Qualitative and Quantitative Research on Graphs via Matrices: Gram Mates, Fiedler Vectors, Kemeny's Constant, and Perfect State Transfer

by

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Abstract

A fundamental mathematical approach uses graphs to understand networks representing objects with their interrelationships. This thesis is dedicated to qualitative and quantitative research through a bridge—the connections in a graph—with Gram mates arising in social networks; Fiedler vectors in networks; Kemeny's constant in road networks; and perfect state transfer in quantum spin networks. We use techniques from graph theory together with matrix theory—combinatorial matrix theory, algebraic graph theory, and spectral graph theory.

Our main work is to examine two-mode networks retaining their information under the conversion approach in social networks. We characterize the relationship of two-mode networks (Gram mates) with the same single-mode networks via their singular values and vectors. So, we produce pairs of Gram mates that inform the retention of the information of two-mode networks. Furthermore, we provide Gram mates under mathematical restrictions.

Our next goal is to inspect the robustness of the usage of Fiedler vectors in networks. One popular technique for detecting community structures is based on spectral bisection that uses Fiedler vectors for graph partitioning. We examine graphs where the partite sets resulting from spectral bisection are extremely different in size. We discuss pathological graphs where any choice of Fiedler vectors produces the bisection where one is a singleton and the other the rest. We furnish some classes of graphs that are potentially pathological.

Our third task is to explain Braess' paradox in road networks. Kemeny's constant for a Markov chain can be used to measure the travel time of vehicles between two randomly chosen places. We present graphs where the insertion of an edge increases Kemeny's constant. We provide tools for identifying such an edge with examples of graphs, and produce families of graphs with such edges.

Our goal of the final research is to switch interactions between qubits in a quantum spin network corresponding to a hypercube, in order for the manipulated spin network to become insensitive to external environments under perfect state transfer (PST). We investigate differences and similarities between hypercubes and the resulting graphs regarding the graph structure, PST, and the sensitivity of PST.

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Contributions of Authors

In Chapter 3, Sections 3.2–3.4 are a version of a journal article co-authored with Steve Kirkland submitted for publication in Linear Algebra and its Applications. I am the primary author.

Chapter 4 is a version of a journal article co-authored with Steve Kirkland accepted in the Czechoslovak Mathematical Journal. I am the primary author.

Chapter 5 is a version of a journal article submitted for publication in the Electronic Journal of Linear Algebra. I am the sole author.

The contents in Chapter 6 are original to this thesis. I am the sole author.

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J	an all ones matrix
$\mathbf{1}$	a column vector of all ones
$\mathbf{e}_k$	the column vector whose k^{th} component is 1 and zeros elsewhere
$A^\dagger$	the Moore–Penrose inverse of A
$am(\lambda)$	the algebraic multiplicity of an eigenvalue λ
$A \otimes B$	the Kronecker product of A and B
$\mathrm{Row}(A)$	the row space of a matrix A
$\mathrm{Col}(A)$	the column space of a matrix A
$\mathrm{rank}(A)$	the rank of a matrix A
$A[\alpha, \beta]$	the submatrix of A whose rows and columns are indexed by α and β where α (resp. β) is a set of some row (resp. column) indices
$\mathbf{x} \succ \mathbf{y}$	a vector $\mathbf{x}$ majorizes a vector $\mathbf{y}$
$V(G)$	the vertex set of a graph G
$E(G)$	the edge set of a graph G
$v \sim w$	the edge between vertices v and w
$N_G(v)$	the set of neighbours of a vertex v in a graph G
$N_X(v)$	the set of neighbours of a vertex v in a graph G that belong to X where X is a subset of $V(G)$
$\deg_G(v)$	the degree of a vertex v in a graph G
$d_G(v, w)$	the distance between vertices v ans w in a graph G
$e_G(v)$	the eccentricity of a vertex v in a graph G
$\mathrm{diam}(G)$	the diameter of a graph G
$v(G)$	the vertex connectivity of a graph G
$\bar{G}$	the complement of a graph G
$G_1 + G_2$	the disjoint union of graphs G_1 and G_2
$G_1 \vee G_2$	the join of graphs G_1 and G_2
$G_1 \Box G_2$	the Cartesian product of graphs G_1 and G_2

$\mathcal{U}(R,S)$	the set of $(0,1)$ matrices with row and column sum vectors R and S
$\mathcal{S}_n$	the symmetric group on $\{1,\ldots,n\}$
$L(G)$	the Laplacian matrix of a graph G
$A(G)$	the adjacency matrix of a graph G
$S(L(G))$	the sequence of eigenvalues of $L(G)$ in non-increasing order
$S(A(G))$	the sequence of eigenvalues of $A(G)$ in non-increasing order
$\alpha(G)$	the algebraic connectivity of a graph G
$\delta(G)$	the minimum degree of a graph G
$i(\mathbf{x})$	minimum of the number of negative entries and positive entries in $\mathbf{x}$ where $\mathbf{x}$ is a Fiedler vector
$i(G)$	the minimum number of negative entries in a Fiedler vector among all Fiedler vectors of G
$\kappa(G)$	Kemeny's constant for the transition matrix of the random walk on a graph G
N_k	the graph that consists of k vertices with no edges
K_n	the complete graph of order n
C_n	the cycle of length n
S_n	the star of order n
m_G	the number of edges of a graph G
$\mathbf{d}_G$	the column vector whose i^{th} entry is the degree of i^{th} vertex of a graph G where a labelling of $V(G)$ is given
τ_G	the number of spanning trees of a graph G
$\mathcal{F}_G(i;j)$	the set of 2-tree spanning forests of a graph G such that one of the two trees contains a vertex i of G, and the other has a vertex j of G
F_G	the matrix whose (i,j)-entry is the cardinality of $\mathcal{F}_G(i;j)$
$\Gamma(A)$	the automorphism group of the graph associated to a matrix A
$S_r(X)$	the set of vertices v in a graph G such that $d(v,x)=r$ for all $x\in X$ where X is a subset of $V(G)$
G/π	the quotient graph of a graph G with respect to an equitable partition π
$\widehat{G/\pi}$	the symmetrized quotient graph of a graph G with respect to an equitable partition π
$G^{(M_\tau)}$	the equidistant switched graph via an equidistant switch M_τ
Q_n	the hypercube of dimension n or the n-cube
$\widetilde{Q}_n$	the $(2,2,2;\{3\})$-switched n-cube

1

Introduction

A graph is a tool to model a *network*—the representation of a system that consists of objects with their interrelationships. In order to understand the essential and intrinsic features of a network, analysis and transformation of the connections in a graph are used to provide qualitative information from quantitative information, and vice versa. In this thesis, we study Gram mates, Fiedler vectors, Kemeny's constant, and perfect state transfer that arise from qualitative questions in social networks, road networks, and quantum spin networks, using graph theory together with matrix theory—combinatorial matrix theory, algebraic graph theory and spectral graph theory.

We consider graph connectedness for these four topics as follows. We study Gram mates and perfect state transfer by transforming the connections in a graph, and we analyse Fiedler vectors and Kemeny's constant that provide algebraic measures of graph connectedness. In Gram mates, we investigate two bipartite graphs corresponding to the so-called two-mode networks, where one can be obtained from the other by perturbing its edges while preserving its degree sequence. Secondly, Fiedler vectors of a graph can be used to partition the graph into two subgraphs while minimizing the number of edges between the two subgraphs, by using the signs of the entries in a Fiedler vector. That is, Fiedler vectors generate partitions of the graph for which two subgraphs are not 'well connected'. We analyse Fiedler vectors with unbalanced sign patterns. Next, Kemeny's constant provides an overall measure of connectedness of a graph in the context of a random walk on a graph—'well connected' graphs have 'low' Kemeny's constants. We study graphs where adding an edge results in an increase of Kemeny's constant. Finally, in perfect state transfer, manipulating the connectedness of a graph, we shall obtain other graph whose fidelity of perfect state transfer between vertices becomes less sensitive to changes of edge weight. So, we conduct a sensitivity analysis for certain quantum spin networks that are related by switching edges and changing the weight of an edge.

Here we describe our motivation and quantitative approaches for the following qualitative questions:

(1) When does a two-mode network retain its information in the conversion approach in social networks?

(2) Is spectral bisection a robust technique for detecting community structures in networks?

(3) When does Braess's paradox occur in networks?

(4) How can a quantum spin network become insensitive to external environments when it exhibits perfect state transfer?

The present thesis is comprised as follows. We explain background information on each of these questions in the remaining sections of this chapter. We deal with the necessary background and notation for each question in Chapter 2. Then, we produce quantitative and qualitative information for the proposed questions throughout Chapters 3–6. We conclude this thesis in Chapter 7 by restating the problems and conjectures described in Chapters 3–6 with brief comments.

1.1 Two-mode networks retaining their information

A *two-mode network* is a network with two different sets of vertices (a set of actors and a set of events) and with edges (actions on events) only between vertices belonging to different sets—that is, it corresponds to a bipartite graph. Then, the relations within a set of actors and within a set of events are called *single-mode networks* of the two-mode network. As an example, one vertex set in a two-mode network consists of students at the University of Manitoba, and the other consists of social events, where edges are given by students' participation in events; by examining patterns of which students participate in which events, one can infer which events are influential and how those events may affect students' decision (see [37] for the further background and details). The two-mode network of this example can be thought of as a $(0, 1)$ matrix in the following way: rows represent students and columns represent events, with a 1 in the corresponding position of the matrix if a student joins an event, and a 0 otherwise. In this manner, every two-mode network can be expressed as a $(0,1)$ matrix A, and vice versa. In this setting, A is known as the *bi-adjacency matrix* for the bipartite graph. Then, both AA^T and A^TA represent its single-mode networks. One of the basic approaches to the study of two-mode networks is the *conversion approach* [7], which investigates the patterns from single-mode networks. Naturally, this raises a question [30] whether the pair of single-mode networks uniquely specifies the original two-mode network. In other words, is it possible for two different $(0,1)$ matrices A and B to have the property that $AA^T = BB^T$ and $A^TA = B^TB$ (called *Gram mates*)? Such A and B can be thought as the bi-adjacency matrices of two bipartite graphs, as described in the earlier part of this chapter, where one can be obtained from the other by modifying its edges.

Further, two-mode networks corresponding to Gram mates can have the same structure—that is, there exists an isomorphism of two bipartite graphs corresponding to the two-mode networks, which preserves adjacency between the two-mode networks. To resolve that question, the existence of an isomorphism provides a clue [30, 44] if a two-mode network exhibits data-loss in the conversion approach. In Chapter 3, we study two-mode networks (Gram mates) with the same single-mode networks, and the existence of isomorphisms between them.

1.2 Fiedler vectors for spectral bisection

The state of connectedness of a graph is inherent in Fiedler vectors used to detect community structures in networks.

For example, a community structure in a social network is a set of groups of individuals in the network obtained by clustering them according to friendships or other acquaintances (connection) between them. Considering the network as a graph, the state of connectedness between two groups in the community structure can be measured as how many edges there are between the corresponding subsets of the vertex set, whose deletion results in a disconnected subgraph. By minimizing the number of such edges, community structures can be obtained [55].

A graph bisection is a partition of the vertex set of a graph into two subsets whose sizes differ by at most 1. In particular, the fewer edges between two partitioned sets there are, the less the two parts are related. One of the popular techniques for the bisection is *spectral bisection*, which uses a Fiedler vector [32] of a graph G so that the edges between two vertices valuated by different signs of the Fiedler vector are cut in order to have the graph G partitioned into two connected subgraphs. Spectral bisection is iteratively used for detecting community structures in [55]. However, according to [2], many algorithms based on spectral bisection have no proof for why they show empirical successes. In Chapter 4, we study Fiedler vectors with unbalanced sign patterns to examine the robustness of spectral bisection.

1.3 Kemeny's constant and Braess' paradox

The extent of connectedness of a road network informs the travel time of vehicles between two randomly chosen points in the network.

One can expect the trip time of vehicles to be shorter as the extent of connectedness increases in a road network. Considering the network as a graph, this anticipation can be examined. The level of connectedness can be regarded as the number of edges in the graph—as more edges are inserted into the graph, there is a higher probability that there are more routes with shorter distances to arrive at a random destination from a randomly chosen initial place.

Imagine a situation where adding roads to a road network in order to reduce traffic congestion results in, contrary to one's expectation, slowing down overall traffic flow (this is called Braess' paradox [9]). Random walks on graphs can also exhibit a version of this paradox. Random walks on undirected graphs are a special family of Markov chains. A random walk on an undirected graph can be described by the transition matrix for a finite, discrete, time-homogeneous Markov chain, where the transition probability from one initial state to another is given by the inverse of the degree of the vertex corresponding to the initial state.

The parameter known as Kemeny's constant can be used to measure the average time for travel of a Markov chain between two randomly chosen states. Hence, Kemeny's constant can serve as a proxy for identifying an edge exhibiting the version of the paradox, by examining an edge whose insertion into an undirected graph increases Kemeny's constant for random walks on the graph (such an edge is called a *Braess edge*). In Chapter 5, we study under what circumstances graphs can have a Braess edge in order to see what type of graphs exhibit the version of the paradox.

1.4 Sensitivity of perfect state transfer

A quantum spin network describes quantum states and interactions between qubits (coupling strengths) in the interior of a quantum computer. A quantum state is not definite—it can exist in multiple states simultaneously—(called quantum superposition of states) in contrast to the states related to a random walk. Qubits (short for quantum bit) can exhibit quantum entanglement that allows them to interact with each other regardless of their distance. These features enable quantum computers to outperform classical computers for some particular tasks. For the construction of quantum computers, a crucial task is to transfer a quantum state from one location to another.

Continuous-time quantum walks play an important role in achieving perfect state transfer (PST): an initial quantum state at one location along the walk for a specified length of time is found as the same state at a different location. An undirected graph can be used to model a quantum spin network by considering qubits as vertices and their interactions as edges. A continuous-time quantum walk can be represented by a transition operator $U(t) = e^{itA}$ [16, 46], where t is readout time and A is the adjacency matrix of the undirected graph. The square of the modulus of the entry in i^{th} row and j^{th} column of $U(t)$ indicates the *fidelity* (probability) of state transfer from i to j. Hence, $U(t)$ provides information for PST.

Isolating a spin network completely from external environments is a necessary task in order to keep quantum superposition of states and couplings between qubits—this is one of the challenges for the construction of quantum computers. Being affected by external environments can be considered by quantifying the extent of connectedness as perturbations in edge weight (coupling strength). In order to reduce external effects between particular places, one could manipulate the network. Then, manipulation of the state of connectedness can be considered as switching edges (changing interaction between qubits) in the corresponding graph. In Chapter 6, we study edge-switches on hypercubes and the graphs obtained from hypercubes by those edge-switches, and compare the derivatives of the fidelity under PST with respect to the weight of an edge (also with respect to readout time) between hypercubes and the resulting graphs.

2

Preliminaries

We first introduce basic notation and terminologies in graph theory and matrix theory. Then, we elaborate necessary definitions and background knowledge with further notation, topic by topic.

2.1 Basic notation and terminologies

Throughout this thesis, we assume familiarity with basic material on graph theory and matrix theory. We refer the reader to [17] and [38] for the necessary background.

2.1.1 Graph theory

A *graph* G is a pair that consists of a finite non-empty set $V(G)$ of objects called *vertices* together with a set $E(G)$ of pairs of vertices in $V(G)$ called *edges*. We say that $V(G)$ is the *vertex set* of G, and $E(G)$ is the *edge set* of G. The *order* of G is the number of vertices. Two vertices v and w are *adjacent* if $\{v, w\} \in E(G)$. The *subgraph of G induced* by a subset S of $V(G)$ is the graph with vertex set S, where two vertices in S are adjacent if and only if they are adjacent in G. An edge of the form $\{v, v\}$ is called a *loop*. If $E(G)$ is not a multi-set and does not contain any loops, then G is called a *simple graph*. If $E(G)$ is a set of unordered (resp. ordered) pairs of $V(G)$, then G is called an *undirected graph* (resp. a *directed* graph). For a directed graph G, we call the ordered pairs (v, w) in $E(G)$ *arcs*. We say that for an arc (v, w) in $E(G)$, v is *adjacent to w*. A *weighted graph* is a graph each of whose edges (or arcs) is assigned a real number, called the *weight* of the edge (or the arc).

Unless stated otherwise in this thesis, we assume all graphs to be simple, undirected and unweighted though a few graphs are non-simple, directed or weighted.

Let G be a graph of order n. Let m_G be defined as $|E(G)|$. We use $u \sim v$ to denote an edge $\{u, v\}$ of G. For an edge $e = u \sim v$ of G, e is said to *join* u and v. Two edges are *incident* if they share a common vertex. A *matching* in G is a set of pairwise non-incident edges. A vertex w is a *neighbour* of v if v and w are adjacent. We denote the set of neighbours of v in G by $N_G(v)$. For a vertex v of G and a subset X of $V(G)$, $N_X(v)$ denotes the set of neighbours of v that belong to X. The *degree*, denoted $\deg_G(v)$, of a vertex v in G is the number of neighbours of v. We denote the minimum degree of a graph G by $\delta(G)$. A vertex v is a *dominating vertex* if v is adjacent to all the other vertices in G. A vertex v is said to be *pendent* if $\deg_G(v) = 1$. Given a labelling of $V(G)$, we use $\mathbf{d}_G$ to denote the column vector whose i^{th} component is $\deg_G(v_i)$ for $1 \leq i \leq n$, where v_i is the i^{th} vertex in $V(G)$.

Let G be a graph. A *walk* of length k in G is a sequence of $k+1$ vertices $v_1, \ldots, v_{k+1}$ such that v_i and v_{i+1} are adjacent for $i = 1, \ldots, k$. One may consider a walk as a finite sequence of edges. A *path* is a walk in which all vertices are distinct. A path is called an (x, y)-path if x and y are the pendent vertices in the path. We say that G is *connected* if, for any two vertices v and w in G, there is a (v, w)-path. A *cycle* of length ℓ is a walk $(v_1, \ldots, v_{\ell+1})$ such that $v_1, \ldots, v_\ell$ are distinct and $v_1 = v_{\ell+1}$. The *distance* $d_G(v, w)$ between vertices v and w in G is the length of a shortest (v, w)-path in G. For a connected graph G, a distance d_G on $V(G)$ is a function from $V(G)$ to $V(G)$ that satisfies the following: (i) $d_G(v, w) \geq 0$ for $v, w \in V(G)$ with $d_G(v, w) = 0$ if and only if $v = w$, (ii) $d_G(v, w) = d_G(w, v)$ for $v, w \in V(G)$, and (iii) $d_G(v, w) \leq d_G(v, x) + d_G(x, w)$ for $v, w, x \in V(G)$ (the *triangle inequality*). Hence $d_G(\cdot, \cdot)$ is a metric on G. For a connected graph G with a vertex v, the *eccentricity* $e_G(v)$ of v is $e_G(v) = \max\{d_G(v, w) | w \in V(G)\}$. The *diameter*, denoted $\operatorname{diam}(G)$, of G is $\operatorname{diam}(G) = \max\{e_G(v) | v \in V(G)\}$. Two vertices v and w of G are called *antipodal vertices* if $d_G(v, w) = \operatorname{diam}(G)$. We also say that v is an antipodal vertex of w, and vice versa.

We omit the sub-index G in $\deg_G$, d_G, and e_G if G is clear from the context.

Let us introduce several types of graphs. The *empty graph*, denoted N_k, on k vertices consists of k vertices with no edges. The *trivial graph* is a graph of order 1. A graph G is called *bipartite* if $V(G)$ is partitioned into two subsets U and W (called *partite sets*) so that each edge of G joins one vertex in U and the other in W. A graph is *r-regular* if each vertex of the graph has degree r. A *complete graph* K_n is the $(n-1)$-regular graph on n vertices. The *line graph* of a graph G is the graph whose vertices are the edges of G, where two vertices are adjacent if and only if their corresponding edges are incident in G. We denote a cycle of length n by

C_n, and a path on n vertices by P_n. A *tree* is a connected graph that has no cycles. A *star* S_n is a tree on n vertices with one vertex of degree $n-1$. For $n \geq 3$, v is called the *centre vertex* of S_n if $\deg_{S_n}(v) = n-1$. For $n > k \geq 1$, a *broom* $\mathcal{B}_{n,k}$ is a tree constructed from a path on k vertices by adding $n-k$ pendent vertices to one pendent vertex on the path.

For $v \in V(G)$, we use $G - v$ to denote the graph obtained from G by the deletion of v. A vertex v of a connected graph G is called a *cut-vertex* of G if $G - v$ is disconnected. The *vertex connectivity*, denoted $v(G)$, of a connected graph G is the minimum number of vertices whose removal disconnects G. The *complement* $\bar{G}$ of a graph G is a graph with the vertex set $V(G)$ where two vertices are adjacent in $\bar{G}$ if and only if the two vertices are not adjacent in G. For two graphs G_1 and G_2 on disjoint vertex sets, the *disjoint union* $G_1 + G_2$ of G_1 and G_2 is defined as the graph $(V(G_1) \cup V(G_2), E(G_1) \cup E(G_2)))$. The *join* of G_1 and G_2, denoted as $G_1 \vee G_2$, is the graph obtained from $G_1 + G_2$ by joining every vertex in $V(G_1)$ to every vertex in $V(G_2)$. Furthermore, $\vee_{i=1}^{k} G$ is defined as $\underbrace{G \vee \cdots \vee G}_{k \text{ times}}$. It is straightforward to see that $G_1 \vee (G_2 \vee G_3) = (G_1 \vee G_2) \vee G_3$ and $G_1 \vee G_2 = G_2 \vee G_1$. The *Cartesian product* $G_1 \square G_2$ of graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$, and two vertices (v_1, v_2) and (w_1, w_2) are adjacent if and only if either $v_1 = w_1$ and $v_2 \sim w_2 \in E(G_2)$ or $v_2 = w_2$ or $v_1 \sim w_1 \in E(G_1)$.

2.1.2 Matrix theory

Throughout this thesis, we use boldface lowercase letters to denote column vectors.

Let us consider some notation and terminology in matrix theory. Let A be an $m \times n$ matrix. We denote the transpose of A by A^T. Let $\alpha \subset \{1, \ldots, m\}$ and $\beta \subset \{1, \ldots, n\}$. We denote by $A[\alpha, \beta]$ the submatrix of A whose rows and columns are indexed by α and β, respectively. Let α^c denote the complement of α. We use $(A)_{ij}$ to denote the (i,j)-entry of A. We denote by $\mathbf{1}_n$ the all ones column vector of size n, by I_n the identity matrix of size $n \times n$, and by $J_{n,m}$ the all ones matrix of size $n \times m$. If $k = n = m$, then we denote $J_{n,m}$ by J_k. The subscripts of $\mathbf{1}_n$, I_n, $J_{n,m}$ and J_k are omitted if their sizes are clear from the context. We also use $\mathbf{0}_n$ to denote the all zeros column vector of size n. We write $\mathbf{0}_n$ as 0 if no confusion arises. The column vector whose component in k^{th} position is 1 and zeros elsewhere is denoted as $\mathbf{e}_k$. We use $\text{diag}(A_1, \ldots, A_k)$ to denote the block diagonal matrix consisting of the main diagonal blocks $A_1, \ldots, A_k$ which are square matrices, and zeros elsewhere. In particular, if all the main diagonal blocks are scalars, it is a diagonal matrix.

For a subset X in $\mathbb{R}^n$, we denote the subspace spanned by X as $\text{span}(X)$. We use $\text{Row}(A)$ and $\text{Col}(A)$ to denote the row space of A and the column space of A, respectively. The rank of A is denoted as $\text{rank}(A)$. Given an eigenvalue λ of a square matrix A, the *algebraic multiplicity* of λ is its multiplicity as a root of the characteristic polynomial of A. We use $am(\lambda)$ to denote the algebraic multiplicity of an eigenvalue λ of a matrix. The *spectrum* of a square matrix A is the multi-set of eigenvalues of A. In Chapter 4, we particularly use the spectrum as the sequence of eigenvalues in non-increasing order.

Let A be an $m \times n$ matrix and B be a $p \times q$ matrix. The *Kronecker product* $A \otimes B$ of A and B is the $mp \times nq$ matrix

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \cdots & a_{1,n}B \\ \vdots & \ddots & \vdots \\ a_{m,1}B & \cdots & a_{m,n}B \end{bmatrix}$$

where $A = [a_{ij}]$. Then, it is straightforward to see that if B and C are of the same size, then $A \otimes (B + C) = A \otimes B + A \otimes C$ and $(B + C) \otimes A = B \otimes A + C \otimes A$. Furthermore, the following properties can be found in [27]. Given matrices A and B, we have $(A \otimes B)^T = A^T \otimes B^T$. Let A, B, C and D be matrices of compatible sizes for AB and CD to be defined. Then, $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.

Let G be a directed, weighted graph on n vertices. The *adjacency matrix* $A(G) = [a_{i,j}]_{1 \le i,j \le n}$ of G is the $n \times n$ matrix given by

$$a_{i,j} = \begin{cases} w_{i,j}, & \text{if } i \text{ is adjacent to } j \text{, and } w_{i,j} \text{ is the weight of the arc from } i \text{ to } j, \\ 0, & \text{if there is no arc from } i \text{ to } j. \end{cases}$$

If G is an unweighted graph, then the adjacency matrix of G is defined as that of the directed, weighted graph obtained from G by assigning weight 1 to each arc of G; if G is undirected, then the adjacency matrix of G is defined as that of the directed, weighted graph obtained from G by transforming each edge $i \sim j$ with its weight in G into two arcs from i to j, and vice versa, with the same weight. Then, the adjacency matrix of an undirected graph is symmetric.

2.2 Gram mates

Definition 2.2.1. Let A and B be $(0, 1)$ matrices. The matrices A and B are *Gram mates* and A is called a *Gram mate to* B if $AA^T = BB^T$, $A^TA = B^TB$ and $A \neq B$.

The vertex set of a two-mode network consists of a set of actors and a set of events. Permuting rows and columns of the corresponding matrix is equivalent to relabelling actors and events. Hence, we use the following definition in Chapter 3.

Definition 2.2.2. Let A and B be $(0,1)$ matrices. The matrices A and B are *isomorphic* if there exist permutation matrices P and Q such that $B = PAQ$.

Example 2.2.3. Let $A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$. It can be verified that A and B are Gram mates, and they are isomorphic.

It is readily verified that: (i) A and B are Gram mates if and only if, for any permutation matrices P and Q of the appropriate sizes, PAQ and PBQ are Gram mates; and (ii) A and B are Gram mates if and only if A^T and B^T are Gram mates. So, those statements are used when we need to simplify some hypotheses of a claim in terms of Gram mates to focus on particular cases without the loss of the generality of the claim.

Let A be a $(0,1)$ matrix. We say that $A\mathbf{1}$ (resp. $\mathbf{1}^T A$) is the *row sum vector* of A (resp. the *column sum vector* of A). We have a basic observation [44] that Gram mates A and B must have the same row sum vectors and the same column sum vectors. Thus, both $A - B$ and $B - A$ are $(0,1,-1)$ matrices such that their row sum and column sum vectors are 0.

Definition 2.2.4. Let E be a $(0,1,-1)$ matrix such that $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0$. The matrix E is said to be *realizable (with respect to Gram mates)* if there is a pair of Gram mates A and $A+E$. We say that A and B are *Gram mates via* E if A and B are Gram mates, and either $A - B = E$ or $B - A = E$.

Evidently, any zero matrix is not realizable. It is easily seen that E is realizable if and only if for any permutation matrices P and Q of the appropriate sizes, PEQ is realizable; E is realizable if and only if E^T is realizable. Furthermore, every pair of Gram mates is a pair via some unique realizable matrix up to sign.

The following are used in Section 3.2.

Proposition 2.2.5. *[38] Let $\ell \geq 1$, and let $D = \operatorname{diag}(d_1 I_{k_1}, \ldots, d_\ell I_{k_\ell})$ where $d_1, \ldots, d_\ell$ are distinct and $k_i \geq 1$ for $i = 1, \ldots, \ell$. Suppose that A commutes with D, and A is orthogonal. Then, A is a block diagonal matrix compatible with the partition of D such that each of the main diagonal blocks of A is orthogonal.*

Proposition 2.2.6. *[65] Let A and B be matrices of compatible sizes for AB to be defined. Then,*

$$\begin{aligned}
&\mathrm{Col}(AA^T) = \mathrm{Row}(AA^T) = \mathrm{Col}(A),\\
&\mathrm{Col}(A^TA) = \mathrm{Row}(A^TA) = \mathrm{Row}(A),\\
&\mathrm{Col}(AB) \subseteq \mathrm{Col}(A).
\end{aligned}$$

Furthermore, if AB is of rank k, then there are k columns $\mathbf{a}_1, \ldots, \mathbf{a}_k$ of A that comprise a basis of $\mathrm{Col}(AB)$.

We briefly introduce the singular value decomposition (the SVD) [38] which is a factorization of a real (or complex) matrix. We also state a basic observation regarding change of signs of some positive singular values. Our interest lies in zero-one matrices, so we assume our matrices to be real. Given an $m \times n$ matrix A, there exist $m \times m$ and $n \times n$ orthogonal matrices U and V, respectively, such that $A = U\Sigma V$ for some $m \times n$ diagonal matrix Σ whose entries on the main diagonal are non-negative in non-increasing order. The diagonal entries of Σ are called singular values of A. The columns of U and the columns of V are called the left and right singular vectors of A, respectively. Note that the number of positive singular values of A equals $\mathrm{rank}(A)$.

Suppose that B is obtained from A by changing signs of some positive singular values. Then, B can be written as $B = US\Sigma V^T$, where S is a diagonal matrix the main diagonal entries of which consist of r -1's and $m - r$ ones, for some number r. Let $\widetilde{U} = US$. Clearly, $\widetilde{U}$ is an orthogonal matrix, so $\widetilde{U}\Sigma V^T$ is a singular value decomposition of B. Since $S\Sigma\Sigma^T S^T = \Sigma\Sigma^T$ and $\Sigma^T S^T S\Sigma = \Sigma^T\Sigma$, we have $AA^T = BB^T$ and $A^TA = B^TB$. Furthermore, since $A - B = U(\Sigma - S\Sigma)V^T$ and $\Sigma - S\Sigma \neq 0$, we have $A - B \neq 0$.

Remark 2.2.7. Continuing with A and $B = US\Sigma V^T$ above, S gives different interpretations for the relationship between A and B. For example, if S is given by $S = \mathrm{diag}(-1, -1, 1, \ldots, 1)$, then we can say that A is obtained from B by changing the signs of the first two singular values; or of the first two either left or right singular vectors; or of the first (resp. second) left and the second (resp. first) right singular vectors. In order to avoid confusion from the choices of singular vectors for sign change, we adopt the interpretation 'changing signs of singular values' despite the fact that A and B have the same singular values.

Lemma 2.2.8. *Let A be an $m \times n$ $(0,1)$ matrix. If B is obtained from A by changing signs of some positive singular values of A, then $AA^T = BB^T$, $A^TA = B^TB$ and $A \neq B$.*

Remark 2.2.9. For the result of Lemma 2.2.8, if B is not a zero-one matrix, then A and B are not Gram mates.

2.3 Fiedler vectors with unbalanced sign patterns

Let G be a graph of order n. The *Laplacian matrix* $L(G)$ of G is $L(G) = D(G) - A(G)$ where $A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of vertex degrees. The *spectrum* of $L(G)$, $S(L(G)) = (\lambda_1(G), \dots, \lambda_n(G))$, is defined as the sequence of eigenvalues of $L(G)$ in non-increasing order. It is well known that $L(G)$ is symmetric and positive semi-definite. In particular, $L(G)\mathbf{1} = 0$, so $\lambda_n(G) = 0$. Similarly, the *spectrum* of $A(G)$, $S(A(G)) = (\mu_1(G), \dots, \mu_n(G))$, is defined as the sequence of eigenvalues of $A(G)$ in non-increasing order. Moreover, $\lambda_i(G)$ and $\mu_i(G)$ are written as λ_i and μ_i if G is clear from the context. The *algebraic connectivity* $\alpha(G)$ of a graph G is defined as $\lambda_{n-1}(G)$. It is proven in [31] that $\alpha(G) \leq v(G)$ for a non-complete graph G. We refer the reader to [31] for more properties of $\alpha(G)$. Since $v(G) \leq \delta(G)$, we have $\alpha(G) \leq \delta(G)$ for a non-complete graph G. An eigenvector associated with $\alpha(G)$ is called a *Fiedler vector*. Let $V(G) = \{v_1, \dots, v_n\}$ and $\mathbf{x} = [x_i]$ be a Fiedler vector of G. For $1 \leq i \leq n$, a vertex v_i is said to be *valuated* by x_i if x_i is assigned to v_i.

Suppose that $\mathbf{x} = [x_j]$ is an eigenvector associated to an eigenvalue λ of $L(G)$ or $A(G)$. We define $i_\lambda(\mathbf{x}) = \min\{|\{x_j | x_j > 0\}|, |\{x_j | x_j < 0\}|\}$. To distinguish between $L(G)$ and $A(G)$, we define

$$i_\lambda(G) := \min_{\mathbf{x} \neq 0} \{i_\lambda(\mathbf{x}) | L(G)\mathbf{x} = \lambda \mathbf{x}\} \text{ and } i^*_\mu(G) := \min_{\mathbf{x} \neq 0} \{i_\mu(\mathbf{x}) | A(G)\mathbf{x} = \mu \mathbf{x}\}.$$

In particular, $i_{\alpha(G)}(\mathbf{x})$ and $i_{\alpha(G)}(G)$ are denoted as $i(\mathbf{x})$ and $i(G)$, respectively.

Example 2.3.1. Consider the Laplacian matrix $L(C_4)$ of the cycle C_4:

$$L(C_4) = \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix}.$$

One can verify from computation that $\alpha(C_4) = 2$ and $am(\alpha(C_4)) = 2$; further, two linearly independent Fiedler vectors are given by

$$\mathbf{x}_1^T = \begin{bmatrix}1 & 0 & -1 & 0\end{bmatrix}^T \text{ and } \mathbf{x}_2^T = \begin{bmatrix}0 & 1 & 0 & -1\end{bmatrix}^T.$$

Then, $i(C_4) = i(\mathbf{x}_1) = i(\mathbf{x}_2) = 1$. Similarly, considering the least eigenvalue -2 of the adjacency matrix $A(C_4)$, one can check $i^*_{-2}(C_4) = 2$.

We introduce the spectral properties of a join of graphs. Consider two graphs G_1 and G_2 on disjoint sets of p and q vertices, respectively. Let $S(L(G_1)) = (\lambda_1(G_1), \dots, \lambda_p(G_1))$ and $S(L(G_2)) = (\lambda_1(G_2), \dots, \lambda_q(G_2))$. It is known (see [53]) that the (multi-)set of all eigenvalues of $L(G_1 \vee G_2)$ is

$$\{0, \lambda_1(G_1) + q, \dots, \lambda_{p-1}(G_1) + q, \lambda_1(G_2) + p, \dots, \lambda_{q-1}(G_2) + p, p + q\}.$$

To see this, label the indices of rows and columns of $L(G_1 \vee G_2)$ in order of $V(G_1)$ followed by $V(G_2)$. If $\mathbf{x}$ is an eigenvector orthogonal to $\mathbf{1}_p$ corresponding to $\lambda_i(G_1)$ for $1 \le i \le p-1$, then $\begin{bmatrix}\mathbf{x}^T & \mathbf{0}^T\end{bmatrix}^T$ is an eigenvector of $L(G_1 \vee G_2)$. Similarly, for an eigenvector $\mathbf{y}$ orthogonal to $\mathbf{1}_q$ corresponding to $\lambda_i(G_2)$ for $1 \le i \le q-1$, we have $\begin{bmatrix}\mathbf{0}^T & \mathbf{y}^T\end{bmatrix}^T$ as an eigenvector of $L(G_1 \vee G_2)$. Furthermore, $\mathbf{1}_{p+q}$ and $\begin{bmatrix}-q\mathbf{1}^T & p\mathbf{1}^T\end{bmatrix}^T$ are eigenvectors associated with 0 and $p+q$, respectively.

2.4 Families of graphs with the Braess edge on twin pendent paths

A *forest* is a graph whose connected components are trees. A *spanning tree* (resp. a *spanning forest*) of a graph G is a subgraph that is a tree (resp. a forest) and includes all of the vertices of G. A *k-tree spanning forest* of G is a spanning forest that consists of k trees. If $G - v$ has k connected components $G_1, \dots, G_k$ for some $k \ge 2$ (that is, v is a cut-vertex), then the subgraph induced by $V(G_i) \cup \{v\}$ for $1 \le i \le k$ is called a *branch* of G at v. Two vertices are called *twin pendent vertices* if they are pendent vertices with a common neighbour.

Let G be a graph. Let $P_{k_1} = (v_0, \dots, v_{k_1})$ and $P_{k_2} = (w_0, \dots, w_{k_2})$ where k_1 and k_2 are non-negative integers with $k_1 + k_2 \ge 2$. Suppose that $\widetilde{G}$ is the graph obtained from G, P_{k_1}, and P_{k_2} by identifying a vertex v of G, v_0, and w_0. We say that the paths $(v, v_1, \dots, v_{k_1})$ and $(v, w_1 \dots, w_{k_2})$ in $\widetilde{G}$ are *twin pendent paths*. Then, the pendent vertices of the twin pendent paths in $\widetilde{G}$ are v_{k_1} and w_{k_2}.

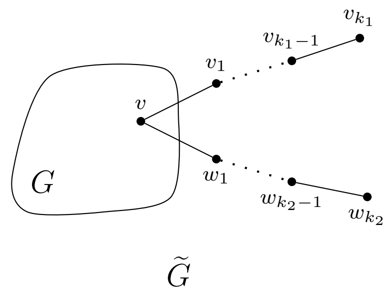


Figure 2.1: An illustration of twin pendent paths in $\widetilde{G}$.

A Markov chain is a stochastic model of a system where at any given time, transitions at the next step depend only on the current state of the system, according to prescribed transition probabilities. Given a discrete, finite, time-homogeneous Markov chain whose finite state space is $\{1, \dots, n\}$, the Markov chain can be represented by the $n \times n$ transition matrix M whose entries are the transition probabilities. We refer the reader to [63] for the necessary background on Markov chains. Then, *Kemeny's constant* $\kappa(M)$ is defined as $\sum_{j\neq i}^{n} m_{i,j}w_j$, where $m_{i,j}$ is the mean first passage time from state i to state j, and w_j is the j^{th} entry of the stationary distribution. Note that Kemeny's constant is independent of i. It is found in [51] that $\kappa(M) + 1 = \sum_{i=1}^{n}\sum_{j=1}^{n} w_i m_{i,j} w_j$. This admits the interpretation of Kemeny's constant in terms of the expected number of steps from a randomly-chosen initial state to a randomly-chosen final state. Alternatively, $\kappa(M)$ can be expressed as $\kappa(M) = \sum_{j=2}^{n} \frac{1}{1-\lambda_j}$ where $1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of M. For the details, the reader may refer to [41].

For our work, we use the combinatorial expression for Kemeny's constant for a random walk on a connected and undirected graph in [47]. In order to emphasize that we are dealing with random walks on connected and undirected graphs, given a connected graph G, we use $\kappa(G)$ to denote Kemeny's constant for the transition matrix of the random walk on G. We denote by τ_G the number of spanning trees of G, and by $\mathcal{F}_G(i;j)$ the set of 2-tree spanning forests of G such that one of the two trees contains a vertex i of G, and the other has a vertex j of G. Define F_G to be the matrix given by $F_G = [f_{i,j}^G]$ where $f_{i,j}^G = |\mathcal{F}_G(i;j)|$. Then,

$$\kappa(G) = \frac{\mathbf{d}_G^T F_G \mathbf{d}_G}{4 m_G \tau_G}.$$

We denote by $\mathbf{f}_G^j$ the j^{th} column of F_G. A non-edge e of G is called a *Braess edge* for G if $\kappa(G) < \kappa(G \cup e)$ where $G \cup e$ is the graph obtained from G by adding e to G. A

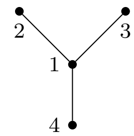


Figure 2.2: The star on 4 vertices used in Example 2.4.1.

connected graph G is said to be *paradoxical* [21] if there exists a Braess edge for G.

