Research Article

Hariprasad Manjunath*

Block diagonalization of (*p*, *q*)-tridiagonal matrices

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Abstract: In this article, we study the block diagonalization of (p, q)-tridiagonal matrices and derive closed-form expressions for the number and structure of diagonal blocks as functions of the parameters p, q, and n. This reduction enables efficient computation of eigenvalues and eigenvectors by decomposing the matrix into smaller subproblems. We extend the method to more general $(\mathcal{P}, \mathcal{Q})$-tridiagonal matrices, where $\mathcal{P}$ and $\mathcal{Q}$ are sets of positive integers, covering general banded structures. We also examine special cases such as bidiagonal and triangular block reductions along with supporting algorithms and numerical examples.

Keywords: k-tridiagonal matrices, p, q-tridiagonal matrices, upper Hessenberg, eigenvalues

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1 Introduction

An $n \times n$ matrix is a (p, q)-tridiagonal matrix if it is of the form

$$T_n^{(p,q)} = \begin{array}{c} \\ 1 \\ 2 \\ \vdots \\ q+1 \\ q+2 \\ \vdots \\ n \end{array} \begin{array}{c} \begin{array}{ccccccc} 1 & 2 & \cdots & p+1 & p+2 & \cdots & n \end{array} \\ \begin{pmatrix} a_1 & & & b_1 & & & \\ & a_2 & & & b_2 & & \\ & & \ddots & & & \ddots & \\ c_1 & & & \ddots & & & b_{n-p} \\ & c_2 & & & \ddots & & \\ & & \ddots & & & \ddots & \\ & & & c_{n-q} & & & a_n \end{pmatrix} \end{array}. \quad (1)$$

When $p = q = 1$, the matrix is tridiagonal. When $p = q = k$, they are known as k-tridiagonal matrices. The inverses of k tridiagonal matrices are studied in [14]. In [18] and [14], explicit construction of permutation matrices was given fork diagonalization of k-tridiagonal matrices. da Fonseca et al. [4] explained the historical connection with trigonometric polynomials and the development of algorithms for k-tridiagonal matrices and (p, q) -penta-diagonal matrices. da Fonseca et al. [4] also mentioned the graph-theoretic approach, which we follow in this study. da Fonseca and Yılmaz [6] derived the determinant spectra and inversion of k-tridiagonal matrices.

As an extension of k-tridiagonal matrices, when $p = k, q = k + 1$, the $(k, k + 1)$-tridiagonal matrices are studied in [19]. Takahira et al. [19] derived the bidiagonalization using a permutation matrix. The $(k, k + 1)$ tridiagonal matrices arise in discrete hungry Lotka-Volterra models [10]. In particular, when $\lceil \frac{n}{2} \rceil \leq p < q$, a

*** Corresponding author: Hariprasad Manjunath**, School of Mathematics and Natural Sciences, Chanakya University, Bengaluru, Karnataka, India, e-mail: mhariprasadkansur@gmail.com

bidiagonal reduction of $T_n^{(p,q)}$ is possible by a permutation matrix. Recently, a bidiagonalization reduction of (p, q)-tridiagonal matrices was investigated in [12]. The bidiagonalization was further used to compute the inverse of these matrices. The bidiagonalization of the blocks for the k-tridiagonal block matrices is studied in [13]. In general, we do not have the bidiagonal reduction of (p, q)-tridiagonal matrices. The determinants and their properties are studied in [7]. The eigenvalues of double-banded matrices are studied in [16]. These structured tridiagonal matrices are applied in boundary value problems [9], and in the discretization of differential equations [1]. They are also of interest in number theory [5].

2 Notations

The greatest common divisor of two integers a, b is denoted by $\mathrm{GCD}(a, b)$. The identity matrix of order n is denoted by I_n (or I in the absence of ambiguity). The adjacency matrix of a directed *cycle* is denoted by C,

Table 1: Number of blocks in the block diagonal reduction of $T_n^{(p,q)}$ and nature of the blocks for even n (for odd n, the number of blocks can be deduced by Theorem 9)

Condition on p and q	**Number of blocks**	**Nature of blocks**
$p + q \leq n$, $d = \mathrm{GCD}(p, q)$	d	Each block is (p', q')-tridiagonal with $p' = \frac{p}{d}$, $q' = \frac{q}{d}$
$p = \frac{n}{2}, q > p$ $2q > 3p$	$q - p$	$n - q$ paths with four vertices each $2q - 3p$ paths containing two vertices
$p = \frac{n}{2}, q > p$ $2q < 3p$ $(q - p)k + r = \frac{n}{2}$	$q - p$	r paths with $(2k + 2)$ vertices each $q - p - r$ paths containing $2k$ vertices
$p, q > \frac{n}{2}$	$p + q - n$	$2p - n$ isolated vertices, nature of remaining blocks to be deduced from rows two and three of this table depending on values of $p' = n - p, q' = n + q - 2p, n' = 2n - 2p$
$p + q > n$ $p < \frac{n}{2}$ $p \mid q$	p	$n - q$ cycles of length $1 + \frac{q}{p}$ $p + q - n$ paths of length $\frac{q}{p}$
$p + q > n$ $p < \frac{n}{2}$ $r = n \bmod p, n = pt + r,$ $r > 2(n - q) - 1$	$p + q - n$	$p - r$ paths have t vertices $r - 2(n - q)$ paths have $t + 1$ vertices $n - q$ paths have $2t + 2$ vertices
$p + q > n$ $p < \frac{n}{2}$ $r = n \bmod p, n = pt + r,$ $(n - q) < r \leq 2(n - q) - 1$	$p + q - n$	$p - r$ paths have t vertices length of remaining paths depends on $r, n - q$
$p + q > n$ $p < \frac{n}{2}$ $r = n \bmod p, n = pt_1 + r$ $r < n - q,$ $r > 2(n - q) - p - 1$ $r = t_2(r - (n - q)) + r_2$	$p + q - n$	$r - (n - q - r_2)$ paths with $t_2(t_1 + 1)$ vertices each r_2 paths with $(t_1 + 1)(t_2 + 1)$ vertices each $(p - r)$ paths with t_1 vertices each
$p + q > n$ $p < \frac{n}{2}$ $r = n \bmod p, n = pt + r$ $r < n - q, r \leq 2(n - q) - p - 1$ $d = \mathrm{GCD}(p, q)$	d if $d \geq p + q - n$ $p + q - n$ if $d < p + q - n$	$d - (p + q - n)$ of them are cycles, while remaining are paths

which is $C = \begin{bmatrix} \mathbf{0} & 1 \\ I_{n-1} & \mathbf{0} \end{bmatrix}$. Throughout, a *path* refers to a path in the directed graph defined by the adjacency matrix.

