^{-1}(i)-1} & T'_{\sigma^{-1}(i),\sigma^{-1}(i)} \end{pmatrix} = \begin{pmatrix} d_{k+i} & 0 \\ a_i & d_i \end{pmatrix}, \qquad i = 1, 2, \ldots, n-k. \tag{20}$$

Proof. We write τ and T for σ^{-1} and $T_n^{(k,k+1)}$, respectively. For the main diagonal of the matrix T', we focus on the 2-by-2 submatrix whose lower right element is $T'_{\tau(1),\tau(1)}$. Because T' is a bidiagonal matrix, a submatrix of T' is a lower bidiagonal matrix. From Lemma 2, the form of the submatrix is

$$\begin{pmatrix} T'_{\tau(1)-1,\tau(1)-1} & 0 \\ T'_{\tau(1),\tau(1)-1} & T'_{\tau(1),\tau(1)} \end{pmatrix} = \begin{pmatrix} T_{\sigma(\tau(1)-1),\sigma(\tau(1)-1)} & 0 \\ T_{\sigma(\tau(1)),\sigma(\tau(1)-1)} & T_{\sigma(\tau(1)),\sigma(\tau(1))} \end{pmatrix},$$
$$= \begin{pmatrix} T_{\sigma(\tau(1)-1),\sigma(\tau(1)-1)} & 0 \\ T_{1,\sigma(\tau(1)-1)} & T_{1,1} \end{pmatrix}. \tag{21}$$

The nonzero elements in the first row of T are d_1 and a_1. From $T_{1,1} = d_1$, it follows that $T_{1,\sigma(\tau(1)-1)} = a_1 = T_{1,k+1}$ because the subdiagonals of T' are all nonzero when $n = 2k$. Thus, we have $\sigma(\tau(1)-1) = k+1$. Therefore, we can rewrite equation (21) as

$$\begin{pmatrix} T'_{\tau(1)-1,\tau(1)-1} & 0 \\ T'_{\tau(1),\tau(1)-1} & T'_{\tau(1),\tau(1)} \end{pmatrix} = \begin{pmatrix} d_{k+1} & 0 \\ a_1 & d_1 \end{pmatrix}. \tag{22}$$

The cases $i = 2, 3, \ldots, n-k$ follow similarly, which proves the lemma. □

Lemma 9. *Let $T_n^{(k,k+1)}$ be the n-by-n $(k, k+1)$-tridiagonal matrix in Eq.(1) and let P be the n-by-n permutation matrix as in Eq.(4). If $n = 2k$ and P bidiagonalizes $T_n^{(k,k+1)}$, then the matrix $T' = P^{\mathrm{T}} T_n^{(k,k+1)} P$ has the following 2-by-2 submatrices whose lower left element is b_i:*

$$\begin{pmatrix} T'_{\sigma^{-1}(i),\sigma^{-1}(i)} & 0 \\ T'_{\sigma^{-1}(i)+1,\sigma^{-1}(i)} & T'_{\sigma^{-1}(i)+1,\sigma^{-1}(i)+1} \end{pmatrix} = \begin{pmatrix} d_i & 0 \\ b_i & d_{k+i+1} \end{pmatrix}, \qquad i = 1, 2, \ldots, n-k-1. \tag{23}$$

Proof. The proof is similar to that of Lemma 8. □

We now show the nonzero structure of the bidiagonal matrix T' in Lemma 8 and Lemma 9.

Proposition 10. *Let $T_n^{(k,k+1)}$ be the n-by-n $(k, k+1)$-tridiagonal matrix in Eq.(1) and let P be the permutation matrix in Eq.(4). If $n = 2k$ and P bidiagonalizes $T_n^{(k,k+1)}$, then the matrix $T' = P^{\mathrm{T}} T_n^{(k,k+1)} P$ is a bidiagonal matrix of the form*

$$T' = P^{\mathrm{T}} T_n^{(k,k+1)} P = \sum_{i=1}^{n-k} (d_{i+k}\boldsymbol{e}_{2i-1}\boldsymbol{e}_{2i-1}^{\mathrm{T}} + d_i\boldsymbol{e}_{2i}\boldsymbol{e}_{2i}^{\mathrm{T}}) + \sum_{i=1}^{n-k} a_i\boldsymbol{e}_{2i}\boldsymbol{e}_{2i-1}^{\mathrm{T}} + \sum_{i=1}^{n-k-1} b_i\boldsymbol{e}_{2i+1}\boldsymbol{e}_{2i}^{\mathrm{T}}. \tag{24}$$

Proof. From Eqs.(20) and (23), we have the following 3-by-3 bidiagonal submatrices of T':

$$\begin{pmatrix} T'_{\tau(i)-1,\tau(i)-1} & 0 & 0 \\ T'_{\tau(i)-1,\tau(i)} & T'_{\tau(i),\tau(i)} & 0 \\ 0 & T'_{\tau(i),\tau(i)+1} & T'_{\tau(i)+1,\tau(i)+1} \end{pmatrix} = \begin{pmatrix} d_{i+k} & 0 & 0 \\ a_i & d_i & 0 \\ 0 & b_i & d_{i+1+k} \end{pmatrix}, \quad i = 1, 2, \ldots, n-k-1. \tag{25}$$

The elements of $T_n^{(k,k+1)}$ are not divided into two parts by the transformation. For example, d_1 is the only element of T'. Therefore, we have $\tau(i) + 1 = \tau(i+1) - 1$ for $i = 1, 2, \ldots, n-k-1$. Considering the submatrix (20) for $i = n-k$, the sequence on the main diagonal of T' is $d_{1+k}, d_1, d_{2+k}, d_2, \ldots, d_{n-k}, d_n$. Moreover, the sequence on the subdiagonal of T' is $a_1, b_1, a_2, b_2, \ldots, a_{n-k-1}, b_{n-k-1}, a_{n-k}$. □

A.3 Derivation of the permutation matrix

We now derive an explicit representation of the permutation matrix P when $n = 2k$. Proposition 10 suggests a permutation matrix of the form $P = \sum_{i=1}^{n} \boldsymbol{e}_{\sigma(i)}\boldsymbol{e}_i^{\mathrm{T}}$, where σ is the permutation. From the proof of the proposition, the sequence on the main diagonal of T' when $n = 2k$ is $d_{k+1}, d_1, d_{k+2}, d_2, \ldots, d_n, d_{n-k}$. Moreover, from Lemma 7, the (i, i) element of T' is the $(\sigma(i), \sigma(i))$ element of $T_n^{(k,k+1)}$. Thus, we have $k+1 = \sigma(1)$, $1 = \sigma(2)$, $k+2 = \sigma(3)$, $2 = \sigma(4), \ldots, n = \sigma(n-1)$, $n-k = \sigma(n)$. Namely, when $n = 2k$, we have the permutation matrix

$$P = \sum_{j=1}^{n-k} (\boldsymbol{e}_{k+j}\boldsymbol{e}_{2j-1}^{\mathrm{T}} + \boldsymbol{e}_j\boldsymbol{e}_{2j}^{\mathrm{T}}). \tag{26}$$

We summarize this in the following proposition.

Proposition 11. *The permutation matrix P that bidiagonalizes the n-by-n $(k, k+1)$-tridiagonal matrix $T_n^{(k,k+1)}$ when $n = 2k$ is the matrix in Eq.(26).*

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