Example 2.4.1. Consider the star S_4 in Figure 2.2. Then, $m_{S_4} = 3$, $\tau_{S_4} = 1$, $\mathbf{d}_{S_4}^T = \begin{bmatrix} 3 & 1 & 1 & 1 \end{bmatrix}^T$, and $F_{S_4} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 2 & 2 \\ 1 & 2 & 0 & 2 \\ 1 & 2 & 2 & 0 \end{bmatrix}$. By simple computation, we have $\kappa(S_4) = \frac{5}{2}$. Let $\widehat{S_4}$ be the graph obtained from S_4 by adding edge $2 \sim 3$. Then, $m_{\widehat{S_4}} = 4$, $\tau_{\widehat{S_4}} = 3$, $\mathbf{d}_{\widehat{S_4}}^T = \begin{bmatrix} 3 & 2 & 2 & 1 \end{bmatrix}^T$, and $F_{\widehat{S_4}} = \begin{bmatrix} 0 & 2 & 2 & 3 \\ 2 & 0 & 2 & 5 \\ 2 & 2 & 0 & 5 \\ 3 & 5 & 5 & 0 \end{bmatrix}$. One can check $\kappa(\widehat{S}_4) = \frac{122}{48} > \kappa(S_4)$. Therefore, $2 \sim 3$ is a Braess edge for S_4, and S_4 is paradoxical.

2.5 Equidistant switched hypercubes: their properties and sensitivity analysis under PST

We introduce hypercubes and their basic properties; these and other details can be found in [12] and [17]. The *hypercube* Q_n (also called the *n-cube*) of dimension n is the graph whose vertex set is the set of ordered n-tuples $(x_1, \ldots, x_n)$ (called *binary strings* of length n) where $x_i \in \{0, 1\}$ for $1 \leq i \leq n$, and two vertices are adjacent if and only if their corresponding ordered n-tuples differ at exactly one coordinate. We denote by $x_1 \ldots x_n$ an ordered n-tuple $(x_1, \ldots, x_n)$. Evidently, $|V(Q_n)| = 2^n$. The n-cube Q_n is a regular graph, each vertex of which is of degree n. The distance between v and w in Q_n is the number of positions in which v and w differ. The n-cube Q_n is bipartite. For any vertex x of Q_n, there is a unique vertex y such that $d_{Q_n}(x, y) = n$. Furthermore, $\mathrm{diam}(Q_n) = n$. So, we denote by x^* the antipodal vertex of x.

An *automorphism* of a graph G is a bijection f from $V(G)$ to $V(G)$ such that two vertices v and w are adjacent if and only if $f(v)$ and $f(w)$ are adjacent. Let

$\mathcal{S}_n$ denote the set of all permutations of $\{1, \ldots, n\}$ (called the *symmetric* group on $\{1, \ldots, n\}$).

Proposition 2.5.1. *[66] Let Q_n be a hypercube for $n \geq 1$. Then, the following properties hold:*

(i) For any two vertices v and w, there exists an automorphism f of Q_n such that $f(v) = w$. We say that Q_n is vertex-transitive*.*

(ii) For any two paths (v_1, v_2, v_3) and (w_1, w_2, w_3) of length 2, there exists an automorphism f of Q_n such that $f(v_i) = w_i$ for $i = 1, 2, 3$. We say that Q_n is P_3-transitive*.*

(iii) For any vertices v, w, x and y such that $d(v, w) = d(x, y)$, there exists an automorphism f of Q_n such that $f(v) = x$ and $f(w) = y$. We say that Q_n is distance-transitive*.*

Let $A(G)$ be the adjacency matrix of a weighted (or unweighted) graph G. Let $U(t) = e^{itA}$ where $t > 0$. The *fidelity of state transfer* from v to w at time t in G is given by $p_G(t) = |(U(t))_{v,w}|^2$. If G is clear in the context, we write $p(t)$. If $p_G(t_0) = 1$, we say that there is *perfect state transfer (PST)* between v and w at time t_0, or equivalently that v and w pair up to exhibit (have) PST, or that G exhibits (has) PST.

Proposition 2.5.2. *[20] Let $n \geq 1$, and Q_n be the hypercube. Then, for $x \in V(Q_n)$, Q_n admits PST between x and x^* at time $\frac{\pi}{2}$.*

A *partition* of a set X is a set of non-empty subsets $X_1, \ldots, X_k$ of X such that $X = X_1 \cup \cdots \cup X_k$ and $X_i \cap X_j = \emptyset$ whenever $i \neq j$. The subsets in the partition are called *cells*. We denote a partition $\{X_1, \ldots, X_k\}$ of X by $(X_1, \ldots, X_k)$. Given a labelling of X, we define the *characteristic matrix* of a partition $(X_1, \ldots, X_k)$ to be the $|X| \times k$ matrix whose j^{th} column for $1 \leq j \leq k$ is $\sum_{x \in X_j} \mathbf{e}_x$.

Let G be a graph with or without loops. A partition $\pi = (C_1, \ldots, C_k)$ of $V(G)$ is said to be *equitable* if for any $i, j \in \{1, \ldots, k\}$, $|N_{C_j}(v)|$ is constant for all $v \in C_i$. If π is equitable, we denote $|N_{C_j}(v)|$ for $v \in C_i$ by c_{ij}. Note that c_{ij} is not necessarily the same as c_{ji}.

Given a graph G with an equitable partition $\pi = (C_1, \ldots, C_k)$, the *quotient graph*, denoted G/π, of G with respect to π is the directed weighted graph with vertex set $\{C_1, \ldots, C_k\}$, where there is an arc from vertex C_i to vertex C_j under weight c_{ij} if and only if $c_{ij} > 0$. The *symmetrized quotient graph*, denoted $\widehat{G/\pi}$, of G with respect to π is the undirected weighted graph with vertex set $\{C_1, \ldots, C_k\}$, where vertex C_i is adjacent to C_j under weight $\sqrt{c_{ij}c_{ji}}$ if and only if $c_{ij}c_{ji} > 0$. We note that if $A(G/\pi)$ is symmetric, then $A(G/\pi) = A(\widehat{G/\pi})$.

Proposition 2.5.3. *[35] Let G be a graph, and let π be an equitable partition of G, with characteristic matrix P. Then, $A(G/\pi) = (P^TP)^{-1}P^TA(G)P$ and $A(G)P = PA(G/\pi)$. This implies that if $\mathbf{x}$ is an eigenvector of $A(G/\pi)$ associated to λ, then $P\mathbf{x}$ is an eigenvector of $A(G)$ associated to λ. Furthermore, if there exists a matrix B such that $A(G)P = PB$, then π is equitable, and $B = A(G/\pi)$.*

Theorem 2.5.4. *[5] Let G be a graph with an equitable partition π where v and w belong to singleton cells. Then, G admits PST from a vertex v to a vertex w at time t if and only if $\widehat{G/\pi}$ admits PST from $\{v\}$ to $\{w\}$ at time t.*

Given a graph G with a subset X of $V(G)$, we use $S_r(X)$ to denote the set of vertices v in G such that $d(v,x) = r$ for all $x \in X$. If X is a singleton, say $X = \{x\}$, then we write $S_r(\{x\})$ as $S_r(x)$. The *distance partition* of a connected graph G with respect to $v \in V(G)$ is a partition that consists of the subsets $S_0(v), \ldots, S_k(v)$ where k is the eccentricity of v.

The definition of distance-regular graph can be found in [10] and [35]. Moreover, hypercubes are distance-regular [10].

Theorem 2.5.5. *[35] The distance partition of a graph G with respect to v is equitable for every $v \in V(G)$ if and only if G is distance-regular.*

Here are some properties of hypercubes regarding the distance partition.

Proposition 2.5.6. *[66] Let $\pi = (S_0(v), S_1(v), \ldots, S_n(v))$ be the distance partition of Q_n with respect to a vertex v. Then, the following hold:*

(i) Every vertex in $S_i(v)$ for $1 \leq i \leq n$ is adjacent to exactly i vertices in $S_{i-1}(v)$.

(ii) Every vertex in $S_i(v)$ for $0 \leq i \leq n-1$ is adjacent to exactly $n-i$ vertices in $S_{i+1}(v)$.

Example 2.5.7. Let us consider the 3-cube Q_3 where

$$V(Q_3) = \{000, 001, 010, 100, 011, 101, 110, 111\}.$$

Consider a partition $\pi = (C_1, \ldots, C_k)$ of $V(Q_3)$ where $C_1 = \{000\}$, $C_2 = \{001, 010, 100\}$, $C_3 = \{011, 101, 110\}$, and $C_4 = \{111\}$. As an example, we can see that $|N_{C_3}(v)| = 2$

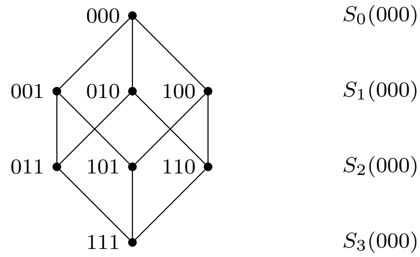


Figure 2.3: The distance partition of Q_3 with respect to 000.

for all $v \in C_2$. In this way, it can be seen that π is equitable. So, we have

$$A(Q_3/\pi) = \begin{bmatrix} 0 & 3 & 0 & 0 \\ 1 & 0 & 2 & 0 \\ 0 & 2 & 0 & 1 \\ 0 & 0 & 3 & 0 \end{bmatrix} \text{ and } A(\widehat{Q_3/\pi}) = \begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}.$$

One can check that $A(Q_3)P = PA(Q_3/\pi)$ where

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}^T$$

is the characteristic matrix of π. Furthermore, π is the distance partition of Q_3 with respect to 000. Note that $\operatorname{diam}(Q_3) = 3$ and $d_{Q_3}(000, 111) = 3$. By Proposition 2.5.2, 000 and 111 pair up to exhibit PST at time $\frac{\pi}{2}$ in Q_3. Further, from Theorem 2.5.4, $\widehat{Q_3/\pi}$ admits PST between vertices C_1 and C_4 at time $\frac{\pi}{2}$.

3

Gram mates

Every two-mode network can be represented by a $(0,1)$ matrix A, and its single-mode networks by AA^T and A^TA. In what follows, we consider $(0,1)$ matrices instead of using the term 'two-mode networks'. This chapter is a study of pairs of distinct $(0,1)$ matrices A and B such that $AA^T = BB^T$ and $A^TA = B^TB$—that is, a study of pairs of Gram mates. Recall that $(0,1)$ matrices A and B are isomorphic if there exist permutation matrices P and Q such that $B = PAQ$.

Sections 3.2–3.4 are based on a version of a journal article co-authored with Steve Kirkland submitted for publication in Linear Algebra and its Applications.

3.1 Introduction

A study of pairs of Gram mates arises from a question in [30] as to whether the conversion approach loses structural features of a two-mode network; the topic is discussed further in [44]. In [30], it is shown how to recover a $(0,1)$ matrix A from AA^T and A^TA under certain circumstances, and how non-isomorphic Gram mates A and B can cause 'data loss of the information for A'. To be clear about our work in this chapter, we briefly introduce the way of recovering A from AA^T and A^TA. For the recovery of A from AA^T and A^TA, the singular value decomposition is used as follows: under the assumption that A has distinct positive singular values, for fixed singular vectors of A (which are uniquely determined up to sign), we change some signs of singular values until a $(0,1)$ matrix is obtained from a singular value decomposition, or until no $(0,1)$ matrix is produced. It is speculated in [30] that there is a very high probability that matrices from this reconstruction are isomorphic.

Kirkland [44] presents techniques for a systematic study of a pair of Gram mates. One of those techniques is to consider a realizable matrix E and to investigate Gram mates A and $A + E$. We use that technique in order to understand the relation between $(0, 1)$ matrices A and B, where B is obtained from A by changing signs of some positive singular values. Furthermore, regarding the speculation, we provide an infinite family of pairs of non-isomorphic Gram mates with that relation.

In addition to the works motivated by [30], we study families of pairs of Gram mates. One of the works of Kirkland [44] is that given two $(0, 1)$ matrices at random of the same large size, the probability that they are Gram mates is 'very' small. For that reason, we furnish infinite families of pairs of Gram mates according to the rank of their difference, or in classes of particular $(0, 1)$ matrices. Moreover, from those families, we give tools to construct other families.

In the present chapter, we discuss the following in each section. We characterize matrices from the reconstruction regardless of whether they have all distinct positive singular values in Section 3.2 (Theorem 3.2.9 and Corollary 3.2.10). Section 3.3 establishes all pairs of Gram mates A and B where the rank of $A - B$ is at most 2 (Theorems 3.3.7, 3.3.15 and 3.3.22). Moreover, we provide equivalent conditions for A being obtained from B by changing signs of at most two positive singular values of A (Theorems 3.3.7, 3.3.19 and 3.3.36). Section 3.4 exhibits families of pairs of non-isomorphic Gram mates A and B, with some extra conditions, where the rank of $A-B$ is 1 (Proposition 3.4.5 and Theorem 3.4.11). In Section 3.5, we provide several tools for attaining pairs of Gram mates via realizable matrices of rank more than 2. In Section 3.6, we mainly focus on circulant Gram mates and realizable matrices. We also study a few types of Gram mates related to tournament matrices. Finally, in Section 3.7, we introduce an analogous approach as we analyse Gram mates via realizable matrices, and we examine $(0, 1)$ matrices A such that A and UA are Gram mates where U is the so-called *discrete Fourier transform matrix*.

3.2 Gram mates and the SVD

Proposition 3.2.1. *Let A and B be $m \times n$ real matrices, and let $\sigma_1, \dots, \sigma_\ell$ be distinct singular values (not necessarily in non-increasing order) of A where $\ell \geq 1$. Then, $AA^T = BB^T$ and $A^TA = B^TB$ if and only if there exist conformable orthogonal matrices U_1, U_2, some orthogonal V, and some rectangular diagonal matrix Σ such that $A = U_1\Sigma V^T$, $B = U_2\Sigma V^T$, and $U_1 = U_2\mathrm{diag}(W_1, \dots, W_\ell)$, where for $i = 1, \dots, \ell$, W_i is an $m_i \times m_i$ orthogonal matrix, and m_i is the multiplicity of σ_i as a singular value. (Here the multiplicity of 0 as a singular value coincides with that of 0 as an eigenvalue of AA^T.)*

Proof. By the singular value decomposition, we find from $A^TA = B^TB$ that there exists an $n \times n$ orthogonal matrix V such that $A = U_1\Sigma V^T$ and $B = U_2\Sigma V^T$ for some $m \times n$ rectangular diagonal matrix Σ, and $m \times m$ orthogonal matrices U_1 and U_2. Since $AA^T = BB^T$, we have $U_2^TU_1\Sigma\Sigma^T = \Sigma\Sigma^TU_2^TU_1$. By Proposition 2.2.5, our desired conclusion is obtained.

It is straightforward to prove the converse. □

Remark 3.2.2. In the proof of Proposition 3.2.1, considering $AA^T = BB^T$ first instead of $A^TA = B^TB$, we can fix the same left singular vectors for A and B. So, it can be deduced that there exist conformable orthogonal matrices V_1, V_2, some orthogonal U, and some rectangular diagonal matrix Σ such that $A = U\Sigma V_1^T$, $B = U\Sigma V_2^T$, $V_1 = V_2\text{diag}(W_1, \ldots, W_\ell)$, where ℓ is the number of distinct singular values, W_i is an $m_i \times m_i$ orthogonal matrix, and m_i is the multiplicity of σ_i as a singular value for $i = 1, \ldots, \ell$. (Here the multiplicity of 0 as a singular value coincides with that of 0 as an eigenvalue of A^TA.)

Proposition 3.2.3. *Let E be a realizable matrix, and $(A, A+E)$ be a pair of Gram mates. For $\mathbf{x} \in \text{Row}(E)$, we have $A\mathbf{x} \in \text{Col}(E)$, and for $\mathbf{y} \in \text{Col}(E)$, $A^T\mathbf{y} \in \text{Row}(E)$.*

Proof. Since $AA^T = (A+E)(A+E)^T$, we have $AE^T = -E(A^T + E^T)$. It follows that for any i^{th} row vector $\mathbf{x}_i^T$ of E, $A\mathbf{x}_i \in \text{Col}(E)$. Similarly, $A^TE = -E^T(A+E)$ implies that for any i^{th} column vector $\mathbf{y}_i$ of E, $A^T\mathbf{y}_i \in \text{Row}(E)$. Therefore, we obtain our desired results. □

Lemma 3.2.4. *Let E be a realizable matrix of rank k, and $(A, A+E)$ be a pair of Gram mates. Then, there exist k positive singular values of A such that the set of their corresponding right (resp. left) singular vectors is a basis of $\text{Row}(E)$ (resp. $\text{Col}(E)$).*

Proof. By Proposition 3.2.1, there exist orthogonal matrices U_1, U_2 and V such that $A = U_1\Sigma V^T$ and $A + E = U_2\Sigma V^T$ for some rectangular diagonal matrix Σ. Then, $EV = (U_2 - U_1)\Sigma$. Since $A^TA = (A+E)^T(A+E)$, we have $E^TE = -A^TE - E^TA$. Substituting $V\Sigma^TU_1^T$ and $V\Sigma^T(U_2 - U_1)^T$ for A^T and E^T, respectively, in $-A^TE - E^TA$, we have

$$E^TE = V(-\Sigma^TU_1^TE - \Sigma^T(U_2 - U_1)^TA).$$

By Lemma 2.2.6, $\text{Col}(E^TE) = \text{Row}(E)$. Since $\text{rank}(E) = k$, $\text{rank}(E^TE) = k$. Again by Lemma 2.2.6, the column space of $V(-\Sigma^TU_1^TE - \Sigma^T(U_2 - U_1)^TA)$ is spanned by

k columns $\mathbf{v}_1, \ldots, \mathbf{v}_k$ of V; thus, the vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ comprise a basis of $\mathrm{Row}(E)$. Moreover, for any right singular vector $\mathbf{v} \notin \mathrm{Row}(E)$, $\mathbf{v}$ is orthogonal to $\mathrm{Row}(E)$. Thus, $E\mathbf{v} = 0$. The rank of EV is k, so $E\mathbf{v}_i \neq 0$ for $i = 1, \ldots, k$. Considering $EV = (U_2 - U_1)\Sigma$, for $i = 1, \ldots, k$ the singular value corresponding to $\mathbf{v}_i$ must be positive.

By Proposition 3.2.3, $A\mathbf{v}_i \in \mathrm{Col}(E)$ for $i = 1, \ldots, k$. Note that $AV = U_1\Sigma$. Since $A\mathbf{v}_1, \ldots, A\mathbf{v}_k$ are linearly independent and $\mathrm{rank}(E) = k$, the set of $A\mathbf{v}_1, \ldots, A\mathbf{v}_k$ is a basis of $\mathrm{Col}(E)$. Our desired conclusion follows. $\square$

Given a $(0,1)$ matrix A, let B be a $(0,1)$ matrix obtained from A by changing signs of some positive singular values. Since A and B are $(0,1)$ matrices, by Lemma 2.2.8 A and B are Gram mates. Suppose that $\mathbf{v}$ is a right singular vector corresponding to one of those singular values. Then, $A\mathbf{v} = -B\mathbf{v}$ and so, $(A+B)\mathbf{v} = 0$. Considering Lemma 3.2.4, either $\mathbf{v} \in \mathrm{Row}(A-B)$ or $\mathbf{v} \notin \mathrm{Row}(A-B)$. We shall investigate the relation between $\mathbf{v}$ and $\mathrm{Row}(A-B)$.

Remark 3.2.5. Suppose that B is obtained from A by changing the signs of positive singular values $\sigma_1, \ldots, \sigma_k$ of A for some $k \geq 1$. We can find from Remark 2.2.7 that in the context of obtaining B from A, converting the signs of $\sigma_1, \ldots, \sigma_k$ is equivalent to changing the sign of one of the left and right singular vectors of A corresponding to σ_i for $i = 1, \ldots, k$.

Proposition 3.2.6. *Let E be an $m \times n$ realizable matrix of rank k, and let A be a $(0,1)$ matrix such that $A + E$ is a $(0,1)$ matrix. Then, the following are equivalent:*

(a) $(A, A+E)$ is a pair of Gram mates and $(2A+E)E^T = 0$,

(b) $A+E$ is obtained from A by changing the signs of some positive singular values.

Furthermore, if one of (a) and (b) holds, then the following are satisfied:

(i) the number of positive singular values whose signs are changed is $\mathrm{rank}(E)$*,*

(ii) the positive singular values of A whose signs are changed are the same as the k positive singular values of $-\frac{1}{2}E$, and

(iii) the corresponding left (resp. right) singular vectors of A can be obtained from the corresponding left (resp. right) singular vectors of $-\frac{1}{2}E$. This implies that the corresponding left (resp. right) singular vectors of A comprise a basis of $\mathrm{Col}(E)$ *(resp.* $\mathrm{Row}(E)$*).*

Proof. Suppose that $(A, A+E)$ is a pair of Gram mates and $(2A+E)E^T = 0$. By Proposition 3.2.1, there exist orthogonal matrices U_1, U_2 and V such that $A = U_1\Sigma V^T$ and $A+E = U_2\Sigma V^T$ for some rectangular diagonal matrix Σ. Let $k = \operatorname{rank}(E)$. By Lemma 3.2.4, there exist right singular vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ of A corresponding to positive singular values $\sigma_1, \dots, \sigma_k$ that form a basis of $\operatorname{Row}(E)$. Since $(2A+E)E^T = 0$, we have $(2A+E)\mathbf{v}_i = 0$ for $i = 1, \dots, k$. Then, we have $E\mathbf{v}_i = -2A\mathbf{v}_i = -2\sigma_i\mathbf{u}_i$ where $\mathbf{u}_i$ is a left singular vector of A corresponding to σ_i. Furthermore, for any right singular vector $\mathbf{v} \notin \operatorname{Row}(E)$, $E\mathbf{v} = 0$. Then, without loss of generality, we have

$$EV = -2\begin{bmatrix}\mathbf{u}_1 & \cdots & \mathbf{u}_k & 0\end{bmatrix}\Sigma.$$

Since $E = (U_2 - U_1)\Sigma V^T$, we have $(U_2 - U_1)\Sigma = -2\begin{bmatrix}\mathbf{u}_1 & \cdots & \mathbf{u}_k & 0\end{bmatrix}\Sigma$. If AA^T is singular, then we may choose the same left singular vectors corresponding to the singular value 0 for A and $A+E$. Hence, $U_2 - U_1 = -2\begin{bmatrix}\mathbf{u}_1 & \cdots & \mathbf{u}_k & 0\end{bmatrix}$. It follows from Remark 3.2.5 that $A+E$ is obtained from A by changing the signs of $\sigma_1, \dots, \sigma_k$. Furthermore, applying the Gram–Schmidt process to a basis of the orthogonal complement of $\operatorname{Row}(E)$, we obtain an orthonormal basis, say $\{\tilde{\mathbf{u}}_{k+1}, \dots, \tilde{\mathbf{u}}_m\}$. Then,

$$-E = \begin{bmatrix}\mathbf{u}_1 & \cdots & \mathbf{u}_k & \tilde{\mathbf{u}}_{k+1} & \cdots & \tilde{\mathbf{u}}_m\end{bmatrix}(2\widetilde{\Sigma})V^T$$

where $\widetilde{\Sigma} = \operatorname{diag}(\sigma_1, \dots, \sigma_k, 0, \dots, 0)$. Rearranging the diagonal entries of $\widetilde{\Sigma}$ in non-decreasing order, one can obtain a singular value decomposition of $-E$. Therefore, $2\sigma_1, \dots, 2\sigma_k$ are the positive singular values of $-E$.

Suppose that $A+E$ is obtained from A by changing the signs of ℓ positive singular values for some $\ell > 0$. By Lemma 2.2.8, A and $A+E$ are Gram mates. By Remark 3.2.5, there exist orthogonal matrices U, $\widetilde{U}$ and V such that $A = U\Sigma V^T$ and $A+E = \widetilde{U}\Sigma V^T$ for some rectangular diagonal matrix Σ, where $\widetilde{U}$ is obtained from U by changing the signs of, without loss of generality, the first ℓ columns $\mathbf{u}_1, \dots, \mathbf{u}_\ell$ of U. Let $\sigma_1, \dots, \sigma_\ell$ be the corresponding positive singular values. Then, $E = (\widetilde{U} - U)\Sigma V^T = -2\begin{bmatrix}\mathbf{u}_1 & \cdots & \mathbf{u}_\ell & 0\end{bmatrix}\Sigma V^T$. So, each row of E is a linear combination of the first ℓ rows $\mathbf{v}_1^T, \dots, \mathbf{v}_\ell^T$ of V^T. Hence, $\operatorname{Row}(E) = \operatorname{span}\{\mathbf{v}_1 \dots, \mathbf{v}_\ell\}$, and this implies $\ell = k = \operatorname{rank}(E)$. Moreover, since $EV = (\widetilde{U} - U)\Sigma$, we have $E\mathbf{v}_i = -2\sigma_i\mathbf{u}_i = -2A\mathbf{v}_i$ for $i = 1, \dots, k$. So, $(2A+E)\mathbf{v}_i = 0$ for $i = 1, \dots, k$. Therefore, $(2A+E)E^T = 0$. Furthermore, applying the same argument above for finding the singular value decomposition of $-E$, we can find that (ii) and (iii) hold. $\square$

Remark 3.2.7. By a similar argument as in the proof of Proposition 3.2.6, one can establish that $(A, A+E)$ is a pair of Gram mates, $E^T(2A+E) = 0$, and $k = \operatorname{rank}(E)$ if and only if for a $(0,1)$ matrix A, a $(0,1)$ matrix $A+E$ is obtained from A by changing the signs of k positive singular values. For the proof of the converse, one can begin with $A = U\Sigma V^T$ and $A + E = U\Sigma\widetilde{V}^T$ for some orthogonal matrices U, V, and $\widetilde{V}$, where $\widetilde{V}$ is obtained from V by changing the signs of k columns of V corresponding to the k positive singular values.

Remark 3.2.8. Let E be an $m \times n$ realizable matrix of rank k, and $(A, A+E)$ be a pair of Gram mates. Suppose that $(2A+E)E^T = 0$. Then, $\operatorname{rank}(2A+E) \leq n-k$. There are k right singular vectors of A that correspond to positive singular values and comprise a basis of $\operatorname{Row}(E)$. So, we have $E\mathbf{v} = 0$ for any right singular vector $\mathbf{v} \notin \operatorname{Row}(E)$. It follows that $E\mathbf{x} = 0$ for $\mathbf{x} \notin \operatorname{Row}(E)$. Therefore, A^TA is singular if and only if $\operatorname{rank}(2A+E) < n-k$. Furthermore, $\operatorname{rank}(2A+E) = n-k-l$ where l is the nullity of A^TA.

Theorem 3.2.9. *Let E be a realizable matrix of rank k, and let A be a $(0,1)$ matrix such that $A+E$ is a $(0,1)$ matrix. Then, the following are equivalent:*

(i) $(A, A+E)$ is a pair of Gram mates and $(2A+E)E^T = 0$.

(ii) $(A, A+E)$ is a pair of Gram mates and $E^T(2A+E) = 0$.

(iii) $A+E$ is obtained from A by changing the signs of k positive singular values of A. (Here the k positive singular values are the same as those of $-\frac{1}{2}E$.)

(iv) There exist k right singular vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ of A corresponding to positive singular values such that the vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ form a basis of $\operatorname{Row}(E)$ and $\mathbf{v}_i$ is a null vector of $2A+E$ for $i = 1, \ldots, k$. (Here $\mathbf{v}_1, \ldots, \mathbf{v}_k$ can be obtained from right singular vectors corresponding to the positive singular values of $-\frac{1}{2}E$.)

(v) There exist k left singular vectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ of A corresponding to positive singular values such that the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ form a basis of $\operatorname{Col}(E)$ and $\mathbf{u}_i$ is a null vector of $(2A+E)^T$ for $i = 1, \ldots, k$. (Here $\mathbf{u}_1, \ldots, \mathbf{u}_k$ can be obtained from left singular vectors corresponding to the positive singular values of $-\frac{1}{2}E$.)

(vi) $(A, A+E)$ is a pair of Gram mates and AE^T is symmetric.

(vii) $(A, A+E)$ is a pair of Gram mates and A^TE is symmetric.

Proof. (i) $\Leftrightarrow$ (ii) $\Leftrightarrow$ (iii): It is clear from Proposition 3.2.6 and Remark 3.2.7.

(i) $\Leftrightarrow$ (iv) and (ii) $\Leftrightarrow$ (v): Using Lemma 3.2.4 and Proposition 3.2.6, the proof is straightforward.

(i) $\Leftrightarrow$ (vi) and (ii) $\Leftrightarrow$ (vii): Since $AA^T = (A+E)(A+E)^T$, we have $AE^T + EA^T + EE^T = 0$. Hence, $(2A+E)E^T = 0$ implies $EA^T = AE^T$, and vice versa. Similarly, from $A^TA = (A+E)^T(A+E)$, we find (ii) $\Leftrightarrow$ (vii). $\square$

Theorem 3.2.9 can be recast with respect to Gram mates A and B.

Corollary 3.2.10. *Let A and B be $(0,1)$ matrices with $A \neq B$, and let $k = \operatorname{rank}(A-B)$. Then, the following are equivalent:*

(i) (A,B) is a pair of Gram mates and $(A+B)(A-B)^T = 0$.

(ii) (A,B) is a pair of Gram mates and $(A-B)^T(A+B) = 0$.

(iii) B is obtained from A by changing the signs of k positive singular values. (Here the k positive singular values are the same as those of $\frac{1}{2}(A-B)$.)

(iv) There exist k right singular vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ of A corresponding to positive singular values such that the vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ form a basis of $\operatorname{Row}(A-B)$ and $\mathbf{v}_i$ is a null vector of $A+B$ for $i = 1, \dots, k$. (Here $\mathbf{v}_1, \dots, \mathbf{v}_k$ are obtained from right singular vectors corresponding to the positive singular values of $\frac{1}{2}(A-B)$.)

(v) There exist k left singular vectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ of A corresponding to positive singular values such that the vectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ form a basis of $\operatorname{Col}(A-B)$ and $\mathbf{u}_i$ is a null vector of $(A+B)^T$ for $i = 1, \dots, k$. (Here $\mathbf{u}_1, \dots, \mathbf{u}_k$ are obtained from left singular vectors corresponding to the positive singular values of $\frac{1}{2}(A-B)$.)

(vi) (A,B) is a pair of Gram mates and $A(A-B)^T$ is symmetric.

(vii) (A,B) is a pair of Gram mates and $A^T(A-B)$ is symmetric.

Definition 3.2.11. Let A be a rectangular $(0,1)$ matrix. The matrix A is said to be *convertible* (to B) if there exists a $(0,1)$ matrix B obtained from A by changing the signs of k positive singular values (possibly with repetition) for some $k \geq 1$. Such A and B are called *convertible Gram mates.* We say that the k positive singular values of A are the *Gram singular values* of Gram mates A (and B). The matrix A is said to *have Gram singular values* if A is convertible.

Remark 3.2.12. In order to clarify Definition 3.2.11, consider a $(0,1)$ matrix A convertible to B. Even though the signs of k positive singular values of A for some $k \geq 1$ are changed for obtaining B, by Remark 3.2.5 A and B have the same singular values. By converting the signs of the k singular values of B, we can obtain A from B. So, B is convertible to A. Hence, we may use the term 'convertible Gram mates'.

Let $A = U\Sigma V^T$ where U and V are orthogonal matrices and Σ is a rectangular diagonal matrix. Suppose that there exist two ways of obtaining B from A by changing the signs of k positive diagonal entries of Σ, say $B = U\Sigma_1 V^T$ and $B = U\Sigma_2 V^T$. Clearly, $\Sigma_1 = \Sigma_2$. Thus, if A is convertible to B, then the k positive singular values of A whose signs are changed and their corresponding singular vectors are uniquely determined. Thus, we may use the term 'the Gram singular values of A and B'. Furthermore, if there are repeated values among the Gram singular values, then we need to indicate which positions on the main diagonal of Σ corresponding to the repeated values are chosen for the sign changes. Therefore, if the Gram singular values are not distinct, then we need to specify corresponding right singular vectors (or left singular vectors).

Remark 3.2.13. Let A and B be $(0,1)$ matrices with $A \neq B$. If one of the conditions in Corollary 3.2.10 holds, then A and B are convertible Gram mates; furthermore, all singular vectors of A corresponding to the Gram singular values of A and B can be obtained from those corresponding to all positive singular values of $\frac{1}{2}(A - B)$. One can establish analogous results with respect to Gram mates A and $A + E$ via a realizable matrix E by using Theorem 3.2.9.

Example 3.2.14. Suppose that a $(0,1)$ matrix Q is a Gram mate to the identity matrix I. Clearly, $Q \neq I$ and Q is a permutation matrix. By (vi) of Corollary 3.2.10, Q is convertible to I if and only if $I(I - Q)^T$ is symmetric, *i.e.,* Q is symmetric. Therefore, any non-convertible Gram mate to I is a non-symmetric permutation matrix.

Example 3.2.15. Let $A = \begin{bmatrix} A_1 & A_2 \\ A_2 & A_1 \end{bmatrix}$ be a $(0,1)$ matrix where A_1 and A_2 have the same size and $A_1 \neq A_2$. It can be checked that $B = \begin{bmatrix} A_2 & A_1 \\ A_1 & A_2 \end{bmatrix}$ is a Gram mate to A. Furthermore, one can verify that $(A + B)(A - B)^T = 0$. Since the condition (i) of Corollary 3.2.10 holds, A and B are convertible Gram mates. Furthermore, it follows from the structure of $A - B$ that the Gram singular values of A and B can be obtained from the k positive singular values of $A_1 - A_2$ where $k = \text{rank}(A_1 - A_2)$.

3.3 Gram mates via realizable matrices of rank 1 and 2

In this section, we shall completely characterize Gram mates A and B where the rank of $A-B$ is 1 or 2. We also investigate convertible Gram mates A and B, their Gram singular values, and corresponding singular vectors.

Recall that given a realizable matrix E and a pair of Gram mates $(A, A+E)$, PAQ and $P(A+E)Q$ are Gram mates for any appropriately sized permutation matrices P and Q. Hence, we may consider a $(0,1,-1)$ matrix $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ such that $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$.

Proposition 3.3.1 ([44, Lemma 2.1])**.** *Let $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ be realizable, and let $A = \begin{bmatrix} \widetilde{A} & X_1 \\ X_2 & X_3 \end{bmatrix}$ be compatible with the partition of E. Then, A and $A+E$ are Gram mates if and only if $(\widetilde{A}, \widetilde{A}+\widetilde{E})$ is a pair of Gram mates, $\widetilde{E}X_2^T = 0$ and $\widetilde{E}^T X_1 = 0$.*

Remark 3.3.2. Note that $X_1^T \widetilde{E} = 0$ and $\widetilde{E}X_2^T = 0$ if and only if columns of X_1 are $(0,1)$ left null vectors of $\widetilde{E}$, and rows of X_2 are $(0,1)$ right null vectors of $\widetilde{E}$.

Proposition 3.3.3. *Let $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ be a $(0,1,-1)$ matrix such that $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$. Then, E is realizable if and only if $\widetilde{E}$ is realizable.*

Proof. Suppose that $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ is realizable. Then, there exists a $(0,1)$ matrix $A = \begin{bmatrix} \widetilde{A} & X_1 \\ X_2 & X_3 \end{bmatrix}$ that is compatible with the partition of E, and is a Gram mate to $A+E$. By Proposition 3.3.1, $(\widetilde{A}, \widetilde{A}+\widetilde{E})$ is a pair of Gram mates, and so $\widetilde{E}$ is realizable. Conversely, assume that $\widetilde{E}$ is realizable. Then, for a pair $(\widetilde{A}, \widetilde{A}+\widetilde{E})$ of Gram mates, $\begin{bmatrix} \widetilde{A} & 0 \\ 0 & 0 \end{bmatrix}$ and $\begin{bmatrix} \widetilde{A}+\widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ are Gram mates. Hence, E is realizable. $\square$

Proposition 3.3.4. *Let $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ be realizable, and let $A = \begin{bmatrix} \widetilde{A} & X_1 \\ X_2 & X_3 \end{bmatrix}$ be compatible with the partition of E. Suppose that A and $A+E$ are Gram mates. Then, $AE^T = EA^T$ if and only if $\widetilde{A}\widetilde{E}^T = \widetilde{E}\widetilde{A}^T$. This implies that if A is convertible to $A+E$, so is $\widetilde{A}$ to $\widetilde{A}+\widetilde{E}$, and vice versa.*

Proof. From Proposition 3.3.1, we have $\widetilde{E}X_2^T = 0$. It can be readily checked from computation that $AE^T = EA^T$ if and only if $\widetilde{A}\widetilde{E}^T = \widetilde{E}\widetilde{A}^T$. By Remark 3.2.13, the desired conclusion follows. $\square$

Proposition 3.3.5. *Let* $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ *be realizable, and let* $A = \begin{bmatrix} \widetilde{A} & X_1 \\ X_2 & X_3 \end{bmatrix}$ *be compatible with the partition of* E*. Suppose that* A *and* $A+E$ *are Gram mates. We may assume (by Lemma 3.2.4) that* $\tilde{\mathbf{v}}_1, \ldots, \tilde{\mathbf{v}}_k$ *form a basis of* $\mathrm{Row}(\widetilde{E})$*, where* $\tilde{\mathbf{v}}_i$ *is a right singular vector associated to a positive singular value* σ_i *of* $\widetilde{A}$ *for* $i = 1, \ldots, k$*. Furthermore, suppose that for* $i = 1, \ldots, k$*,* $\tilde{\mathbf{u}}_i$ *is the corresponding left singular vector. Then,* $\begin{bmatrix} \tilde{\mathbf{v}}_i \\ 0 \end{bmatrix}$ $\left(\textit{resp.} \begin{bmatrix} \tilde{\mathbf{u}}_i \\ 0 \end{bmatrix} \right)$ *is a right (resp. left) singular vector corresponding to* σ_i *of* A *for* $i = 1, \ldots, k$*.*

Proof. Using Proposition 3.3.1, we have $\widetilde{E}X_2^T = 0$ and $\widetilde{E}^T X_1 = 0$, *i.e.*, $\mathrm{Row}(\widetilde{E})$ and $\mathrm{Col}(\widetilde{E})$ are orthogonal to $\mathrm{Row}(X_2)$ and $\mathrm{Col}(X_1)$, respectively. Let $\tilde{\mathbf{v}}$ be a right singular vector corresponding to a positive singular value σ of $\widetilde{A}$ such that $\tilde{\mathbf{v}} \in \mathrm{Row}(\widetilde{E})$. Since $\widetilde{E}X_2^T = 0$, we have $X_2\tilde{\mathbf{v}} = 0$. For $\sigma\tilde{\mathbf{u}} = \widetilde{A}\tilde{\mathbf{v}}$ where $\tilde{\mathbf{u}}$ is the corresponding left singular vector of $\widetilde{A}$, we have $A \begin{bmatrix} \tilde{\mathbf{v}} \\ 0 \end{bmatrix} = \begin{bmatrix} \widetilde{A}\tilde{\mathbf{v}} \\ X_2\tilde{\mathbf{v}} \end{bmatrix} = \sigma \begin{bmatrix} \tilde{\mathbf{u}} \\ 0 \end{bmatrix}$. Since $\tilde{\mathbf{v}} \in \mathrm{Row}(\widetilde{E})$, by Proposition 3.2.3 we obtain $\sigma\tilde{\mathbf{u}} = \widetilde{A}\tilde{\mathbf{v}} \in \mathrm{Col}(\widetilde{E})$. We find from $\widetilde{E}^T X_1 = 0$ that $X_1^T(\sigma\tilde{\mathbf{u}}) = X_1^T\widetilde{A}\tilde{\mathbf{v}} = 0$. Note that $\widetilde{A}^T\tilde{\mathbf{u}} = \sigma\tilde{\mathbf{v}}$. Hence, $A^T \begin{bmatrix} \tilde{\mathbf{u}} \\ 0 \end{bmatrix} = \begin{bmatrix} \widetilde{A}^T\tilde{\mathbf{u}} \\ X_1^T\tilde{\mathbf{u}} \end{bmatrix} = \sigma \begin{bmatrix} \tilde{\mathbf{v}} \\ 0 \end{bmatrix}$. Therefore, our desired result is obtained. $\square$

Corollary 3.3.6. *Let* $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ *be realizable, and let* $A = \begin{bmatrix} \widetilde{A} & X_1 \\ X_2 & X_3 \end{bmatrix}$ *be compatible with the partition of* E*. Suppose that* A *and* $A+E$ *are Gram mates. If* $\widetilde{A}$ *is convertible to* $\widetilde{A}+\widetilde{E}$*, then* A *is convertible to* $A+E$*; the Gram singular values of* A *and* $A+E$ *are the same as those of* $\widetilde{A}$ *and* $\widetilde{A}+\widetilde{E}$*; and the corresponding singular vectors of* A *are obtained from those of* $\widetilde{A}$ *by adjoining a column of zeros.*

Proof. Combining Propositions 3.3.4 and 3.3.5, the conclusion is straightforward. $\square$

Summarizing Propositions 3.3.1–3.3.5 and Corollary 3.3.6, given a realizable matrix $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$, characterizing realizability of $\widetilde{E}$, Gram mates via $\widetilde{E}$, convertible Gram mates via $\widetilde{E}$, and their Gram singular values and corresponding singular vectors endows E with the same properties except that we need the extra conditions in Proposition 3.3.1 to find Gram mates via E.