3 Summary of the results

In Table 1, we summarize our results on block diagonal reduction of (p, q)-tridiagonal matrices for even n. For odd n, the number of blocks can be deduced from the number of blocks in $T_{n-1}^{(p,q)}$ using Theorem 9. Table 1 gives the relation between p, q, n and the corresponding number of irreducible blocks in the block diagonalization and the nature of the individual blocks. The different support graphs of the individual blocks lead to the nine distinct cases outlined in Table 1.

We present an algorithm for the bidiagonal reduction of $T_n^{(p,q)}$ when $\frac{n}{2} \le p < q$. In Section 6, we prove that an upper or lower triangular reduction of $T_n^{(\mathcal{P},\mathcal{Q})}$ is possible when $\mathcal{P} = \{p_1 < p_2 < \ldots < p_k\}$ and $\mathcal{Q} = \{q_1 < q_2 < \ldots < q_l\}$ with $\frac{n}{2} \le p_1 < \ldots < p_k < q_1 < \ldots < q_l$.

4 Block diagonal reduction of (p, q)-tridiagonal matrices and their nature

Let $A^{(p,q)}$ denote the matrix with ones along the pth upper diagonal and qth lower diagonal, i.e. $A(i,j) = 1$ if $i - j = p$ or $j - i = q$. The matrix $A^{(p,q)}$ is the support of the non-diagonal entries of $T_n^{(p,q)}$. We consider the directed graph represented by the adjacency (incidence) matrix $A^{(p,q)}$. $A^{(p,q)}(i,j) = 1$, if there is an edge from vertex i to vertex j. Let $[n] = \{1, 2, 3, \ldots, n\}$.

Starting with a vertex s, from the matrix $A^{(p,q)}$, it has out neighbour $v_1 = s + p$, $v_2 = s - q$ and in neighbours $v_3 = s - p$, $v_4 = s + q$ given $1 \le v_i \le n$ for $i = 1, 2, 3, 4$. If any of the neighbour $v_j \notin [n]$ it is not a neighbour of s in the graph.

Then, to obtain the connected component corresponding to vertex s, we consider $(i,j) \in \mathbb{Z}^2$ and $r \in [n]$ such that

$$pi + qj + s = r,$$

where (i,j) is either $(0, 0)$ (the vertex s itself) or (i,j) is **connected** to $(0, 0)$. We say $(i,j) \in \mathbb{Z}^2$ is connected to $(0, 0)$ if there is a path $\mathcal{L}$ of feasible vertices ($1 \le px + qy + s \le n, \forall (x,y) \in \mathcal{L}$) formed by either moving right or left (vertices $(x \pm 1, y)$) or moving up or down (vertices $(x, y \pm 1)$), connecting (i,j) to $(0, 0)$.

Let

$$C_s = \{r | pi + qj + s = r \text{ for } (i,j) \text{ connected to } (0,0)\}.$$

Then, we have the disjoint union

$$[n] = \bigsqcup_{s \in S} C_s.$$

Let the number of equivalent classes be k ($|S| = k$).

Let e_r be rth canonical basis vector in $\mathbb{R}^n$. Let the columns of the matrices P_s be $e_r \in \mathbb{R}^n$ for $r \in C_s$. We arrange the columns of P_s in the lexicographic order of (i,j).

Let P be the permutation matrix such that

$$P = [P_{s_1} \quad P_{s_2} \quad P_{s_3} \quad \ldots \quad P_{s_k}]. \tag{2}$$

Then, we have the following theorem.

Theorem 1. *The matrix $P^T T_n^{(p,q)} P$ is block-diagonal with k blocks and each block is of size $|C_s|$ for $s \in S$.*

Proof. Consider the directed graph corresponding to $A^{(p,q)}$. Then, the set C_s defines a connected component that starts with the vertex s. Thus, the similarity transform by P will rearrange the vertices such that the connected components are next to each other. Thus, reducing the matrix into a block diagonal form. Since $A^{(p,q)}$ is support of $T_n^{p,q}$ on non-diagonal entries, the matrix P also block diagonalizes $T_n^{(p,q)}$. □

Consider a situation when a connected component is a directed path. Define the "*matrix order*" to be the order of the vertices according to the adjacency matrix $A^{(p,q)}$. Let the "*latent order*" be the order of vertices in such a way that they form a directed path starting from left to right. We intend to find a permutation for converting matrix order to the latent order.

The following Lemma 1 gives a situation when every connected component is a path.

Lemma 1. *If $p + q \geq n$, then every connected component of $A^{(p,q)}$ is either a path or a loop (cycle). Further when $\frac{n}{2} \leq p < q$ every connected component is a path.*

Proof. Since $n - p < q$, rows 1 to $n - p$ have a single one each and rows $q + 1$ to n have single one each. Therefore, in the graph corresponding to A, every vertex has at most one incoming edge. Similarly, columns 1 to $n - q$ have a single one each, and columns $p + 1$ to n have a single one each. Therefore, every vertex has at most one outgoing edge.

Starting with an arbitrary vertex in a connected component, one can move right (in the direction of the arrow) or left (against the direction of the arrow). If we continue this traversal and the two ends meet, then we obtain a directed cycle. Otherwise, we obtain a directed path.

Let $q > p \geq \frac{n}{2}$, and assume there is a cycle. Then, to move right from an arbitrary position in the latent order, we have $r + p, r + p - q, r + 2p - q, r + 2p - 2q, \ldots$. If we move left in the latent order, $r + q, r + q - p, r + 2q - p, r + 2q - 2p, \ldots$ The first sequence is of the form $r + k(p - q), r + k(p - q) + p$, the second sequence is of the form $r + l(q - p), r + l(q - p) + q$. If there is a loop, then these two sequences must meet at some point. If

$$
\begin{aligned}
r + kp - (k - 1)q &= r + lq - (l - 1)p, \\
(k + l - 1)p &= (k + l - 1)q, \\
p &= q.
\end{aligned}
$$

This leads to a contradiction. On the other hand, if $r - k(q - p) + p = r + l(q - p)$ Then, we obtain $p = (k + l)(q - p)$. We also have $r + k(q - p) \in [n]$ since $r - k(q - p) + p \in [n]$. Therefore, we obtain $r \geq 1 + k(q - p)$. Similarly, we have $r + (l - 1)(q - p) + q \leq n$. This implies

$$
\begin{aligned}
1 + (k + l - 1)(q - p) + q &\leq n, \\
1 + p + q &\leq n + (q - p), \\
1 + 2p + (q - p) &\leq n + (q - p).
\end{aligned}
$$

Since we know $2p \geq n$, this also gives a contradiction. Therefore, when $\frac{n}{2} \leq p < q$, we do not obtain a cycle in a connected component. □

Algorithm 1. Obtain connected components

Input : n, p, q, marked vertices $M = \phi$
Output: Connected components C_s Lexicographic order Q_s.
while $[n] \backslash M \neq \phi$ **do**
  take $s \in [n] \backslash M$.
  $C_s, Q_{s_i} = LDFS(n, p, q, s)$
  $M = M \cup C_s$.