3.3.1 Gram mates via matrices of rank 1

Suppose that a realizable matrix E is of rank 1. Without loss of generality,

$$E = \begin{bmatrix} J_{k_1,k_2} & -J_{k_1,k_2} & 0 \\ -J_{k_1,k_2} & J_{k_1,k_2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

for some $k_1, k_2 > 0$. Let $\widetilde{E} = \begin{bmatrix} J_{k_1,k_2} & -J_{k_1,k_2} \\ -J_{k_1,k_2} & J_{k_1,k_2} \end{bmatrix}$. It is straightforward that $\widetilde{A} = \begin{bmatrix} 0 & J_{k_1,k_2} \\ J_{k_1,k_2} & 0 \end{bmatrix}$ and $\widetilde{A} + \widetilde{E}$ are the only pair of Gram mates via E. Thus, $\widetilde{E}$ is realizable. Furthermore, $\widetilde{A}\widetilde{E}^T = \widetilde{E}\widetilde{A}^T$. This implies that $\widetilde{A}$ is convertible to $\widetilde{A} + \widetilde{E}$. Since $\operatorname{rank}(\widetilde{E}) = 1$, there is only one positive singular value of $-\frac{1}{2}\widetilde{E}$, which is the Gram singular value of $\widetilde{A}$ and $\widetilde{A} + \widetilde{E}$. One can find that the positive singular value of $-\frac{1}{2}\widetilde{E}$ is $\sqrt{k_1 k_2}$ and the corresponding left and the corresponding right singular vector are $\frac{1}{\sqrt{2k_1}} \begin{bmatrix} -\mathbf{1}_{k_1} \\ \mathbf{1}_{k_1} \end{bmatrix}$ and $\frac{1}{\sqrt{2k_2}} \begin{bmatrix} \mathbf{1}_{k_2} \\ -\mathbf{1}_{k_2} \end{bmatrix}$ up to sign, respectively.

Theorem 3.3.7. *Suppose that E is a realizable matrix of rank 1:*

$$E = \begin{bmatrix} J_{k_1,k_2} & -J_{k_1,k_2} & 0 \\ -J_{k_1,k_2} & J_{k_1,k_2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

for some $k_1, k_2 > 0$. Let $A = \begin{bmatrix} 0 & J_{k_1,k_2} & X_1 \\ J_{k_1,k_2} & 0 & X_2 \\ X_3 & X_4 & Y \end{bmatrix}$ be a $(0,1)$ matrix compatible with the partition of E. Then, we have the following:

(i) A and $A + E$ are Gram mates if and only if $\mathbf{1}^T X_1 = \mathbf{1}^T X_2$ and $X_3\mathbf{1} = X_4\mathbf{1}$.

(ii) E is realizable.

(iii) For any Gram mates via E, A and $A + E$ are convertible into each other.

(iv) For any Gram mates via E, their Gram singular value is $\sqrt{k_1 k_2}$, and the corresponding left and right singular vectors are (up to sign) $\frac{1}{\sqrt{2k_1}} \begin{bmatrix} -\mathbf{1}_{k_1} \\ \mathbf{1}_{k_1} \\ 0 \end{bmatrix}$ and

$\frac{1}{\sqrt{2k_2}}\begin{bmatrix}\mathbf{1}_{k_2}\\-\mathbf{1}_{k_2}\\0\end{bmatrix}$, *respectively.*

Proof. Applying Proposition 3.3.1, we have

$$\begin{bmatrix}J_{k_2,k_1} & -J_{k_2,k_1}\\ -J_{k_2,k_1} & J_{k_2,k_1}\end{bmatrix}\begin{bmatrix}X_1\\X_2\end{bmatrix}=0,\ \begin{bmatrix}X_3 & X_4\end{bmatrix}\begin{bmatrix}J_{k_2,k_1} & -J_{k_2,k_1}\\ -J_{k_2,k_1} & J_{k_2,k_1}\end{bmatrix}=0.$$

Since J_{k_1,k_2} is an all ones matrix, we have $\mathbf{1}^T X_1 = \mathbf{1}^T X_2$ and $X_3\mathbf{1} = X_4\mathbf{1}$. Applying Propositions 3.3.3–3.3.5 and Corollary 3.3.6 with the argument immediately preceding this theorem, the desired conclusions follow. □

Remark 3.3.8. Consider A and $A+E$ in Theorem 3.3.7. Let $B = A+E$ and $k = k_1 = k_2$. One can check that $AB = BA$ if and only if A and B are Gram mates. Suppose that A and B are diagonalisable. It is known (see [38]) that A and B are simultaneously diagonalisable. Since $\text{rank}(A-B) = 1$, we have $|\sigma(A) - \sigma(B)| = 1$ where $\sigma(A)$ and $\sigma(B)$ are multisets of eigenvalues of A and B, respectively. It follows that $\sigma(A) - \sigma(B) = \{-k\}$ and $\sigma(B) - \sigma(A) = \{k\}$.

Example 3.3.9. Let

$$A = \left[\begin{array}{cc|cc|ccc}0&0&1&1&1&1&0\\0&0&1&1&0&0&1\\\hline 1&1&0&0&1&1&1\\1&1&0&0&0&0&0\\\hline 1&0&1&0&1&1&1\\1&0&1&0&1&1&1\\0&1&1&0&1&1&1\end{array}\right],\ E = \left[\begin{array}{cc|cc|ccc}1&1&-1&-1&0&0&0\\1&1&-1&-1&0&0&0\\\hline -1&-1&1&1&0&0&0\\-1&-1&1&1&0&0&0\\\hline 0&0&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&0\end{array}\right].$$

Clearly, E has rank 1. By Theorem 3.3.7, A and $A+E$ are Gram mates, and the Gram singular value is 2. Moreover, $\frac{1}{2}\begin{bmatrix}\mathbf{1}_2\\-\mathbf{1}_2\\\mathbf{0}_3\end{bmatrix}$ is a corresponding right singular vector.

3.3.2 Gram mates via matrix of rank 2

We first show that given a $(0,1,-1)$ matrix $E = \begin{bmatrix}\widetilde{E} & 0\\0 & 0\end{bmatrix}$ of rank 2 with $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$, $\widetilde{E}$ is in one of the following forms (M1)–(M5). Unless stated otherwise, we assume that all the indices of each block in matrices of types (M1)–(M5) are nonnegative and each of their row and column sum vectors is zero.

(M1) $\begin{bmatrix} J_{k,a} & J_{k,b} & -J_{k,b} & -J_{k,a} \\ -J_{k,a} & -J_{k,b} & J_{k,b} & J_{k,a} \\ J_{l,a} & -J_{l,b} & J_{l,b} & -J_{l,a} \\ -J_{l,a} & J_{l,b} & -J_{l,b} & J_{l,a} \end{bmatrix}$ where all indices of each block are positive.

(M2) $\begin{bmatrix} J_{k,e} & -J_{k,f} & 0 & 0 \\ -J_{k,e} & J_{k,f} & 0 & 0 \\ 0 & 0 & J_{l,g} & -J_{l,h} \\ 0 & 0 & -J_{l,g} & J_{l,h} \end{bmatrix}$ where all indices of each block are positive.

(M3) $\begin{bmatrix} J_{k,a} & J_{k,b} & -J_{k,c} & -J_{k,d} & J_{k,e} & -J_{k,f} \\ -J_{k,a} & -J_{k,b} & J_{k,c} & J_{k,d} & -J_{k,e} & J_{k,f} \\ J_{l,a} & -J_{l,b} & J_{l,c} & -J_{l,d} & 0 & 0 \\ -J_{l,a} & J_{l,b} & -J_{l,c} & J_{l,d} & 0 & 0 \end{bmatrix}$ where $k, l > 0$, $e + f > 0$ and $a + b + c + d > 0$.

(M4) $\begin{bmatrix} J_{k,a} & J_{k,b} & -J_{k,c} & -J_{k,d} & J_{k,e} & -J_{k,f} & 0 & 0 \\ -J_{k,a} & -J_{k,b} & J_{k,c} & J_{k,d} & -J_{k,e} & J_{k,f} & 0 & 0 \\ J_{l,a} & -J_{l,b} & J_{l,c} & -J_{l,d} & 0 & 0 & J_{l,g} & -J_{l,h} \\ -J_{l,a} & J_{l,b} & -J_{l,c} & J_{l,d} & 0 & 0 & -J_{l,g} & J_{l,h} \end{bmatrix}$ where $k, l > 0$, $a + b + c + d > 0$, $e + f > 0$, and $g + h > 0$.

(M5) $\begin{bmatrix} J_{k,a} & -J_{k,b} & J_{k,c} & -J_{k,d} & 0 & 0 \\ -J_{l,a} & J_{l,b} & -J_{l,c} & J_{l,d} & 0 & 0 \\ J_{p,a} & -J_{p,b} & 0 & 0 & J_{p,e} & -J_{p,f} \\ -J_{q,a} & J_{q,b} & 0 & 0 & -J_{q,e} & J_{q,f} \\ 0 & 0 & J_{r,c} & -J_{r,d} & -J_{r,e} & J_{r,f} \\ 0 & 0 & -J_{s,c} & J_{s,d} & J_{s,e} & -J_{s,f} \end{bmatrix}$ where $a + b$, $c + d$, $e + f$, $k + l$, $p + q$ and $r + s$ are positive.

As done in Subsection 3.3.1, we examine properties related to Gram mates via $\widetilde{E}$ for types (M4) and (M5). We also show that the types (M1)–(M3) inherit the same properties from the type (M4). For ease of exposition, we only present an interpretation from the viewpoint of the null space in order to find Gram mates via E by using Gram mates via $\widetilde{E}$ with Proposition 3.3.1.

Unless stated otherwise, we assume that a $(0, 1, -1)$ matrix E has neither a row of zeros nor a column of zeros. Suppose that a $(0, 1, -1)$ matrix E with $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$ is of rank 2. Then, there are two $(0, 1, -1)$ rows $\mathbf{x}_1^T$ and $\mathbf{x}_2^T$ of E that form a basis of $\mathrm{Row}(E)$. Without loss of generality,

$$\begin{aligned}\mathbf{x}_1^T &= \left[\begin{array}{cccc|cccc} \mathbf{1}_{\alpha_1}^T & \mathbf{1}_{\alpha_2}^T & -\mathbf{1}_{\alpha_3}^T & -\mathbf{1}_{\alpha_4}^T & \mathbf{1}_{\beta_1}^T & -\mathbf{1}_{\beta_2}^T & \mathbf{0}_{\beta_3}^T & \mathbf{0}_{\beta_4}^T \end{array}\right], \\ \mathbf{x}_2^T &= \left[\begin{array}{cccc|cccc} \mathbf{1}_{\alpha_1}^T & -\mathbf{1}_{\alpha_2}^T & \mathbf{1}_{\alpha_3}^T & -\mathbf{1}_{\alpha_4}^T & \mathbf{0}_{\beta_1}^T & \mathbf{0}_{\beta_2}^T & \mathbf{1}_{\beta_3}^T & -\mathbf{1}_{\beta_4}^T \end{array}\right]\end{aligned}$$

where $\alpha_1 + \alpha_2 + \beta_1 = \alpha_3 + \alpha_4 + \beta_2 > 0$, $\alpha_1 + \alpha_3 + \beta_3 = \alpha_2 + \alpha_4 + \beta_4 > 0$, $\alpha_i, \beta_i \geq 0$ for $i = 1, 2, 3, 4$.

Consider further conditions for the indices and pairs (α, β) such that $\alpha\mathbf{x}_1 + \beta\mathbf{x}_2$ is a $(0, 1, -1)$ vector for the following three cases: (i) $\beta_1 + \beta_2 > 0$ and $\beta_3 + \beta_4 > 0$, (ii) either $\beta_1 + \beta_2 = 0$ or $\beta_3 + \beta_4 = 0$, (iii) $\beta_i = 0$ for $i = 1, \ldots, 4$.

• Suppose that $\beta_1 + \beta_2 > 0$ and $\beta_3 + \beta_4 > 0$. Evidently, $\mathbf{x}_1$ and $\mathbf{x}_2$ are linearly independent. Since $\alpha\mathbf{x}_1 + \beta\mathbf{x}_2$ is a $(0, 1, -1)$ vector, we have $\alpha, \beta \in \{0, 1, -1\}$. Considering $\mathbf{x}_1^T\mathbf{1} = \mathbf{x}_2^T\mathbf{1} = 0$ and possible $(0, 1, -1)$ linear combinations of $\mathbf{x}_1$ and $\mathbf{x}_2$, we have three subcases:

(C1) Suppose that $\alpha_1 + \alpha_4 > 0$ and $\alpha_2 + \alpha_3 > 0$. If $\alpha, \beta \in \{1, -1\}$, then $\alpha\mathbf{x}_1 + \beta\mathbf{x}_2$ is not a $(0, 1, -1)$ vector. So, $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1)\}$. Moreover, we have $\alpha_1 + \alpha_2 + \beta_1 = \alpha_3 + \alpha_4 + \beta_2$, $\alpha_1 + \alpha_3 + \beta_3 = \alpha_2 + \alpha_4 + \beta_4$.

(C2) If without loss of generality $\alpha_1 + \alpha_4 > 0$ and $\alpha_2 + \alpha_3 = 0$, then $\alpha_2 = \alpha_3 = 0$, $\alpha_1 + \beta_1 = \alpha_4 + \beta_2$, $\alpha_1 + \beta_3 = \alpha_4 + \beta_4$ and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm 1, \mp 1)\}$.

(C3) If $\alpha_1 + \alpha_4 = 0$ and $\alpha_2 + \alpha_3 = 0$, then $\alpha_i = 0$ for $i = 1, \ldots, 4$, $\beta_1 = \beta_2$, $\beta_3 = \beta_4$ and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm 1, \pm 1), (\pm 1, \mp 1)\}$.

• Suppose that either $\beta_1 + \beta_2 = 0$ or $\beta_3 + \beta_4 = 0$. Without loss of generality, $\beta_1 + \beta_2 > 0$ and $\beta_3 + \beta_4 = 0$. For $\mathbf{x}_1$ and $\mathbf{x}_2$ to be linearly independent, $\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 > 0$. Considering $\mathbf{x}_1^T\mathbf{1} = \mathbf{x}_2^T\mathbf{1} = 0$ and possible $(0, 1, -1)$ linear combinations of $\mathbf{x}_1$ and $\mathbf{x}_2$, we have two subcases:

(C4) Let $\alpha_1 + \alpha_4 > 0$ and $\alpha_2 + \alpha_3 > 0$. By an analogous argument as in (C1), $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1)\}$. Furthermore, $\alpha_1 + \alpha_2 + \beta_1 = \alpha_3 + \alpha_4 + \beta_2$, $\alpha_1 + \alpha_3 = \alpha_2 + \alpha_4$.

(C5) If without loss of generality, $\alpha_1 + \alpha_4 > 0$ and $\alpha_2 + \alpha_3 = 0$, then $\alpha_2 = \alpha_3 = 0$, $\alpha_1 = \alpha_4$, $\beta_1 = \beta_2$ and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm 1, \mp 1)\}$.

- Assume that $\beta_i = 0$ for $i = 1, \ldots, 4$. Then, we have a single subcase:

(C6) Obviously, $\alpha_1 = \alpha_4$ and $\alpha_2 = \alpha_3$. Since $\mathbf{x}_1$ and $\mathbf{x}_2$ are linearly independent, $\alpha_i > 0$ for $i = 1, \ldots, 4$. Moreover, $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm\frac{1}{2}, \pm\frac{1}{2}), (\pm\frac{1}{2}, \mp\frac{1}{2})\}$.

Summarizing the conditions for the indices and pairs (α, β) in each of the six subcases, they can be recast as:

(C1) $\alpha_1 + \alpha_4 > 0$, $\alpha_2 + \alpha_3 > 0$, $\beta_1 + \beta_2 > 0$, $\beta_3 + \beta_4 > 0$, $\alpha_1 + \alpha_2 + \beta_1 = \alpha_3 + \alpha_4 + \beta_2$, $\alpha_1 + \alpha_3 + \beta_3 = \alpha_2 + \alpha_4 + \beta_4$ and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1)\}$;

(C2) $\alpha_1 + \alpha_4 > 0$, $\alpha_2 = \alpha_3 = 0$, $\beta_1 + \beta_2 > 0$, $\beta_3 + \beta_4 > 0$, $\alpha_1 + \beta_1 = \alpha_4 + \beta_2$, $\alpha_1 + \beta_3 = \alpha_4 + \beta_4$, and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm 1, \mp 1)\}$;

(C3) $\alpha_i = 0$ for $i = 1, \ldots, 4$, $\beta_1 = \beta_2 > 0$, $\beta_3 = \beta_4 > 0$, and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm 1, \pm 1), (\pm 1, \mp 1)\}$;

(C4) $\alpha_1 + \alpha_4 > 0$, $\alpha_2 + \alpha_3 > 0$, $\beta_1 + \beta_2 > 0$, $\beta_3 = \beta_4 = 0$, $\alpha_1 + \alpha_2 + \beta_1 = \alpha_3 + \alpha_4 + \beta_2$, $\alpha_1 + \alpha_3 = \alpha_2 + \alpha_4$, and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1)\}$;

(C5) $\alpha_1 = \alpha_4 > 0$, $\alpha_2 = \alpha_3 = 0$, $\beta_1 = \beta_2 > 0$, $\beta_3 = \beta_4 = 0$, and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm 1, \mp 1)\}$;

(C6) $\alpha_1 = \alpha_4 > 0$, $\alpha_2 = \alpha_3 > 0$, $\beta_i = 0$ for $i = 1, \ldots, 4$, and $(\alpha, \beta) \in \{(\pm 1, 0), (0, \pm 1), (\pm\frac{1}{2}, \pm\frac{1}{2}), (\pm\frac{1}{2}, \mp\frac{1}{2})\}$.

Now, we shall see that any $(0, 1, -1)$ matrix E with each of the conditions (C1)–(C6) corresponds to one of the following types (M1)–(M5) (up to transposition and permutation of rows and columns).

Let us consider $\mathbf{x}_1^T$ and $\mathbf{x}_2^T$ where the condition (C6) holds. Suppose that $\alpha \mathbf{x}_1^T + \beta \mathbf{x}_2^T$ is a $(0, 1, -1)$ vector for some α and β. Since

$$(\alpha, \beta) \in \left\{(\pm 1, 0), (0, \pm 1), \left(\pm\frac{1}{2}, \pm\frac{1}{2}\right), \left(\pm\frac{1}{2}, \mp\frac{1}{2}\right)\right\},$$

we have four distinct $(0, 1, -1)$ rows up to sign as follows:

$$\begin{aligned}
\mathbf{x}_1^T &= \begin{bmatrix} \mathbf{1}_{\alpha_1}^T & \mathbf{1}_{\alpha_2}^T & -\mathbf{1}_{\alpha_2}^T & -\mathbf{1}_{\alpha_1}^T \end{bmatrix}, \ \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2)^T = \begin{bmatrix} \mathbf{1}_{\alpha_1}^T & \mathbf{0}_{\alpha_2}^T & \mathbf{0}_{\alpha_2}^T & -\mathbf{1}_{\alpha_1}^T \end{bmatrix}, \\
\mathbf{x}_2^T &= \begin{bmatrix} \mathbf{1}_{\alpha_1}^T & -\mathbf{1}_{\alpha_2}^T & \mathbf{1}_{\alpha_2}^T & -\mathbf{1}_{\alpha_1}^T \end{bmatrix}, \ \frac{1}{2}(\mathbf{x}_1 - \mathbf{x}_2)^T = \begin{bmatrix} \mathbf{0}_{\alpha_1}^T & \mathbf{1}_{\alpha_2}^T & -\mathbf{1}_{\alpha_2}^T & \mathbf{0}_{\alpha_1}^T \end{bmatrix}.
\end{aligned}$$

Consider all possible combinations of the four row vectors that span the row space of a $(0, 1, -1)$ matrix E such that $\mathrm{rank}(E) = 2$, $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$. Suppose that

$\mathbf{x}_1^T$ and $\frac{1}{2}(\mathbf{x}_1+\mathbf{x}_2)^T$ are the only distinct rows in E up to sign. Then, we generate E' from E by permuting rows as follows:

$$E' = \begin{bmatrix} J_{\gamma_1,\alpha_1} & J_{\gamma_1,\alpha_2} & -J_{\gamma_1,\alpha_2} & -J_{\gamma_1,\alpha_1} \\ -J_{\gamma_2,\alpha_1} & -J_{\gamma_2,\alpha_2} & J_{\gamma_2,\alpha_2} & J_{\gamma_2,\alpha_1} \\ J_{\gamma_3,\alpha_1} & 0 & 0 & -J_{\gamma_3,\alpha_1} \\ -J_{\gamma_4,\alpha_1} & 0 & 0 & J_{\gamma_4,\alpha_1} \end{bmatrix}$$

for some $\gamma_i \geq 0$ for $i=1,\ldots,4$. Since $\mathbf{1}^T E' = 0^T$, we have $\gamma_1 = \gamma_2$ and $\gamma_3 = \gamma_4$. By $\text{rank}(E') = 2$, $\gamma_i > 0$ for $i = 1,\ldots,4$. Taking the transpose of E' and permuting rows of $(E')^T$, we find that the resulting matrix is of type (M3). Similarly, one can check that for the other choices among the four rows, E must be of one of types (M1)–(M4) (up to transposition and permutation of rows and columns).

Given $\mathbf{x}_1^T$ and $\mathbf{x}_2^T$ with (C2), we have $(\alpha,\beta) \in \{(\pm1,0),(0,\pm1),(\pm1,\mp1)\}$ so that there are three distinct rows up to sign:

$$\begin{aligned} \mathbf{x}_1^T &= \begin{bmatrix} \mathbf{1}_{\alpha_1}^T & -\mathbf{1}_{\alpha_4}^T & \mathbf{1}_{\beta_1}^T & -\mathbf{1}_{\beta_2}^T & \mathbf{0}_{\beta_3}^T & \mathbf{0}_{\beta_4}^T \end{bmatrix}, \\ \mathbf{x}_2^T &= \begin{bmatrix} \mathbf{1}_{\alpha_1}^T & -\mathbf{1}_{\alpha_4}^T & \mathbf{0}_{\beta_1}^T & \mathbf{0}_{\beta_2}^T & \mathbf{1}_{\beta_3}^T & -\mathbf{1}_{\beta_4}^T \end{bmatrix}, \\ (\mathbf{x}_1-\mathbf{x}_2)^T &= \begin{bmatrix} \mathbf{0}_{\alpha_1}^T & \mathbf{0}_{\alpha_4}^T & \mathbf{1}_{\beta_1}^T & -\mathbf{1}_{\beta_2}^T & -\mathbf{1}_{\beta_3}^T & \mathbf{1}_{\beta_4}^T \end{bmatrix}. \end{aligned}$$

Then, if the rows of E consist of rows $\pm\mathbf{x}_1^T$ and $\pm\mathbf{x}_2^T$, then E is of form (M4); if E consists of rows $\pm\mathbf{x}_1^T$, $\pm\mathbf{x}_2^T$ and $\pm(\mathbf{x}_1-\mathbf{x}_2)^T$, then E is of form (M5).

In this manner, one can verify that any $(0,1,-1)$ matrix E whose either row space or column space spanned by $\mathbf{x}_1$ and $\mathbf{x}_2$ with (C1) is in type (M4); E with (C3) is in one of types(M1)–(M4); E with (C4) is in type (M3); and E with (C5) is in one of types (M2)–(M4).

Here is a useful lemma for characterizing Gram mates via E of rank 2.

Lemma 3.3.10. *Let X_1, X_2, Y_1 and Y_2 be matrices of sizes $k\times a$, $k\times b$, $l\times c$ and $l\times d$, respectively. Then, $J_{k,c}Y_1^T + J_{k,d}Y_2^T + X_1J_{a,l} + X_2J_{b,l} = \alpha J_{k,l}$ if and only if $X_1\mathbf{1}_a + X_2\mathbf{1}_b = x\mathbf{1}_k$ and $Y_1\mathbf{1}_c + Y_2\mathbf{1}_d = y\mathbf{1}_l$, where $x+y=\alpha$.*

Proof. Consider the sufficiency of the statements. Suppose that $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{y}_1$ and $\mathbf{y}_2$ are row sum vectors of X_1, X_2, Y_1 and Y_2, respectively. Then, we have $\begin{bmatrix} \mathbf{y}_1^T+\mathbf{y}_2^T \\ \vdots \\ \mathbf{y}_1^T+\mathbf{y}_2^T \end{bmatrix} +$ $\begin{bmatrix} \mathbf{x}_1+\mathbf{x}_2 & \cdots & \mathbf{x}_1+\mathbf{x}_2 \end{bmatrix} = \alpha J$. Let $(\mathbf{x})_i$ be the i^{th} component of $\mathbf{x}$. Considering the j^{th} columns of the both sides, $\mathbf{x}_1+\mathbf{x}_2+(\mathbf{y}_1+\mathbf{y}_2)_j\mathbf{1} = \alpha\mathbf{1}$. Then, $\mathbf{x}_1+\mathbf{x}_2 = x\mathbf{1}$ for some x. Similarly, from the rows of both sides, it can be deduced that $\mathbf{y}_1 + \mathbf{y}_2 = y\mathbf{1}$ for some y. Hence, the equation $J_{k,c}Y_1^T + J_{k,d}Y_2^T + X_1J_{a,l} + X_2J_{b,l} = \alpha J_{k,l}$ can be recast as $yJ + xJ = \alpha J$, and so $x + y = \alpha$.

The converse is straightforward. $\square$

3.3.2.1 Realizable matrices in the form (M1)–(M4)

Here, we first focus on Gram mates via a matrix of the form (M4). It is shown that the cases (M1)–(M3) are special cases of (M4).

Lemma 3.3.11. *Let A and B be $m \times n$ $(0,1)$ matrices such that $A+B = J$. Then, $AA^T = BB^T$ if and only if n is even, and $A\mathbf{1} = B\mathbf{1} = \frac{n}{2}\mathbf{1}$. Similarly, $A^TA = B^TB$ if and only if m is even, and $\mathbf{1}^TA = \mathbf{1}^TB = \frac{m}{2}\mathbf{1}^T$.*

Proof. Suppose that $AA^T = BB^T$ and $A + B = J$. Since $(0,1)$ matrices A and B have the same row sum vector, n is even and $A\mathbf{1} = B\mathbf{1} = \frac{n}{2}\mathbf{1}$. Conversely, assume that n is even, and $A\mathbf{1} = B\mathbf{1} = \frac{n}{2}$. Then,

$$\begin{aligned} AA^T &= (J - B)(J - B)^T \\ &= JJ^T - BJ^T - JB^T + BB^T = nJ - \frac{n}{2}J - \frac{n}{2}J + BB^T = BB^T. \end{aligned}$$

Similarly, one can deduce the remaining conclusions. $\square$

Remark 3.3.12. Suppose that E is of form (M1). By Lemma 3.3.11, $(A, B) = (\frac{1}{2}(J + E), \frac{1}{2}(J - E))$ is a pair of Gram mates. Moreover, it is the only pair of Gram mates such that $A - B = E$.

Lemma 3.3.13. *Let $A = \begin{bmatrix} A_1 & A_2 & X \\ A_3 & Y & A_4 \end{bmatrix}$ and $B = \begin{bmatrix} B_1 & B_2 & X \\ B_3 & Y & B_4 \end{bmatrix}$ be $(0,1)$ matrices. Suppose that $(A - B)\mathbf{1} = 0$, and $\mathbf{1}^TA_i = \mathbf{1}^TB_i$, $A_i + B_i = J$ for $i = 1, \ldots 4$. Then, A and B are Gram mates if and only if*

$$(B_2 - A_2)Y^T + X(B_4^T - A_4^T) = A_1J^T + JA_3^T - JJ^T \tag{3.3.1}$$

$$(B_1^T - A_1^T)X = 0, \tag{3.3.2}$$

$$(B_3^T - A_3^T)Y = 0, \tag{3.3.3}$$

$$(B_2^T - A_2^T)X + Y^T(B_4 - A_4) = 0. \tag{3.3.4}$$

Proof. Since $(A - B)\mathbf{1} = 0$, we have

$$\begin{bmatrix} A_1 & A_2 \end{bmatrix}\mathbf{1} = \begin{bmatrix} B_1 & B_2 \end{bmatrix}\mathbf{1} \text{ and } \begin{bmatrix} A_3 & A_4 \end{bmatrix}\mathbf{1} = \begin{bmatrix} B_3 & B_4 \end{bmatrix}\mathbf{1}.$$

Applying Lemma 3.3.11 to pairs $(\begin{bmatrix} A_1 & A_2 \end{bmatrix}, \begin{bmatrix} B_1 & B_2 \end{bmatrix})$ and $(\begin{bmatrix} A_3 & A_4 \end{bmatrix}, \begin{bmatrix} B_3 & B_4 \end{bmatrix})$, we obtain $A_1A_1^T + A_2A_2^T = B_1B_1^T + B_2B_2^T$ and $A_3A_3^T + A_4A_4^T = B_3B_3^T + B_4B_4^T$. Let the numbers of rows of A_1 and A_3 be k and l, respectively. Since $\mathbf{1}^T A_i = \mathbf{1}^T B_i$ and $A_i + B_i = J$ for $i = 1, \ldots 4$, the numbers k and l are even, $\mathbf{1}^T A_1 = \mathbf{1}^T A_2 = \frac{k}{2}\mathbf{1}^T$ and $\mathbf{1}^T A_3 = \mathbf{1}^T A_4 = \frac{l}{2}\mathbf{1}^T$. From $B_i = J - A_i$ for $i = 1, \ldots 4$, we have

$$B_1B_3^T - A_1A_3^T = (J - A_1)(J - A_3)^T - A_1A_3^T = JJ^T - A_1J^T - JA_3^T, \tag{3.3.5}$$
$$B_1^TB_2 - A_1^TA_2 = (J - A_1)^T(J - A_2) - A_1^TA_2 = J^TJ - A_1^TJ - J^TA_2 = 0, \tag{3.3.6}$$
$$B_3^TB_4 - A_3^TA_4 = (J - A_3)^T(J - A_4) - A_3^TA_4 = J^TJ - A_3^TJ - J^TA_4 = 0. \tag{3.3.7}$$

Furthermore, using Lemma 3.3.11 for each pair (A_i, B_i) for $i = 1, \ldots, 4$, we obtain $A_i^TA_i = B_i^TB_i$.

One can check that $AA^T = BB^T$ if and only if

$$\begin{aligned} A_1A_1^T + A_2A_2^T + XX^T &= B_1B_1^T + B_2B_2^T + XX^T, \\ A_1A_3^T + A_2Y^T + XA_4^T &= B_1B_3^T + B_2Y^T + XB_4^T, \\ A_3A_3^T + A_4A_4^T + YY^T &= B_3B_3^T + B_4B_4^T + YY^T. \end{aligned}$$

Using (3.3.5), $A_1A_1^T + A_2A_2^T = B_1B_1^T + B_2B_2^T$ and $A_3A_3^T + A_4A_4^T = B_3B_3^T + B_4B_4^T$, we find that $AA^T = BB^T$ if and only if $(B_2 - A_2)Y^T + X(B_4^T - A_4^T) = A_1J^T + JA_3^T - JJ^T$.

One can verify that $A^TA = B^TB$ if and only if

$$\begin{aligned} &A_1^TA_1 + A_3^TA_3 = B_1^TB_1 + B_3^TB_3,\ A_2^TA_2 + Y^TY = B_2^TB_2 + Y^TY, \\ &A_4^TA_4 + X^TX = B_4^TB_4 + X^TX,\ A_1^TA_2 + A_3^TY = B_1^TB_2 + B_3^TY, \\ &A_1^TX + A_3^TA_4 = B_1^TX + B_3^TB_4,\ A_2^TX + Y^TA_4 = B_2^TX + Y^TB_4. \end{aligned}$$

By (3.3.6), (3.3.7) and the fact that $A_i^TA_i = B_i^TB_i$ for $i = 1, \ldots, 4$, the desired conclusion follows. $\square$

Remark 3.3.14. Let C and D be Gram mates, and let α and β be sets of some row and column indices, respectively. Then, $C[\alpha, \beta]$ and $D[\alpha, \beta]$ are not necessarily Gram mates. That is, the submatrices do not necessarily inherit properties of being Gram mates from C and D. However, the matrices with the hypothesis in Lemma 3.3.13 yield the following submatrices with inherited properties in the matrices.

Let $A = \begin{bmatrix} A_1 & A_2 \\ A_3 & Y \end{bmatrix}$ and $B = \begin{bmatrix} B_1 & B_2 \\ B_3 & Y \end{bmatrix}$. Suppose that $(A - B)\mathbf{1} = 0$, and $\mathbf{1}^T A_i = \mathbf{1}^T B_i$, $A_i + B_i = J$ for $i = 1, 2, 3$. It can be found from the definition of Gram mates that A and B are Gram mates if and only if $(B_2 - A_2)Y^T = A_1J^T + JA_3^T - JJ^T$ and $(B_3^T - A_3^T)Y = 0$. Then, the equivalent condition for Gram mates A and B is the same as that obtained from the conditions (3.3.1)–(3.3.4) in Lemma 3.3.13 by removing the terms containing A_4, B_4 or X.

Similarly, given $A = \begin{bmatrix} A_2 & X \\ Y & A_4 \end{bmatrix}$ and $B = \begin{bmatrix} B_2 & X \\ Y & B_4 \end{bmatrix}$ where $A_i\mathbf{1} = B_i\mathbf{1}$, $\mathbf{1}^TA_i = \mathbf{1}^TB_i$ and $A_i + B_i = J$ for $i = 2, 4$, we can find from the definition of Gram mates that A and B are Gram mates if and only if $(B_2 - A_2)Y^T + X(B_4^T - A_4^T) = 0$ and $(B_2^T - A_2^T)X + Y^T(B_4 - A_4) = 0$. Then, the equivalent condition for Gram mates A and B can be also obtained by annihilating the terms having A_1, A_3, B_1 or B_3 in the conditions (3.3.1)–(3.3.4) in Lemma 3.3.13.

Therefore, equivalent conditions for Gram mates via matrices of forms (M2) and (M3) can be induced by those for Gram mates via matrices of form (M4).

Theorem 3.3.15. *Let*

$$E = \begin{bmatrix} J_{k,a} & J_{k,b} & -J_{k,c} & -J_{k,d} & J_{k,e} & -J_{k,f} & 0 & 0 \\ -J_{k,a} & -J_{k,b} & J_{k,c} & J_{k,d} & -J_{k,e} & J_{k,f} & 0 & 0 \\ J_{l,a} & -J_{l,b} & J_{l,c} & -J_{l,d} & 0 & 0 & J_{l,g} & -J_{l,h} \\ -J_{l,a} & J_{l,b} & -J_{l,c} & J_{l,d} & 0 & 0 & -J_{l,g} & J_{l,h} \end{bmatrix}$$

where any column index in each block is a nonnegative integer, and $k, l > 0$, $a + b + c + d > 0$, $e + f > 0$, $g + h > 0$, $E\mathbf{1} = 0$ and $\mathbf{1}^TE = 0^T$. Let

$$A = \begin{bmatrix} 0 & 0 & J_{k,c} & J_{k,d} & 0 & J_{k,f} & X_{11} & X_{12} \\ J_{k,a} & J_{k,b} & 0 & 0 & J_{k,e} & 0 & X_{21} & X_{22} \\ 0 & J_{l,b} & 0 & J_{l,d} & Y_{11} & Y_{12} & 0 & J_{l,h} \\ J_{l,a} & 0 & J_{l,c} & 0 & Y_{21} & Y_{22} & J_{l,g} & 0 \end{bmatrix} \tag{3.3.8}$$

where each block of A is a $(0,1)$ matrix. Then, A and $A+E$ are Gram mates if and only if the following conditions are satisfied:

(i) $\mathbf{1}^TX_{1i} = \mathbf{1}^TX_{2i}$ *and* $\mathbf{1}^TY_{1i} = \mathbf{1}^TY_{2i}$ *for* $i = 1, 2$*;*

(ii) $\begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \frac{g-h}{2} \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix}$ *and* $\begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \frac{e-f}{2} \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix}$ *where $g - h$ and $e - f$ are even.*

Proof. Let $A_1 = \begin{bmatrix} 0 & 0 & J_{k,c} & J_{k,d} \\ J_{k,a} & J_{k,b} & 0 & 0 \end{bmatrix}$, $A_3 = \begin{bmatrix} 0 & J_{l,b} & 0 & J_{l,d} \\ J_{l,a} & 0 & J_{l,c} & 0 \end{bmatrix}$, $A_2 = \begin{bmatrix} 0 & J_{k,f} \\ J_{k,e} & 0 \end{bmatrix}$

and $A_4 = \begin{bmatrix} 0 & J_{l,h} \\ J_{l,g} & 0 \end{bmatrix}$. Set $X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$, $Y = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix}$ and $B_i = J - A_i$ for $i = 1, \ldots, 4$.

Applying Lemma 3.3.13 to our setup, it is enough to show that our desired conditions (i) and (ii) are deduced from the conditions (3.3.1)–(3.3.4). From the condition (3.3.2), which is $(B_1^T - A_1^T)X = 0$, we have

$$\begin{bmatrix} J_{k,a} & J_{k,b} & -J_{k,c} & -J_{k,a} \\ -J_{k,a} & -J_{k,b} & J_{k,c} & J_{k,d} \end{bmatrix}^T \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} = 0.$$

Since $a + b + c + d > 0$, there is at least one row in $B_1^T - A_1^T$ that is $\begin{bmatrix} \mathbf{1}^T & -\mathbf{1}^T \end{bmatrix}$ or $\begin{bmatrix} -\mathbf{1}^T & \mathbf{1}^T \end{bmatrix}$. Hence, $\mathbf{1}^T X_{1i} = \mathbf{1}^T X_{2i}$ for $i = 1, 2$. Conversely, $\mathbf{1}^T X_{1i} = \mathbf{1}^T X_{2i}$ for $i = 1, 2$ implies $(B_1^T - A_1^T)X = 0$. Similarly, we can find that the condition (3.3.3) is equivalent to $\mathbf{1}^T Y_{1i} = \mathbf{1}^T Y_{2i}$ for $i = 1, 2$. Since $k, l > 0$, each of $B_2^T - A_2^T$ and $B_4^T - A_4^T$ consists of rows that are $\pm \begin{bmatrix} \mathbf{1}^T & -\mathbf{1}^T \end{bmatrix}$. Thus, $\mathbf{1}^T X_{1i} = \mathbf{1}^T X_{2i}$ and $\mathbf{1}^T Y_{1i} = \mathbf{1}^T Y_{2i}$ for $i = 1, 2$ imply (3.3.4).