Algorithm 2. Lexicographic depth-first search (LDFS)

n, p, q, s, marked vertices $M = \phi$, stack St

Connected component C_s Lexicographic order Q_s.

Append$(Q_s, (0,0))$

Append(M, s).

push($Neighbours(s, (0,0)), St$)

while Stack St is not empty **do**

  $v, (i, j)$= pop(St)

  if $v \cap M = \phi$ **then**

    Append(M, v), Append$(Q_s, (i, j))$.

    push($Neighbours(v, (i, j)), St$)

$C_s = M$.

Sort vertices in C_s according to the lexicographic order given in Q_s.

Algorithm 3. Neighbour$(v, (i, j))$

v, p, q.

$N_s = \phi$, $Q_s = \phi$, l_1, l_2, r_1, r_2.

if $v - p > 0$ **then**

  $l_1 = v - p, dl_1 = (i - 1, j)$.

  Append(N_s, l_1)

  Append(Q_s, dl_1)

if $v - q > 0$ **then**

  $l_2 = v - q$, $dl_2 = (i, j + 1)$.

  Append(N_s, l_2)

  Append(Q_s, dl_2)

if $v + p \leq n$ **then**

  $r_1 = v + p$, $dr_1 = (i + 1, j)$.

  Append(N_s, r_1)

  Append(Q_s, dr_1)

if $v + q \leq n$ **then**

  $r_2 = v + q$, $dr_2 = (i, j - 1)$.

  Append(N_s, r_2)

  Append(Q_s, dr_2)

Return N_s, Q_s

Theorem 2. *When the indices (i, j) determining the columns of P_s are in lexicographic order and the corresponding e_r form the columns of P_s, we obtain the bidiagonalization when a connected component is a path.*

Proof. In the lexicographic Depth First Search, starting with an arbitrary vertex $r = (0,0)$, we move right in the latent order, in steps of p, it will increase the first coordinate (Figure 1, we move starting from the origin in the positive p axis). If the vertex $(i, 0)$ does not have any vertex to the right in the matrix order, then we move left in the matrix order in steps of q, this will increase the second coordinate (the second axis is $-q$, in Figure 1, we move from C to D increasing $-q$). Then, we reach (i, j), which does not have any vertex to the left in the matrix order, we again move right by increasing p, till we reach a vertex with degree one (E_1 in Figure 1). Now, the left neighbour of (0, 0) is either (−1, 0) or (0, −1). Thus, we move left by decreasing the first coordinate $(-i, 0)$ and then, decreasing the second coordinate, etc. In conclusion, moving right in the latent order will increase the coordinates in the $p, -q$ plane, and moving left will decrease the coordinates. Thus, the lexicographic order will preserve the path. □

As a corollary of the above theorem, we have block bidiagonalization when $\lceil \frac{n}{2} \rceil \leq p < q < n$.

Corollary 1. *When $\lceil \frac{n}{2} \rceil \leq p < q < n$, and the permutation matrix P is constructed according to the LDFS, we obtain $P^T T_n^{(p,q)} P$ as a block bidiagonal matrix.*

Next we look at the number of diagonal blocks and their nature in the block diagonal reduction of $T_n^{(p,q)}$.

Remark. Unless otherwise stated, we assume n is even in the following theorems. For odd n, Theorem 9 relates this to the number of blocks for $T_{n-1}^{(p,q)}$.

Theorem 3. *If $p + q < n$, then we have $d = \mathrm{GCD}(p, q)$ many diagonal blocks.*

Proof. Consider equivalence classes $C_1, C_2, \ldots C_d$. Now, we need to prove that $C_s \neq C_t$ for any $i, j \in [d-1]$. Suppose $C_s = C_t$, then we have for some index $r \in C_s$.

$$s + ip + jq = t + ap + bq$$
$$s - t = (a - i)p + (b - j)q.$$

Now, d divides $(a - i)p + (b - j)q$ so it should divide $s - t$. But we have $|s - t| < d$. So $s = t$. This proves that there are at least d diagonal blocks.

From any arbitrary vertex, we can trace back to a vertex number $r \leq p$ via the pth upper diagonal. Then, it is sufficient to prove that every element of $[p]$ belongs to one of C_s for $s < d$.

Let $p = wd$. Without loss of generality, we show that every vertex $md + 1$ for $m = 0, 1, \ldots w$ is reachable to C_1. From the Euclid's algorithm, we have $md = mk_1 p - mk_2 q$. With $m, k_1, k_2 \geq 0$. So md is represented by $(mk_1, -mk_2)$. Now, we can go to the right by the amount q because $md + q \leq n$. Thus, the tuple reduces to $(mk_1, -(mk_2 - 1))$. Now, we can continue going to the right by q or going to the left by p depending on the

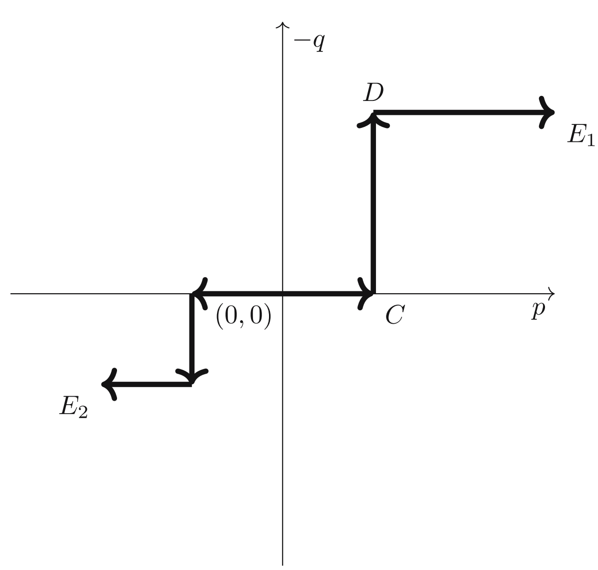

Figure 1: Depth-first search starting at (0, 0) marks the nodes in the path along the arrow in the upper right quadrant ((0, 0) to E_1) and then again visits the left neighbour and traces the arrow in the lower left quadrant ((0, 0) to E_2). Ordering the nodes lexicographically along the $(p, -q)$ axis will trace the nodes in the path (E_2 to E_1).

resulting number. Let $(i, -j)$ be an intermediate stage, if $i, j > 1$, then we can always go right by p or go left by q, otherwise, we obtain $p + q > n$, which is a contradiction. The procedure ends only at the index (0, 0), which corresponds to vertex 1. □

Remark 1. The above theorem gives a simple procedure to reduce the $T_n^{(p,q)}$ to block banded matrices when $p + q < n$ and $d = \mathrm{GCD}(p, q)$. Starting with the first vertex, consider vertices $1, d+1, 2d+1, 3d+1, \ldots$, they form a connected component. Similarly, the vertices $r, r+d, r+2d, r+3d, \ldots$ form a connected component for $1 \le r \le d$.

From Remark 1, each block diagonal matrix is (p', q')-tridiagonal with $p' = \frac{p}{d}$ and $q' = \frac{q}{d}$. Let $n' = \lfloor \frac{n}{d} \rfloor$, we have $p' + q' \le n'$. In addition, we have $\mathrm{GCD}(p', q') = 1$, implying that no further block diagonal reduction is possible.

Example 1. Consider $A^{(2,4)} = \begin{bmatrix} 0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&1&0&0&0&0\\ 1&0&0&0&0&0&1&0&0&0\\ 0&1&0&0&0&0&0&1&0&0\\ 0&0&1&0&0&0&0&0&1&0\\ 0&0&0&1&0&0&0&0&0&1\\ 0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&0&1&0&0 \end{bmatrix}_{10\times 10}$. We have $GCD(2, 4) = 2$ and $2 + 4 < 10$. As per Remark 1, we can have $C_1 = \{1, 3, 5, 7, 9\}$ and $C_2 = \{2, 4, 6, 8, 10\}$. Let e_j be the jth canonical basis vector. The permutation matrix $P = [e_1\ e_3\ e_5\ e_7\ e_9\ e_2\ e_4\ e_6\ e_8\ e_{10}]$ will give the block diagonal reduction

$$P^T A^{(2,4)} P = \begin{bmatrix} T_1 & \\ & T_2 \end{bmatrix} = \begin{bmatrix} 0&0&1&&&&&&&\\ 1&0&0&1&&&&&&\\ &1&0&0&1&&&&&\\ &&1&0&0&&&&&\\ &&&1&0&&&&&\\ &&&&&0&0&1&&\\ &&&&&1&0&0&1&\\ &&&&&&1&0&0&1\\ &&&&&&&1&0&0\\ &&&&&&&&1&0 \end{bmatrix}.$$

Example 2. For the eigenvalue computation, we consider the block diagonal reduction of $T_n^{(p,q)}$ with n varying over the set $\{2^4, 2^5, \ldots, 2^{12}\}$, and corresponding values of $p \in \{2, 2^2, 2^3, \ldots, 2^{10}\}$ and $q \in \{2^2, 2^3, \ldots, 2^{11}\}$. Figure 2(a) demonstrates that the time taken by the block diagonal reduction is significantly lower compared to the unreduced case. This can be understood as follows: if we solve a fixed-size problem of size k exactly n/k times, and the method used has a complexity of $O(n^\alpha)$ for some constant α, then the total computational cost becomes $O((n/k) \cdot k^\alpha) = O(n \cdot k^{\alpha-1})$. Since both k and α are constants, this results in an overall linear complexity in n. In Figure 2(b), n varies as before, but the parameters are fixed at $p = 2$ and $q = 4$. This setup affects only the constant factor in the computational complexity. As a result, the logarithmic plot in Figure 2(b) shows two approximately parallel lines, which is consistent with the expected theoretical complexity.

Theorem 4. *When $p = \frac{n}{2}$, and $q > p$, then there are $q - p$ blocks.*

Proof. Start with the block $A^{(p,q)}(p+1 : q, p+1 : q)$, and trace back in anticlockwise order in the matrix. Then, we can see that all the blocks are connected. The vertices inside the block are disconnected. Thus, we have $q - p$ connected components. The proof is illustrated in Figure 3. □

Theorem 5. *If $p, q > \frac{n}{2}$, then there are $q + p - n$ blocks.*

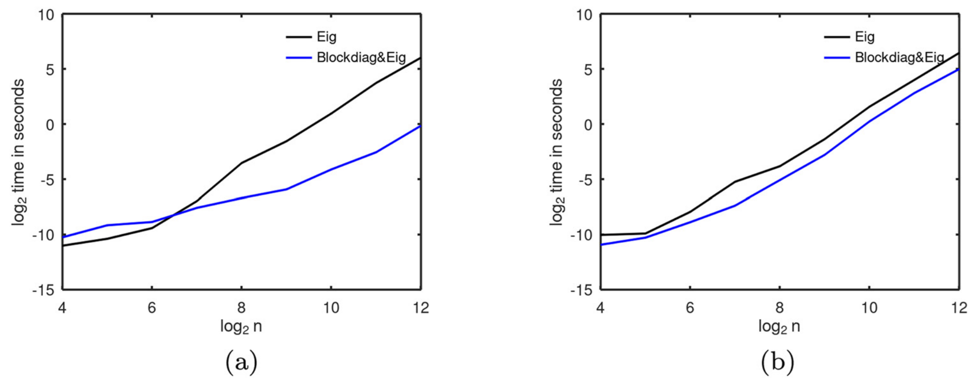

Figure 2: For n varying as a power of 2, (a) increases p and q respectively in the power of two and (b) keeps $p = 2$ and $q = 2$ constant while n is varied in power of two. (a) Varying block size and (b) constant blocksize.