Consider the condition (3.3.1). Then, it can be checked that (3.3.1) is equivalent to

$$\begin{bmatrix} J_{k,e} & -J_{k,f} \\ -J_{k,e} & J_{k,f} \end{bmatrix} \begin{bmatrix} Y_{11}^T & Y_{21}^T \\ Y_{12}^T & Y_{22}^T \end{bmatrix} + \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} J_{g,l} & -J_{g,l} \\ -J_{h,l} & J_{h,l} \end{bmatrix} = \begin{bmatrix} (d-a)J_{k,l} & (c-b)J_{k,l} \\ (b-c)J_{k,l} & (a-d)J_{k,l} \end{bmatrix}.$$

It follows from Lemma 3.3.10 that the condition (3.3.1) is equivalent to $Y_{11}\mathbf{1}_e - Y_{12}\mathbf{1}_f = y_1\mathbf{1}_l$, $X_{11}\mathbf{1}_g - X_{12}\mathbf{1}_h = x_1\mathbf{1}_k$ and $Y_{21}\mathbf{1}_e - Y_{22}\mathbf{1}_f = y_2\mathbf{1}_l$, $X_{21}\mathbf{1}_g - X_{22}\mathbf{1}_h = x_2\mathbf{1}_k$ where $x_1 + y_1 = x_2 + y_2 = d - a$ and $y_2 - x_1 = y_1 - x_2 = c - b$. Furthermore, premultiplying both sides of $Y_{11}\mathbf{1}_e - Y_{12}\mathbf{1}_f = y_1\mathbf{1}_l$ and $Y_{21}\mathbf{1}_e - Y_{22}\mathbf{1}_f = y_2\mathbf{1}_l$ by $\mathbf{1}_l^T$, respectively, we have

$$\mathbf{1}_l^T Y_{11}\mathbf{1}_e - \mathbf{1}_l^T Y_{12}\mathbf{1}_f = y_1\mathbf{1}_l^T\mathbf{1}_l = y_1 l \text{ and } \mathbf{1}_l^T Y_{21}\mathbf{1}_e - \mathbf{1}_l^T Y_{22}\mathbf{1}_f = y_2\mathbf{1}_l^T\mathbf{1}_l = y_2 l.$$

Since $\mathbf{1}_l^T Y_{1i} = \mathbf{1}_l^T Y_{2i}$ for $i = 1, 2$, from subtraction of the two equations, we obtain $(y_1 - y_2)l = 0$ and so $y_1 = y_2$. Similarly, using $X_{11}\mathbf{1}_g - X_{12}\mathbf{1}_h = x_1\mathbf{1}_k$ and $X_{21}\mathbf{1}_g - X_{22}\mathbf{1}_h = x_2\mathbf{1}_k$, it can be checked that $x_1 = x_2$. It follows from $E\mathbf{1} = 0$ that $x_1 = \frac{-a+b-c+d}{2} = \frac{g-h}{2}$ and $y_1 = \frac{-a-b+c+d}{2} = \frac{e-f}{2}$. Furthermore, since x_1 and y_1 are integers, $g - h$ and $e - f$ must be even. $\square$

Corollary 3.3.16. *Let E be a $(0, 1, -1)$ matrix of form (M4). Then, E is realizable if and only if $g - h$ and $e - f$ are even.*

Proof. Suppose that E is realizable. By Theorem 3.3.15, the conclusion is straightforward. Conversely, let $g-h$ and $e-f$ be even. We only need to show the existence of $X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$ and $Y = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix}$ satisfying (i) and (ii) of Theorem 3.3.15. If $g-h=0$, then our desired matrix can be obtained by choosing $X=0$. We can also obtain X with (i) and (ii) by choosing $X_{11} = X_{21} = \begin{bmatrix} J_{k,\frac{g-h}{2}} & 0 \end{bmatrix}$ and $X_{12} = X_{22} = 0$ if $g-h>0$, and choosing $X_{11} = X_{21} = 0$ and $X_{12} = X_{22} = \begin{bmatrix} J_{k,\frac{h-g}{2}} & 0 \end{bmatrix}$ if $g-h<0$. In this manner, we can also construct Y satisfying (i) and (ii). $\square$

Remark 3.3.17. Consider a $(0,1,-1)$ matrix E of form (M3). Then, $E\mathbf{1} = 0$ implies $c-b = d-a = \frac{e-f}{2}$. The matrix E can be regarded as a matrix of form (M4) by setting $g=0$ and $h=0$. From Remark 3.3.14, equivalent conditions for Gram mates via E can be induced by those for Gram mates via matrices of form (M4), annihilating the conditions related to X in (i) and (ii) of Theorem 3.3.15. Hence, A and $A+E$ are Gram mates where A is in form (3.3.8) with $g=h=0$ if and only if $\mathbf{1}^T Y_{1i} = \mathbf{1}^T Y_{2i}$ for $i=1,2$ and $\begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \frac{e-f}{2} \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix}$ where $e-f$ is even. Furthermore, E is realizable if and only if $e-f$ is even.

Let E be a $(0,1,-1)$ matrix of form (M2). Then, $E\mathbf{1} = 0$ implies $e=f>0$ and $g=h>0$. By an analogous argument with Remark 3.3.14, we can find that A and $A+E$ are Gram mates where A is in form (3.3.8) with $a=b=c=d=0$ if and only if $\begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = 0$, $\begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = 0$, $\mathbf{1}^T X_{1i} = \mathbf{1}^T X_{2i}$ and $\mathbf{1}^T Y_{1i} = \mathbf{1}^T Y_{2i}$ for $i=1,2$. Since $e-f = g-h = 0$, E is realizable for any $e,f,g,h>0$.

Finally, from Remark 3.3.12, there is only one pair of Gram mates via E of form (M1), and so E is realizable. Thus, one may consider E as a matrix of form (M4) by setting $e=f=g=h=0$.

Remark 3.3.18. Let $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ be a realizable matrix where $\widetilde{E}$ is of one of types (M1)–(M4), and let $\widetilde{A}$ and $\widetilde{E}$ be Gram mates. Suppose that $A = \begin{bmatrix} \widetilde{A} & X_1 \\ X_2 & X_3 \end{bmatrix}$ is a $(0,1)$ matrix compatible with the partition of E. By Proposition 3.3.1 and Remark 3.3.2, completely determining Gram mates via E is equivalent to finding all left and right $(0,1)$ null vectors of $\widetilde{E}$ for X_1 and X_2.

Let E be a matrix of form (M4). Suppose that A and $A+E$ are Gram mates where A is in the form (3.3.8). Then,

$$2A+E=\begin{bmatrix} J_{k,a} & J_{k,b} & J_{k,c} & J_{k,d} & J_{k,e} & J_{k,f} & 2X_{11} & 2X_{12} \\ J_{k,a} & J_{k,b} & J_{k,c} & J_{k,d} & J_{k,e} & J_{k,f} & 2X_{21} & 2X_{22} \\ J_{l,a} & J_{l,b} & J_{l,c} & J_{l,d} & 2Y_{11} & 2Y_{12} & J_{l,g} & J_{l,h} \\ J_{l,a} & J_{l,b} & J_{l,c} & J_{l,d} & 2Y_{21} & 2Y_{22} & J_{l,g} & J_{l,h} \end{bmatrix} \tag{3.3.9}$$

where $e+f$ and $g+h$ are positive even numbers, $k,l>0$ and $a+b+c+d>0$. Consider two vectors $\mathbf{x}_1^T$ and $\mathbf{x}_2^T$ that form a basis of $\mathrm{Row}(E)$:

$$\begin{aligned} \mathbf{x}_1^T &= \begin{bmatrix} \mathbf{1}_a^T & \mathbf{1}_b^T & -\mathbf{1}_c^T & -\mathbf{1}_d^T & \mathbf{1}_e^T & -\mathbf{1}_f^T & \mathbf{0}_g^T & \mathbf{0}_h^T \end{bmatrix}, \\ \mathbf{x}_2^T &= \begin{bmatrix} \mathbf{1}_a^T & -\mathbf{1}_b^T & \mathbf{1}_c^T & -\mathbf{1}_d^T & \mathbf{0}_e^T & \mathbf{0}_f^T & \mathbf{1}_g^T & -\mathbf{1}_h^T \end{bmatrix}. \end{aligned} \tag{3.3.10}$$

From $E\mathbf{1}=0$, we have $a+b+e=c+d+f$ and $a+c+g=b+d+h$. By Theorem 3.3.15, $2(X_{i1}\mathbf{1}_g-X_{i2}\mathbf{1}_h)=g-h$ and $2(Y_{i1}\mathbf{1}_e-Y_{i2}\mathbf{1}_f)=e-f$ for $i=1,2$. It follows from a computation that $(2A+E)\mathbf{x}_j=0$ for $j=1,2$. Since $\mathrm{Row}(E)=\mathrm{span}\{\mathbf{x}_1,\mathbf{x}_2\}$, we obtain $(2A+E)E^T=0$. By Theorem 3.2.9, $A+E$ is obtained from A by changing the signs of 2 positive singular values. Hence, A is convertible to $A+E$. Furthermore, for E' in each of types (M1), (M2) and (M3), we may consider $e=f=g=h=0$, $a=b=c=d=0$ and $g=h=0$, respectively, in (3.3.9) and (3.3.10). One can readily check for each case we have $(2A'+E')(E')^T=0$ where A' is a Gram mate to $A'+E'$. Therefore, for any pair of Gram mates A and $A+E$ via E in any form among (M1)–(M4), A and $A+E$ are convertible Gram mates.

We now consider right singular vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ corresponding to the Gram singular values of A and $A+E$. Since $\mathrm{Row}(E)=\mathrm{span}\{\mathbf{x}_1,\mathbf{x}_2\}$, we have $\mathrm{span}\{\mathbf{x}_1,\mathbf{x}_2\}=\mathrm{span}\{\mathbf{v}_1,\mathbf{v}_2\}$. Using $a+b-c-d+e-f=0$, $a-b+c-d+g-h=0$ and the conditions (i) and (ii) in Theorem 3.3.15, one can verify from computations that

$$A^TA\mathbf{x}_1=\begin{bmatrix} (k(a+b+e)+\frac{1}{2}l(a-b-c+d))\mathbf{1}_a \\ (k(a+b+e)-\frac{1}{2}l(a-b-c+d))\mathbf{1}_b \\ (-k(a+b+e)+\frac{1}{2}l(a-b-c+d))\mathbf{1}_c \\ (-k(a+b+e)-\frac{1}{2}l(a-b-c+d))\mathbf{1}_d \\ k(a+b+e)\mathbf{1}_e \\ -k(a+b+e)\mathbf{1}_f \\ \frac{1}{2}l(a-b-c+d)\mathbf{1}_g \\ -\frac{1}{2}l(a-b-c+d)\mathbf{1}_h \end{bmatrix},\ A^TA\mathbf{x}_2=\begin{bmatrix} (\frac{1}{2}k(a-b-c+d)+l(a+c+g))\mathbf{1}_a \\ (\frac{1}{2}k(a-b-c+d)-l(a+c+g))\mathbf{1}_b \\ (-\frac{1}{2}k(a-b-c+d)+l(a+c+g))\mathbf{1}_c \\ (-\frac{1}{2}k(a-b-c+d)-l(a+c+g))\mathbf{1}_d \\ \frac{1}{2}k(a-b-c+d)\mathbf{1}_e \\ -\frac{1}{2}k(a-b-c+d)\mathbf{1}_f \\ l(a+c+g)\mathbf{1}_g \\ -l(a+c+g)\mathbf{1}_h \end{bmatrix}.$$

Consider an equation $A^TA(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2)=\lambda(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2)$ where ζ_1, ζ_2 and λ are real numbers. Set $a_1=k(a+b+e)$, $a_2=k(a-b-c+d)$, $a_3=l(a+c+g)$ and

$a_4 = l(a-b-c+d)$. Then,

$$A^TA(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2) = \begin{bmatrix} (\zeta_1(a_1+\frac{1}{2}a_4)+\zeta_2(\frac{1}{2}a_2+a_3))\mathbf{1}_a \\ (\zeta_1(a_1-\frac{1}{2}a_4)+\zeta_2(\frac{1}{2}a_2-a_3))\mathbf{1}_b \\ (\zeta_1(-a_1+\frac{1}{2}a_4)+\zeta_2(-\frac{1}{2}a_2+a_3))\mathbf{1}_b \\ (\zeta_1(-a_1-\frac{1}{2}a_4)+\zeta_2(-\frac{1}{2}a_2-a_3))\mathbf{1}_d \\ (\zeta_1 a_1+\frac{1}{2}\zeta_2 a_2)\mathbf{1}_e \\ (-\zeta_1 a_1-\frac{1}{2}\zeta_2 a_2)\mathbf{1}_f \\ (\frac{1}{2}\zeta_1 a_4+\zeta_2 a_3)\mathbf{1}_g \\ (-\frac{1}{2}\zeta_1 a_4-\zeta_2 a_3)\mathbf{1}_h \end{bmatrix} = \lambda \begin{bmatrix} (\zeta_1+\zeta_2)\mathbf{1}_a \\ (\zeta_1-\zeta_2)\mathbf{1}_b \\ (-\zeta_1+\zeta_2)\mathbf{1}_b \\ (-\zeta_1-\zeta_2)\mathbf{1}_d \\ \zeta_1\mathbf{1}_e \\ -\zeta_1\mathbf{1}_f \\ \zeta_2\mathbf{1}_g \\ -\zeta_2\mathbf{1}_h \end{bmatrix}.$$

This implies that $\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2$ is an eigenvector of A^TA corresponding to an eigenvalue λ if and only if (ζ_1,ζ_2) is a solution to the system of equations $a_1\zeta_1+\frac{1}{2}a_2\zeta_2=\lambda\zeta_1$ and $\frac{1}{2}a_4\zeta_1+a_3\zeta_2=\lambda\zeta_2$. Hence, for an eigenvector (ζ_1,ζ_2) of the matrix $\begin{bmatrix} a_1 & \frac{1}{2}a_2 \\ \frac{1}{2}a_4 & a_3 \end{bmatrix}$ associated to an eigenvalue λ, a normalized vector of $\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2$ is a right singular vector corresponding to a Gram singular value $\sqrt{\lambda}$ of A. Furthermore, for E' in each of types (M1), (M2) and (M3), considering the extra conditions $e=f=g=h=0$, $a=b=c=d=0$ and $g=h=0$, respectively, one can find that analogous results are established for right singular vectors associated to the Gram singular values of Gram mates via E'. Therefore, we have the following result.

Theorem 3.3.19. *Let E be a realizable matrix of rank 2 corresponding to one of forms (M1)–(M4). Let*

$$M = \begin{bmatrix} k(a+b+e) & \frac{1}{2}k(a-b-c+d) \\ \frac{1}{2}l(a-b-c+d) & l(a+c+g) \end{bmatrix}$$

where the entries in M correspond to the sub-indices in (M1)–(M4). Suppose that A and $A+E$ are Gram mates via E. Then, A and $A+E$ are convertible, and their Gram singular values are the square roots of the eigenvalues λ of M. Furthermore, a right singular vector corresponding to $\sqrt{\lambda}$ is a normalized vector of $\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2$, where $\mathbf{x}_1$ and $\mathbf{x}_2$ are the vectors in (3.3.10) *and (ζ_1,ζ_2) is an eigenvector of M associated to λ.*

3.3.2.2 Realizable matrices in the form (M5)

We now investigate Gram mates via matrices of the form (M5). Furthermore, we shall show that there exist non-convertible Gram mates via matrices of the form

(M5), while any Gram mates via matrices in any form among (M1)–(M4) have Gram singular values.

Lemma 3.3.20. *Let*

$$A = \begin{bmatrix} A_1 & A_2 & X \\ A_3 & Y & A_4 \\ Z & A_5 & A_6 \end{bmatrix}, \; B = \begin{bmatrix} B_1 & B_2 & X \\ B_3 & Y & B_4 \\ Z & B_5 & B_6 \end{bmatrix}$$

be $(0,1)$ *matrices such that* $(A-B)\mathbf{1} = 0$, $\mathbf{1}^T(A-B) = 0^T$, *and* $A_i + B_i = J$ *for* $i = 1, \dots 6$. *Then,* $AA^T = BB^T$ *if and only if*

$$\begin{aligned} (B_2 - A_2)Y^T + X(B_4^T - A_4^T) &= A_1A_3^T - B_1B_3^T, \\ (B_1 - A_1)Z^T + X(B_6^T - A_6^T) &= A_2A_5^T - B_2B_5^T, \\ (B_3 - A_3)Z^T + Y(B_5^T - A_5^T) &= A_4A_6^T - B_4B_6^T. \end{aligned}$$

Furthermore, $A^TA = B^TB$ *if and only if*

$$\begin{aligned} (B_2^T - A_2^T)X + Y^T(B_4 - A_4) &= A_5^TA_6 - B_5^TB_6, \\ (B_1^T - A_1^T)X + Z^T(B_6 - A_6) &= A_3^TA_4 - B_3^TB_4, \\ (B_3^T - A_3^T)Y + Z^T(B_5 - A_5) &= A_1^TA_2 - B_1^TB_2. \end{aligned}$$

Proof. From $(A-B)\mathbf{1} = 0$, we have $\begin{bmatrix} A_1 & A_2 \end{bmatrix}\mathbf{1} = \begin{bmatrix} B_1 & B_2 \end{bmatrix}\mathbf{1}$, $\begin{bmatrix} A_3 & A_4 \end{bmatrix}\mathbf{1} = \begin{bmatrix} B_3 & B_4 \end{bmatrix}\mathbf{1}$, and $\begin{bmatrix} A_5 & A_6 \end{bmatrix}\mathbf{1} = \begin{bmatrix} B_5 & B_6 \end{bmatrix}\mathbf{1}$. Moreover, $A_i + B_i = J$ for $i = 1, \dots 6$. By Lemma 3.3.11, $A_1A_1^T + A_2A_2^T = B_1B_1^T + B_2B_2^T$, $A_3A_3^T + A_4A_4^T = B_3B_3^T + B_4B_4^T$ and $A_5A_5^T + A_6A_6^T = B_5B_5^T + B_6B_6^T$. Similarly, one can deduce from $\mathbf{1}^T(A-B) = 0^T$ that $A_1^TA_1 + A_3^TA_3 = B_1^TB_1 + B_3^TB_3$, $A_2^TA_2 + A_5^TA_5T = B_2^TB_2 + B_5^TB_5$ and $A_4^TA_4 + A_6^TA_6 = B_4^TB_4 + B_6^TB_6$. Considering $AA^T = BB^T$ and $A^TA = B^TB$, the desired conclusion is straightforward. □

Remark 3.3.21. Continuing with the notation and hypothesis of Lemma 3.3.20, consider A that is a 3×3 block partitioned matrix. Let n_i be the number of columns in the i^{th} column partition of A for $i = 1, 2, 3$. Then, $(A-B)\mathbf{1} = 0$ and $A_i + B_i = J$ imply that $n_1 + n_2$, $n_1 + n_3$ and $n_2 + n_3$ are even. Hence, n_i is either even for $i = 1, 2, 3$ or odd for $i = 1, 2, 3$. Similarly, the number of rows in each row partition of A has the same parity.

Theorem 3.3.22. *Let*

$$E = \begin{bmatrix} J_{k,a} & -J_{k,b} & J_{k,c} & -J_{k,d} & 0 & 0 \\ -J_{l,a} & J_{l,b} & -J_{l,c} & J_{l,d} & 0 & 0 \\ J_{p,a} & -J_{p,b} & 0 & 0 & J_{p,e} & -J_{p,f} \\ -J_{q,a} & J_{q,b} & 0 & 0 & -J_{q,e} & J_{q,f} \\ 0 & 0 & J_{r,c} & -J_{r,d} & -J_{r,e} & J_{r,f} \\ 0 & 0 & -J_{s,c} & J_{s,d} & J_{s,e} & -J_{s,f} \end{bmatrix}$$

where $E\mathbf{1} = 0$, $\mathbf{1}^T E = 0^T$, *and* $a+b$, $c+d$, $e+f$, $k+l$, $p+q$ *and* $r+s$ *are positive. Let*

$$A = \begin{bmatrix} 0 & J_{k,b} & 0 & J_{k,d} & X_{11} & X_{12} \\ J_{l,a} & 0 & J_{l,c} & 0 & X_{21} & X_{22} \\ 0 & J_{p,b} & Y_{11} & Y_{12} & 0 & J_{p,f} \\ J_{q,a} & 0 & Y_{21} & Y_{22} & J_{q,e} & 0 \\ Z_{11} & Z_{12} & 0 & J_{r,d} & J_{r,e} & 0 \\ Z_{21} & Z_{22} & J_{s,c} & 0 & 0 & J_{s,f} \end{bmatrix} \tag{3.3.11}$$

be a $(0,1)$ *matrix conformally partitioned with* E. *Suppose that* $X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$, $Y = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix}$ *and* $Z = \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix}$. *Then,* A *and* $A+E$ *are Gram mates if and only if* X, Y *and* Z *satisfy the following conditions:*

(i) there are integers x_1, x_2, y_1, y_2, z_1 *and* z_2 *such that* $X \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \begin{bmatrix} x_1\mathbf{1} \\ x_2\mathbf{1} \end{bmatrix}$, $Y \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \begin{bmatrix} y_1\mathbf{1} \\ y_2\mathbf{1} \end{bmatrix}$, $Z \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \begin{bmatrix} z_1\mathbf{1} \\ z_2\mathbf{1} \end{bmatrix}$ *and* $x_1 = y_2 = -z_2$, $x_2 = y_1 = -z_1$, $x_1+x_2 = y_1+y_2 = -(z_1+z_2) = e-f$; *and*

(ii) there are integers $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1$ *and* γ_2 *such that* $X^T \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \begin{bmatrix} \alpha_1\mathbf{1} \\ \alpha_2\mathbf{1} \end{bmatrix}$, $Y^T \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \begin{bmatrix} \beta_1\mathbf{1} \\ \beta_2\mathbf{1} \end{bmatrix}$, $Z^T \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \begin{bmatrix} \gamma_1\mathbf{1} \\ \gamma_2\mathbf{1} \end{bmatrix}$ *and* $\gamma_1 = \beta_2 = -\alpha_2$, $\gamma_2 = \beta_1 = -\alpha_1$, $\gamma_1+\gamma_2 = \beta_1+\beta_2 = -(\alpha_1+\alpha_2) = l-k$.

In particular, (i) and (ii) imply (a) $e\alpha_1 - f\alpha_2 = kx_1 - lx_2$, $c\beta_1 - d\beta_2 = py_1 - qy_2$, *and* $a\gamma_1 - b\gamma_2 = rz_1 - sz_2$.

Proof. Let $A = \begin{bmatrix} A_1 & A_2 & X \\ A_3 & Y & A_4 \\ Z & A_5 & A_6 \end{bmatrix}$ and $E = \begin{bmatrix} E_1 & E_2 & 0 \\ E_3 & 0 & E_4 \\ 0 & E_5 & E_6 \end{bmatrix}$. Set $B = A+E$. By Lemma 3.3.20, $AA^T = BB^T$ if and only if

$$\begin{bmatrix} J_{k,c} & -J_{k,d} \\ -J_{l,c} & J_{l,d} \end{bmatrix} Y^T + X \begin{bmatrix} J_{p,e} & -J_{p,f} \\ -J_{q,e} & J_{q,f} \end{bmatrix}^T = \begin{bmatrix} (b-a)J_{k,p} & 0 \\ 0 & (a-b)J_{l,q} \end{bmatrix}, \tag{3.3.12}$$

$$\begin{bmatrix} J_{k,a} & -J_{k,b} \\ -J_{l,a} & J_{l,b} \end{bmatrix} Z^T + X \begin{bmatrix} -J_{r,e} & J_{r,f} \\ J_{s,e} & -J_{s,f} \end{bmatrix}^T = \begin{bmatrix} (d-c)J_{k,r} & 0 \\ 0 & (c-d)J_{l,s} \end{bmatrix}, \tag{3.3.13}$$

$$\begin{bmatrix} J_{p,a} & -J_{p,b} \\ -J_{q,a} & J_{q,b} \end{bmatrix} Z^T + Y \begin{bmatrix} J_{r,c} & -J_{r,d} \\ -J_{s,c} & J_{s,d} \end{bmatrix}^T = \begin{bmatrix} 0 & (f-e)J_{p,s} \\ (e-f)J_{q,r} & 0 \end{bmatrix}. \tag{3.3.14}$$

From (3.3.12), we have

$$\begin{aligned} &J_{k,c}Y_{11}^T - J_{k,d}Y_{12}^T + X_{11}J_{e,p} - X_{12}J_{f,p} = (b-a)J_{k,p}, \\ &-J_{l,c}Y_{11}^T + J_{l,d}Y_{12}^T + X_{21}J_{e,p} - X_{22}J_{f,p} = 0, \\ &J_{k,c}Y_{21}^T - J_{k,d}Y_{22}^T - X_{11}J_{e,q} + X_{12}J_{f,q} = 0, \\ &-J_{l,c}Y_{21}^T + J_{l,d}Y_{22}^T - X_{21}J_{e,q} + X_{22}J_{f,q} = (a-b)J_{l,q}. \end{aligned}$$

By Lemma 3.3.10, (3.3.12) is equivalent to the conditions that $X_{11}\mathbf{1}_e - X_{12}\mathbf{1}_f = x_1\mathbf{1}_k$, $X_{21}\mathbf{1}_e - X_{22}\mathbf{1}_f = x_2\mathbf{1}_l$, $Y_{11}\mathbf{1}_c - Y_{12}\mathbf{1}_d = y_1\mathbf{1}_p$ and $Y_{21}\mathbf{1}_c - Y_{22}\mathbf{1}_d = y_2\mathbf{1}_q$ where $x_1+y_1 = x_2+y_2 = b-a$ and $x_1-y_2 = x_2-y_1 = 0$. Similarly, applying Lemma 3.3.10 to (3.3.13) and (3.3.14), we find that (3.3.13) is equivalent to $z_1-x_1 = z_2-x_2 = d-c$ and $z_2+x_1 = z_1+x_2 = 0$ where $Z_{11}\mathbf{1}_a - Z_{12}\mathbf{1}_b = z_1\mathbf{1}_r$ and $Z_{21}\mathbf{1}_a - Z_{22}\mathbf{1}_b = z_2\mathbf{1}_s$; (3.3.14) is equivalent to $z_2-y_1 = z_1-y_2 = f-e$ and $z_1+y_1 = z_2+y_2 = 0$. Note that $x_1-y_2 = x_2-y_1 = z_2+x_1 = z_1+x_2 = z_1+y_1 = z_2+y_2 = 0$ if and only if $x_1 = y_2 = -z_2$ and $x_2 = y_1 = -z_1$. Since $E\mathbf{1} = 0$ and $\mathbf{1}^TE = 0^T$, we have $a-b = d-c = f-e$. It follows that $x_1+x_2 = y_1+y_2 = -(z_1+z_2) = e-f$.

Applying an analogous argument to the equivalent conditions for $A^TA = B^TB$ from Lemma 3.3.20, it can be found that $\gamma_1 = \beta_2 = -\alpha_2$, $\gamma_2 = \beta_1 = -\alpha_1$, $\gamma_1+\gamma_2 = \beta_1+\beta_2 = -(\alpha_1+\alpha_2) = l-k$ where $X_{11}^T\mathbf{1}_k - X_{21}^T\mathbf{1}_l = \alpha_1\mathbf{1}_e$, $X_{12}^T\mathbf{1}_k - X_{22}^T\mathbf{1}_l = \alpha_2\mathbf{1}_f$, $Y_{11}^T\mathbf{1}_p - Y_{21}^T\mathbf{1}_q = \beta_1\mathbf{1}_c$, $Y_{12}^T\mathbf{1}_p - Y_{22}^T\mathbf{1}_q = \beta_2\mathbf{1}_d$, $Z_{11}^T\mathbf{1}_r - Z_{21}^T\mathbf{1}_s = \gamma_1\mathbf{1}_a$, and $Z_{12}^T\mathbf{1}_r - Z_{22}^T\mathbf{1}_s = \gamma_2\mathbf{1}_b$.

On the other hand, subtracting $\mathbf{1}_l^TX_{21}\mathbf{1}_e - \mathbf{1}_l^TX_{22}\mathbf{1}_f = x_2\mathbf{1}_l^T\mathbf{1}_l$ from $\mathbf{1}_k^TX_{11}\mathbf{1}_e -$

$\mathbf{1}_k^T X_{12} \mathbf{1}_f = x_1 \mathbf{1}_k^T \mathbf{1}_k$, we have

$$(\mathbf{1}_k^T X_{11} - \mathbf{1}_l^T X_{21})\mathbf{1}_e - (\mathbf{1}_k^T X_{12} - \mathbf{1}_l^T X_{22})\mathbf{1}_f = x_1 \mathbf{1}_k^T \mathbf{1}_k - x_2 \mathbf{1}_l^T \mathbf{1}_l.$$

Hence, $e\alpha_1 - f\alpha_2 = kx_1 - lx_2$. Similarly, we can find $c\beta_1 - d\beta_2 = py_1 - qy_2$ from $\mathbf{1}_p^T Y_{11} \mathbf{1}_c - \mathbf{1}_p^T Y_{12} \mathbf{1}_d = y_1 \mathbf{1}_p^T \mathbf{1}_p$ and $\mathbf{1}_q^T Y_{21} \mathbf{1}_c - \mathbf{1}_q^T Y_{22} \mathbf{1}_d = y_2 \mathbf{1}_q^T \mathbf{1}_q$; and $a\gamma_1 - b\gamma_2 = rz_1 - sz_2$ from $\mathbf{1}_r^T Z_{11} \mathbf{1}_a - \mathbf{1}_r^T Z_{12} \mathbf{1}_b = z_1 \mathbf{1}_r^T \mathbf{1}_r$ and $\mathbf{1}_s^T Z_{21} \mathbf{1}_a - \mathbf{1}_s^T Z_{22} \mathbf{1}_b = z_2 \mathbf{1}_s^T \mathbf{1}_s$. Again by a similar argument, one can verify that (i) implies (a). $\square$

Remark 3.3.23. Let us continue the notation and result of Theorem 3.3.22. Suppose $q = 0$. This is equivalent to the fourth row partition of E being annihilated. Since Y_{21} and Y_{22} in the corresponding A are removed, the parameter y_2 does not appear for this case. Furthermore, examining the proof of Theorem 3.3.22, in order to attain the equivalent condition for A and $A + E$ to be Gram mates, we only need to modify the conditions as follows: $x_1 = -z_2$, $x_2 = y_1 = -z_1$ and $x_1 + x_2 = -(z_1 + z_2) = e - f$; that is, we can obtain the equivalent condition by annihilating the constraints involved with y_2 in (i) and (ii). In this manner, one can check that if the sub-indices indicating positions of row or column partitions in E are zero, then the equivalent condition is achieved by removing the constraints involved with the parameters in (i) and (ii) that do not appear, due to the resulting matrix being obtained from E by deleting row or column partitions corresponding to the sub-indices.

Example 3.3.24. Maintaining the notation and result of Theorem 3.3.22, for $n \geq 1$, set $k = a = s = f = n+1$, $l = b = r = e = n$, $p = c = 0$, and $q = d = 1$. By Remark 3.3.23, we obtain the equivalent condition for A and $A+E$ to be Gram mates, from (i) and (ii) by modifying as follows: $x_1 = y_2 = -z_2$, $x_2 = -z_1$, $x_1 + x_2 = -(z_1 + z_2) = -1$, $\gamma_1 = \beta_2 = -\alpha_2$, $\gamma_2 = -\alpha_1$, $\gamma_1 + \gamma_2 = -(\alpha_1 + \alpha_2) = -1$. Since $p = c = 0$ and $q = d = 1$, we have $Y = -y_2 = -\beta_2$. For ease of exposition, permuting the 4$^{\text{th}}$ and 5$^{\text{th}}$ row partitions and the 4$^{\text{th}}$ and 5$^{\text{th}}$ column partitions, we have

$$E = \left[\begin{array}{cc|c|cc} J_{n+1} & -J_{n+1,n} & -\mathbf{1}_{n+1} & \multicolumn{2}{c}{\multirow{2}{*}{0}} \\ -J_{n,n+1} & J_n & \mathbf{1}_n & & \\ \hline -\mathbf{1}_{n+1}^T & \mathbf{1}_n^T & 0 & \mathbf{1}_{n+1}^T & -\mathbf{1}_n^T \\ \hline \multicolumn{2}{c|}{\multirow{2}{*}{0}} & \mathbf{1}_{n+1} & -J_{n+1} & J_{n+1,n} \\ & & -\mathbf{1}_n & J_{n,n+1} & -J_n \end{array}\right].$$

Then, one can verify from the equivalent condition that A is a Gram mate to $A + E$

if and only if A is of the form as follows:

$$A = \left[\begin{array}{cc|c|cc} 0 & J_{n+1,n} & \mathbf{1}_{n+1} & \multicolumn{2}{c}{\multirow{2}{*}{M_1}} \\ J_{n,n+1} & 0 & 0 & & \\ \hline \mathbf{1}_{n+1}^T & 0 & m & 0 & \mathbf{1}_n^T \\ \hline \multicolumn{2}{c|}{\multirow{2}{*}{M_2}} & 0 & J_{n+1} & 0 \\ & & \mathbf{1}_n & 0 & J_n \end{array}\right]$$

where for $m \in \{0,1\}$, M_1 and M_2 are $(2n+1)\times(2n+1)$ matrices such that $M_i \begin{bmatrix} \mathbf{1}_{n+1} \\ -\mathbf{1}_n \end{bmatrix} = \begin{bmatrix} m\mathbf{1}_{n+1} \\ (1-m)\mathbf{1}_n \end{bmatrix}$ and $M_i^T \begin{bmatrix} \mathbf{1}_{n+1} \\ -\mathbf{1}_n \end{bmatrix} = \begin{bmatrix} m\mathbf{1}_{n+1} \\ (1-m)\mathbf{1}_n \end{bmatrix}$ for $i \in \{1,2\}$.

Remark 3.3.25. Let $E = \begin{bmatrix} \widetilde{E} & 0 \\ 0 & 0 \end{bmatrix}$ be a realizable matrix where $\widetilde{E}$ is of type (M5). Then, Gram mates via E can be characterized as in Remark 3.3.18.

Remark 3.3.26. Continuing the hypotheses and notation in Theorem 3.3.22, let us consider $e\alpha_1 - f\alpha_2 = kx_1 - lx_2$, $c\beta_1 - d\beta_2 = py_1 - qy_2$ and $a\gamma_1 - b\gamma_2 = rz_1 - sz_2$ where $x_1 = y_2 = -z_2$, $x_2 = y_1 = -z_1$, $\gamma_1 = \beta_2 = -\alpha_2$, $\gamma_2 = \beta_1 = -\alpha_1$, $x_1 + x_2 = e - f$ and $\alpha_1 + \alpha_2 = k - l$. Then,

$$\begin{aligned} e\alpha_1 - f\alpha_2 &= kx_1 - lx_2, \\ -c\alpha_1 + d\alpha_2 &= px_2 - qx_1, \\ -a\alpha_2 + b\alpha_1 &= -rx_2 + sx_1. \end{aligned}$$

Furthermore, we obtain a linear system

$$\begin{aligned} (e+f)\alpha_1 - (k+l)x_1 &= f(k-l) - l(e-f), \\ (c+d)\alpha_1 - (p+q)x_1 &= d(k-l) - p(e-f), \\ (a+b)\alpha_1 - (r+s)x_1 &= a(k-l) - r(e-f). \end{aligned} \tag{3.3.15}$$

Note that the equations $(e+f)(p+q) = (k+l)(c+d)$, $(e+f)(r+s) = (k+l)(a+b)$ and $(c+d)(r+s) = (p+q)(a+b)$, which are from the determinant of the coefficient matrix of each pair of equations in (3.3.15), are equivalent to $\frac{e+f}{k+l} = \frac{c+d}{p+q} = \frac{a+b}{r+s}$, *i.e.*, the ratios of the numbers of rows and columns of X, Y and Z are in proportion. For such case, the sizes of X, Y and Z are said to be *proportional*.

We observe that a pair of α_1 and x_1 completely determine the integers in (i) and (ii). Using $a - b = d - c = f - e$ and $k - l = q - p = s - r$ from $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$, respectively, it can be checked that $(\alpha_1, x_1) = (\frac{k-l}{2}, \frac{e-f}{2})$ is a solution to the linear system (3.3.15). Then, $\alpha_1 = \alpha_2$ and $x_1 = x_2$. Considering $(0,1)$ matrices, $k-l$ and $e-f$ are even whenever there exist Gram mates A of form (3.3.11) and $A+E$ with $(\alpha_1, x_1) = (\frac{k-l}{2}, \frac{e-f}{2})$.

Suppose that there are two matrices among X, Y and Z such that their sizes are not proportional. Then, the system (3.3.15) has a unique solution $(\alpha_1, x_1) = (\frac{k-l}{2}, \frac{e-f}{2})$. So, if $k-l$ or $e-f$ is odd, then there are no $(0,1)$ matrices X, Y and Z satisfying (i) and (ii). In other words, if E is realizable, then $k-l$ and $e-f$ both are even.

Assume that the sizes of X, Y and Z are proportional. Considering the equation $(e+f)\alpha_1 - (k+l)x_1 = f(k-l) - l(b-a)$ with a solution $(\alpha_1, x_1) = (\frac{k-l}{2}, \frac{e-f}{2})$, we obtain $(\alpha_1, x_1) = t(k+l, e+f) + (\frac{k-l}{2}, \frac{e-f}{2})$ for any t as the solutions to (3.3.15). Set $t = \frac{1}{2}$. Then, $(\alpha_1, x_1) = (k, e)$. So, $x_1 = y_2 = -z_2 = e$, $x_2 = y_1 = -z_1 = -f$, $\gamma_1 = \beta_2 = -\alpha_2 = l$ and $\gamma_2 = \beta_1 = -\alpha_1 = -k$. This particular solution is used for showing that E is realizable under the condition that $k-l$ or $e-f$ is odd.

Continuing the hypotheses and notation in Theorem 3.3.22, by Remark 3.3.21 the number of rows (resp. columns) in each of X, Y and Z has the same parity. Let X be an $m \times n$ $(0,1)$ matrix. We shall establish the equivalent condition for E to be realizable (Theorem 3.3.35) by considering two cases: m and n are even (Lemma 3.3.28), and m or n is odd (Lemma 3.3.33). Note that we only need to show the existence of X, Y and Z satisfying (i) and (ii) of Theorem 3.3.22.