Proof. The columns $n - q + 1$ to p have only diagonal entries. The rows in $n - p + 1$, to q will have only the diagonal entry. If $p < q$, then we have the indices $n - p + 1$ to p corresponding to only diagonal entries. So, $2p - n$ entries correspond to entries as diagonal blocks. Now, the remaining problem reduces to that of $n' = 2n - (2p)$, with $p' = n - p$, $q' = n + q - 2p$. We can see that $p' + q' = 2n - 3p + q > n'$ and $p' = \frac{n'}{2}$. Then, from theorem 4, we obtain $q' - p' = q - p$ additional blocks. □

Theorem 6. *When $p < \frac{n}{2}$, $p + q > n$, and $p|q$, then there are p blocks.*

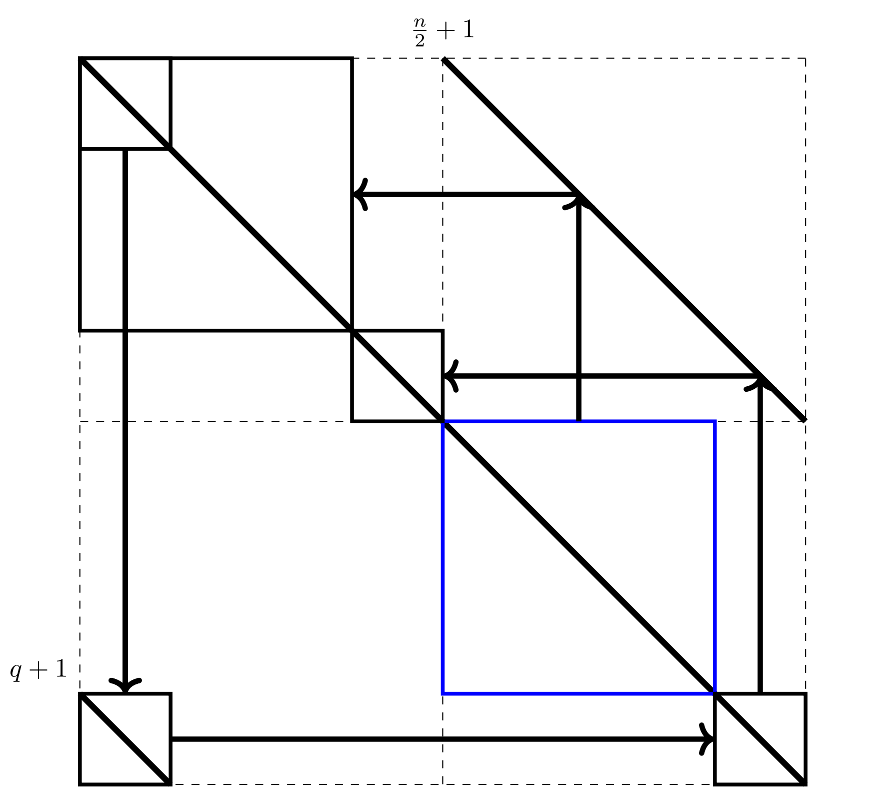

Figure 3: When $p = \frac{n}{2}$ and $q > p$, the connectivity of $(p - q) \times (p - q)$ block (in blue) with the rest of the diagonal entries, is obtained by tracing in the anticlockwise direction along the arrow. Thus, we obtain $p - q$ connected components. There are $n - q$ paths of length four and $q - p - (n - q) = 2q - 3p$ paths of length two.

Proof. Consider the $p \times p$ block $(1:p, 1:p)$, the block is connected to every other $p \times p$ blocks along the diagonal via pth upper diagonal. Via the qth lower diagonal, the first block is connected to the remaining $n-q$ vertices. The proof is illustrated in Figure 4. □

Theorem 7. *When $p < \frac{n}{2}$, $p+q > n$, $r = n \bmod p$, and $r > 2(n-q)-1$, then we have $p+q-n$ blocks. Each of them is a path. If $n-q < r \le 2(n-q)-1$, then we have $p+q-n$ blocks.*

Proof. Let $v \in \{1, 2, \ldots, p\}$. The node v is connected to a node of the form $tp+v$ via the pth upper diagonal. Let $r = n \bmod p$ and $r + tp = n$. They form p distinct paths. Then, the paths ending at $n-q$th to nth vertices are connected back to the paths starting at vertex 1 to vertex $n-q$, respectively. If $r > n-q$, these paths are $r-(n-q)+1, r-(n-q)+2, \ldots, r$. If we have $n-q < r-(n-q)+1$, then we have $p-(n-q) = p+q-n$ connected components. Among them, $p-r$ paths have t vertices and $r-2(n-q)$ paths have $t+1$ vertices and $n-q$ paths have $2t+2$ vertices.

If $n-q \le r-(n-q)+1$, then we have path $r-(n-q)+1$ connected to path 1, $r-(n-q)+2$ path connected to path 2, etc., and path r connected to path $n-q$. So, we obtain $r-(n-q)$ components from these paths. In total, this also leaves with $p+q-n$ connected components. These two situations are shown in Figure 5. □

Theorem 8. *When $p < \frac{n}{2}$, $p+q > n$, $r = n \bmod p$, and $r < n-q$, and $r > 2(n-q)-p-1$, then there are $p+q-n$ blocks. If $r \le 2(n-q)-p-1$ and $d = \mathrm{GCD}(p,q) < p+q-n$, then there are $p+q-n$ blocks, if $d > p+q-n$, then there are d blocks.*

Proof. Let $v \in \{1, 2, \ldots p\}$. The node v is connected to a node of the form $tp+v$ via the pth upper diagonal. Let $r = n \bmod p$. They form p distinct paths. Then, the paths ending at $n-q$th to nth vertices are connected

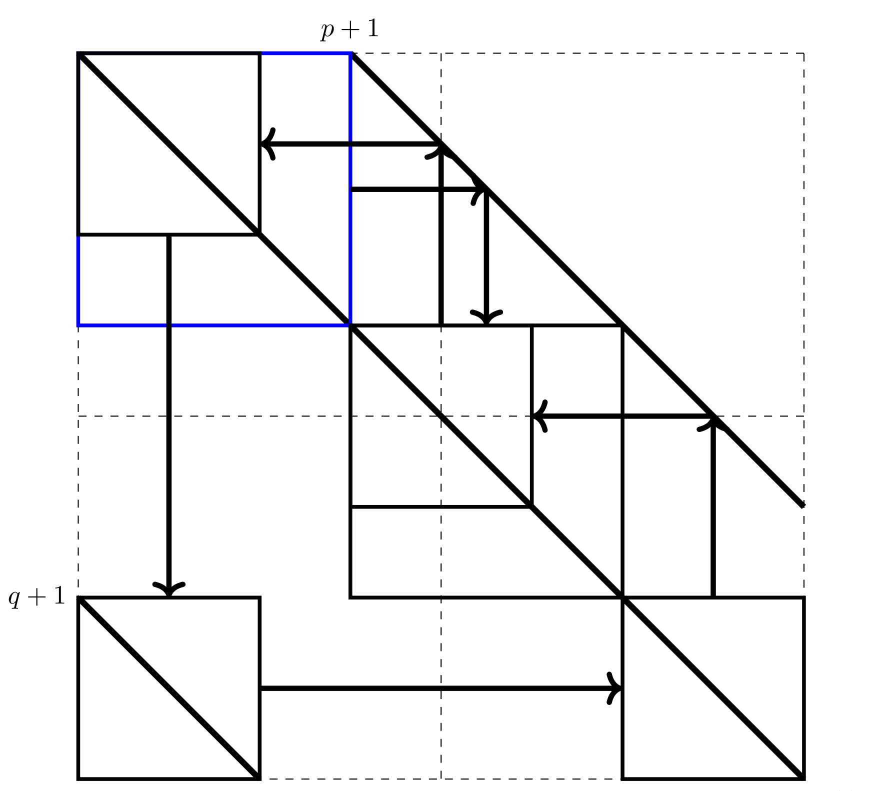

Figure 4: When $n - q < p$ and $p < \frac{n}{2}$, $p|q$, the top left $p \times p$ block (blue) is connected to all the blocks of size $p \times p$ along the diagonal (tracing clockwise). By tracing the top left $(n-q) \times (n-q)$ block anticlockwise, we can see there are cycles of length $1 + \frac{q}{p}$. and there are $p+q-n$ paths of length $\frac{q}{p}$.