Lemma 3.3.27. *Let $m_1, m_2, n_1, n_2 > 0$. Let $X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$ be a $(0,1)$ matrix where X_{11} and X_{22} are $m_1 \times n_1$ and $m_2 \times n_2$ matrices, respectively. Suppose that $X \begin{bmatrix} \mathbf{1}_{n_1} \\ -\mathbf{1}_{n_2} \end{bmatrix} = \begin{bmatrix} a_1 \mathbf{1}_{m_1} \\ a_2 \mathbf{1}_{m_2} \end{bmatrix}$ and $X^T \begin{bmatrix} \mathbf{1}_{m_1} \\ -\mathbf{1}_{m_2} \end{bmatrix} = \begin{bmatrix} b_1 \mathbf{1}_{n_1} \\ b_2 \mathbf{1}_{n_2} \end{bmatrix}$. For $X_1 = \begin{bmatrix} X_{12} & X_{11} \\ X_{22} & X_{21} \end{bmatrix}$, we have $X_1 \begin{bmatrix} \mathbf{1}_{n_2} \\ -\mathbf{1}_{n_1} \end{bmatrix} = \begin{bmatrix} -a_1 \mathbf{1}_{m_1} \\ -a_2 \mathbf{1}_{m_2} \end{bmatrix}$ and $X_1^T \begin{bmatrix} \mathbf{1}_{m_1} \\ -\mathbf{1}_{m_2} \end{bmatrix} = \begin{bmatrix} b_2 \mathbf{1}_{n_2} \\ b_1 \mathbf{1}_{n_1} \end{bmatrix}$. Furthermore, given $X_2 = \begin{bmatrix} X_{22} & X_{21} \\ X_{12} & X_{11} \end{bmatrix}$, we have $X_2 \begin{bmatrix} \mathbf{1}_{n_2} \\ -\mathbf{1}_{n_1} \end{bmatrix} = \begin{bmatrix} -a_2 \mathbf{1}_{m_2} \\ -a_1 \mathbf{1}_{m_1} \end{bmatrix}$ and $X_2^T \begin{bmatrix} \mathbf{1}_{m_2} \\ -\mathbf{1}_{m_1} \end{bmatrix} = \begin{bmatrix} -b_2 \mathbf{1}_{n_2} \\ -b_1 \mathbf{1}_{n_1} \end{bmatrix}$.*

Lemma 3.3.28. *Let $m_1, m_2, n_1, n_2 > 0$. Suppose that $m_1 + m_2$ and $n_1 + n_2$ are even. Then, there exists an $(m_1+m_2) \times (n_1+n_2)$ $(0,1)$ matrix $X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$, where X_{11} and X_{22} are $m_1 \times n_1$ and $m_2 \times n_2$ matrices, respectively, such that $X \begin{bmatrix} \mathbf{1}_{n_1} \\ -\mathbf{1}_{n_2} \end{bmatrix} = \frac{n_1 - n_2}{2} \begin{bmatrix} \mathbf{1}_{m_1} \\ \mathbf{1}_{m_2} \end{bmatrix}$ and $X^T \begin{bmatrix} \mathbf{1}_{m_1} \\ -\mathbf{1}_{m_2} \end{bmatrix} = \frac{m_1 - m_2}{2} \begin{bmatrix} \mathbf{1}_{n_1} \\ \mathbf{1}_{n_2} \end{bmatrix}$.*

Proof. If $m_1 = m_2$ and $n_1 = n_2$, then X can be chosen as the zero matrix. By Lemma 3.3.27, we only need to consider two cases: (i) $m_1 > m_2$ and $n_1 = n_2$, (ii) $m_1 > m_2$ and $n_1 > n_2$. If $m_1 > m_2$ and $n_1 = n_2$, then $X = \begin{bmatrix} J_{\frac{m_1-m_2}{2}, n_1+n_2} \\ 0 \end{bmatrix}$ is one of our desired matrices. Suppose $m_1 > m_2$ and $n_1 > n_2$. Let $\alpha = \frac{m_1-m_2}{2}$ and $\beta = \frac{n_1-n_2}{2}$. Then, it is straightforward to check that the following matrix can be our desired matrix:

$$X = \left[\begin{array}{ccc|c} J_{\alpha,\beta} & 0 & 0 & 0 \\ 0 & 0 & J_{m_2,\beta} & 0 \\ 0 & J_{\alpha,n_2} & J_{\alpha,\beta} & J_{\alpha,n_2} \\ \hline 0 & 0 & J_{m_2,\beta} & 0 \end{array}\right].$$

□

Let $n > 0$, and let $\alpha = (\alpha_1, \ldots, \alpha_n)$ and $\beta = (\beta_1, \ldots, \beta_n)$ be real vectors. Suppose that $\alpha' = (\alpha'_1, \ldots, \alpha'_n)$ and $\beta' = (\beta'_1, \ldots, \beta'_n)$ are obtained from α and β, respectively, by rearrangements such that $\alpha'_1 \geq \cdots \geq \alpha'_n$ and $\beta'_1 \geq \cdots \geq \beta'_n$. The vector α *majorizes* β, denoted by $\alpha \succ \beta$, if $\sum_{i=1}^k \alpha'_i \geq \sum_{i=1}^k \beta'_i$ for all $1 \leq k \leq n$, and $\sum_{i=1}^n \alpha'_i = \sum_{i=1}^n \beta'_i$. For nonnegative integers $\alpha_1, \ldots, \alpha_n$, define $\alpha^*_i = |\{\alpha_j | \alpha_j \geq i, j = 1, \ldots, n\}|$ for $i = 1, \ldots, n$. The vector $\alpha^* := (\alpha^*_1, \ldots, \alpha^*_n)$ is said to be *conjugate* to α. For instance, if $\alpha = (3, 3, 3, 3, 3)$, then $\alpha^* = (5, 5, 5, 0, 0)$.

Let $\mathcal{U}(R, S)$ denote the set of all $(0, 1)$ matrices with row sum vector R and column sum vector S. Let $R = (r_1, \ldots, r_m)$ and $S = (s_1, \ldots, s_n)$ be nonnegative integral vectors. In the context of majorization, we may adjoin zeros to S (resp. R) if $m > n$ (resp. $m < n$).

Theorem 3.3.29. *[58](the Gale–Ryser theorem) Let $R = (r_1, \ldots, r_m)$ and $S = (s_1, \ldots, s_n)$ be nonnegative integral vectors. Then, there exists a $(0, 1)$ matrix in $\mathcal{U}(R, S)$ if and only if $S \prec R^*$ and $r_i \leq n$ for $i = 1, \ldots, m$.*

We refer the reader to [58] for the construction of a matrix in $\mathcal{U}(R, S)$. From Theorem 3.3.29, we immediately have two lemmas as follows.

Lemma 3.3.30. *Let $R = (r, \ldots, r)$ and $S = (s, \ldots, s)$ be nonnegative integral vectors of size $m(\geq s)$ and $n(\geq r)$, respectively. Then, $rm = sn$ if and only if there exists a matrix in $\mathcal{U}(R, S)$.*

Lemma 3.3.31. *Let $S = (s_1, \ldots, s_n)$ be a nonnegative integral vector where $\sum_{i=1}^n s_i = \ell$. Let m be a positive integer such that $s_i \leq m$ for all $i = 1, \ldots n$ and $\ell = qm + r$*

for some $q \geq 0$ and $0 \leq r \leq m-1$. Suppose

$$R = (\underbrace{q+1, \dots, q+1}_{r \text{ times}}, \underbrace{q, \dots, q}_{m-r \text{ times}}).$$

Then, there exists a matrix $A \in \mathcal{U}(R, S)$.

Proof. Evidently, $l \leq mn$, so $q+1 \leq n$ whenever $r > 0$. Since we have $R^* = (m, \dots, m, r, 0, \dots, 0)$ where m appears q times, we can see that $S \prec R^*$. By Theorem 3.3.29, our desired result is obtained. $\square$

Given a nonnegative integral vector $R = (r_1, \dots, r_m)$ where $\sum_{i=1}^m r_i = \ell$, we shall establish an analogous result for Lemma 3.3.31 by constructing a concrete matrix. Let n be a positive integer such that $r_i \leq n$ for all $i = 1, \dots, m$. Choose $q \geq 0$ so that $\ell = qn + r$ for some $0 \leq r \leq n-1$. Let $r_0 = 0$, and let A_0 be the $m \times n(q+1)$ matrix such that if $r_i > 0$, then the i^{th} row of A_0 consists of 1's from the $(1 + \sum_{j=1}^i r_{j-1})^{\text{th}}$ position to the $(\sum_{j=1}^i r_j)^{\text{th}}$ position and 0's elsewhere; if $r_i = 0$, then the i^{th} row of A_0 is a row of zeros. Then, A_0 can be partitioned into $(q+1)$ submatrices $A_1, \dots, A_{q+1}$ so that for $1 \leq i \leq q+1$, A_i is an $m \times n$ submatrix of A_0 whose columns are indexed by $(i-1)n+1, \dots, (i-1)n+n$.

Let $A = A_1 + \cdots + A_{q+1}$. It is clear that the row sum vector of A is R. Since ones in each row of A_0 appear consecutively and each row contains at most n ones, A must be a $(0,1)$ matrix. Furthermore, every column of A_i for $i = 1, \dots, q$ contains precisely a single one, and each of the first r columns of A_{q+1} contains a single one. Therefore, $A \in \mathcal{U}(R, S)$ where

$$S = (\underbrace{q+1, \dots, q+1}_{r \text{ times}}, \underbrace{q, \dots, q}_{n-r \text{ times}}). \tag{3.3.16}$$

Example 3.3.32. Let $R = (3, 3, 0, 2, 3)$. Consider the described matrix A_0 above:

$$A_0 = \left[\begin{array}{cccc|cccc|cccc} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{array}\right].$$

As explained above, we obtain

$$A = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}.$$

Continuing with the hypotheses and notation in Theorem 3.3.22, assume that E is a $(0, 1, -1)$ matrix of the form (M5) and A is a $(0, 1)$ matrix of the form (3.3.11). Recall from Remark 3.3.26 that given that the number of rows or columns of X in A is odd, if E is realizable, then necessarily the sizes X, Y and Z in A are proportional.

We now claim that the converse holds. In order to establish the claim, we shall construct $(0, 1)$ matrices X, Y and Z satisfying (i) and (ii) of Theorem 3.3.22, under the condition that the sizes of X, Y and Z are in proportion in absence of the parities of their size. Since the sizes of X and Y are proportional, if the number of rows of Y is bigger than that of rows of X, then the number of columns of Y is bigger than that of columns of X, and vice versa. Hence, we may assume that X has the smallest size. Then, it is enough to show that the existence of X implies that of Y. Considering the last paragraph of Remark 3.3.26, we shall find X and Y with the condition that $x_1 = y_2 = e$, $x_2 = y_1 = -f$, $\beta_2 = -\alpha_2 = l$ and $\beta_1 = -\alpha_1 = -k$. Then, one of the desired matrices for X can be obtained as $\begin{bmatrix} J_{k,e} & 0 \\ 0 & J_{l,f} \end{bmatrix}$.

If the size of Y is the same as that of X, then we choose $Y = X$. Suppose $p + q > k + l$ and $c + d > e + f$. Since the sizes of X and Y are proportional, $\frac{c+d}{p+q} = \frac{e+f}{k+l}$. From $E\mathbf{1} = 0$ and $\mathbf{1}^T E = 0^T$, we have $q - p = k - l$ and $c - d = e - f$. We need to construct a $(0, 1)$ matrix Y such that

$$Y \begin{bmatrix} \mathbf{1}_c \\ -\mathbf{1}_d \end{bmatrix} = \begin{bmatrix} -f\mathbf{1}_p \\ e\mathbf{1}_q \end{bmatrix} \text{ and } Y^T \begin{bmatrix} \mathbf{1}_p \\ -\mathbf{1}_q \end{bmatrix} = \begin{bmatrix} -k\mathbf{1}_c \\ l\mathbf{1}_d \end{bmatrix}.$$

By Lemma 3.3.27, we may prove that there exists a $(0, 1)$ matrix Y_1 such that

$$Y_1 \begin{bmatrix} \mathbf{1}_c \\ -\mathbf{1}_d \end{bmatrix} = \begin{bmatrix} e\mathbf{1}_q \\ -f\mathbf{1}_p \end{bmatrix} \text{ and } Y_1^T \begin{bmatrix} \mathbf{1}_q \\ -\mathbf{1}_p \end{bmatrix} = \begin{bmatrix} k\mathbf{1}_c \\ -l\mathbf{1}_d \end{bmatrix}.$$

Lemma 3.3.33. *Let $a_1, a_2, b_1, b_2 > 0$. Suppose that m_1, m_2, n_1 and n_2 are positive integers such that $m_1 + m_2 > a_1 + a_2$, $n_1 + n_2 > b_1 + b_2$, $m_1 - m_2 = a_1 - a_2$,*

$n_1 - n_2 = b_1 - b_2$ *and* $\frac{n_1+n_2}{m_1+m_2} = \frac{b_1+b_2}{a_1+a_2}$. *Then, there exists a* $(0,1)$ *matrix* Y *of size* $(m_1+m_2) \times (n_1+n_2)$ *such that*

$$Y \begin{bmatrix} \mathbf{1}_{n_1} \\ -\mathbf{1}_{n_2} \end{bmatrix} = \begin{bmatrix} b_1\mathbf{1}_{m_1} \\ -b_2\mathbf{1}_{m_2} \end{bmatrix}, Y^T \begin{bmatrix} \mathbf{1}_{m_1} \\ -\mathbf{1}_{m_2} \end{bmatrix} = \begin{bmatrix} a_1\mathbf{1}_{n_1} \\ -a_2\mathbf{1}_{n_2} \end{bmatrix}.$$

Proof. We shall construct a $(0,1)$ matrix $Y = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix}$ with our desired property where Y_{11} and Y_{22} are $m_1 \times n_1$ and $m_2 \times n_2$ matrices, respectively. Here, for $i, j \in \{1, 2\}$, we denote the row sum and column sum vectors of Y_{ij} by R_{ij} and S_{ij}, respectively.

Using $m_1 - m_2 = a_1 - a_2$, $n_1 - n_2 = b_1 - b_2$, we find from $m_1 + m_2 > a_1 + a_2$ and $n_1 + n_2 > b_1 + b_2$ that $m_1 > a_1$, $m_2 > a_2$, $n_1 > b_1$ and $n_2 > b_2$; and we see from $\frac{n_1+n_2}{m_1+m_2} = \frac{b_1+b_2}{a_1+a_2}$ that $m_1b_1 + m_2b_2 = n_1a_1 + n_2a_2$. Suppose that $m_1b_1 = n_1a_1$. Then, $m_2b_2 = n_2a_2$. By Lemma 3.3.30, there exist $Y_{11} \in \mathcal{U}(R_{11}, S_{11})$ and $Y_{22} \in \mathcal{U}(R_{22}, S_{22})$ such that $R_{11} = b_1\mathbf{1}_{m_1}$, $S_{11} = a_1\mathbf{1}_{n_1}$, $R_{22} = b_2\mathbf{1}_{m_2}$ and $S_{22} = a_2\mathbf{1}_{n_2}$. Choosing $Y_{12} = 0$ and $Y_{21} = 0$, our desired matrix is obtained.

Considering the transpose of Y, we may assume that $m_1b_1 > n_1a_1$. Set $Y_{12} = 0$. Let $\ell = m_1b_1 - n_1a_1$. We first construct Y_{11}. Choose $q_1 \geq 0$ such that $\ell = n_1q_1 + r_1$ for some $0 \leq r_1 < n_1$. Let $\widetilde{S} = (q_1+1, \ldots, q_1+1, q_1, \ldots, q_1)$ where $q_1 + 1$ and q_1 appear r_1 times and $n_1 - r_1$ times in $\widetilde{S}$, respectively. Let $S_{11} = a_1\mathbf{1}_{n_1} + \widetilde{S}$ and $R_{11} = b_1\mathbf{1}_{m_1}$. Since $\ell = m_1b_1 - n_1a_1$, the sum of the entries of S_{11} is the same as the sum for R_{11}. We shall show that each entry in S_{11} is not greater than m_1. From $n_1 > b_1$, we have

$$\begin{aligned} m_1 - (a_1 + q_1) &= m_1 - \frac{n_1a_1 + \ell - r_1}{n_1} \\ &= m_1 - \frac{m_1b_1 - r_1}{n_1} = \frac{m_1(n_1 - b_1) + r_1}{n_1} > 0. \end{aligned}$$

So, $m_1 - (q_1 + 1 + a_1) \geq 0$. Furthermore, $R_{11}^* \succ S_{11}$. By Theorem 3.3.29, there exists a matrix $Y_{11} \in \mathcal{U}(R_{11}, S_{11})$.

Now, we shall construct Y_{21} with a column sum vector as $\widetilde{S}$. Then, we need to show $m_2 \geq q_1 + 1$. From $m_1 - m_2 = a_1 - a_2$ and $n_1 > b_1$, we have

$$\begin{aligned} m_2 - q_1 &= \frac{m_2n_1 - \ell + r_1}{n_1} \\ &= \frac{m_2n_1 - m_1b_1 + n_1a_1 + r_1}{n_1} = \frac{m_1(n_1 - b_1) + n_1a_2 + r_1}{n_1} > 0. \end{aligned}$$

So, $m_2 \geq q_1 + 1$. Choose $q_2 \geq 0$ such that $\ell = m_2 q_2 + r_2$ for some $0 \leq r_2 < m_2$. Applying Lemma 3.3.31 with $\widetilde{S}$, there exists $Y_{21} \in \mathcal{U}(R_{21}, S_{21})$ such that $S_{21} = \widetilde{S}$ and $R_{21} = (q_2 + 1, \ldots, q_2 + 1, q_2, \ldots, q_2)$ where $q_2 + 1$ and q_2 appear r_2 times and $m_2 - r_2$ times in R_{21}, respectively.

Let $R_{22} = b_2 \mathbf{1}_{m_2} + R_{21}$ and $S_{22} = a_2 \mathbf{1}_{n_2}$. Then, the sum of the entries of R_{22} is equal to the sum for S_{22}. Using $\ell = m_1 b_1 - n_1 a_1$, $m_1 b_1 + m_2 b_2 = n_1 a_1 + n_2 a_2$ and $m_2 > a_2$, we obtain

$$n_2 - (b_2 + q_2) = n_2 - \frac{m_2 b_2 + \ell - r_2}{m_2} = \frac{n_2(m_2 - a_2) + r_2}{m_2} > 0.$$

Then, $n_2 - (q_2 + 1 + b_2) \geq 0$. Moreover, $S_{22}^* \succ R_{22}$. By Theorem 3.3.29, there exists $Y_{22} \in \mathcal{U}(R_{22}, S_{22})$. Therefore, the conclusion follows. $\square$

Example 3.3.34. Let $a_1 = 4$, $a_2 = 6$, $b_1 = 5$, $b_2 = 3$, $m_1 = 9$, $m_2 = 11$, $n_1 = 9$ and $n_2 = 7$. One can check that the indices satisfy the hypothesis of Lemma 3.3.33. We use the results and notation in the proof of Lemma 3.3.33. Then, $m_1 b_1 - n_1 a_1 = 9$ and so $\widetilde{S} = \mathbf{1}_9$. It can be found that we have $Y_{11} \in \mathcal{U}(R_{11}, S_{11})$ where $R_{11} = 5\mathbf{1}_9$ and $S_{11} = 4\mathbf{1}_9 + \widetilde{S}$; $Y_{21} \in \mathcal{U}(R_{21}, S_{21})$ where $R_{21}^T = (\mathbf{1}_9^T, 0, 0)$ and $S_{21} = \widetilde{S}$; and $Y_{22} \in \mathcal{U}(R_{22}, S_{22})$ where $R_{22} = R_{21} + 3\mathbf{1}_{11}$ and $S_{22} = 6\mathbf{1}_7$. As in the construction described in Example 3.3.32, we can obtain $Y_{21} = \begin{bmatrix} I_9 \\ 0 \end{bmatrix}$. (One can obtain Y_{11} and Y_{22} by using the process illustrated in [58].)

Applying Lemmas 3.3.28 and 3.3.33, the following result is established.

Theorem 3.3.35. *Let E be a $(0, 1, -1)$ matrix of form (M5). Then, E is realizable if and only if one of the following conditions is satisfied:*

(i) $a + b$, $c + d$, $e + f$, $k + l$, $p + q$ and $r + s$ are all even, and

(ii) three numbers $a + b$, $c + d$ and $e + f$ are all odd or three numbers $k + l$, $p + q$ and $r + s$ are all odd; and $\frac{e+f}{k+l} = \frac{c+d}{p+q} = \frac{a+b}{r+s}$.

Assume that A and $A + E$ are Gram mates via a $(0, 1, -1)$ matrix E of the form

(M5). We use the results and notation in Theorem 3.3.22. Consider

$$2A+E = \begin{bmatrix} J_{k,a} & J_{k,b} & J_{k,c} & J_{k,d} & 2X_{11} & 2X_{12} \\ J_{l,a} & J_{l,b} & J_{l,c} & J_{l,d} & 2X_{21} & 2X_{22} \\ J_{p,a} & J_{p,b} & 2Y_{11} & 2Y_{12} & J_{p,e} & J_{p,f} \\ J_{q,a} & J_{q,b} & 2Y_{21} & 2Y_{22} & J_{q,e} & J_{q,f} \\ 2Z_{11} & 2Z_{12} & J_{r,c} & J_{r,d} & J_{r,e} & J_{r,f} \\ 2Z_{21} & 2Z_{22} & J_{s,c} & J_{s,d} & J_{s,e} & J_{s,f} \end{bmatrix}.$$

Let

$$\begin{aligned} \mathbf{x}_1^T &= \begin{bmatrix} \mathbf{1}_a^T & -\mathbf{1}_b^T & \mathbf{1}_c^T & -\mathbf{1}_d^T & \mathbf{0}_e^T & \mathbf{0}_f^T \end{bmatrix}, \\ \mathbf{x}_2^T &= \begin{bmatrix} \mathbf{1}_a^T & -\mathbf{1}_b^T & \mathbf{0}_c^T & \mathbf{0}_d^T & \mathbf{1}_e^T & -\mathbf{1}_f^T \end{bmatrix}. \end{aligned} \tag{3.3.17}$$

From $E\mathbf{1}=0$, we have $b-a=c-d=e-f$. So,

$$(2A+E)\mathbf{x}_1 = \begin{bmatrix} 0 \\ 0 \\ (f-e+2y_1)\mathbf{1}_p \\ (f-e+2y_2)\mathbf{1}_q \\ (2z_1+e-f)\mathbf{1}_r \\ (2z_2+e-f)\mathbf{1}_s \end{bmatrix}, \ (2A+E)\mathbf{x}_2 = \begin{bmatrix} (f-e+2x_1)\mathbf{1}_k \\ (f-e+2x_2)\mathbf{1}_l \\ 0 \\ 0 \\ (2z_1+e-f)\mathbf{1}_r \\ (2z_2+e-f)\mathbf{1}_s \end{bmatrix}.$$

Since A and $A+E$ are Gram mates, the condition (i) in Theorem 3.3.22 holds, so we have $x_1=y_2=-z_2$, $x_2=y_1=-z_1$ and $x_1+x_2=y_1+y_2=-(z_1+z_2)=e-f$. Note that $\mathbf{x}_1$ and $\mathbf{x}_2$ form a basis of Row(E). Hence, $(2A+E)E^T=0$ if and only if $x_1=\frac{e-f}{2}$. Therefore, by Theorem 3.2.9, A and $A+E$ are convertible if and only if $x_1=\frac{e-f}{2}$.

Suppose that $x_1=\frac{e-f}{2}$. Since (α_1,x_1) is a solution to the system (3.3.15) in Remark 3.3.26, we have $\alpha_1=\frac{k-l}{2}$. Hence, from $E\mathbf{1}=0$, $\mathbf{1}^TE=0^T$ and the conditions (i) and (ii) of Theorem 3.3.22, for $i=1,2$, $x_i=y_i=-z_i=\frac{e-f}{2}=\frac{c-d}{2}=\frac{b-a}{2}$ and $\gamma_i=\beta_i=-\alpha_i=\frac{l-k}{2}=\frac{p-q}{2}=\frac{r-s}{2}$. We now find the Gram singular values of A and

$A+E$ and the corresponding right singular vectors. It can be computed that

$$A^TA\begin{bmatrix}\mathbf{1}_a\\-\mathbf{1}_b\\\mathbf{1}_c\\-\mathbf{1}_d\\0\\0\end{bmatrix}=\begin{bmatrix}(l(a+c)+q(a+y_2))\mathbf{1}_a+(z_1-d)Z_{11}^T\mathbf{1}_r+(z_2+c)Z_{21}^T\mathbf{1}_s\\(k(-b-d)+p(-b+y_1))\mathbf{1}_b+(z_1-d)Z_{12}^T\mathbf{1}_r+(z_2+c)Z_{22}^T\mathbf{1}_s\\(l(a+c)+s(z_2+c))\mathbf{1}_c+(-b+y_1)Y_{11}^T\mathbf{1}_p+(a+y_2)Y_{21}^T\mathbf{1}_q\\(k(-b-d)+r(z_1-d))\mathbf{1}_d+(-b+y_1)Y_{12}^T\mathbf{1}_p+(a+y_2)Y_{22}^T\mathbf{1}_q\\(q(a+y_2)+r(z_1-d))\mathbf{1}_e+(-b-d)X_{11}^T\mathbf{1}_k+(a+c)X_{21}^T\mathbf{1}_l\\(p(-b+y_1)+s(z_2+c))\mathbf{1}_f+(-b-d)X_{21}^T\mathbf{1}_k+(a+c)X_{22}^T\mathbf{1}_l\end{bmatrix}.$$

Substituting $\frac{d-c}{2}$ into z_1 and z_2 in the first entry of the right side, we have $-\frac{1}{2}(c+d)Z_{11}^T\mathbf{1}_r+\frac{1}{2}(c+d)Z_{21}^T\mathbf{1}_s=-\gamma_1(c+d)\mathbf{1}_a$. So, from $y_2=\frac{b-a}{2}$, we find $(l(a+c)+\frac{1}{2}q(a+b)+\gamma_1(c+d))\mathbf{1}_a$ in the first entry. Applying a similar argument for the remaining entries of the right side, it follows that

$$A^TA\begin{bmatrix}\mathbf{1}_a\\-\mathbf{1}_b\\\mathbf{1}_c\\-\mathbf{1}_d\\0\\0\end{bmatrix}=\begin{bmatrix}(l(a+c)+\frac{1}{2}q(a+b)-\frac{1}{2}\gamma_1(c+d))\mathbf{1}_a\\(-k(a+c)-\frac{1}{2}p(a+b)-\frac{1}{2}\gamma_2(c+d))\mathbf{1}_b\\(l(a+c)+\frac{1}{2}s(c+d)-\frac{1}{2}\beta_1(a+b))\mathbf{1}_c\\(-k(a+c)-\frac{1}{2}r(c+d)-\frac{1}{2}\beta_2(a+b))\mathbf{1}_d\\(\frac{1}{2}q(a+b)-\frac{1}{2}r(c+d)-\alpha_1(b+d))\mathbf{1}_e\\(-\frac{1}{2}p(a+b)+\frac{1}{2}s(c+d)-\alpha_2(b+d))\mathbf{1}_f\end{bmatrix}.$$

Similarly, one can verify that

$$A^TA\begin{bmatrix}\mathbf{1}_a\\-\mathbf{1}_b\\0\\0\\\mathbf{1}_e\\-\mathbf{1}_f\end{bmatrix}=\begin{bmatrix}(\frac{1}{2}l(a+b)+q(a+e)+\frac{1}{2}\gamma_1(e+f))\mathbf{1}_a\\(-\frac{1}{2}k(a+b)-p(a+e)+\frac{1}{2}\gamma_2(e+f)\mathbf{1}_b\\(\frac{1}{2}l(a+b)-\frac{1}{2}s(e+f)-\beta_1(b+f))\mathbf{1}_c\\(-\frac{1}{2}k(a+b)+\frac{1}{2}r(e+f)-\beta_2(b+f))\mathbf{1}_d\\(q(a+e)+\frac{1}{2}r(e+f)-\frac{1}{2}\alpha_1(a+b))\mathbf{1}_e\\(-p(a+e)-\frac{1}{2}s(e+f)-\frac{1}{2}\alpha_2(a+b))\mathbf{1}_f\end{bmatrix}.$$

Consider an equation $A^TA(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2)=\lambda(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2)$ where ζ_1, ζ_2 and λ are real numbers. Using $\gamma_i=\beta_i=\alpha_i=\frac{l-k}{2}=\frac{p-q}{2}=\frac{r-s}{2}$, it can be checked that the equations from the first, third and fifth row blocks are identical with those from the second, fourth and sixth row blocks, respectively. Moreover, we can find that the equation from the first row block is the same as the addition of two equations from the third and fifth row blocks. Hence, $A^TA(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2)=\lambda(\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2)$ is equivalent to a linear system of two equations from the third and fifth row blocks:

$$\zeta_1\left(l(a+c)+\frac{1}{2}s(c+d)-\frac{1}{2}\beta_1(a+b)\right)+\zeta_2\left(\frac{1}{2}l(a+b)-\frac{1}{2}s(e+f)-\beta_1(b+f)\right)=\lambda\zeta_1,$$
$$\zeta_1\left(\frac{1}{2}q(a+b)-\frac{1}{2}r(c+d)-\alpha_1(b+d)\right)+\zeta_2\left(q(a+e)+\frac{1}{2}r(e+f)-\frac{1}{2}\alpha_1(a+b)\right)=\lambda\zeta_2.$$

Therefore, we have the following result.

Theorem 3.3.36. *Let E be a realizable matrix of form (M5), and let*

$$A=\begin{bmatrix} 0 & J_{k,b} & 0 & J_{k,d} & X_{11} & X_{12}\\ J_{l,a} & 0 & J_{l,c} & 0 & X_{21} & X_{22}\\ 0 & J_{p,b} & Y_{11} & Y_{12} & 0 & J_{p,f}\\ J_{q,a} & 0 & Y_{21} & Y_{22} & J_{q,e} & 0\\ Z_{11} & Z_{12} & 0 & J_{r,d} & J_{r,e} & 0\\ Z_{21} & Z_{22} & J_{s,c} & 0 & 0 & J_{s,f}\end{bmatrix}$$

be a $(0,1)$ matrix conformally partitioned with E. Suppose that A and $A+E$ are Gram mates. Then, A and $A+E$ are convertible if and only if one of the following hold: (i) $(X_{i1}-X_{i2})\mathbf{1}=\frac{e-f}{2}\mathbf{1}$ for $i=1,2$; (ii) $(X_{i1}^T-X_{i2}^T)\mathbf{1}=\frac{k-l}{2}\mathbf{1}$ for $i=1,2$; (iii) $(Y_{i1}-Y_{i2})\mathbf{1}=\frac{c-d}{2}\mathbf{1}$ for $i=1,2$; (iv) $(Y_{i1}^T-Y_{i2}^T)\mathbf{1}=\frac{p-q}{2}\mathbf{1}$ for $i=1,2$; (v) $(Z_{i1}-Z_{i2})\mathbf{1}=\frac{a-b}{2}\mathbf{1}$ for $i=1,2$; and (vi) $(Z_{i1}^T-Z_{i2}^T)\mathbf{1}=\frac{r-s}{2}\mathbf{1}$ for $i=1,2$. Furthermore, if A is convertible to $A+E$, then the Gram singular values of A and $A+E$ are the square roots of the eigenvalues λ of M where

$$M=\begin{bmatrix} l(a+c)+\frac{1}{2}s(c+d)+\frac{1}{4}(k-l)(a+b) & \frac{1}{2}l(a+b)-\frac{1}{2}s(e+f)+\frac{1}{2}(k-l)(a+e)\\ \frac{1}{2}q(a+b)-\frac{1}{2}r(c+d)+\frac{1}{2}(p-q)(a+c) & q(a+e)+\frac{1}{2}r(e+f)+\frac{1}{4}(p-q)(a+b)\end{bmatrix}.$$

Further, a right singular vector associated to $\sqrt{\lambda}$ is a normalized vector of $\zeta_1\mathbf{x}_1+\zeta_2\mathbf{x}_2$, where $\mathbf{x}_1$ and $\mathbf{x}_2$ are the vectors in (3.3.17) and (ζ_1,ζ_2) is an eigenvector of M associated to λ.

3.4 Non-isomorphic Gram mates via realizable matrices of rank 1

Here we revisit the speculative statement in [30]: if Gram mates A and B with distinct positive singular values are convertible, then A and B are isomorphic with very high probability. We characterize non-isomorphic square Gram mates with all distinct singular values—in particular the multiplicity of 0 as a singular value is 1, if Gram mates are singular—via a realizable matrix of rank 1. As seen in Subsection 3.3.1, those Gram mates are convertible.

Let A and B be Gram mates such that $\mathrm{rank}(A - B) = 1$. Let α (resp. β) be the set of row indices (resp. column indices) such that there is a nonzero entry in the corresponding rows (resp. columns) of $A - B$. Then, $A[\alpha^c, \beta^c] = B[\alpha^c, \beta^c]$. The submatrix $A[\alpha^c, \beta^c]$ is said to be the *remaining matrix* of Gram mates A and B. Rearranging rows in order of α and α^c and columns in order of β and β^c, we can obtain isomorphic matrices to A and B, respectively, as we preserve the structure of the remaining matrix. Without loss of generality, by Theorem 3.3.7,

$$A = \begin{bmatrix} 0 & J_{k_1,k_2} & X_1 \\ J_{k_1,k_2} & 0 & X_2 \\ X_3 & X_4 & Y \end{bmatrix}, \; B = \begin{bmatrix} J_{k_1,k_2} & 0 & X_1 \\ 0 & J_{k_1,k_2} & X_2 \\ X_3 & X_4 & Y \end{bmatrix} \tag{3.4.1}$$

$\mathbf{1}^T X_1 = \mathbf{1}^T X_2$ and $X_3\mathbf{1} = X_4\mathbf{1}$ where $k_1, k_2 > 0$. Note that Y is the remaining matrix of A and B.

We now consider sets of particular permutation matrices in order to establish families of non-isomorphic Gram mates (Proposition 3.4.5 and Theorem 3.4.11). Let Z_i be an $m \times n$ $(0,1)$ matrix for $i = 1, \ldots, 4$. Define $\mathcal{R}_{Z_1,Z_2}$ to be the set of all 3-tuples (P_1, P_2, Q), where P_1, P_2 and Q are permutation matrices such that $Z_2 = P_1 Z_1 Q$ and $Z_1 = P_2 Z_2 Q$. We also define $\mathcal{L}_{Z_3,Z_4}$ as the set of all 3-tuples (P, Q_3, Q_4), where P, Q_3 and Q_4 are permutation matrices such that $Z_3 = P Z_3 Q_3$ and $Z_4 = P Z_4 Q_4$.

If there exist $(P_1, P_2, Q) \in \mathcal{R}_{X_1,X_2}$ and $(P, Q_3, Q_4) \in \mathcal{L}_{X_3,X_4}$ such that $Y = PYQ$, then

$$\begin{bmatrix} 0 & P_2 & 0 \\ P_1 & 0 & 0 \\ 0 & 0 & P \end{bmatrix} A \begin{bmatrix} Q_3 & 0 & 0 \\ 0 & Q_4 & 0 \\ 0 & 0 & Q \end{bmatrix} = \begin{bmatrix} J_{k_1,k_2} & 0 & P_2 X_2 Q \\ 0 & J_{k_1,k_2} & P_1 X_1 Q \\ P X_3 Q_3 & P X_4 Q_4 & PYQ \end{bmatrix} = B.$$

So, A and B are isomorphic. Similarly, if there exist $(P_1, P_2, Q) \in \mathcal{R}_{X_3^T,X_4^T}$ and $(P, Q_3, Q_4) \in \mathcal{L}_{X_1^T,X_2^T}$ such that $Y^T = PY^TQ$, then

$$\begin{bmatrix} Q_3^T & 0 & 0 \\ 0 & Q_4^T & 0 \\ 0 & 0 & Q^T \end{bmatrix} A \begin{bmatrix} 0 & P_1^T & 0 \\ P_2^T & 0 & 0 \\ 0 & 0 & P^T \end{bmatrix} = B.$$

Hence, A is isomorphic to B. The remaining matrix Y of A and B is said to be *fixable* if there exist permutation matrices P and Q such that $Y = PYQ$ and one of two cases holds:

(i) $(P_1, P_2, Q) \in \mathcal{R}_{X_1,X_2}$ and $(P, Q_3, Q_4) \in \mathcal{L}_{X_3,X_4}$ for some P_1, P_2, Q_3, Q_4; and

(ii) $(Q_3, Q_4, P^T) \in \mathcal{R}_{X_3^T,X_4^T}$ and $(Q^T, P_1, P_2) \in \mathcal{L}_{X_1^T,X_2^T}$ for some P_1, P_2, Q_3, Q_4.

The following proposition immediately follows.

Proposition 3.4.1. *Suppose that A and B are Gram mates and* $\operatorname{rank}(A - B) = 1$. *If the remaining matrix of A and B is fixable, then A is isomorphic to B.*

Remark 3.4.2. Let Z_1 and Z_2 be $(0, 1)$ matrices of the same size. We have $(I, I, I) \in \mathcal{L}_{Z_1,Z_2}$. If Z_1 and Z_2 are not isomorphic, then $\mathcal{R}_{Z_1,Z_2}$ and $\mathcal{R}_{Z_1^T,Z_2^T}$ are empty. For the matrices A and B in (3.4.1), if $\mathcal{R}_{X_1,X_2}$ and $\mathcal{R}_{X_3^T,X_4^T}$ both are empty, then Y is not fixable.

Example 3.4.3. Here we revisit Example 3.3.9:

$$A = \left[\begin{array}{cc|cc|ccc} 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ \hline 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 1 \end{array}\right], \quad B = \left[\begin{array}{cc|cc|ccc} 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 1 \end{array}\right]$$

where A and B are conformally partitioned with the matrices in (3.4.1), and we use the same notation in (3.4.1). Since X_1 and X_2 are not isomorphic, $\mathcal{R}_{X_1,X_2}$ is empty. Similarly, $\mathcal{R}_{X_3^T,X_4^T}$ is also empty. So, the remaining matrix is not fixable.

We claim that A and B are not isomorphic. The multi-sets of row sums and column sums of a matrix are invariant under permutation of rows and columns in the matrix. The row and column sum vectors for A and B are $(4, 3, 5, 2, 5, 5, 5)$. So, if A and B are isomorphic, then necessarily $A[\alpha, \alpha]$ is isomorphic to $B[\alpha, \alpha]$ where $\alpha = \{3, 5, 6, 7\}$. However, $A[\alpha, \alpha]$ contains fewer ones than $B[\alpha, \alpha]$. Hence, A and B are not isomorphic.

We shall consider the converse of Proposition 3.4.1 under some circumstances motivated by Example 3.4.3.

Remark 3.4.4. Let $A = \begin{bmatrix} 0 & J_{k_1,k_2} \\ J_{k_1,k_2} & 0 \end{bmatrix}$ and $B = \begin{bmatrix} J_{k_1,k_2} & 0 \\ 0 & J_{k_1,k_2} \end{bmatrix}$ where $k_1, k_2 > 0$. One can verify that for any permutation matrices P and Q such that $B = PAQ$, a pair (P, Q) is either $\left(\begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix}, \begin{bmatrix} 0 & Q_1 \\ Q_1 & 0 \end{bmatrix} \right)$ or $\left(\begin{bmatrix} 0 & P_1 \\ P_2 & 0 \end{bmatrix}, \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix} \right)$ for some permutation matrices P_1, P_2, Q_1 and Q_2.

Proposition 3.4.5. *Let A and B be Gram mates of the form* (3.4.1)*. Let R and S be the row and column sum vectors of A, and conformally partitioned with the rows and the columns of A as $R = (R_1, R_2, R_3)$ and $S = (S_1, S_2, S_3)$, respectively. Suppose that for $i = 1, 2$, the set of all entries of R_i (resp. S_i) does not have any element in common with that of R_3 (resp. S_3). Then, A is isomorphic to B if and only if the remaining matrix is fixable.*

Proof. Suppose that A and B are isomorphic, say $B = PAQ$ for some permutation matrices P and Q. Since the multi-sets of row sums and column sums of a matrix are preserved by permutation, for $i = 1, 2$, any row of A indexed by an entry in R_i cannot turn into some row indexed by an entry in R_3 in order to obtain B by permutation. Similarly, one can find an analogous result with respect to columns by using S_1, S_2, and S_3. Hence, considering Remark 3.4.4, a pair (P, Q) must be one of the following:

$$\left(\begin{bmatrix} P_1 & 0 & 0 \\ 0 & P_2 & 0 \\ 0 & 0 & P_3 \end{bmatrix}, \begin{bmatrix} 0 & Q_1 & 0 \\ Q_2 & 0 & 0 \\ 0 & 0 & Q_3 \end{bmatrix} \right) \text{ and } \left(\begin{bmatrix} 0 & P_1 & 0 \\ P_2 & 0 & 0 \\ 0 & 0 & P_3 \end{bmatrix}, \begin{bmatrix} Q_1 & 0 & 0 \\ 0 & Q_2 & 0 \\ 0 & 0 & Q_3 \end{bmatrix} \right). \tag{3.4.2}$$

Let (P, Q) be the former of the two cases. From $B = PAQ$, one can check that $X_3 = P_3X_4Q_2$, $X_4 = P_3X_3Q_1$, $X_1 = P_1X_1Q_3$, $X_2 = P_2X_2Q_3$ and $Y = P_3YQ_3$. Hence, Y is fixable. The other case of (P, Q) can be easily checked. Hence, the remaining matrix is fixable.

The converse of the proof follows from Proposition 3.4.1. $\square$

Example 3.4.6. Let $E = \begin{bmatrix} J_3 & -J_3 & 0 \\ -J_3 & J_3 & 0 \\ 0 & 0 & 0 \end{bmatrix}$. Consider

$$A = \begin{bmatrix} 0 & J_3 & X_1 \\ J_3 & 0 & X_2 \\ X_3 & X_4 & Y \end{bmatrix} = \left[\begin{array}{ccc|ccc|cccc} 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 \\ \hline 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ \hline 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \end{array}\right].$$

Since $\mathbf{1}^T X_1 = \mathbf{1}^T X_2$ and $X_3\mathbf{1} = X_4\mathbf{1}$, A and $A + E$ are Gram mates. Moreover, $(P_1, P_2, Q) \in \mathcal{R}_{X_1,X_2}$ where P_1, P_2 and Q correspond to permutations $(1,3)$, $(1,3)$ and $(2,3)$ in cycle notation, respectively. Note that $(I, I, I) \in \mathcal{L}_{X_3,X_4}$. Since Y is invariant under the column permutation corresponding to $(2,3)$, the remaining matrix of A is fixable. The row and column sum vectors of A are $(5\mathbf{1}_6^T, 7, 9, 8, 8)$ and $(6\mathbf{1}_6^T, 5, 8, 8, 5)$, respectively. By Proposition 3.4.5, A and B are isomorphic.

Let square matrices A and B be Gram mates, where $\operatorname{rank}(A - B) = 1$. Suppose that all singular values of A are distinct. We claim that if the remaining matrix of A is not fixable, then A and B are not isomorphic. To establish the claim, we consider that for the adjacency matrix X of a (multi-)graph, the *automorphism group* of X, denoted $\Gamma(X)$, is defined as the set of all permutation matrices P such that $PXP^T = X$. We refer the interested reader to [24] for properties of $\Gamma(X)$ regarding spectrum of X, and to [35] for an introduction to the automorphism group of a connected simple graph regarding group action.

Let A and B (not necessarily square) be Gram mates. Suppose that A and B are isomorphic. Then, there exist permutation matrices P and Q such that $B = PAQ$. Since A and B are Gram mates, we have $PAA^TP^T = AA^T$ and $Q^TA^TAQ = A^TA$. Therefore, $P \in \Gamma(AA^T)$ and $Q \in \Gamma(A^TA)$. However, the converse does not hold.

Example 3.4.7. Non-isomorphic symmetric balanced incomplete block designs A and B can be found in [69]. Since $AA^T = A^TA = aI + bJ$ for some $a, b > 0$, $\Gamma(AA^T)$ and $\Gamma(A^TA)$ are isomorphic to the symmetric group.

Problem 3.4.8. *As seen above, for a $(0,1)$ matrix A, we could understand non-isomorphic Gram mates to A by studying the automorphism groups $\Gamma(AA^T)$ and $\Gamma(A^TA)$. Since AA^T is an integral matrix, AA^T can be expressed as $AA^T = \alpha_1 X_1 + \cdots + \alpha_k X_k$ for some $k \geq 1$, where α_i and X_i for $1 \leq i \leq k$ are a scalar and a $(0,1)$ symmetric matrix, respectively, and $\alpha_j \neq \alpha_l$ and $X_j \circ X_l = 0$ whenever $j \neq l$ (where $\circ$ denotes the Hadamard product of matrices). It follows that $\Gamma(AA^T) = \bigcap_{i=1}^{k} \Gamma(X_i)$. If there exists an index j such that the graph associated to X_j is asymmetric—that is, $\Gamma(X_j) = \emptyset$, then $\Gamma(AA^T) = \emptyset$. This provides information that if A and B with $A \neq B$ are isomorphic Gram mates and $\Gamma(AA^T) = \emptyset$, then B must be obtained from A only by permuting columns of A. From this observation, characterize $(0,1)$ matrices A such that $\Gamma(AA^T) = \emptyset$. Further, we may study $(0,1)$ matrices X such that $\Gamma(X) = \emptyset$.*

Theorem 3.4.9. *[24, 54] Let X be the adjacency matrix of a multigraph. Suppose that X has all distinct eigenvalues. Then, for any $P \in \Gamma(X)$, $P^2 = I$. Furthermore, this implies $\Gamma(X)$ is abelian.*

Corollary 3.4.10. *Let $n \times n$ matrices A and B be Gram mates with all distinct singular values. If A and B are isomorphic, then B is obtained from A by permuting rows and columns according to permutations, any cycle in which is of length at most 2.*

Theorem 3.4.11. *Let $n \times n$ $(0,1)$ matrices A and B be Gram mates of form* (3.4.1) *with all distinct singular values where* $\text{rank}(A - B) = 1$. *Then, A and B are isomorphic if and only if the remaining matrix is fixable.*

Proof. Assume for contradiction that A and B are isomorphic and the remaining matrix is not fixable, say $B = P_0 A Q_0$ where P_0 and Q_0 are permutation matrices. By Corollary 3.4.10, $P_0^2 = Q_0^2 = I$. Let σ_0 and τ_0 be permutations corresponding to P_0 and Q_0, respectively. Adopting the notation in (3.4.1) for A and B, let $\alpha_1 = \{1, \ldots, k_1\}$, $\alpha_2 = \{k_1 + 1, \ldots, 2k_1\}$, $\alpha_3 = \{2k_1 + 1, \ldots, n\}$, $\beta_1 = \{1, \ldots, k_2\}$, $\beta_2 = \{k_2 + 1, \ldots, 2k_2\}$ and $\beta_3 = \{2k_2 + 1, \ldots, n\}$. Let $\widetilde{A}$ be the resulting matrix after applying the permutation σ_0 to rows of A, and let B be the resulting matrix after applying τ_0 to columns of $\widetilde{A}$. Consider

$$A = \begin{bmatrix} 0 & J_{k_1,k_2} & X_1 \\ J_{k_1,k_2} & & X_2 \\ X_3 & X_4 & Y \end{bmatrix} \xrightarrow{\sigma_0} \widetilde{A} = \begin{bmatrix} \widetilde{A}_{11} & \widetilde{A}_{12} & \widetilde{X}_1 \\ \widetilde{A}_{21} & \widetilde{A}_{22} & \widetilde{X}_2 \\ \widetilde{X}_3 & \widetilde{X}_4 & \widetilde{Y} \end{bmatrix} \xrightarrow{\tau_0} B = \begin{bmatrix} J_{k_1,k_2} & 0 & X_1 \\ 0 & J_{k_1,k_2} & X_2 \\ X_3 & X_4 & Y \end{bmatrix}.$$

Suppose to the contrary that $\sigma_0(a) \in \alpha_3$ for all $a \in \alpha_3$. We consider three cases: (a) $\sigma_0(\alpha_1) \neq \alpha_1$ and $\sigma_0(\alpha_1) \neq \alpha_2$, (b) $\sigma_0(\alpha_1) = \alpha_1$, (c) $\sigma_0(\alpha_1) = \alpha_2$. Let the condition (a) hold. Then, $|\{x \in \alpha_1 | \sigma_0(x) \in \alpha_1\}| > 0$. So, neither $\begin{bmatrix} \widetilde{A}_{11} \\ \widetilde{A}_{21} \end{bmatrix}$ nor $\begin{bmatrix} \widetilde{A}_{12} \\ \widetilde{A}_{22} \end{bmatrix}$ contains the columns $\begin{bmatrix} \mathbf{1}_{k_1} \\ \mathbf{0}_{k_1} \end{bmatrix}$ or $\begin{bmatrix} \mathbf{0}_{k_1} \\ \mathbf{1}_{k_1} \end{bmatrix}$. Note that any cycle of τ_0 is of length either 1 or 2. In order to obtain B from $\widetilde{A}$, the first column $\tilde{\mathbf{x}}_1$ of $\widetilde{A}$ must be swapped with some j^{th} column $\tilde{\mathbf{x}}_j$ of $\widetilde{A}$ for some $j \in \beta_3$. Then, the subvector $\tilde{\mathbf{x}}_j[\alpha_1 \cup \alpha_2]$ must be $\begin{bmatrix} \mathbf{1}_{k_1} \\ \mathbf{0}_{k_1} \end{bmatrix}$. So, for the j^{th} column $\mathbf{x}_j$ of A, we have $\mathbf{x}_j[\alpha_1 \cup \alpha_2] \xrightarrow{\sigma_0} \begin{bmatrix} \mathbf{1}_{k_1} \\ \mathbf{0}_{k_1} \end{bmatrix}$. Further, we can readily find $\begin{bmatrix} \mathbf{0}_{k_1} \\ \mathbf{1}_{k_1} \end{bmatrix} \xrightarrow{\sigma_0} \tilde{\mathbf{x}}_1[\alpha_1 \cup \alpha_2]$. Since $j \in \beta_3$, the j^{th} columns of A and B must coincide, *i.e.*, $\mathbf{x}_j[\alpha_1 \cup \alpha_2] = \tilde{\mathbf{x}}_1[\alpha_1 \cup \alpha_2]$. Hence, we obtain

$$\begin{bmatrix} \mathbf{0}_{k_1} \\ \mathbf{1}_{k_1} \end{bmatrix} \xrightarrow{\sigma_0} \tilde{\mathbf{x}}_1[\alpha_1 \cup \alpha_2] = \mathbf{x}_j[\alpha_1 \cup \alpha_2] \xrightarrow{\sigma_0} \begin{bmatrix} \mathbf{1}_{k_1} \\ \mathbf{0}_{k_1} \end{bmatrix}.$$

However, the mapping contradicts the fact that σ_0^2 is the identity. Therefore, the case (a) does not hold.

Consider the case (b) that $\sigma_0(\alpha_1) = \alpha_1$. Since $\mathbf{1}^T X_1 = \mathbf{1}^T X_2$, there are no columns in $\widetilde{A}[\alpha_1 \cup \alpha_2, \beta_3]$ that are $\begin{bmatrix} \mathbf{1}_{k_1} \\ \mathbf{0}_{k_1} \end{bmatrix}$ or $\begin{bmatrix} \mathbf{0}_{k_1} \\ \mathbf{1}_{k_1} \end{bmatrix}$. This implies that $\tau_0(\beta_1) = \beta_2$, $\tau_0(\beta_2) = \beta_1$ and $\tau_0(\beta_3) = \beta_3$. Then, a pair (P, Q) corresponds to the former in (3.4.2). By the argument of the proof in 3.4.5, Y is fixable, which is a contradiction to the hypothesis. Finally, suppose that $\sigma_0(\alpha_1) = \alpha_2$. Since $\mathbf{1}^T X_1 = \mathbf{1}^T X_2$, we have $\tau_0(\beta_1) = \beta_1$, $\tau_0(\beta_2) = \beta_2$ and $\tau_0(\beta_3) = \beta_3$. Using an analogous argument as for case (b), we have a contradiction for the case (c). Therefore, there exists $a \in \alpha_3$ such that $\sigma_0(a) \notin \alpha_3$.

We now suppose that there exists $j \in \alpha_3$ such that $\sigma_0(j) \notin \alpha_3$. Let $i = \sigma_0(j)$. Then, $i \in \alpha_1 \cup \alpha_2$, say $i \in \alpha_1$. Let $\mathbf{a}_i^T$ and $\mathbf{a}_j^T$ be the i^{th} and j^{th} rows of A, respectively, where $\mathbf{a}_i^T = \begin{bmatrix} \mathbf{0}_{k_1}^T & \mathbf{1}_{k_1}^T & \mathbf{x}_1^T \end{bmatrix}$, $\mathbf{a}_j^T = \begin{bmatrix} \mathbf{x}_3^T & \mathbf{x}_4^T & \mathbf{y}^T \end{bmatrix}$ and $\mathbf{a}_j^T$ is compatible with the partition of $\mathbf{a}_i^T$. Since each cycle of σ_0 is of length either 1 or 2, $\mathbf{a}_j^T$ and $\mathbf{a}_i^T$ are mapped to the i^{th} row $\tilde{\mathbf{a}}_i^T$ and the j^{th} row $\tilde{\mathbf{a}}_j^T$ of $\widetilde{A}$, respectively, after applying the row permutation σ_0. After permuting columns of $\tilde{\mathbf{a}}_i^T$ and $\tilde{\mathbf{a}}_j^T$ according to τ_0, we must have $\mathbf{b}_i^T$ and $\mathbf{b}_j^T$ that are the i^{th} and j^{th} rows of B:

$$\begin{bmatrix} \tilde{\mathbf{a}}_i^T \\ \tilde{\mathbf{a}}_j^T \end{bmatrix} = \begin{bmatrix} \mathbf{x}_3^T & \mathbf{x}_4^T & \mathbf{y}^T \\ \mathbf{0}^T & \mathbf{1}^T & \mathbf{x}_1^T \end{bmatrix} \xrightarrow{\tau_0} \begin{bmatrix} \mathbf{b}_i^T \\ \mathbf{b}_j^T \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T & \mathbf{0}^T & \mathbf{x}_1^T \\ \mathbf{x}_3^T & \mathbf{x}_4^T & \mathbf{y}^T \end{bmatrix}.$$

Since A and B are Gram mates, the row sums of $\mathbf{x}_3^T$ and $\mathbf{x}_4^T$ are the same, say ℓ. Permuting columns of $\begin{bmatrix} \tilde{\mathbf{a}}_i^T \\ \tilde{\mathbf{a}}_j^T \end{bmatrix}$ and $\begin{bmatrix} \mathbf{b}_i^T \\ \mathbf{b}_j^T \end{bmatrix}$ simultaneously, we can obtain

$$Z_1 = \begin{bmatrix} \mathbf{1}_\ell^T & \mathbf{0}_{k-\ell}^T & \mathbf{1}_\ell^T & \mathbf{0}_{k-\ell}^T & \mathbf{y}^T \\ \mathbf{0}_\ell^T & \mathbf{0}_{k-\ell}^T & \mathbf{1}_\ell^T & \mathbf{1}_{k-\ell}^T & \mathbf{x}_1^T \end{bmatrix} \xrightarrow{\tau_0} Z_2 = \begin{bmatrix} \mathbf{1}_\ell^T & \mathbf{1}_{k-\ell}^T & \mathbf{0}_\ell^T & \mathbf{0}_{k-\ell}^T & \mathbf{x}_1^T \\ \mathbf{1}_\ell^T & \mathbf{0}_{k-\ell}^T & \mathbf{1}_\ell^T & \mathbf{0}_{k-\ell}^T & \mathbf{y}^T \end{bmatrix}.$$

Suppose that $\ell > 0$. Note that if the kth column of Z_1 for $k \in \beta_3$ is $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$, so is the kth column of Z_2. Considering that each cycle in τ_0 is of length either 1 or 2, the first column $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ of Z_1 must be swapped with some k_0^{th} column $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ of Z_2 where $k_0 \in \beta_3$. Then, $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is the k_0^{th} column of Z_2, which is a contradiction. Similarly, applying an analogous argument of the case $\ell > 0$ to the case $\ell = 0$, one can obtain a contradiction. Therefore, our desired result is established.

For the proof of the converse, apply Proposition 3.4.1. □

Conjecture 3.4.12. *Let A and B be Gram mates of form* (3.4.1) *where* $\operatorname{rank}(A - B) = 1$. *Then, A and B are isomorphic if and only if the remaining matrix is fixable.*

The following result could be used for proving the conjecture 3.4.12 with an extra condition that the multiplicity of each singular value of Gram mates is at most 2.

Proposition 3.4.13. *Let A be a* $(0,1)$ *matrix. Suppose that each eigenvalue of AA^T is of multiplicity at most* 2. *Then, for any $P \in \Gamma(AA^T)$, $P^4 = I$.*

Proof. Since AA^T is a real symmetric matrix, there exists an orthogonal matrix U and a diagonal matrix $D = \operatorname{diag}(d_1 I_{k_1}, \ldots, d_s I_{k_s})$ for some s, where $1 \le k_i \le 2$ for $i = 1, \ldots, s$, such that $AA^T = UDU^T$. Let $P \in \Gamma(AA^T)$. Then, $PAA^TP^T = AA^T$ implies that $U^TPUD = DU^TPU$. Since U^TPU and D commute, by Proposition 2.2.5, $U^TPU = \operatorname{diag}(B_1, \ldots, B_s)$ where B_i is a $k_i \times k_i$ orthogonal matrix for $1 \le i \le s$. In particular, if $k_j = 1$ for some $1 \le j \le s$, then $B_j = \pm 1$. We may assume $k_1 = 2$. Then, it is enough to show that $B_1^4 = I$ in order to obtain the conclusion.

Note that since B_1 is orthogonal, there exist real numbers a and b such that either $B_1 = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}$ or $B_1 = \begin{bmatrix} a & b \\ b & -a \end{bmatrix}$ where $a^2 + b^2 = 1$. Let $\mathbf{u}$ be an eigenvector of AA^T associated to the eigenvalue d_1. Then,

$$AA^T P\mathbf{u} = PAA^T\mathbf{u} = P(d_1\mathbf{u}) = d_1 P\mathbf{u}.$$

So, $\mathbf{u}$ and $P\mathbf{u}$ are eigenvectors of AA^T. We consider two cases: $\mathbf{u}$ and $P\mathbf{u}$ are linearly independent, or not.

Suppose that $\mathbf{u}$ and $P\mathbf{u}$ are linearly independent. From $PU = U\text{diag}(B_1, \ldots, B_s)$, we have $P\begin{bmatrix} \mathbf{u} & P\mathbf{u} \end{bmatrix} = \begin{bmatrix} \mathbf{u} & P\mathbf{u} \end{bmatrix} B_1$. Consider $B_1 = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}$. Then, $P\mathbf{u} = (aI + bP)\mathbf{u}$, $P^2\mathbf{u} = (-bI + aP)\mathbf{u}$. We recast $P\mathbf{u} = (aI + bP)\mathbf{u}$ as $(1-b)P\mathbf{u} = a\mathbf{u}$. Since $\mathbf{u}$ and $P\mathbf{u}$ are linearly independent, we have $a = 0$ and $b = 1$. Similarly, it can be checked that if $B_1 = \begin{bmatrix} a & b \\ b & -a \end{bmatrix}$, then $a = 0$ and $b = 1$.

Assume that $\mathbf{u}$ and $P\mathbf{u}$ are linearly dependent. Then, there are linearly independent vectors $\mathbf{u}_1$ and $\mathbf{u}_2$ such that $P\begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 \end{bmatrix} B_1$ and $P\mathbf{u}_i = \pm\mathbf{u}_i$ for $i = 1, 2$. Consider $B_1 = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}$. Then, $P\mathbf{u}_1 = a\mathbf{u}_1 + b\mathbf{u}_2$, $P\mathbf{u}_2 = -b\mathbf{u}_1 + a\mathbf{u}_2$. If $P\mathbf{u}_i = \mathbf{u}_i$ for $i = 1, 2$, then $(1-a)\mathbf{u}_1 = b\mathbf{u}_2$ and $(1-a)\mathbf{u}_2 = -b\mathbf{u}_1$; since $\mathbf{u}_1$ and $\mathbf{u}_2$ are linearly independent, $a = 1$ and $b = 0$. If $P\mathbf{u}_1 = \mathbf{u}_1$ and $P\mathbf{u}_2 = -\mathbf{u}_2$, then $(1-a)\mathbf{u}_1 = b\mathbf{u}_2$ and $(1+a)\mathbf{u}_2 = b\mathbf{u}_1$; so, there are no desired values of a and b. In this manner, it can be checked that $a = \pm 1$ and $b = 0$. Applying an analogous argument to the case $B_1 = \begin{bmatrix} a & b \\ b & -a \end{bmatrix}$, one can verify that $a = \pm 1$ and $b = 0$.

Summing up all the cases, any 2×2 block diagonal matrix in $\text{diag}(B_1, \ldots, B_s)$ is one of the following matrices:

$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \text{ or } \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Evidently, $B_1^4 = I$ for all cases. Therefore, the conclusion follows. □

3.5 Construction of Gram mates

In this section, using given pairs of Gram mates, we provide several tools for constructing other pairs. Similarly, with given realizable matrices, we construct others; and we discuss realizable matrices of rank more than 2.

Proposition 3.5.1. *Let A and B be Gram mates. Then, $J-A$ and $J-B$ are Gram mates.*

Proof. Since A and B are Gram mates, $A\mathbf{1} = B\mathbf{1}$ and $\mathbf{1}^T A = \mathbf{1}^T B$. From $A\mathbf{1} = B\mathbf{1}$, we have

$$\begin{aligned}(J-A)(J-A)^T &= J^2 - JA^T - AJ^T + AA^T \\ &= J^2 - JB^T - BJ^T + BB^T = (J-B)(J-B)^T.\end{aligned}$$

By a similar argument with $\mathbf{1}^T A = \mathbf{1}^T B$, we can find that $(J-A)^T(J-A) = (J-B)^T(J-B)$. □

Proposition 3.5.2. *Suppose that (A_1, B_1) and (A_2, B_2) are pairs of Gram mates (that are not necessarily square matrices). Then, we have the following pairs of Gram mates:*

$$\left(\begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}, \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}\right) \text{ and } \left(\begin{bmatrix} A_1 & J \\ J & A_2 \end{bmatrix}, \begin{bmatrix} B_1 & J \\ J & B_2 \end{bmatrix}\right).$$

Proof. For $i = 1, 2$, A_i and B_i have the same row sum vector and the same column sum vector. Then, it is straightforward to establish the desired results. □

Proposition 3.5.3. *Suppose that (A_1, B_1) and (A_2, B_2) are pairs of Gram mates. Then, $A_1 \otimes B_1$ and $A_2 \otimes B_2$ are Gram mates.*

Proof. Since (A_1, B_1) and (A_2, B_2) are pairs of Gram mates, we have

$$(A_1 \otimes B_1)(A_1 \otimes B_1)^T = A_1 A_1^T \otimes B_1 B_1^T = A_2 A_2^T \otimes B_2 B_2^T = (A_2 \otimes B_2)(A_2 \otimes B_2)^T.$$

Similarly, it can be checked that $(A_1 \otimes B_1)^T (A_1 \otimes B_1) = (A_2 \otimes B_2)^T (A_2 \otimes B_2)$. □

Remark 3.5.4. In analogy to graph operations, one might regard ways of the constructions for Gram mates in Propositions 3.5.1–3.5.3 as the complement of a graph, the disjoint union of two graphs and the join of two graphs, and the Cartesian product of two graphs, respectively.

We can apply analogous approaches with Propositions 3.5.2 and 3.5.3 to realizable matrices. Given realizable matrices E_1 and E_2, it follows from Proposition 3.5.2 that $\begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$ is realizable.

Proposition 3.5.5. *Let E be a realizable, and let X be a $(0,1)$ matrix. Then, $X \otimes E$ and $E \otimes X$ are realizable.*

Proof. Let A and $A+E$ be Gram mates via E. Since $E\mathbf{1} = 0$, we have $(X \otimes E)\mathbf{1} = X\mathbf{1} \otimes E\mathbf{1} = X\mathbf{1} \otimes 0 = 0$. Similarly, $\mathbf{1}^T(X \otimes E) = 0$. By Proposition 3.5.3, we have

$$\begin{aligned}(X \otimes A + X \otimes E)(X \otimes A + X \otimes E)^T =& (X \otimes (A+E))(X \otimes (A+E))^T \\ =& (X \otimes A)(X \otimes A)^T\end{aligned}$$

In a similar way, we can find that $(X \otimes A + X \otimes E)^T(X \otimes A + X \otimes E) = (X \otimes A)^T(X \otimes A)$. Therefore, $X \otimes E$ is realizable. An analogous argument establishes that $E \otimes X$ is realizable. □

Remark 3.5.6. With the aid of the results in this section, we can construct Gram mates via realizable matrices of rank more than 2 from those of rank at most 2 that we studied in Section 3.3. As an example, let us consider a realizable matrix E of rank 2. For a $(0,1)$ matrix X of rank $k > 0$, $X \otimes E$ is realizable, and its rank is $2k$.

Problem 3.5.7. *Regarding the construction of Gram mates, we can pose the following question: given non-negative integral vectors R and S, does there exist a pair of Gram mates in $\mathcal{U}(R,S)$?*

We can approach this question under specific circumstances. Here we revisit Example 3.2.15: we have Gram mates $A = \begin{bmatrix} A_1 & A_2 \\ A_2 & A_1 \end{bmatrix}$ and $B = \begin{bmatrix} A_2 & A_1 \\ A_1 & A_2 \end{bmatrix}$ where A_1 and A_2 are $(0,1)$ matrices of the same size with $A_1 \neq A_2$. We note that A_1 and A_2 can be chosen arbitrarily. Examining the row and column sum vectors R and S of A, each distinct integer in R (resp. S) appears an even number of times.

Motivated by the example, we have the following problem. Let R and S be non-negative integral vectors. Suppose that each distinct integer in R (resp. S) appears an even number of times. Prove or disprove that if $R^* \succ S$, then there exists a pair of Gram mates A and B in $\mathcal{U}(R,S)$ with $A \neq B$. One could check if such Gram mates A and B can be constructed as $A = \begin{bmatrix} A_1 & A_2 \\ A_2 & A_1 \end{bmatrix}$ and $B = \begin{bmatrix} A_2 & A_1 \\ A_1 & A_2 \end{bmatrix}$ for some A_1 and A_2 with $A_1 \neq A_2$.

3.6 Several types of Gram mates

In this section, we deal with Gram mates related to tournament matrices or circulant matrices.

An $n \times n$ $(0,1)$ matrix A is called a *tournament matrix* if $A + A^T = J - I$. An $n \times n$ tournament matrix A is called *regular* if n is odd and $A\mathbf{1} = \frac{n-1}{2}$. It is found in [14] that given a tournament matrix A, the following are equivalent: (i) A is regular, (ii) $JA = AJ$, (iii) $AA^T = A^TA$. An $n \times n$ tournament matrix A is called a *Hadamard tournament matrix* if $n \equiv 3 \pmod 4$, A is regular and $AA^T = \frac{n+1}{4}I + \frac{n-3}{4}J$.

Proposition 3.6.1. *Let A_1 and B_1 be $n \times n$ Hadamard tournament matrices. Then,* $A = \begin{bmatrix} \mathbf{1}^T & 0 \\ A_1 & J - A_1 \end{bmatrix}$ *and* $B = \begin{bmatrix} 0 & \mathbf{1}^T \\ J - B_1 & B_1 \end{bmatrix}$ *are Gram mates.*

Proof. Let $A_2 = J - A_1$ and $B_2 = J - B_1$. Direct computation shows that $AA^T = BB^T$ if and only if $\mathbf{1}^T A_1^T = \mathbf{1}^T B_1^T$ and $A_1A_1^T + A_2A_2^T = B_2B_2^T + B_1B_1^T$; and $A^TA = B^TB$ if and only if $J + A_1^TA_1 = B_2^TB_2$, $A_1^TA_2 = B_2^TB_1$, and $A_2^TA_2 = J + B_1^TB_1$. Since A_1 and A_2 are regular, $A_1A_1^T = A_1^TA_1 = B_1B_1^T = B_1^TB_1$. From $A_1A_1^T = \frac{n+1}{4}I + \frac{n-3}{4}J$, one can check that $A_2A_2^T = A_2^TA_2 = B_2B_2^T = B_2^TB_2 = \frac{n+1}{4}I + \frac{n+1}{4}J$. Since $B_1\mathbf{1} = \frac{n-1}{2}\mathbf{1}$, we have $B_2\mathbf{1} = \frac{n+1}{2}\mathbf{1}$. Then, we can find that $A_1^T(J - A_1) = B_2^T(J - B_2)$. So, $A_1^TA_2 = B_2^TB_1$. The desired conclusion follows. $\square$

Remark 3.6.2. One can illustrate Proposition 3.6.1 with the Hadamard designs and their complements [69].

Remark 3.6.3. Let $E = \begin{bmatrix} \mathbf{1}_n^T & -\mathbf{1}_n^T \\ -I_n & I_n \end{bmatrix}$ where $n \geq 1$. Then, it is found in [44] that any Gram mates A and $A + E$ via E are given by $A = \begin{bmatrix} 0^T & \mathbf{1}^T \\ M + I & M^T \end{bmatrix}$ and $A + E$ for some regular tournament M. We note that Gram mates in Proposition 3.6.1 are not necessarily via E.

Proposition 3.6.4. *Let A and B be $(0,1)$ matrices such that $A + B = J - I$ and $A \neq B$. Then, A and B are Gram mates if and only if $B = A^T$ and $AA^T = A^TA$, i.e. A is a regular tournament.*

Proof. Suppose that A and B are Gram mates. Then, $(A - B)\mathbf{1} = 0$ and $\mathbf{1}^T(A - B) = 0$. Since there is a single zero in each row and column, n is odd and each column of A and B has $\frac{n-1}{2}$ ones. Assume to the contrary that $B \neq A^T$. Then, there is a pair (i, j) with $i \neq j$ such that either $a_{ij} = a_{ji} = 0$ or $a_{ij} = a_{ji} = 1$. If $a_{ij} = a_{ji} = 0$, then we have $b_{ij} = b_{ji} = 1$. So, we may assume $a_{ij} = a_{ji} = 1$. Let $\mathbf{a}_i$ and $\mathbf{a}_j$ be the i^{th} and j^{th} columns of A, respectively. Then, $\mathbf{1} - \mathbf{e}_i - \mathbf{a}_i$ and $\mathbf{1} - \mathbf{e}_j - \mathbf{a}_j$ are the i^{th} and j^{th} columns of B. Since $a_{ij} = a_{ji} = 1$, we have $(\mathbf{1} - \mathbf{e}_j)^T\mathbf{a}_i = (\mathbf{1} - \mathbf{e}_i)^T\mathbf{a}_j = \frac{n-3}{2}$. Hence,

$$((\mathbf{1} - \mathbf{e}_i) - \mathbf{a}_i)^T((\mathbf{1} - \mathbf{e}_j) - \mathbf{a}_j) = (n - 2) - (n - 3) + \mathbf{a}_i^T\mathbf{a}_j = 1 + \mathbf{a}_i^T\mathbf{a}_j.$$

We have $(BB^T)_{ij} = (AA^T)_{ij} + 1$, a contradiction to $AA^T = BB^T$. Thus, $B = A^T$. Since A and B are Gram mates, we have $AA^T = BB^T = A^TA$.

The converse follows readily. $\square$

3.6.1 Circulant Gram mates and realizable matrices

Throughout this subsection, we assume that all sub-indices indicating positions of entries in matrices or vectors are in $\mathbb{Z}_m = \{0, \ldots, m-1\}$, where m is given by the number of rows or columns in the context, and $\mathbb{Z}_m$ is the set of integers modulo m. An $n \times n$ matrix C of the form

$$C = \begin{bmatrix} c_0 & c_1 & \cdots & c_{n-2} & c_{n-1} \\ c_{n-1} & c_0 & \cdots & c_{n-3} & c_{n-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_2 & c_3 & \cdots & c_0 & c_1 \\ c_1 & c_2 & \cdots & c_{n-1} & c_0 \end{bmatrix}$$

is a *circulant matrix*. We denote C by $\mathrm{circ}(c_0, \ldots, c_{n-1})$. Given two row vectors $\mathbf{a}^T$ and $\mathbf{b}^T$ of the same size, we have $\mathrm{circ}(\mathbf{a}^T) + \mathrm{circ}(\mathbf{b}^T) = \mathrm{circ}(\mathbf{a}^T + \mathbf{b}^T)$. In this subsection, let P_n denote the $n \times n$ circulant matrix $\mathrm{circ}(0, 1, 0, \ldots, 0)$. Let H_n be the $n \times n$ matrix given by:

$$H_n := \begin{bmatrix} 0 & \cdots & 0 & 1 \\ \vdots & \iddots & 1 & 0 \\ 0 & \iddots & \iddots & \vdots \\ 1 & 0 & \cdots & 0 \end{bmatrix}.$$

We write P_n and H_n as P and H, respectively, if the size is clear from the context. It can be readily checked that $P^T = P^{-1}$, $H^2 = I$ and $HP^iH = P^{-i}$ for $i \in \mathbb{Z}$. Then, C can be recast as

$$C = \begin{bmatrix} \mathbf{c}^T P^0 \\ \vdots \\ \mathbf{c}^T P^{n-1} \end{bmatrix} = \left[\begin{array}{c|c|c|c} P^{n-1} H\mathbf{c} & \cdots & PH\mathbf{c} & H\mathbf{c} \end{array}\right]$$

where $\mathbf{c}^T = (c_0, \ldots, c_{n-1})$.

An *interchange* in a $(0,1)$ matrix A is a transformation that changes a submatrix

$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ of A into $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. One of the works of Ryser [59] is that given A and B in $\mathcal{U}(R, S)$, A can be transformed into B by a finite sequence of interchanges. Kirkland [44] applied this idea to Gram mates by considering a realizable matrix, without loss of generality, $E = \begin{bmatrix} E' & 0 \\ 0 & 0 \end{bmatrix}$ where $E' = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$. That is, Gram mates via E can be regarded as two matrices where one is obtained from the other by an interchange with the property of being Gram mates. Furthermore, Kirkland [44] generalised the notion of an interchange by considering E' as the difference of two permutation matrices such that their Hadamard product is zero. Then, characterizing Gram mates via such generalised realizable matrices can be simplified as finding Gram mates via the direct sum of realizable matrices in form $P - I$ (see [44] for the details). Motivated by the fact that $P - I$ is a circulant matrix, we therefore explore circulant Gram mates and circulant realizable matrices.

Proposition 3.6.5. *[44] Let* $\mathbf{e}^T = (-1, 1, 0, \dots, 0)$. *Then,* $\operatorname{circ}(\mathbf{a}^T)$ *and* $\operatorname{circ}(\mathbf{a}^T + \mathbf{e}^T)$ *are Gram mates if and only if there exists scalars* $a_2, \dots, a_{n-1} \in \{0, 1\}$ *with* $a_j = a_{n+1-j}$ *for* $j = 2, \dots, n-1$ *such that* $\mathbf{a}^T = \operatorname{circ}(1, 0, a_2, \dots, a_{n-1})$.

Example 3.6.6. Let $\mathbf{e}^T = \operatorname{circ}(-1, 0, 0, 0, 1, 0, 0, 0)$. Then, A and $A + \operatorname{circ}(\mathbf{e}^T)$ are Gram mates where

$$A = \left[\begin{array}{cccc|cccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right].$$

Example 3.6.6 tells that given a circulant realizable matrix E, Gram mates via E are not necessarily circulant unlike the result of Proposition 3.6.5.

Remark 3.6.7. The paper [44] illustrates how to find all Gram mates via $E = P_n^k - I_n$ where $n \geq 3$ and $2 \leq k \leq n - 1$.

Now, we consider $(0, 1)$ circulant matrices A and B with $A \neq B$. From commutativity of multiplication for circulant matrices, it suffices to consider $AA^T = BB^T$ in order to see if A and B are Gram mates. We note that every circulant matrix is completely determined by its first row. Therefore, we only need to compare the first rows of AA^T and BB^T.

Theorem 3.6.8. *Let* $\mathbf{a}^T$ *and* $\mathbf{b}^T$ *be* $(0,1)$ *row vectors with* $\mathbf{a}^T \neq \mathbf{b}^T$*. Then,* $\mathrm{circ}(\mathbf{a}^T)$ *and* $\mathrm{circ}(\mathbf{b}^T)$ *are Gram mates if and only if* $\mathbf{a}^T P^i \mathbf{a} = \mathbf{b}^T P^i \mathbf{b}$ *for* $i \in \mathbb{Z}_n$*.*

Proof. Note that $A^T = \begin{bmatrix} (P^0)^T\mathbf{a} & \cdots & (P^{n-1})^T\mathbf{a} \end{bmatrix}$. Considering the first rows of AA^T and BB^T, we can readily see that $AA^T = BB^T$ if and only if $\mathbf{a}^T P^i \mathbf{a} = \mathbf{b}^T P^i \mathbf{b}$ for $i = 0, \dots, n-1$. The conclusion follows. □

Remark 3.6.9. In Theorem 3.6.8, since $\mathbf{a}^T P^i \mathbf{a} = \mathbf{a}^T P^{-i} \mathbf{a}$ for $i \in \mathbb{Z}_n$, it suffices to have $\mathbf{a}^T P^i \mathbf{a} = \mathbf{b}^T P^i \mathbf{b}$ for $0 \le i \le \lfloor \frac{n}{2} \rfloor$ in order that $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{b}^T)$ are Gram mates.

The *centralizer* of a subset S of a group G is defined to be

$$C_G(S) = \{g \in G | gs = sg \text{ for all } s \in S\}.$$

Recall that $\mathcal{S}_n$ denotes the symmetric group of degree n. Here we use a permutation in $\mathcal{S}_n$ as a bijection from $\mathbb{Z}_n$ to $\mathbb{Z}_n$. Let $\mathscr{P}_n$ denote the set of all $n \times n$ permutation matrices, and let $\mathscr{F}_n := \{P^i \in \mathscr{P}_n | i = 0, \dots, n-1\}$. Then, P corresponds to the cyclic permutation $\sigma = (0\ 1\ \dots\ n-1)$. It can be found in [28] that $C_{\mathcal{S}_n}(\sigma) = \{\sigma^1, \dots, \sigma^n\}$. Furthermore, $\sigma^i\sigma^j = \sigma^j\sigma^i$. Hence, we have $C_{\mathscr{P}_n}(\mathscr{F}_n) = \mathscr{F}_n$. Therefore, for $(0,1)$ row vectors $\mathbf{a}^T$ and $\mathbf{b}^T$ with $\mathbf{a}^T \neq \mathbf{b}^T$, if there exists $Q \in C_{\mathscr{P}_n}(\mathscr{F}_n)$ such that $\mathbf{b}^T = \mathbf{a}^T Q$, then $\mathbf{a}^T P^k \mathbf{a} = \mathbf{b}^T P^k \mathbf{b}$ for $k = 0, \dots, n-1$; so, $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{b}^T)$ are Gram mates.

The *normalizer* of a subset S of a group G is defined to be

$$N_G(S) = \{g \in G | gS = Sg\}.$$

It can be found in [28] that $N_{\mathscr{P}_n}(\mathscr{F}_n) \cong \mathbb{Z}_n \rtimes \mathrm{Aut}(\mathbb{Z}_n)$ where $\rtimes$ denotes the semidirect product. It is well-known that $\mathrm{Aut}(\mathbb{Z}_n) = \{\sigma \in \mathcal{S}_n | \sigma(1) = k \text{ where } \gcd(k,n) = 1\}$ (see [28]) where $\gcd(a,b)$ for $a, b \in \mathbb{Z}$ denotes the greatest common divisor of a and b. Given a permutation $\sigma \in \mathcal{S}_n$, Q_σ denotes the permutation matrix where $(Q_\sigma)_{i,j} = (Q)_{\sigma(i),j}$. Then,

$$N_{\mathscr{P}_n}(\mathscr{F}_n) = \{P^i Q_\sigma | 0 \le i \le n-1, \sigma \in \mathrm{Aut}(\mathbb{Z}_n)\}.$$

Let $\mathscr{C}_n$ denote the set of all $n \times n$ $(0,1)$ circulant matrices. Given a $(0,1)$ row vector $\mathbf{a}^T$, let $\mathscr{C}_{\mathbf{a}^T}$ denote the set of all circulant matrices that each of them is either $\mathrm{circ}(\mathbf{a}^T)$ or a Gram mate to $\mathrm{circ}(\mathbf{a}^T)$. Suppose that $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{b}^T)$ are Gram mates. Let $Q \in N_{\mathscr{P}_n}(\mathscr{F}_n)$. Then, $\mathscr{F}_n = \{QP^iQ^T | i = 0, \dots, n-1\}$. Hence, we obtain that for $0 \leq i \leq n-1$, $\mathbf{a}^T P^i \mathbf{a} = \mathbf{b}^T P^i \mathbf{b}$ if and only if $\mathbf{a}^T Q P^i Q^T \mathbf{a} = \mathbf{b}^T Q P^i Q^T \mathbf{b}$. It follows from Theorem 3.6.8 that for any $Q \in N_{\mathscr{P}_n}(\mathscr{F}_n)$, there is a bijection between $\mathscr{C}_{\mathbf{a}^T}$ and $\mathscr{C}_{\mathbf{a}^T Q}$. Therefore, we may identify $\mathscr{C}_{\mathbf{a}^T}$ with $\mathscr{C}_{\mathbf{a}^T Q}$.