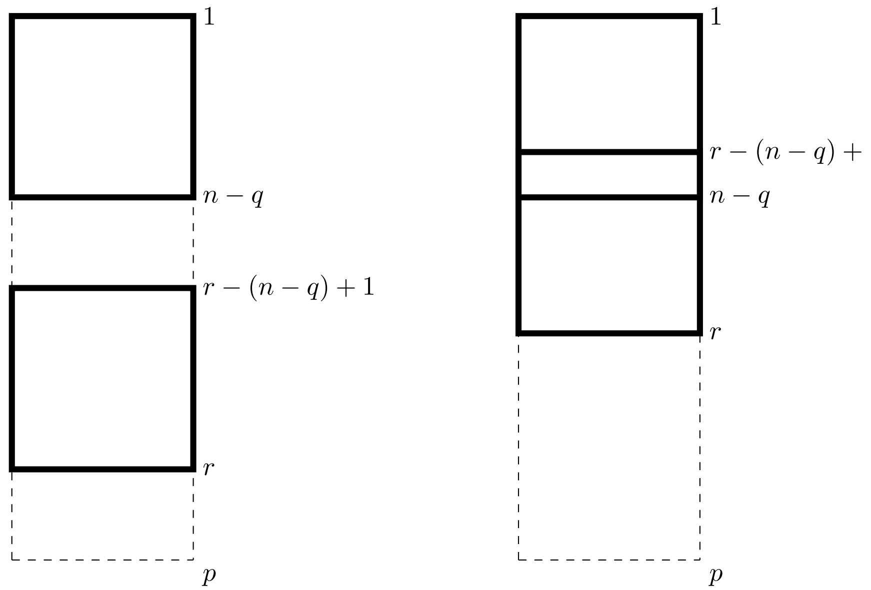

Figure 5: Two cases when $r > n - q$.

back to the paths starting at vertex 1 to vertex $n - q$, respectively. If $r < n - q$, these paths are $p - (n - q - r) + 1, p - (n - q - r) + 2, \dots, p, 1, 2, \dots, r$. So, 1 to $n - q$ is respectively divided into a set, 1 to $n - q - r$ and $n - q - r + 1$ to $n - q$. Let $n - q < p - (n - q - r) + 1$. Note that path r is connected to path $n - q$, $r - 1$ is connected to path $n - q - 1$, etc. This leaves us with $n - q - r$ connected components from the total $n - q$ paths.

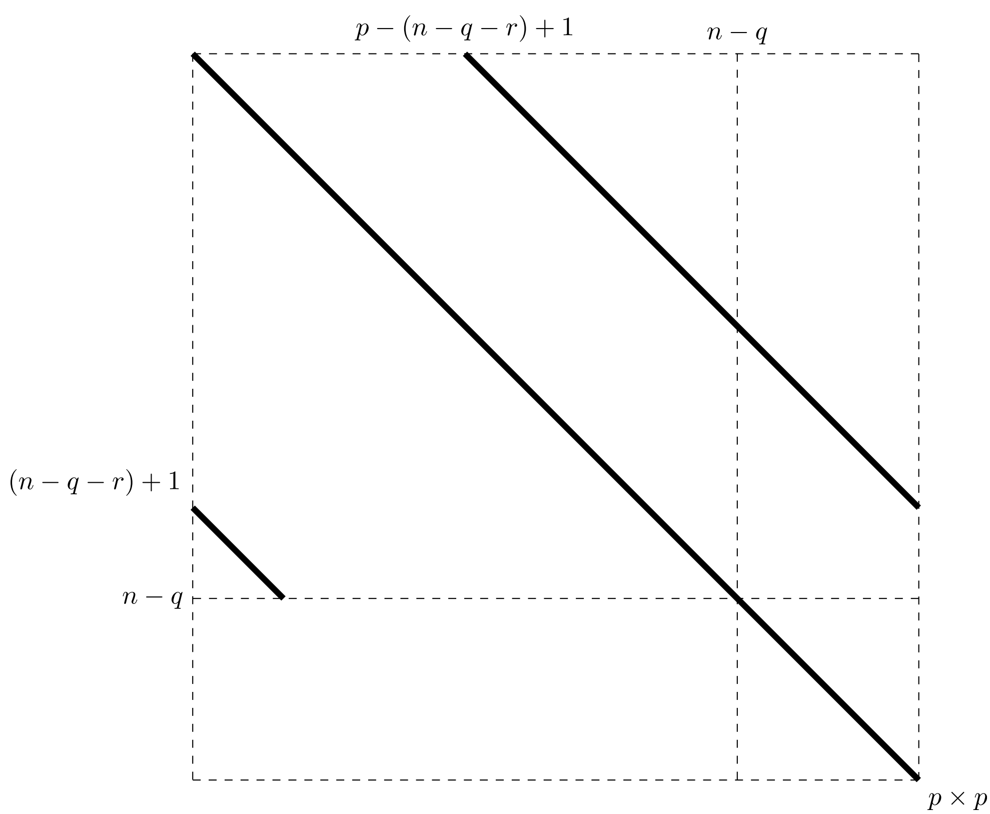

Figure 6: The structure of the connections when $r < n - q$ and $n - q \geq p - (n - q - r) + 1$.

When $n - q \geq p - (n - q - r) + 1$, the paths 1 to $n - q$ are connected to paths $p - (n - q - r) + 1$ to r in the cyclic fashion. This can be represented in a matrix form represented in Figure 6.

Therefore, if $n - q \geq p - (n - q - r) + 1$, then the number of connected components is equal to the number of components in the subproblem with $n' = n - q$, $p' = p + q + r - n$, and $q' = n - q - r$.

The matrix can be seen as the $(n - q - r)$th, power of the cycle matrix C, multiplied with a diagonal matrix, which will force the rows $n - q$ to p to zero. It can be seen that the power of an $n \times n$ cycle matrix, C^m can be expressed as a direct sum of $d = \mathrm{GCD}(m, n)$ cycles.

Let $d = \mathrm{GCD}(p, p - (n - q - r)) = \mathrm{GCD}(p, q)$. If $p - (n - q) < d$, then, we have d connected components, among them $d - (p - (n - q))$ are cycles, and the remaining are paths.

If $d < p - (n - q)$, then for some k_1 and r_1, we have $k_1 d + r_1 = p + q - n$. Then, if $k_1 \geq 2$, each of the d cycles have k_1 components and r_1 of them have an extra 1 component due to one extra cut. Thus, in total $k_1 d + r_1 = p + q - n$ components. If $k_1 = 1$, then each cycle has reduced to a path, and r_1 of them have extra cut, thus in total $p + q - n$ components. □

Let b_{n-1} be the number of blocks in the block diagonal reduction of the matrix $A_{n-1}^{(p,q)}$. Then, we have the following theorem to determine the number of blocks for odd n.

Theorem 9. *For odd n, the number of blocks in the block diagonal reduction is given by* b_{n-1} *if vertices p and q belong to the same connected component in* $A_{n-1}^{(p,q)}$, $b_{n-1} - 1$ *otherwise.*

Proof. If we remove the vertex 1 in $A_n^{(p,q)}$, we obtain the adjacency matrix $A_{n-1}^{(p,q)}$. After block diagonal reduction of $A_{n-1}^{(p,q)}$, if we add the vertex 1 back, the number of blocks will be unchanged if p, q are already connected in $A_{n-1}^{(p,q)}$. Otherwise they obtain connected and the number of connected components reduce by one. □

5 Description of the algorithm for block diagonalization of (p, q)-tridiagonal matrix

The block diagonalization of a (p, q)-tridiagonal matrix is based on identifying connected components in the matrix's support graph. Each vertex in this graph corresponds to a matrix index, and directed edges reflect the nonzero entries on the pth upper and qth lower diagonals. The connectivity structure is captured by traversing the graph using an LDFS over integer lattice coordinates in the $(p, -q)$ direction. For each unvisited index, the LDFS discovers the full component and records the corresponding indices in lexicographic order.

This ordering is crucial: when a component forms a directed path, lexicographic traversal ensures that the corresponding submatrix becomes bidiagonal under a permutation. After processing all components, the matrix is permuted using the concatenated permutation matrices, yielding a block diagonal form. The overall time complexity of the algorithm is linear in the size of the matrix, since each vertex and edge is visited once. An open-source implementation in Octave is available at: https://github.com/HariprasadManjunath/Block-p-q.

6 Block diagonalization of $(\mathcal{P}, \mathcal{Q})$-tridiagonal matrices

The extension from (p, q)-tridiagonal matrices to (P, Q)-tridiagonal matrices is a natural generalization to a wider class of matrices. While (p, q)-matrices include only one upper and one lower diagonal offset, many problems in numerical linear algebra and scientific computing involve systems with multiple off-diagonal bands ([2],[11], Chapter 8 of [8] on banded matrices). Complex networks-related regular graphs can have such banded structure (Chapter 11 of [3] on configuration models). By using sets $P = \{p_1, \ldots, p_k\}$ and $Q = \{q_1, \ldots, q_l\}$, the (P, Q)-tridiagonal form naturally accommodates such patterns.

Graph-based theoretical tools developed for (p, q)-matrices can be extended to this more general case. Similar multiband or Toeplitz-plus-band matrices have been studied in the context of partial differential equation discretizations and matrix algorithms [15]. This extension allows one to work with a broader class of matrices while preserving structural properties that can be exploited for efficient computation.

In general, when $\mathcal{P} = \{p_1, p_2, \dots, p_k\}$ with $p_1 < p_2 < \dots < p_k$ and $\mathcal{Q} = \{q_1, q_2, \dots, q_l\}$ with $q_1 < q_2 < \dots < q_l$. we have the decomposition of $[n] = \sqcup C_s$. Here the set C_s contains those r,

$$s + \sum_{t=1}^{k} p_t i_t + \sum_{g=1}^{l} q_g j_g = r$$

and the $k + l$ tuple $(i_1, i_2, \dots, i_k, j_1, j_2, \dots, j_l)$ is lexicographically connected to $\mathbf{0}$.

Let the columns of the permutation matrices P_s be e_r for $r \in C_s$. We arrange the columns of P_s in the lexicographic order of (i, j).

Let P be the matrix such that

$$P = [P_{s_1} \quad P_{s_2} \quad P_{s_3} \quad \dots \quad P_{s_k}]. \tag{3}$$

Then, we have the following theorem.

Theorem 10. *The matrix $P^T T_n^{(\mathcal{P},\mathcal{Q})} P$ is block-diagonal with blocks of size $|C_{s_j}|$.*

Proof. The proof follows from the fact that the vertices corresponding to the indices in C_s form a connected component. □

Theorem 10 generalizes block diagonalization of the case of k-tridiagonal matrices. By keeping track of the equivalence classes, we can reduce the matrix into block diagonal form.

This reduces the problem size for eigenvalue and eigenvector algorithms. Thus, further speeding up the parallel computations.

6.1 Triangular reduction of $(\mathcal{P}, \mathcal{Q})$-tridiagonal matrices

Note that, when we have $p_1 > \frac{n}{2}$ and $q_1 > \frac{n}{2}$, a block matrix reduction

$$T_n^{(\mathcal{P},\mathcal{Q})} = \begin{bmatrix} D_1 & B_1 \\ B_2 & D_2 \end{bmatrix}, \tag{4}$$

with diagonal matrices D_1 and D_2 and banded matrices B_1 and B_2.

When we have $q_1 > p_k$, the matrix $B_2 D B_1$ is lower triangular for any diagonal matrix D.

Then, we have the following theorem.