Example 3.6.10. Let $\mathbf{a}^T = (0,0,0,1,0,1,0,0,1,0,0,0)$ and $\sigma = (1\ 5)(2\ 10)(4\ 8)$ in $\mathrm{Aut}(\mathbb{Z}_{12})$. Note that indices indicating positions of entries in vectors are in $\mathbb{Z}_n$. Then, $\mathbf{a}^T Q_\sigma = (0,1,0,1,1,1,0,0,0,0,0,0,0)$. One can check that $\mathbf{a}^T P \mathbf{a} = 0$ and $\mathbf{a}^T Q_\sigma P Q_\sigma^T \mathbf{a} = 1$. Therefore, for $R \in N_{\mathscr{P}_n}(\mathscr{F}_n)$, $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{a}^T R)$ are not necessarily Gram mates.

Proposition 3.6.11. *Let $\mathbf{a}^T$ and $\mathbf{b}^T$ be $(0,1)$ row vectors of size n with $\mathbf{a}^T \neq \mathbf{b}^T$. If there exist indices i and j such that $\mathbf{b}^T = \mathbf{a}^T H^i P^j$, then $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{b}^T)$ are Gram mates.*

Proof. It is enough to show that $\mathbf{a}^T P^k \mathbf{a} = \mathbf{b}^T P^k \mathbf{b}$ for $k = 0, \ldots, n-1$. Since $H^2 = P^n = I$, there are $i \in \{0,1\}$ and $j \in \{0, \ldots, n-1\}$ such that $\mathbf{b}^T = \mathbf{a}^T H^i P^j$. Let $i = 1$. We have $HP^jP^kP^{-j}H = HP^kH = P^{-k}$. So, $\mathbf{b}^T P^k \mathbf{b} = \mathbf{a}^T P^{-k} \mathbf{a} = \mathbf{a}^T P^k \mathbf{a}$. For the case $i = 0$, it is straightforward. $\square$

Let $\mathcal{E}_{n,m}$ denote the set of all $(0,1)$ row vectors of size n with m ones where $n \geq m$. Define a relation $\sim$ on $\mathcal{E}_{n,m}$ as follows: for $\mathbf{a}^T, \mathbf{b}^T \in \mathcal{E}_{n,m}$, $\mathbf{a}^T \sim \mathbf{b}^T$ if and only if either $\mathbf{a}^T = \mathbf{b}^T$ or $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{b}^T)$ are Gram mates. It can be readily verified that the relation $\sim$ is an equivalence relation. So, $\mathcal{E}_{n,m}$ is partitioned into equivalence classes. Let $\mathcal{E}_{n,m}^{\mathbf{a}^T}$ denote the equivalence class of $\mathcal{E}_{n,m}$ containing $\mathbf{a}^T$. Then, $\mathcal{E}_{n,m}^{\mathbf{a}^T}$ may be identified with $\mathscr{C}_{\mathbf{a}^T}$. We note that from Proposition 3.5.1, we may assume $0 \leq m \leq \lfloor \frac{n}{2} \rfloor$.

Now, we introduce a representation of the dihedral group D_{2n} of order $2n$. We refer the reader to [28] for details. The presentation of D_{2n} is $D_{2n} =< r, s | r^n = s^2 = e,\ srs = r^{-1} >$ where e is the identity of D_{2n}. Consider a matrix representation of D_{2n}, *i.e.* a group homomorphism from D_{2n} to $GL_n(\mathbb{R})$ where $GL_n(\mathbb{R})$ is the general linear group of degree n, *i.e.* the set of all $n \times n$ invertible matrices. Then, it can be checked that the dihedral group D_{2n} has a representation ρ on $\mathbb{R}^n$ given by $\rho(r) = P$ and $\rho(s) = H$. Furthermore, we can see that the image of ρ is isomorphic to D_{2n}. We may interchangeably use $D_{2n} =< P, H | P^n = H^2 = I,\ HPH = P^{-1} >$. Any element in D_{2n} can be written as $H^i P^j$ for some $i \in \{0,1\}$ and $j \in \{0, \ldots, n-1\}$. Define a function ϕ from $\mathcal{E}_{n,m}^{\mathbf{a}^T} \times D_{2n}$ to $\mathcal{E}_{n,m}^{\mathbf{a}^T}$ by

$$\phi(\mathbf{b}^T, X) = \mathbf{b}^T X.$$

By Proposition 3.6.11, we have $\mathbf{b}^T \sim \mathbf{b}^T X$. So, ϕ is well defined. For any $\mathbf{b}^T \in \mathcal{E}_{n,m}^{\mathbf{a}^T}$, $\phi(\mathbf{b}^T, I) = \mathbf{b}^T$. Let $X_1, X_2 \in D_{2n}$. Then, $\phi(\mathbf{b}^T, X_1X_2) = \mathbf{b}^T(X_1X_2) = (\mathbf{b}^T X_1)X_2 = \phi(\mathbf{b}^T X_1, X_2)$. Therefore, ϕ is a (right) action of D_{2n} on the set $\mathcal{E}_{n,m}^{\mathbf{a}^T}$. We denote by $\mathcal{O}_{\mathbf{b}^T}$ the orbit of a vector $\mathbf{b}^T$ in $\mathcal{E}_{n,m}^{\mathbf{a}^T}$—that is, $\mathcal{O}_{\mathbf{b}^T} = \{\mathbf{b}^T X | X \in D_{2n}\}$. Furthermore, it is known that $\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n} := \cup_{\mathbf{b}^T \in \mathcal{E}_{n,m}^{\mathbf{a}^T}} \mathcal{O}_{\mathbf{b}^T}$ is a partition of $\mathcal{E}_{n,m}^{\mathbf{a}^T}$.

Example 3.6.12. Let

$$\mathbf{a}^T = (1,1,1,1,0,1,0,0,0,1,0,0,0,0) \text{ and } \mathbf{b}^T = (1,1,1,0,1,0,1,1,0,0,0,0,0,0).$$

One can check from direct computation that $\mathbf{a}^T P^i \mathbf{a} = \mathbf{b}^T P^i \mathbf{b}$ for $0 \le i \le 7$. Hence, $\mathbf{a}^T, \mathbf{b}^T \in \mathcal{E}_{14,6}^{\mathbf{a}^T}$. Since $\mathbf{a}^T$ contains 4 consecutive 1's while $\mathbf{b}^T$ does not, $\mathbf{a}^T \neq \mathbf{b}^T X$ for any $X \in D_{2n}$. So, $\mathbf{b}^T \notin \mathcal{O}_{\mathbf{a}^T}$ and $|\mathcal{E}_{14,6}^{\mathbf{a}^T}/D_{28}| \ge 2$.

We provide a geometric viewpoint for $\mathcal{E}_{n,m}^{\mathbf{a}^T}$ and $\mathcal{O}_{\mathbf{a}^T}$ where $\mathbf{a}^T$ is a $(0,1)$ row vector. Let $\omega_{\mathbf{a}^T} := (\omega_0, \ldots, \omega_{n-1})$ where $\omega_i = \mathbf{a}^T P^i \mathbf{a}$ for $i = 0, \ldots, n-1$. We may consider $\mathbf{a}^T$ as a circular sequence. For example, a row vector $(1,1,1,1,0,1,0,0,0,1,0,0,0,0)$ can be expressed as Figure 3.1. Then, for $i \ge 1$, ω_i is the number of pairs $(1,1)$ in

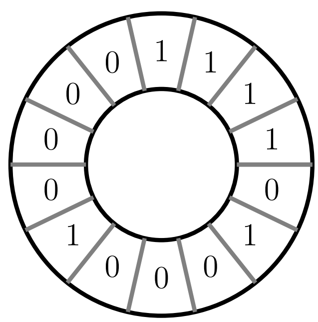


Figure 3.1: A representation of a circular sequence $(1,1,1,1,0,1,0,0,0,1,0,0,0,0)$.

the circular sequence such that there are $i-1$ elements between the pair in either a clockwise or counterclockwise direction. We have several observations. First, $\omega_i = \omega_{n-i}$ for all i. Next, ω_0 is the number of ones in $\mathbf{a}^T$, and $n - \omega_0$ is the number of zeros in $\mathbf{a}^T$. Moreover, $\omega_0 - \omega_1$ is the number of groups consisting of consecutive 1s in the circular sequence; for instance, $\omega_0 - \omega_1 = 6 - 3 = 3$ from the circular sequence in Figure 3.1. Finally, $\mathbf{b}^T \notin \mathcal{O}_{\mathbf{a}^T}$ if and only if a circular sequence corresponding to $\mathbf{b}^T$ cannot be obtained from that corresponding to $\mathbf{a}^T$ by rotations and reflections.

Remark 3.6.13. One can apply the observations above regarding the interpretations of $\omega_0 - \omega_1$ and $\mathbf{b}^T \notin \mathcal{O}_{\mathbf{a}^T}$ to Examples 3.6.10 and 3.6.12, respectively.

Problem 3.6.14. *Let $\mathbf{a}^T$ be a $(0,1)$ row vector of size n, and $\omega_{\mathbf{a}^T} = (\omega_0, \ldots, \omega_{n-1})$. Provide combinatorial interpretations for $\omega_2, \ldots, \omega_{\lfloor \frac{n}{2} \rfloor}$, and bounds on each ω_i for $2 \leq i \leq \lfloor \frac{n}{2} \rfloor$. Develop some algorithms to find a vector $\mathbf{b}^T$ such that $\omega_{\mathbf{a}^T} = \omega_{\mathbf{b}^T}$ and $\mathbf{b}^T \notin \mathcal{O}_{\mathbf{a}^T}$.*

Problem 3.6.15. *We have results by using MATLAB® that for $n \leq 16$ and any $(0,1)$ vector $\mathbf{a}^T$, $|\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n}| \leq 2$ for any $m \leq n$. By increasing n, we are able to find n and m such that $|\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n}| > 2$. From this observation, prove or disprove that $|\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n}| \leq n$. Investigate the relationship between m and $|\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n}|$.*

We shall show an equivalent condition for two circulant matrices to be Gram mates. Spectral properties of circulant matrices can be found in [50]. Let $\varepsilon = e^{\frac{2\pi i}{n}}$. Given an $n \times n$ circulant matrix $C = \mathrm{circ}(\mathbf{c}^T)$ where $\mathbf{c}^T = (c_0, \ldots, c_{n-1})$, n linearly independent eigenvectors can be determined as $\mathbf{x}_\ell^T = \frac{1}{\sqrt{n}}(1, \varepsilon^\ell, \ldots, \varepsilon^{(n-1)\ell})$ for $\ell = 0, \ldots, n-1$. Hence, the unitary matrix $U = \frac{1}{\sqrt{n}}\begin{bmatrix}\mathbf{x}_0 & \cdots & \mathbf{x}_{n-1}\end{bmatrix}$ diagonalises any circulant matrix. Let $f_{\mathbf{c}}(x) := \sum_{i=0}^{n-1} c_i x^i$. Then, the corresponding eigenvalues λ_ℓ are given by $\lambda_\ell = f_{\mathbf{c}}(\varepsilon^\ell)$ for $\ell = 0, \ldots, n-1$.

Proposition 3.6.16. *Let $\mathbf{a}^T$ and $\mathbf{b}^T$ be distinct $(0,1)$ row vectors of size n with m ones. Let $i_0 = j_0 = 0$. Then, $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{b}^T)$ are Gram mates if and only if there are two strictly increasing sequences $(i_1, \ldots, i_m)$ and $(j_1, \ldots, j_m)$ with $0 \leq i_k, j_k \leq n-1$ for $k = 1, \ldots, m$ satisfying the following:*

(i) $a_{i_k} = 1$ *and* $b_{j_k} = 1$ *for* $k = 1, \ldots, m$,

(ii) for $\ell = 0, \ldots, n-1$,

$$\sum_{0 \leq k_1 < k_2 \leq m} \cos\left((i_{k_2} - i_{k_1})\frac{2\pi\ell}{n}\right) = \sum_{0 \leq k_1 < k_2 \leq m} \cos\left((j_{k_2} - j_{k_1})\frac{2\pi\ell}{n}\right).$$

Proof. Let $D_{\mathbf{a}} = \mathrm{diag}(f_{\mathbf{a}}(\varepsilon^0), \ldots, f_{\mathbf{a}}(\varepsilon^{n-1}))$ and $D_{\mathbf{b}} = \mathrm{diag}(f_{\mathbf{b}}(\varepsilon^0), \ldots, f_{\mathbf{b}}(\varepsilon^{n-1}))$. Then, $\mathrm{circ}(\mathbf{a}^T) = UD_{\mathbf{a}}U^*$ and $\mathrm{circ}(\mathbf{b}^T) = UD_{\mathbf{b}}U^*$. Hence, $\mathrm{circ}(\mathbf{a}^T)\mathrm{circ}(\mathbf{a}^T)^T = \mathrm{circ}(\mathbf{b}^T)\mathrm{circ}(\mathbf{b}^T)^T \iff UD_{\mathbf{a}}\bar{D}_{\mathbf{a}}U^* = UD_{\mathbf{b}}\bar{D}_{\mathbf{b}}U^* \iff |f_{\mathbf{a}}(\varepsilon^\ell)| = |f_{\mathbf{b}}(\varepsilon^\ell)|$ for $\ell = 0, \ldots, n-1$. Consider the sequence $(i_1, \ldots, i_m)$ with $0 \leq i_1 < \cdots < i_m \leq n-1$ such that $a_{i_k} = 1$ for $k = 1, \dots, m$. Then, for $\ell = 0, \dots, n-1$,

$$\begin{aligned}
|f_{\mathbf{a}}(\varepsilon^\ell)| &= \left|\sum_{k=1}^{m} \varepsilon^{i_k \ell}\right| \\
&= \left|\sum_{k=1}^{m} \left(\cos\left(i_k \frac{2\pi\ell}{n}\right) + i \sin\left(i_k \frac{2\pi\ell}{n}\right)\right)\right| \\
&= \sqrt{\left(\sum_{k=1}^{m} \cos\left(i_k \frac{2\pi\ell}{n}\right)\right)^2 + \left(\sum_{k=1}^{m} \sin\left(i_k \frac{2\pi\ell}{n}\right)\right)^2} \\
&= \sqrt{m + 2 \sum_{0 \le k_1 < k_2 \le m} \cos\left((i_{k_2} - i_{k_1}) \frac{2\pi\ell}{n}\right)}.
\end{aligned}$$

Similarly, one can find $|f_{\mathbf{b}}(\varepsilon^\ell)|$. From $|f_{\mathbf{a}}(\varepsilon^\ell)| = |f_{\mathbf{b}}(\varepsilon^\ell)|$, the conclusion follows. $\square$

We now consider circulant realizable matrices. Let $\mathbf{e}^T = (e_0, \dots, e_{n-1})$ be a $(0, 1, -1)$ row vector such that $\mathbf{e}^T \mathbf{1} = 0$. Then, $\mathbf{1}^T \mathrm{circ}(\mathbf{e}^T) = 0$ and $\mathrm{circ}(\mathbf{e}^T)\mathbf{1} = 0$. We use $\mathscr{C}^p_{\mathbf{e}^T}$ to denote the set of all pairs of circulant Gram mates via $\mathrm{circ}(\mathbf{e}^T)$. A similar argument as in $\mathscr{C}_{\mathbf{a}^T}$ with $N_{\mathscr{P}_n}(\mathscr{F}_n)$ immediately preceding Example 3.6.10 applies for $\mathscr{C}^p_{\mathbf{a}^T}$ with $N_{\mathscr{P}_n}(\mathscr{F}_n)$. So, we can find that for each $Q \in N_{\mathscr{P}_n}(\mathscr{F}_n)$, there is a bijection between $\mathscr{C}^p_{\mathbf{e}^T}$ and $\mathscr{C}^p_{\mathbf{e}^T Q}$. Hence, $\mathscr{C}^p_{\mathbf{e}^T}$ may be identified as $\mathscr{C}^p_{\mathbf{e}^T Q}$.

Example 3.6.17. Consider $\mathbf{e}^T = (-1, 0, 0, 0, 0, 1, 0, 0, 1, -1, 0, 0)$. Then, $\mathbf{e}^T P = (0, -1, 0, 0, 0, 0, 1, 0, 0, 1, -1, 0)$. We have $\sigma = (1\ 5)(2\ 10)(4\ 8)$ in $\mathrm{Aut}(\mathbb{Z}_{12})$. Then,

$$\mathbf{e}^T P Q_\sigma = (0, 0, -1, 0, 0, -1, 1, 0, 0, 1, 0, 0).$$

Therefore, since $PQ_\sigma \in N_{\mathscr{P}_n}(\mathscr{F}_n)$, the set $\mathscr{C}_{\mathbf{e}^T}$ can be identified as $\mathscr{C}_{\mathbf{e}^T P Q_\sigma}$.

The *characteristic vector* of a subset T of a set U is defined as a vector $(x_u)_{u \in U}$ such that $x_u = 1$ if $u \in T$, and $x_u = 0$ if $u \notin T$. Let $\mathbf{e}^T$ be a $(0, 1, -1)$ row vector of size n. Let $N_0 := \{u \in \mathbb{Z}_n | e_u = 0\}$, $N_+ := \{u \in \mathbb{Z}_n | e_u = 1\}$, and $N_- := \{u \in \mathbb{Z}_n | e_u = -1\}$. We use $\mathbf{e}^T_{N_0}$, $\mathbf{e}^T_{N_+}$, and $\mathbf{e}^T_{N_-}$ to denote the characteristic vectors of the subsets N_0, N_+, and N_-, respectively. Then, $\mathbf{e}^T$ can be written as $\mathbf{e}^T = \mathbf{e}^T_{N_+} - \mathbf{e}^T_{N_-}$.

Theorem 3.6.18. *Let* $\mathbf{e}^T = (e_0, \dots, e_{n-1})$ *be a* $(0, 1, -1)$ *row vector with sum* 0. *Let* $\mathbf{a}^T$ *be a* $(0, 1)$ *row vector. Then,* $\mathrm{circ}(\mathbf{a}^T)$ *and* $\mathrm{circ}(\mathbf{a}^T + \mathbf{e}^T)$ *are Gram mates if and only if there exists a* $(0, 1)$ *vector* $\mathbf{x}^T = (x_0, \dots, x_{n-1})$ *with* $x_u = 0$ *for* $u \in N_+ \cup N_-$ *such that* $\mathbf{a}^T = \mathbf{e}^T_{N_-} + \mathbf{x}^T$ *and* $\mathbf{x}$ *is a solution to the following system:*

$$\mathbf{e}^T (P^i + P^{-i}) \mathbf{x} = -\mathbf{e}^T (P^i \mathbf{e}_{N_+} + P^{-i} \mathbf{e}_{N_-}) \text{ for } i \in \mathbb{Z}_n. \tag{3.6.1}$$

Proof. Suppose that $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{a}^T+\mathbf{e}^T)$ are Gram mates. By Theorem 3.6.8, we have that $\mathbf{a}^T P^i \mathbf{a} = (\mathbf{a}+\mathbf{e})^T P^i (\mathbf{a}+\mathbf{e})$ for $i = 0, \dots, n-1$. Since $\mathbf{a}^T P^i \mathbf{e} = \mathbf{e}^T P^{-i} \mathbf{a}$, we can see that

$$\mathbf{e}^T (P^i + P^{-i}) \mathbf{a} = -\mathbf{e}^T P^i \mathbf{e}. \tag{3.6.2}$$

Since $\mathbf{a}^T$ and $\mathbf{a}^T + \mathbf{e}^T$ are $(0,1)$ vectors, there is a $(0,1)$ vector $\mathbf{x}^T = (x_0, \dots, x_{n-1})$ with $x_u = 0$ for $u \in N_+ \cup N_-$ such that $\mathbf{a}^T = \mathbf{e}_{N_-}^T + \mathbf{x}^T$. Setting $\mathbf{a} = \mathbf{e}_{N_-} + \mathbf{x}$ and $\mathbf{e} = \mathbf{e}_{N_+} - \mathbf{e}_{N_-}$ in (3.6.2) and simplifying yield (3.6.1).

The converse is straightforward. $\square$

Remark 3.6.19. From $\mathbf{e}^T = \mathbf{e}_{N_+}^T - \mathbf{e}_{N_-}^T$, the right side $-\mathbf{e}^T(P^i \mathbf{e}_{N_+} + P^{-i}\mathbf{e}_{N_-})$ of the equation in (3.6.1) can be written as $-\mathbf{e}_{N_+}^T P^i \mathbf{e}_{N_+} + \mathbf{e}_{N_-}^T P^i \mathbf{e}_{N_-}$ for $0 \le i \le n-1$. Since $P^{-i} = HP^iH$, we have that $-\mathbf{e}_{N_+}^T P^i \mathbf{e}_{N_+} + \mathbf{e}_{N_-}^T P^{-i} \mathbf{e}_{N_-} = 0$ if and only if $\mathbf{e}_{N_+}^T P^i \mathbf{e}_{N_+} = \mathbf{e}_{N_-}^T H P^i H \mathbf{e}_{N_-}$. Therefore, by Theorem 3.6.8, the linear system (3.6.1) is homogeneous if and only if $\mathrm{circ}(\mathbf{e}_{N_+}^T)$ and $\mathrm{circ}(\mathbf{e}_{N_-}^T H)$ are Gram mates.

Remark 3.6.20. Maintaining the notation of Theorem 3.6.18, consider the linear system (3.6.1). Given any $(0,1)$ vector $\mathbf{x}^T = (x_0, \dots, x_{n-1})$ with $x_u = 0$ for $u \in N_+ \cup N_-$, we have $\mathbf{e}^T \mathbf{x} = 0$. Since $\mathbf{e}_{N_+}^T \mathbf{e}_{N_-} = 0$, we obtain $\mathbf{e}^T(\mathbf{e}_{N_+} + \mathbf{e}_{N_-}) = 0$. So, the equation for $i = 0$ in (3.6.1) holds for $\mathbf{x}$. Furthermore, examining (3.6.2) in the proof of that theorem, we find that the equation for $i = k$ in (3.6.1) is equivalent to that for $i = -k$. Let S be the characteristic matrix of the partition of N_0 each cell of which is a singleton. Then, considering the condition that $x_u = 0$ where $u \in N_+ \cup N_-$, the coefficient matrix of the linear system (3.6.1) can be simplified as

$$\begin{bmatrix} \mathbf{e}^T(P + P^{-1}) \\ \vdots \\ \mathbf{e}^T(P^{\lfloor \frac{n}{2} \rfloor} + P^{-\lfloor \frac{n}{2} \rfloor}) \end{bmatrix} S. \tag{3.6.3}$$

Let $\mathbf{e}^T$ be a $(0,1,-1)$ row vector with the row sum 0. The coefficient matrix of the linear system (3.6.1) is denoted by $M_{\mathbf{e}}$, and the matrix (3.6.3) by $\widetilde{M}_{\mathbf{e}}$.

Proposition 3.6.21. *Let $\mathbf{e}^T$ be a $(0,1,-1)$ row vector with the row sum 0. Suppose $\mathbf{e}^T H = -\mathbf{e}^T$. If there exists a $(0,1)$ vector $\mathbf{x}^T = (x_0, \dots, x_{n-1})$ with $x_u = 0$ for $u \in N_+ \cup N_-$ such that $\mathbf{x}^T H = \mathbf{x}^T$, then $\mathrm{circ}(\mathbf{a}^T)$ and $\mathrm{circ}(\mathbf{a}^T + \mathbf{e}^T)$ are Gram mates where $\mathbf{a} = \mathbf{e}_{N_-} + \mathbf{x}$.*

Proof. Since $(\mathbf{e}_{N_+}^T - \mathbf{e}_{N_-}^T)H = -(\mathbf{e}_{N_+}^T - \mathbf{e}_{N_-}^T)$, we have $\mathbf{e}_{N_+}^T H = \mathbf{e}_{N_-}^T$ and $\mathbf{e}_{N_-}^T H = \mathbf{e}_{N_+}^T$. By Remark 3.6.19, we have $\mathbf{e}^T(P^i \mathbf{e}_{N_+} + P^{-i}\mathbf{e}_{N_-}) = 0$ for $0 \le i \le n-1$. Since

$\mathbf{e}^T P^{-i} = -\mathbf{e}^T H P^{-i} = -\mathbf{e}^T P^i H$ for $0 \le i \le n-1$, we have

$$M_{\mathbf{e}} = L - LH, \text{ where } L = \begin{bmatrix} \mathbf{e}^T P^0 \\ \vdots \\ \mathbf{e}^T P^{n-1} \end{bmatrix}.$$

Hence, $H\mathbf{x} = \mathbf{x}$ implies $M_{\mathbf{e}}\mathbf{x} = 0$. By Theorem 3.6.18, we obtain the desired result. $\square$

Example 3.6.22. Continuing Example 3.6.17, we have

$$\mathbf{f}^T = \mathbf{e}^T P Q_\sigma = (0, 0, -1, 0, 0, -1, 1, 0, 0, 1, 0, 0).$$

Since $\mathbf{f}^T H = -\mathbf{f}$, we have $\mathbf{f}_{N_+}^T H = \mathbf{f}_{N_-}^T$ and $\mathbf{f}_{N_-}^T H = \mathbf{f}_{N_+}^T$. From Remark 3.6.19, the linear system 3.6.1 with respect to $\mathbf{f}^T$ is homogeneous. Furthermore,

$$\widetilde{M}_{\mathbf{f}} = \begin{bmatrix} 0 & -1 & -1 & -1 & 1 & 1 & 1 & 0 \\ -1 & 0 & -1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 1 & -1 & 0 & -1 & 1 \\ 2 & 0 & 2 & 0 & 0 & -2 & 0 & -2 \end{bmatrix}.$$

Direct computation yields the following basis of the null space of $\widetilde{M}_{\mathbf{f}}$:

$$\left\{ \begin{bmatrix} -1 \\ -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ -1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\}.$$

We can see from this example that the converse of Proposition 3.6.21 does not hold.

3.7 Gram mates via orthogonal matrices

Let A and B be Gram mates. Note that $A \neq B$. By Proposition 3.2.1, there exists an orthogonal matrix Q such that $B = QA$. Inspired by the approach that for a given realizable matrix E we have analyzed Gram mates A and $A+E$, we consider the following question: given an orthogonal matrix Q, how can we obtain Gram mates A and B such that $B = QA$? Here Q plays a similar role as E in the sense that B is obtained from A by pre-multiplying by Q, while by adding to E.

Definition 3.7.1. Let Q be an orthogonal matrix. Zero-one matrices A and B are said to be *Gram mates via an orthogonal matrix* Q if $B = QA$, $AA^T = QAA^TQ^T$, and $A \neq QA$.

Remark 3.7.2. Let A and B be distinct $(0,1)$ matrices such that $B = QA$ for some orthogonal matrix Q. Then, $A^TA = B^TB$. So, it suffices to check if $AA^T = QAA^TQ^T$ for A and B being Gram mates via Q.

Remark 3.7.3. We have a basic observation that if A and QA are Gram mates for some orthogonal matrix Q, then necessarily each column of QA has the same number of ones as the corresponding column of A does.

Let Q be an orthogonal matrix. In order to find Gram mates A and AQ, we necessarily consider the condition that AQ is a $(0,1)$ matrix. However, since Q is a real matrix, it is not easy to find information about the structure of the $(0,1)$ matrix A (while a realizable matrix E provides such information that can be developed into the systematic method to obtain Gram mates via E in [44]). Here we indirectly approach our original question by generalising the notion of Gram mates via Q. We shall consider *Gram mates via unitary matrices*—an analogous definition holds as in Definition 3.7.1—since we can obtain further information by checking if the sum of complex numbers is either 0 or 1.

In the remaining of this subsection, we assume that sub-indices indicating positions of entries in matrices or vectors are in $\mathbb{Z}_n = \{0, \dots, n-1\}$, where n is appropriately given according to the number of rows or columns in the context.

We shall narrow our focus to a family of particular unitary matrices. Consider a *discrete Fourier transform matrix (DFT matrix)* [38] defined as

$$U = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \varepsilon & \varepsilon^2 & \cdots & \varepsilon^{n-1} \\ 1 & \varepsilon^2 & \varepsilon^4 & \cdots & \varepsilon^{2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \varepsilon^{n-1} & \varepsilon^{2(n-1)} & \cdots & \varepsilon^{(n-1)^2} \end{bmatrix}$$

where $\varepsilon = e^{\frac{2\pi i}{n}}$. We now investigate Gram mates via a DFT matrix. Suppose that

A and UA are Gram mates. Then, $U\mathbf{a}$ is a $(0, 1)$ vector for each column $\mathbf{a}$ of A. If $\mathbf{a}$ is the zero vector, so is $U\mathbf{a}$. If $\mathbf{a}$ is a non-zero vector, then since the first row of U is $\frac{1}{\sqrt{n}}\mathbf{1}^T$, $\mathbf{a}$ contains exactly $\sqrt{n}$ ones and n must be a perfect square. From Remark 3.7.3, $U\mathbf{a}$ also contains $\sqrt{n}$ ones.

The set of all n^{th} roots of unity forms a group under multiplication, and it is isomorphic to $\mathbb{Z}_n$ [28]. We may regard ε as a generator 1 of the group $\mathbb{Z}_n$. The order of each element x in $\mathbb{Z}_n$ is $\frac{n}{\gcd(x,n)}$. This implies that the number of 1's in j^{th} row of $\sqrt{n}U$ for $1 \leq j \leq n-1$ is $\gcd(j, n)$. Hence, if $\mathbf{e}_{j_0}^T U\mathbf{a} = 1$ for some $1 \leq j_0 \leq n-1$, then $\mathbf{e}_{j_0}^T U$ contains at least $\sqrt{n}$ ones in order that A and UA are Gram mates, and so $\gcd(j_0, n) \geq \sqrt{n}$.

Lemma 3.7.4. *Let $n \geq 2$ and $\varepsilon = e^{\frac{2\pi i}{n}}$. For $1 \leq k \leq n-1$, $\sum_{j=0}^{n-1} \varepsilon^{kj} = 0$.*

Proof. Considering the telescoping sums, we have

$$(1-\varepsilon^k)\sum_{j=0}^{n-1}\varepsilon^{kj} = \sum_{j=0}^{n-1}\varepsilon^{kj} - \sum_{j=1}^{n}\varepsilon^{kj} = \varepsilon^0 - \varepsilon^{kn} = 0.$$

Since $1 - \varepsilon^k \neq 0$, our desired result is obtained. □

The following trivial result is a benefit we can obtain in that DFT matrices are unitary.

Lemma 3.7.5. *Let k be a positive integer, and let $z_1, \ldots, z_k \in \mathbb{C}$. Suppose that $|z_1| = \cdots = |z_k| = 1$. If $z_1 + \cdots + z_k = k$, then $z_1 = \cdots = z_k = 1$.*

Proposition 3.7.6. *Let n be a perfect square, and U be the $n \times n$ DFT matrix. Suppose that $\ell = |\{j | 1 \leq j \leq n,\ \gcd(j, n) \geq \sqrt{n}\}|$ and $\ell_1 = |\{j | 1 \leq j \leq \sqrt{n} - 1,\ \gcd(j, n) = 1\}|$. Assume that $\ell - \ell_1 < \sqrt{n}$. Then, $AA^T = UAA^TU^T$ if and only if $A = UA$ and each column of A is either the zero vector or $\mathbf{1}_{\sqrt{n}} \otimes \mathbf{x}$ where $\mathbf{x} = (1, 0, \ldots, 0)^T$ and $\mathbf{x}$ is of size $\sqrt{n}$. In other words, there is no pair of Gram mates via U.*

Proof. Suppose that A and UA are Gram mates. If $\gcd(m, n) = \sqrt{n}$ for some $1 \leq m \leq n$, then $m = s\sqrt{n}$ for some $1 \leq s \leq \sqrt{n} - 1$ with $\gcd(s, n) = 1$. Hence, there are exactly ℓ_1 rows in U such that each of them contains precisely $\sqrt{n}$ ones in positions $k\sqrt{n}$ for $0 \leq k \leq \sqrt{n} - 1$. Then, $\ell - \ell_1 = |\{j | 1 \leq j \leq n,\ \gcd(j, n) > \sqrt{n}\}|$.

Let $\mathbf{a}$ be a non-zero column of A. Then, $\mathbf{a}$ and $U\mathbf{a}$ contain exactly $\sqrt{n}$ ones. Consider the indices $j_1, \ldots, j_{\sqrt{n}}$ such that $\mathbf{e}_{j_1}^T U\mathbf{a} = \cdots = \mathbf{e}_{j_{\sqrt{n}}}^T U\mathbf{a} = 1$. Since $\ell - \ell_1 < \sqrt{n}$, there must be an index j_k for some $1 \leq k \leq \sqrt{n}$ such that $\gcd(j_k, n) = \sqrt{n}$, that is, $\mathbf{e}_{j_k}^T U$ is one of the ℓ_1 rows with precisely $\sqrt{n}$ ones in positions $k\sqrt{n}$ for $0 \le k \le \sqrt{n}-1$. Since $\mathbf{e}_{j_k}^T U\mathbf{a} = 1$, by Lemma 3.7.5 we have $\mathbf{a} = \mathbf{1}_{\sqrt{n}} \otimes \mathbf{x}$.

For $j = 0, \ldots, n-1$, we have

$$\begin{aligned}
\mathbf{e}_j^T U\mathbf{a} &= \frac{1}{\sqrt{n}}\left(\varepsilon^{0\sqrt{n}j} + \varepsilon^{\sqrt{n}j} + \varepsilon^{2\sqrt{n}j} + \cdots + \varepsilon^{(\sqrt{n}-1)\sqrt{n}j}\right) \\
&= \frac{1}{\sqrt{n}}\left(1 + \left(e^{\frac{2\pi i}{\sqrt{n}}}\right)^j + \left(e^{2\frac{2\pi i}{\sqrt{n}}}\right)^j + \cdots + \left(e^{(\sqrt{n}-1)\frac{2\pi i}{\sqrt{n}}}\right)^j\right).
\end{aligned}$$

If $j \equiv 0 \pmod{\sqrt{n}}$, we have $\mathbf{e}_j^T U\mathbf{a} = 1$. Otherwise, by Lemma 3.7.4 we obtain $\mathbf{e}_j^T U\mathbf{a} = 0$. Hence, $U\mathbf{a} = \mathbf{a}$. If $\mathbf{a}$ is the zero vector, so is $U\mathbf{a}$. Therefore, $A = UA$.

The converse is straightforward. □

Corollary 3.7.7. *Let n be a perfect square, and $\sqrt{n}$ be prime. Let U be the $n \times n$ DFT matrix. Then, there is no pair of Gram mates via U.*

Problem 3.7.8. *Given a unitary (or an orthogonal) matrix U, develop a systematic way to find Gram mates via U.*

Problem 3.7.9. *Let n be a perfect square, and U be the $n \times n$ DFT matrix. Suppose that $|\{j | 1 \le j \le n,\ \gcd(j,n) > \sqrt{n}\}| \ge \sqrt{n}$. Characterize Gram mates via U.*

4

Fiedler vectors with unbalanced sign patterns

This chapter is based on a study of spectral properties of the Laplacian matrix of a graph. We consider the signs of the entries in a Fiedler vector $\mathbf{x}$ of a graph G that is an eigenvector associated to the algebraic connectivity $\alpha(G)$. Recall that $i(\mathbf{x}) = \min\{|\{x_j|x_j > 0\}|, |\{x_j|x_j < 0\}|\}$ and $i(G) = \min_{\mathbf{x}\neq 0}\{i(\mathbf{x})|\ \mathbf{x}$ is a Fiedler vector of $G\}$. Furthermore, the join of graphs and its spectral property are used a lot, so we refer the reader to Section 2.3 for a review.

This chapter is a slight rewording of work with Kirkland accepted for publication [42].

4.1 Introduction

When does spectral bisection work well? The graph partitioning problem, which has applications in scientific computing [57] and VLSI layout [62], is to partition a graph into k subgraphs each of which is similar in size while minimizing the number of edges between each pair of components; even though finding the optimal solution to the problem is an NP-complete problem, spectral bisection is a method to approximately solve the problem. Regarding the robustness of spectral bisection, [64] shows that the technique works well on some classes of particular graphs. On the other hand, [68] provides the result about the maximal error in spectral bisection with respect to the minimal cut while partition sizes are the same.

In contrast to [68], we shall investigate if spectral bisection is a robust technique by considering the partition sizes. The paper [67] of Urschel and Zikatanov provides a generalisation of the work of Miroslav Fiedler [32] with respect to spectral bisection. Specifically, [67] proves the existence of a Fiedler vector such that two induced subgraphs on the two sets of vertices valuated by non-negative signs and positive signs, respectively, are connected. If all Fiedler vectors of a graph G have a sign pattern such that a few vertices are valuated by one sign and possibly 0, and the others are valuated by the other sign, then spectral bisection provides an inadequate partition regarding the graph partitioning problem. This chapter examines such graphs and their properties.

In Section 4.2 we find equivalent conditions for G to have $i(G) = 1$ (Theorem 4.2.8). In Section 4.3, all graphs G with $i(\mathbf{x}) = 1$ for all Fiedler vectors $\mathbf{x}$ are characterized by studying minimum values of $am(\alpha(G))$, according to the number of vertices with minimum degree (Theorem 4.3.19). Furthermore, we characterize the graphs for which the sign patterns of all Fiedler vectors are extremely unbalanced (Theorem 4.3.22). In Section 4.4, threshold graphs with $i(G) = 1$ and graphs with three distinct Laplacian eigenvalues and $i(G) = 1$ are described. Section 4.5 provides a characterization of all regular graphs G with $i(G) = 2$ by investigating sign patterns of eigenvectors corresponding to the least adjacency eigenvalue of the complement of G (Theorem 4.5.14).

4.2 Characterization of graphs with $i(G) = 1$

Proposition 4.2.1. *Let G be a graph of order $n \geq 2$. Then, G is disconnected if and only if $i(G) = 0$.*

Proof. Suppose that G is disconnected. Then, $\alpha(G) = 0$. So, the all ones vector is a Fiedler vector of G. Hence, $i(G) = 0$. Conversely, assume that $i(G) = 0$. Then there exists a non-negative Fiedler vector $\mathbf{x}$. Since $L(G)\mathbf{x} = \alpha(G)\mathbf{x}$, $\mathbf{1}^T L(G)\mathbf{x} = \alpha(G)\mathbf{1}^T\mathbf{x}$ and it follows that $\alpha(G) = 0$. Hence, G is disconnected. □

For a graph G of order 1, we have $i(G) = 0$, but G is connected. So, if G is a graph on n vertices where $n \geq 2$, then $i(G) > 0$ implies that G is connected.

Lemma 4.2.2. *Let G be a non-complete graph of order $n \geq 3$. If $i(G) = 1$, then $\alpha(G) = \delta(G)$.*

Proof. Let $\mathbf{x}$ be a Fiedler vector with $i(\mathbf{x}) = 1$, and we may suppose that $x_1 < 0$. We have $(L(G) - \alpha(G)I)\mathbf{x} = 0$, and considering the first entry, we find that $(\ell_{11} - \alpha(G))x_1 + \sum_{k\neq 1} \ell_{1k}x_k = 0$. Since $x_1 < 0$, $\ell_{1k} \leq 0$ and $x_k \geq 0$ for all $k \neq 1$, it must be the case that $\ell_{11} \leq \alpha(G)$. Hence $\alpha(G) \geq \delta(G)$, and since G is non-complete, $\alpha(G) \leq \delta(G)$. We deduce that $\alpha(G) = \delta(G)$. □

Example 4.2.3. Consider the complete graph K_n. Then, $(1, -1, 0, \ldots, 0)^T$ is an eigenvector of $\alpha(K_n) = n$ and by Proposition 4.2.1, $i(K_n) = 1$. Moreover, $\alpha(G) > \delta(G) = n - 1$.

Now, we shall characterize non-complete connected graphs G with $\alpha(G) = \delta(G)$. A characterization of graphs for which $\alpha(G) = v(G)$ appears in [45]: for a non-complete, connected graph G on n vertices, $\alpha(G) = v(G)$ if and only if there exists a disconnected graph G_1 on $n - v(G)$ vertices and a graph G_2 on $v(G)$ vertices with $\alpha(G_2) \geq 2v(G) - n$ such that $G = G_1 \vee G_2$. Since $\alpha(G) \leq v(G) \leq \delta(G)$, if $\alpha(G) = \delta(G)$, then $\alpha(G) = v(G) = \delta(G)$. So, we begin with a join of a disconnected graph G_1 on $n - \delta(G)$ vertices and a graph G_2 on $\delta(G)$ vertices with $\alpha(G_2) \geq 2\delta(G) - n$.