Theorem 11. *If $\frac{n}{2} < p_1, q_1$ and $q_1 > p_k$, then the eigenvalues of $T_n^{(\mathcal{P},\mathcal{Q})}$ are its diagonal elements.*

Proof. When λ is not the diagonal element of D_1, the determinant

$$\det(T_n^{(\mathcal{P},\mathcal{Q})} - \lambda I) = \det(D_1 - \lambda I)\det(D_2 - \lambda I - B_2(D_1 - \lambda)^{-1} B_1). \tag{5}$$

Since $B_2(D_1 - \lambda)^{-1} B_1$ is completely upper triangular, $\det(D_2 - \lambda I - B_2(D_1 - \lambda)^{-1} B_1) = 0$ for all $\lambda = D_2(i, i)$. Similarly, for all the other eigenvalues

$$\det(T_n^{(\mathcal{P},\mathcal{Q})} - \lambda I) = \det(D_2 - \lambda I)\det(D_1 - \lambda I - B_2(D_2 - \lambda)^{-1} B_1). \tag{6}$$

Then, $\det(D_1 - \lambda I - B_2(D_2 - \lambda)^{-1} B_1) = 0$ for the diagonal elements of D_1. Therefore, we obtain all the eigenvalues of $T_n^{(\mathcal{P},\mathcal{Q})}$ as its diagonal elements. □

Lemma 2. *If $\frac{n}{2} < p_1, q_1$, and $q_1 > p_k$, then there is no directed cycle in the graph corresponding to A.*

Proof. Starting with an arbitrary vertex r, we move right, we obtain the sequence,

$$r, r + p_{a_1}, r + p_{a_1} - q_{b_1}, \ldots, r + \sum_{i=1}^{t} p_{a_i} - q_{b_i}, r + \sum_{i=1}^{t} p_{a_i} - q_{b_i} + p_{a_{t+1}}.$$

By moving left (in the opposite direction of the arrow), we obtain the sequence,

$$r + q_{c_1}, r + q_{c_1} - p_{d_1}, r + q_{c_1} - p_{d_1} + q_{c_2}, \ldots, r + \sum_{j=1}^{w} q_{c_j} - p_{d_j}, r + \sum_{j=1}^{w} q_{c_j} - p_{d_j} + q_{c_{w+1}}.$$

Now, if there is a directed cycle, then any two terms of the above two sequences must be equal. The term $r + \sum_{i=1}^{t} p_{a_i} - q_{b_i}$ is less than every element of the second sequence. Suppose

$$r + \sum_{i=1}^{t} p_{a_i} - q_{b_i} + p_{a_{t+1}} = r + \sum_{j=1}^{w} q_{c_j} - p_{d_j}, \tag{7}$$

then using $r + \sum_{i=1}^{t} p_{a_i} - q_{b_i} \geq 1$, we obtain

$$r \geq 1 + \sum_{i=1}^{t} (q_{b_i} - p_{a_i}). \tag{8}$$

Using $r + \sum_{j=1}^{w-1} q_{c_j} - p_{d_j} + q_{c_w} \leq n$, we obtain

$$r + \sum_{j=1}^{w-1} q_{c_j} - p_{d_j} + q_{c_w} - p_{d_w} \leq n - p_{d_w}. \tag{9}$$

Using (8) and (9) in (7), we obtain

$$1 + p_{a_{t+1}} + p_{d_w} \leq n,$$

which is a contradiction since $p_{a_{t+1}}, p_{d_w} \geq \frac{n}{2}$.

On the other hand, if we have

$$r + \sum_{i=1}^{t} p_{a_i} - q_{b_i} + p_{a_{t+1}} = r + \sum_{j=1}^{w} q_{c_j} - p_{d_j} + q_{c_{w+1}},$$

$$\sum_{i=1}^{t} (p_{a_i} - q_{b_i}) + (p_{a_{t+1}} - q_{c_{w+1}}) + \sum_{j=1}^{w} (p_{d_j} - q_{c_j}) = 0. \tag{10}$$

Equation (10), is a contradiction since we have $p_i < q_j, \ \forall i, j$. □

Lemma 3. *When $\frac{n}{2} < p_1, q_1$, and $q_1 > p_k$, we can put every connected component in an upper triangular form.*

Proof. Let $|C_s| = T$. Starting with an arbitrary vertex r, we move right, we obtain the sequence,

$$r, r + p_{a_1}, r + p_{a_1} - q_{b_1}, \ldots, r + \sum_{i=1}^{t} p_{a_i} - q_{b_i}, r + \sum_{i=1}^{t} p_{a_i} - q_{b_i} + p_{a_{t+1}}.$$

Let this sequence end at a vertex u, then the vertex u has no outgoing edges. We can put the vertex u in the first column. By moving left (in the opposite direction of the arrow), we obtain the sequence,

$$r + q_{c_1}, r + q_{c_1} - p_{d_1}, r + q_{c_1} - p_{d_1} + q_{c_2}, \ldots, r + \sum_{j=1}^{w} q_{c_j} - p_{d_j}, r + \sum_{j=1}^{w} q_{c_j} - p_{d_j} + q_{c_{w+1}}.$$

Let this sequence end at vertex v, then vertex v has no incoming edges. We can put vertex v in the last in the order. Now, we repeat the procedure for $C_s \backslash \{u, v\}$. Thus, reducing the problem to $T - 2$ vertices. □

From Lemma 2, we can conclude that the graph corresponding to $A^{(\mathcal{P},\mathcal{Q})}$, when $\frac{n}{2} < p_1, q_1$ and $q_1 > p_k$, is a directed acyclic graph (DAG). The DAGs have a topological ordering. In topological ordering, every vertex is arranged on a line and all the arrows are in the same direction [17] (Chapter 32 on Directed Graphs).

When P is constructed by keeping the columns of P_{s_j} in the reverse topological sorted order, we have the following theorem,

Theorem 12. *If $\frac{n}{2} < p_1, q_1$ and $q_1 > p_k$, then the similarity transformation $P^T T_n^{(p,q)} P$ reduces the matrix to lower triangular form.*

Proof. Since we keep the reverse topological order for the connected component, we obtain the lower triangular form. Let $\{v_1, v_2, \dots v_s\}$ be the vertices. The first vertex v_1 does not have any outgoing edges. If we remove v_1, the vertex v_2 will not have any outgoing edges, retaining the lower triangular form in the corresponding adjacency matrix. □

7 Conclusion

In this article, we provide a complete characterization of the block diagonal reduction of the (p, q)-tridiagonal matrix $T_n^{(p,q)}$ for even n and establish its relationship to the reduction for $n - 1$ in the case of odd n. The structural analysis of the support graph enables an efficient decomposition into irreducible diagonal blocks, with explicit formulas for their number and configuration.

These results can be leveraged to design fast numerical algorithms for computing determinants, permanents, eigenvalues, and eigenvectors by reducing large banded matrices into smaller independent subproblems. The block structure is also valuable in the context of inverse eigenvalue problems and in the spectral analysis of structured matrices.

The framework extends naturally to $(\mathcal{P}, \mathcal{Q})$-tridiagonal matrices, encompassing a broad class of banded systems. Future work may explore applications to parallel numerical solvers and preconditioners for sparse matrix computations.

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