Lemma 4.2.4. *Let G be a non-complete, connected graph of order $n \geq 3$. Then, $\alpha(G) = \delta(G)$ if and only if G can be expressed as a join of G_1 and G_2 where the graph G_1 on $n - \delta(G)$ vertices has an isolated vertex, and G_2 is a graph on $\delta(G)$ vertices, and $\alpha(G_2) \geq 2\delta(G) - n$.*

Proof. Suppose that $\alpha(G) = \delta(G)$. We will establish the desired conclusion by induction. For order 3, there is only one graph, $N_1 \vee N_2$, that is non-complete and connected; its algebraic connectivity is equal to the minimum degree and it has the desired structure. Let $n \geq 4$. Suppose that a graph G of order n with $\alpha(G) = \delta(G)$ is non-complete and connected. Since $\alpha(G) = v(G) = \delta(G)$, G is expressed as $G_1 \vee G_2$ where G_1 is a disconnected graph of order $n - \delta(G)$, and G_2 is a graph of order $\delta(G)$ with $\alpha(G_2) \geq 2\delta(G) - n$. We have $\deg_G(v) \geq \delta(G)$ for $v \in V(G_1)$ and $\deg_G(w) \geq n - \delta(G)$ for $w \in V(G_2)$. If G_1 has an isolated vertex, we are done. Suppose that G_1 has no isolated vertex. Since $\delta(G_1) > 0$, we have $\deg_G(v) > \delta(G)$ for all $v \in V(G_1)$. So, there exists a vertex $w \in V(G_2)$ such that

$$\deg_G(w) = \deg_{G_2}(w) + (n - \delta(G)) = \delta(G), \text{ and } \deg_{G_2}(w) = \delta(G_2).$$

Since $\deg_{G_2}(w) \geq 0$, we obtain $n - \delta(G) \leq \delta(G)$.

Suppose that $n - \delta(G) = \delta(G)$. Then, $\deg_{G_2}(w) = 0$ so that G_2 has an isolated vertex. Since G_1 is disconnected, $\alpha(G_1) = 0$. Moreover, $\delta(G) = \frac{n}{2}$. By exchanging the roles of G_1 and G_2, we obtain the desired description of G.

Assume that $n - \delta(G) < \delta(G)$. Note that $\delta(G_2) = 2\delta(G) - n$. Since $\alpha(G_2) \geq 2\delta(G) - n$, we obtain $\alpha(G_2) \geq \delta(G_2)$. Suppose that $\delta(G_2) = \delta(G) - 1$. Then, we have $\delta(G) = n - 1$, which contradicts the non-completeness of G. Therefore, G_2 is a non-complete, connected graph of order $\delta(G)$ with $\alpha(G_2) = \delta(G_2)$. By induction, there exists a graph H_1 of order $\delta(G) - \delta(G_2)$ with an isolated vertex and a graph H_2 of order $\delta(G_2)$ such that $G_2 = H_1 \vee H_2$ and $\alpha(H_2) \geq 2\delta(G_2) - \delta(G)$. Hence, $G = G_1 \vee H_1 \vee H_2$. Consider $G_1 \vee H_2$ of order $n - \delta(G) + \delta(G_2)$. Since $\delta(G_2) = 2\delta(G) - n$, the order of $G_1 \vee H_2$ is $\delta(G)$. Furthermore, G_1 is disconnected so that $\alpha(G_1 \vee H_2)$ is either $\delta(G_2)$ or $\alpha(H_2) + n - \delta(G)$. Considering $\alpha(H_2) \geq 2\delta(G_2) - \delta(G)$, it follows that $\alpha(H_2) + n - \delta(G) \geq \delta(G_2)$. So, $\alpha(G_1 \vee H_2) = \delta(G_2) = 2\delta(G) - n$. Therefore, G can be expressed as a join of H_1 and $G_1 \vee H_2$.

Conversely, suppose that G_1 is a graph of order $n - k$ with an isolated vertex where $1 \leq k \leq n - 2$, and G_2 is a graph of order k with $\alpha(G_2) \geq 2k - n$. Since $\alpha(G_2) + n - k \geq k$, we have $\alpha(G_1 \vee G_2) = k$. Let v be an isolated vertex in G_1. Then, $\deg_G(v) = k$. So, $\delta(G) \leq k = \alpha(G)$ implies $\delta(G) = \alpha(G)$. □

Remark 4.2.5. If G is a non-complete connected graph on n vertices, we have $\delta(G) < n - 1$. So, G_1 in Lemma 4.2.4 is of order at least 2. However, G_2 can consist of a single vertex v. Then, the vertex v is a cut-vertex of G, and also a dominating vertex in G.

Considering the fact that $|V(G_1)| \geq 2$ and $G = G_1 \vee G_2$, there is no cut-vertex of G in G_1. Moreover, if G_2 contains a cut-vertex of G, $|V(G_2)| = 1$. Therefore, if $i(G) = 1$, then G has at most one cut-vertex.

Lemma 4.2.6. *Let G be a non-complete, connected graph of order n. Suppose that G can be expressed as a join of G_1 and G_2 where the graph G_1 on $n - \delta(G)$ vertices has an isolated vertex v, G_2 is a graph on $\delta(G)$ vertices, and $\alpha(G_2) \geq 2\delta(G) - n$. Then, $i(G) = 1$.*

Proof. There exists an eigenvector $\mathbf{x}$ corresponding to $\alpha(G)$ where entries corresponding to vertices in G_1 except v are all ones, the entry for v is $-(|V(G_1)| - 1)$ and zeros elsewhere. Therefore, $i(G) = 1$. □

Corollary 4.2.7. *Let G be a non-complete, connected graph. There exists a cut-vertex v and $i(G) = 1$ if and only if v is a dominating vertex that is adjacent to a pendent vertex, that is, $G = (G - v) \vee \{v\}$ where $G - v$ is disconnected, and has an isolated vertex.*

Proof. Suppose that v is a cut-vertex in G and that $i(G) = 1$. By Remark 4.2.5, G is expressed as $G_1 \vee G_2$ where G_1 contains an isolated vertex w and $G_2 = \{v\}$. It is straightforward that v is a dominating vertex and is adjacent to w, which is a pendent vertex.

Conversely, suppose that $v \in V(G)$ is a dominating vertex and is adjacent to a pendent vertex w. Let $G_1 = G - v$ and $G_2 = \{v\}$. Then, w is an isolated vertex in G_1 and $G = G_1 \vee G_2$. By Lemma 4.2.6, we have the desired result. □

Thus, the following theorem is obtained by Lemmas 4.2.2, 4.2.4 and 4.2.6.

Theorem 4.2.8. *Let G be a non-complete, connected graph of order n. Then, the following are equivalent:*

(i) $i(G) = 1$,

(ii) $\alpha(G) = \delta(G)$,

(iii) G can be written as a join of G_1 and G_2 where the graph G_1 on $n - \delta(G)$ vertices has an isolated vertex, G_2 is a graph on $\delta(G)$ vertices, and $\alpha(G_2) \geq 2\delta(G) - n$.

Problem 4.2.9. *In order for a connected graph G to have $i(G) = 1$, G must be expressed as a join of two graphs. Then, G might be regarded as a highly structured graph so that G could be rarely seen in empirical settings. From this speculation, find bounds on the probability of a connected graph G to have $i(G) = 1$. By extension, one could pose a question as follows: given $\varepsilon > 0$, find the probability of a random graph of order n to have $\frac{i(G)}{n} < \varepsilon$, e.g., one could consider graphs in the Erdös–Rényi random graph model.*

Proposition 4.2.10. *Suppose that G is a connected graph of order $n \geq 3$ and $i(G) \neq 1$. Then, we can construct a graph G' such that $i(G') = 1$ and G is an induced subgraph of G' by adding one vertex or two vertices and joining them to some vertices of G. In particular, we need only one vertex if G is a join. Otherwise, we need two vertices.*

Proof. Suppose that G can be expressed as a join of two graphs, say H_1 of order n_1 and H_2 of order n_2 where $n_1 \geq n_2$. Let G' be $(\{v\} + H_1) \vee H_2$ for a new vertex v. Then, $\delta(G') = n_2$. Since $\alpha(G') = \min\{n_2, a(H_2) + n_1\}$, we have $\delta(G') = \alpha(G')$, and $i(G') = 1$.

Assume that G is not a join of some graphs. Let $H_1 = \{v\} + G$ and $H_2 = \{w\}$ where $v \neq w$. Consider $G' = H_1 \vee H_2$. Since H_1 contains an isolated vertex and $\alpha(H_2) = 0 \geq 2\delta(G') - n$, by Theorem 4.2.8, $i(G') = 1$. It remains to show that every graph H obtained from a graph G by adding just one new vertex v and joining it to some vertices does not satisfy $i(H) = 1$. Suppose to the contrary that there exists such a graph H with $i(H) = 1$. By Theorem 4.2.8 and Remark 4.2.5, H is expressed as a join of two graphs G_1 and G_2 where G_1 has an isolated vertex and $|V(G_1)| \geq 2$. Suppose that the new vertex v is in G_1. Since $|V(G_1)| \geq 2$, a removal of v in H results in the graph G that is a join of some graphs, a contradiction. Hence, $v \in V(G_2)$. Furthermore, $G_2 = \{v\}$, for otherwise, G would be written as a join of some graphs. Thus, $G = G_1$ and so G is disconnected. This contradicts the hypothesis that G is connected. Therefore, we need to add at least two vertices; adding two vertices, we obtain a connected graph G' with the desired properties. $\square$

4.3 Algebraic multiplicity of the algebraic connectivity of a graph with $i(G) = 1$

Recall that $i(\mathbf{x})$ is defined as the minimum number of negative components in $\mathbf{x}$ or $-\mathbf{x}$.

Example 4.3.1. Let $G_1 = K_2 + N_1$ and $G_2 = N_1 \vee N_3$. Since G_1 has an isolated vertex and $\alpha(G_2) = 2\delta(G_1 \vee G_2) - 7$, we have $i(G_1 \vee G_2) = 1$ by Theorem 4.2.8. Furthermore, $\alpha(G_1 \vee G_2) = 4$ and $am(\alpha(G_1 \vee G_2)) = 3$. Labelling vertices in order of $V(G_1)$ and $V(G_2)$, there are three linearly independent Fiedler vectors corresponding to $\alpha(G_1 \vee G_2)$:

$$\mathbf{x}_1^T = (1, 1, -2, 0, 0, 0, 0),\ \mathbf{x}_2^T = (0, 0, 0, 0, 1, -1, 0),\ \text{and}\ \mathbf{x}_3^T = (0, 0, 0, 0, 1, 0, -1).$$

Therefore, $i(\mathbf{x}_1 + \mathbf{x}_2) = 2$ and $i(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3) = 3$.

Let G be a non-complete graph of order n with $i(G) = 1$. So, G can be written as $G = G_1 \vee G_2$ where the graph G_1 on $n - \delta(G)$ vertices contains an isolated vertex, and G_2 is a graph on $\delta(G)$ vertices with $\alpha(G_2) \geq 2\delta(G) - n$. We observe from Example 4.3.1 that if $\alpha(G_2) = 2\delta(G) - n$, then $am(\alpha(G_2))$ must be considered to compute $am(\alpha(G))$. Let $\beta(H)$ denote the number of connected components in a graph H. Since the algebraic multiplicity of the eigenvalue 0 of G_1 is $\beta(G_1)$, by considering $G = G_1 \vee G_2$, we have

$$am(\alpha(G)) = \begin{cases} \beta(G_1) - 1 + am(\alpha(G_2)), & \text{if } \alpha(G_2) = 2\delta(G) - n, \\ \beta(G_1) - 1, & \text{if } \alpha(G_2) > 2\delta(G) - n. \end{cases} \tag{4.3.1}$$

Moreover, from Example 4.3.1, we see that for a non-complete connected graph G the condition that $i(G) = 1$ and $am(\alpha(G)) > 1$ does not guarantee that $i(\mathbf{x}) = 1$ for every Fiedler vector $\mathbf{x}$.

Proposition 4.3.2. *Let G be a non-complete graph of order n and $i(G) = 1$. Suppose that $G \neq N_3 \vee G'$ for any graph G' with $\alpha(G') > 2\delta(G) - n$. Then, $am(\alpha(G)) > 1$ if and only if there exists a Fiedler vector $\mathbf{x}$ such that $i(\mathbf{x}) > 1$.*

Proof. Suppose that $am(\alpha(G)) > 1$. Since $i(G) = 1$, there are graphs G_1 and G_2 such that $G = G_1 \vee G_2$ where the graph G_1 on $n - \delta(G)$ vertices contains an isolated vertex and G_2 is a graph of order $\delta(G)$ with $\alpha(G_2) \geq 2\delta(G) - n$. Assume that $\alpha(G_2) > 2\delta(G) - n$. From (4.3.1), we find that there are at least three connected components in G_1. Since $G_1 \neq N_3$, $|V(G_1)| \geq 4$. Choose two components H_1 and H_2 of G_1 such that H_1 and H_2 are the smallest and second smallest orders in G_1. Then, $H_1 = N_1$. Labelling vertices in order of $V(H_1)$, $V(H_2)$, $V(G_1)\backslash(V(H_1) \cup V(H_2))$ and $V(G_2)$, there exists a Fiedler vector

$$\mathbf{x}^T = \begin{bmatrix} -1 & -(\frac{|V(G_1)|-|V(H_1)|-|V(H_2)|-1}{|V(H_2)|})\mathbf{1}^T_{|V(H_2)|} & \mathbf{1}^T_{|V(G_1)|-|V(H_1)|-|V(H_2)|} & \mathbf{0}^T_{|V(G_2)|} \end{bmatrix}.$$

Then, $\mathbf{x}$ and $-\mathbf{x}$ have $|V(H_1)| + |V(H_2)|$ and $|V(G_1)| - |V(H_1)| - |V(H_2)|$ negative components, respectively. It is clear that $|V(H_1)| + |V(H_2)| \geq 2$. Since $G_1 \neq N_3$ and H_1 and H_2 are the components of the smallest and second smallest orders in G_1, we have $|V(G_1)| - |V(H_1)| - |V(H_2)| \geq 2$. Therefore, $i(\mathbf{x}) \geq 2$.

Suppose that $\alpha(G_2) = 2\delta(G) - n$. Let v be an isolated vertex in G_1. Then, we have a Fiedler vector $\mathbf{x}_1 = \begin{bmatrix} \mathbf{1}_{|V(G_1)|} - |V(G_1)|\mathbf{e}_v \\ \mathbf{0}_{|V(G_2)|} \end{bmatrix}$ where $|V(G_1)| \geq 2$. Choose an eigenvector $\mathbf{y}$ corresponding to $\alpha(G_2)$ such that $\mathbf{y}^T\mathbf{1} = 0$ and $i(\mathbf{y}) > 0$. Since $\alpha(G_2) = 2\delta(G) - n$, $\mathbf{x}_2 = \begin{bmatrix} \mathbf{0}_{|V(G_1)|} \\ \mathbf{y} \end{bmatrix}$ is a Fiedler vector of G. Then, $i(\mathbf{x}_1 + \mathbf{x}_2) > 1$.

Suppose that there is a Fiedler vector $\mathbf{x}$ such that $i(\mathbf{x}) > 1$. By hypothesis, there is a Fiedler vector $\mathbf{x}'$ such that $i(\mathbf{x}') = 1$. Evidently, $\mathbf{x}'$ is not a scalar multiple of $\mathbf{x}$, so those two vectors are linearly independent. Hence, $am(\alpha(G)) \geq 2$. $\square$

Proposition 4.3.2 establishes that the condition that $i(G) = 1$ and $am(\alpha(G)) = 1$ forces any Fiedler vector $\mathbf{x}$ to have $i(\mathbf{x}) = 1$. Moreover, the set of all graphs G such that $am(\alpha(G)) > 1$ and $i(\mathbf{x}) = 1$ for all Fiedler vectors $\mathbf{x}$ is

$$\{N_3 \vee G' | G' \text{ is a graph with } \alpha(G') > 2\delta(N_3 \vee G') - |V(N_3 \vee G')|\}.$$

We will characterize graphs with $i(G) = 1$ and $am(\alpha(G)) = 1$ by studying the relation between $am(\alpha(G))$ and the number of vertices of degree $\delta(G)$. Before presenting the characterization, lower bounds on $am(\alpha(G))$ will be derived.

Lemma 4.3.3. *Let G be a non-complete connected graph of order n. There are exactly ℓ vertices of degree $\delta(G)$ and $i(G) = 1$ if and only if for some $k \geq 1$ there are graphs $G_1, \ldots, G_k$ satisfying the following conditions:*

(i) $|V(G_1)| = \cdots = |V(G_k)| = n - \delta(G) \geq 2$*;*

(ii) for $i = 1, \ldots, k$ *each* G_i *contains* $\ell_i (\geq 1)$ *isolated vertices of degree* $\delta(G)$ *in* G*, and* $\ell = \sum_{j=1}^{k} \ell_j$*;*

(iii) G *is described by one of two cases:*

(a) $G = \vee_{j=1}^{k} G_j$ *or*

(b) $G = (\vee_{j=1}^{k} G_j) \vee G'$ *where* G' *is a graph on* $k\delta(G) - (k-1)n$ *vertices such that* $\deg_G(v) > \delta(G)$ *for all* $v \in V(G')$ *and* $\alpha(G') \geq (k+1)\delta(G) - kn$*.*

Proof. We will use induction on ℓ to prove the necessity of conditions (i),(ii) and (iii) in order for G to have exactly ℓ vertices of degree $\delta(G)$ and $i(G) = 1$. The case $\ell = 1$ follows immediately from Theorem 4.2.8. Let $\ell \geq 2$. Since G is non-complete and $i(G) = 1$, G can be written as a join of two graphs $\hat{G}_1$ and $\hat{G}_2$ where $\hat{G}_1$ is a graph on $n - \delta(G)$ vertices with an isolated vertex and $\hat{G}_2$ is a graph on $\delta(G)$ vertices with $\alpha(\hat{G}_2) \geq 2\delta(G) - n$. The order of $\hat{G}_1$ is more than 1 by Remark 4.2.5. If $\hat{G}_1$ contains ℓ isolated vertices, then $\deg_G(v) > \delta(G)$ for all $v \in V(\hat{G}_2)$. By choosing $G_1 = \hat{G}_1$ and $G' = \hat{G}_2$, we have the desired result with $k = 1$, which corresponds to the case (iii)b. Assume that there are ℓ_1 isolated vertices in $\hat{G}_1$ where $\ell_1 < \ell$. Then, $\hat{G}_2$ contains exactly $\hat{\ell}_2 := \ell - \ell_1$ vertices of degree $\delta(G)$ in G. Since $\delta(G)$ is the minimum degree in G, the $\hat{\ell}_2$ vertices are also of the minimum degree in $\hat{G}_2$. We have $\delta(\hat{G}_2) = 2\delta(G) - n$ from the fact that $G = \hat{G}_1 \vee \hat{G}_2$. If $\hat{G}_2$ is complete, then $\delta(\hat{G}_2) = \delta(G) - 1$ and so $\delta(G) = n - 1$, which contradicts the fact that G is non-complete. Hence, $\hat{G}_2$ is a non-complete graph and $\delta(\hat{G}_2) \geq \alpha(\hat{G}_2)$. Since $\delta(\hat{G}_2) = 2\delta(G) - n$ and $\alpha(\hat{G}_2) \geq 2\delta(G) - n$, we have

$$\delta(\hat{G}_2) = \alpha(\hat{G}_2) = 2\delta(G) - n.$$

Assume that $\hat{G}_2$ is disconnected. Then $\alpha(\hat{G}_2) = 0$, which yields $\delta(\hat{G}_2) = 0$ and $\delta(G) = \frac{n}{2}$. Since $\delta(\hat{G}_2) = 0$, the $\hat{\ell}_2$ vertices are the only isolated vertices in $\hat{G}_2$. Moreover, we have $|V(\hat{G}_1)| = |V(\hat{G}_2)|$ since $\delta(G) = \frac{n}{2}$. Setting up $\ell_2 = \hat{\ell}_2$, $G_1 = \hat{G}_1$, $G_2 = \hat{G}_2$, we have the result with $k = 2$, which corresponds to (iii)a.

Suppose now that $\hat{G}_2$ is connected. Then, $i(\hat{G}_2) = 1$ by Theorem 4.2.8. Since $\hat{\ell}_2 < \ell$, by induction, there are graphs $G_2, \ldots, G_k$ for some $k \geq 2$ satisfying the conditions:

1 $|V(G_2)| = \cdots = |V(G_k)| = \delta(G) - \delta(\hat{G}_2) = n - \delta(G) \geq 2$;

2 for $i = 2, \ldots, k$ each G_i contains $\ell_i(\geq 1)$ isolated vertices of degree $\delta(\hat{G}_2)$ in $\hat{G}_2$ with $\hat{\ell}_2 = \sum_{j=2}^{k} \ell_j$; and

3 $\hat{G}_2$ is described by one of two cases:

   (a) $\hat{G}_2 = \vee_{j=2}^{k} G_j$ or

   (b) $\hat{G}_2 = (\vee_{j=2}^{k} G_j) \vee G'$ where G' is a graph on $(k-1)\delta(\hat{G}_2) - (k-2)|V(\hat{G}_2)|$ vertices such that $\deg_{\hat{G}_2}(v) > \delta(\hat{G}_2)$ for all $v \in V(G')$ and $\alpha(G') \geq k\delta(\hat{G}_2) - (k-1)|V(\hat{G}_2)|$.

Clearly, the condition (i) is satisfied. Since the $\hat{\ell}_2$ vertices in $\hat{G}_2$ have degree $\delta(G)$ in G, we have $\ell = \ell_1 + \hat{\ell}_2 = \sum_{j=1}^{k} \ell_j$. So, the condition (ii) is shown. Let $G_1 = \hat{G}_1$. If $\hat{G}_2 = \vee_{j=2}^{k} G_j$, we obtain the case (iii)a. Suppose that $\hat{G}_2 = (\vee_{j=2}^{k} G_j) \vee G'$. Considering the fact that $G = G_1 \vee \hat{G}_2$, $\delta(\hat{G}_2) = 2\delta(G) - n$ and $|V(\hat{G}_2)| = \delta(G)$, it is straightforward to check the remaining conditions in (iii)b. Therefore, our desired description of G is obtained.

For the proof of the converse, suppose that there exists a graph G with $G_1, \ldots, G_k$ for some $k \geq 1$ satisfying the conditions (i) and (ii) in the statement. For the case (iii)a, G contains ℓ vertices of degree $\delta(G)$ by the condition (ii). Consider the case (iii)b. Since $\deg_G(v) > \delta(G)$ for all $v \in V(G')$, G contains exactly ℓ vertices of degree $\delta(G)$. It remains to show $i(G) = 1$. Suppose that G is as in case (iii)b. Note that $\alpha(G') \geq (k+1)\delta(G) - kn$. So, $\alpha(G)$ can be obtained from the eigenvalue 0 in G_1 by computing the spectrum of the join so that

$$\alpha(G) = (k-1)(n - \delta(G)) + |V(G')| = \delta(G).$$

Therefore, by Theorem 4.2.8, $i(G) = 1$. Similarly, for the case (iii)a, it is straightforward to show that $\alpha(G) = \delta(G)$. □

Remark 4.3.4. Continuing with the notation and result of Lemma 4.3.3, we have $|V(G')| = k\delta(G) - (k-1)n$ and $|V(G_1)| = n - \delta(G)$. So,

$$\alpha(G') \geq (k+1)\delta(G) - kn = |V(G')| - |V(G_1)|.$$

Furthermore, we observe that the complement $\bar{G}_i$ of each G_i for $i = 1, \ldots, k$ is connected, so G_i can not be expressed as a join of graphs. Thus, the decomposition of G in terms of joins in Lemma 4.3.3 is unique (up to the ordering of the graphs). In particular, k is uniquely determined.

Definition 4.3.5. Let $\ell \geq 1$. Graphs $H_1, \dots, H_\ell$ are called *elementary* if

(i) $|V(H_1)| = \cdots = |V(H_\ell)| \geq 2$ and

(ii) each H_i for $i = 1, \dots, \ell$ contains at least one isolated vertex.

A graph G is said to be an *elementary k-join* if G can be written as $G = \vee_{j=1}^{k} G_j$ for some $k \geq 2$ such that $G_1, \dots, G_k$ are elementary. The graphs $G_1, \dots, G_k$ are called *elementary* graphs of G.

Definition 4.3.6. A graph G on n vertices is said to be a *combined k-join* if G can be expressed as $G = (\vee_{j=1}^{k} G_j) \vee G'$ for some $k \geq 1$, where $G_1, \dots, G_k$ are elementary and G' is a graph on $k\delta(G) - (k-1)n$ vertices such that $\deg_G(v) > \delta(G)$ for all $v \in V(G')$ and $\alpha(G') \geq |V(G')| - |V(G_1)|$. The graphs $G_1, \dots, G_k$ are called the *elementary* graphs of G, and the graph G' is called the *combined* graph of G.

Remark 4.3.7. If G is an elementary k-join, then $k \geq 2$. Otherwise, G would be disconnected. Considering Remark 4.3.4, an elementary k-join G does not imply that G is a combined k-join, and vice versa.

Definition 4.3.8. A graph G is said to be a *k-join* if G is either an elementary k-join or a combined k-join.

Remark 4.3.9. A k-join is not a complete graph.

The following result is straightforward from Lemma 4.3.3.

Theorem 4.3.10. *Let G be a non-complete connected graph. Then, $i(G) = 1$ if and only if G is a k-join.*

Example 4.3.11. Consider the Shrikhande graph G' with parameters $(16, 6, 2, 2)$, which is a strongly regular graph, see [11]. By computation, $\alpha(G') = 4$ and $am(\alpha(G')) = 6$. Let $G_1 = K_{11} + \{v\}$. Then $i(G_1 \vee G') = 1$ and it has only one vertex with the minimum degree, but $am(\alpha(G_1 \vee G')) = 7$. Moreover, $G_1 \vee G'$ is a combined 1-join.

Theorem 4.3.12. *Suppose that G is an elementary k-join and $G_1, \dots, G_k$ are the elementary graphs of G. Then, $am(\alpha(G)) = \sum_{i=1}^{k} \beta(G_i) - k$. Assume that G is a combined k-join, and $G_1, \dots, G_k$ and G' are the elementary graphs and the combined graph of G, respectively. Then,*

$$am(\alpha(G)) = \begin{cases} \sum_{i=1}^{k} \beta(G_i) - k + am(\alpha(G')), & \text{if } \alpha(G') = 2\delta(G) - n, \\ \sum_{i=1}^{k} \beta(G_i) - k, & \text{if } \alpha(G') > 2\delta(G) - n. \end{cases}$$

Proof. Considering the spectrum of a join of graphs, we immediately obtain the desired result. $\square$

Let $\mathcal{A}_\ell$ be the set of all non-complete graphs G with ℓ vertices of minimum degree $\delta(G)$ such that $i(G) = 1$. For $G \in \mathcal{A}_\ell$, G is a k-join for some $1 \leq k \leq \ell$. Note that if $k = 1$, then G is a combined 1-join. In order to attain the minimum of $am(\alpha(G))$ where $G \in \mathcal{A}_\ell$ is a k-join, by Theorem 4.3.12 we only need to consider elementary k-joins and combined k-joins G where the combined graph G' of G satisfies $\alpha(G') > 2\delta(G) - |V(G)|$. Let $\mathcal{A}_{\ell,k}$ denote the subset of $\mathcal{A}_\ell$ that consists of elementary k-joins and such combined k-joins. Define

$$m_{\ell,k} := \min\{am(\alpha(G))|G \in \mathcal{A}_{\ell,k}\}.$$

We will investigate $m_{\ell,k}$ and families of graphs attaining $m_{\ell,k}$. Then, the greatest lower bound of $\{am(\alpha(G))|G \in \mathcal{A}_\ell\}$ will be derived.

Let $G \in \mathcal{A}_{\ell,k}$ where $1 \leq k \leq \ell$. Let $G_1, \ldots, G_k$ be the elementary graphs of G. For $i = 1, \ldots, k$, each G_i contains at least one isolated vertex, say v_i, so $\beta(G_i) - 1$ is the number of connected components in $G_i - v_i$. Since there are $\ell - k$ isolated vertices left in the disjoint union of $G_1 - v_1, \ldots, G_k - v_k$ by Theorem 4.3.12, we have

$$am(\alpha(G)) = \ell - k + p(G)$$

where $p(G)$ is the total number of components of order more than 1 in the elementary graphs $G_1, \ldots, G_k$ of G. Define

$$p_{\ell,k} := \min\{p(G)|G \in \mathcal{A}_{\ell,k}\}.$$

Therefore, we have

$$m_{\ell,k} = \ell - k + p_{\ell,k}.$$

Then, $m_{\ell,k}$ can be completely determined by considering 3 cases for $1 \leq k \leq \ell$: (i) $k \mid \ell$ where $\ell \geq 2$ and $1 \leq k < \ell$, (ii) $k = \ell$ or $k = \ell - 1 \geq 2$, (iii) $k \nmid \ell$ and $2 \leq k \leq \ell - 2$.

Lemma 4.3.13 (Case (i))**.** *Let $G \in \mathcal{A}_{\ell,k}$ where $\ell \geq 2$ and $1 \leq k < \ell$. Suppose that $G_1, \ldots, G_k$ are the elementary graphs of G. Then, $k \mid \ell$ if and only if $m_{\ell,k} = \ell - k$. In particular, $G_i = N_{a+1}$ for $i = 1 \ldots, k$ where $a \geq 1$ and $\ell = (a+1)k$.*

Proof. Note that $k \mid \ell$ if and only if $k \mid \ell - k$. Assume that $\ell - k = ak$ for some $a \geq 1$. By choosing $G_i = N_{a+1}$ for $i = 1 \ldots, k$, we have $p(G) = 0$. Hence, $p_{\ell,k} = 0$

and $m_{\ell,k} = \ell - k$. Conversely, if $m_{\ell,k} = \ell - k$, then $p_{\ell,k} = 0$ and so each G_i must consist of isolated vertices. Since $|V(G_1)| = \cdots = |V(G_k)| \geq 2$, it follows that there is $a \geq 1$ such that $\ell - k = ak$. Furthermore, $G_i = N_{a+1}$ for $i = 1, \ldots, k$. $\square$

We shall consider an example to illustrate that $p(G)$ depends on how $G_1, \ldots, G_k$ consist of isolated vertices.

Example 4.3.14. Let $G \in \mathcal{A}_{12,5}$, and let $G_1, \ldots, G_5$ be the elementary graphs of G. Note that for $i = 1, \ldots, 5$, G_i has at least one isolated vertex. Consider the configurations of three distributions of 12 isolated vertices in $G_1, \ldots, G_5$ in Figure 4.1; for each case in Figure 4.1, a $\bullet$ indicates an isolated vertex, and the j^{th} column describes how many isolated vertices G_j has. Note that for each case, there are no more isolated vertices in G_j for $1 \leq j \leq 5$; G_j may have disconnected components of order more than 1 under the condition that $|V(G_1)| = \cdots = |V(G_5)| \geq 2$.

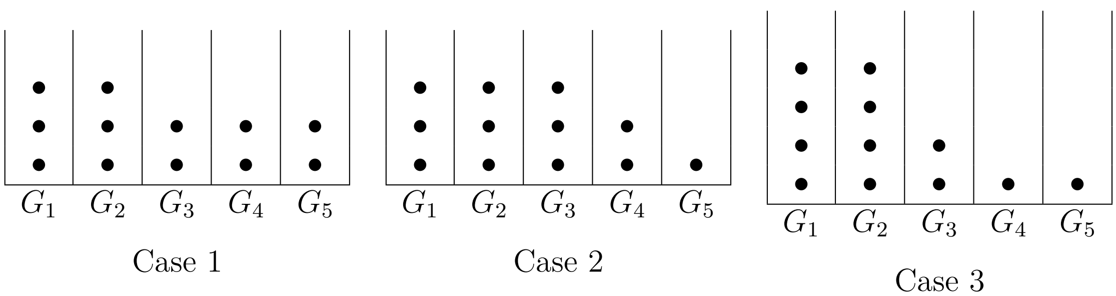


Figure 4.1: The configurations of three distributions of 12 isolated vertices in $G_1, \ldots, G_5$.

Consider Case 1. If $|V(G_i)| = 3$ for $i = 1, \ldots, 5$, then G_3, G_4 and G_5 must have three isolated vertices, a contradiction to $\ell = 12$. In order for G to satisfy the condition that it only has 12 isolated vertices and $|V(G_1)| = \cdots = |V(G_5)| \geq 2$, at least one component of order more than 1 must be added to each G_j. Thus, $p(G) \geq 5$ for Case 1.

Using the same argument for Case 2, it follows that we also need at least five components of order more than 1. Hence, $p(G) \geq 5$ for Case 2.

For Case 3, we minimally need three components: K_2, K_3 and K_3 in G_3, G_4 and G_5, respectively. Thus, $|V(G_1)| = \cdots = |V(G_5)| \geq 4$ and $p(G) \geq 3$.

Let $G \in \mathcal{A}_{\ell,k}$ where $\ell - k \geq 1$. Suppose that $G_1, \ldots, G_k$ are the elementary graphs of G, and v_i is an isolated vertex in G_i for $i = 1, \ldots, k$. Let $c_i(G) \geq 0$ be the number of isolated vertices in $G_i - v_i$ so that $\ell - k = \sum_{i=1}^{k} c_i(G)$. Suppose that

$c_{\max}(G) := \max\{c_1(G), \dots, c_k(G)\}$ and $q(G) := |\{i | c_i(G) = c_{\max}(G) \text{ for } 1 \le i \le k\}|$. Since $\ell - k \ge 1$, we have $c_{\max}(G), q(G) \ge 1$. If G is clear from the context, then $c_i(G)$ and $c_{\max}(G)$ can be written as c_i and $c_{\max}$, respectively. Assume that there is a $G_j - v_j$ such that $c_{\max} - c_j = 1$. Since $|V(G_1)| = \cdots = |V(G_k)|$ and there are only $\ell - k$ isolated vertices in the disjoint union of $G_1 - v_i, \dots, G_k - v_k$, there must be at least one component of order more than 1 in each G_i. Thus, $p(G) \ge k$. Furthermore, choosing $G_j = N_{c_j+1} + K_{s-c_j-1}$ for $j = 1, \dots, k$ where $s \ge c_{\max} + 3$, we have $|V(G_1)| = \cdots = |V(G_k)| = s$ and so $p(G) = k$. On the other hand, suppose that $c_{\max} - c_j \ne 1$ for all $1 \le j \le k$. Choosing

$$G_j = \begin{cases} N_{c_j+1} + K_{c_{\max}-c_j}, & \text{if } c_{\max} - c_j \ge 2, \\ N_{c_{\max}+1}, & \text{if } c_j = c_{\max}, \end{cases}$$

for $1 \le j \le k$, we obtain $|V(G_1)| = \cdots = |V(G_k)| \ge 2$ and so $p(G) = k - q(G)$ where $q(G) \ge 1$.

Let $\mathcal{G}_{\ell,k}$ be the set of graphs $G \in \mathcal{A}_{\ell,k}$ such that for the elementary graphs $G_1, \dots, G_k$, $c_{\max} - c_j \ne 1$ for all $1 \le j \le k$, where $\ell - k \ge 1$. Then, we immediately have the following proposition.

Proposition 4.3.15. *Suppose that $G \in \mathcal{A}_{\ell,k}$ where $\ell - k \ge 1$. If $G \in \mathcal{G}_{\ell,k}$, then $p(G) \ge k - q(G)$ where $q(G) \ge 1$, and there exists a graph $H \in \mathcal{G}_{\ell,k}$ such that $p(H) = k - q(G)$ where $q(G) \ge 1$. If $G \notin \mathcal{G}_{\ell,k}$, then $p(G) \ge k$ and there exists a graph $H \in \mathcal{A}_{\ell,k}$ such that $p(H) = k$.*

Proposition 4.3.15 implies that if $\mathcal{G}_{\ell,k}$ is non-empty, then $p_{\ell,k} < k$. Otherwise, $p_{\ell,k} = k$, and so $m_{\ell,k} = \ell$.

Lemma 4.3.16 (Case (ii))**.** *Let $G \in \mathcal{A}_{\ell,k}$. If $k = \ell$ or $k = \ell - 1 \ge 2$, then $m_{\ell,k} = \ell$.*

Proof. Let $G_1, \dots, G_k$ be the elementary graphs of G. Suppose that $k = \ell$. Note that $|V(G_i)| \ge 2$ for $i = 1, \dots, k$. Since each G_i for $i = 1, \dots, k$ has exactly one isolated vertex, every G_i must have at least one component of order more than 1. Thus, $p_{\ell,\ell} = k$, and so $m_{\ell\ell} = \ell$. If $k = \ell - 1 \ge 2$, there exists a graph G_j for some $1 \le j \le k$ such that $c_{\max} - c_j = 1$. So, $\mathcal{G}_{\ell,k}$ is the empty set, which implies that $m_{\ell,\ell-1} = \ell$. □

Example 4.3.17. Let $G \in \mathcal{A}_{16,5}$, and let $G_1, \dots, G_5$ be the elementary graphs of G. Note that each G_i for $i = 1, \dots, 5$ has at least one isolated vertex.

See the configurations of three distributions of the 16 vertices into $G_1, \dots, G_5$ in Figure 4.2; for each case in Figure 4.2, a • indicates an isolated vertex and the

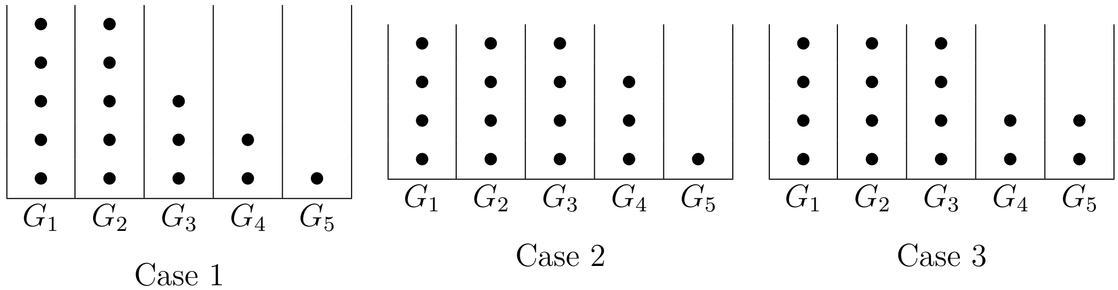


Figure 4.2: The configurations of three distributions of the 16 vertices into $G_1, \ldots, G_5$.

j^{th} column describes how many isolated vertices G_j has.. For Case 1, $G \in \mathcal{G}_{16,5}$ and by Proposition 4.3.15, we may have $p(G) = 3$. Suppose that G corresponds to the configuration of Case 2. Since $c_{\max} - c_4 = 1$, $G \notin \mathcal{G}_{\ell,k}$ and so $p(G) \geq 5$. If G corresponds to Case 3, then $c_{\max} - c_j \neq 1$ for all $1 \leq j \leq 5$ so that we can obtain $p(G) = 2$ by placing K_2 in G_4 and G_5, respectively. Furthermore, there is no graph in $G \in \mathcal{G}_{16,5}$ such that $c_{\max} = 2$, by the pigeonhole principle. Therefore, $p_{16,5} = 2$ and so $m_{16,5} = 13$.

Let $H \in \mathcal{A}_{15,4}$, and let $H_1, \ldots, H_4$ be the elementary graphs of H. Consider the configurations of two distributions of the 15 vertices into $H_1, \ldots, H_4$ in Figure 4.3; for each case in Figure 4.3, a $\bullet$ indicates an isolated vertex and the j^{th} column describes how many isolated vertices H_j has. For Case 4, $H \notin \mathcal{G}_{15,4}$, so $p(H) \geq 4$. For Case 5, we have $p(H) \geq 2$. One can check that $m_{15,4} = 13$.

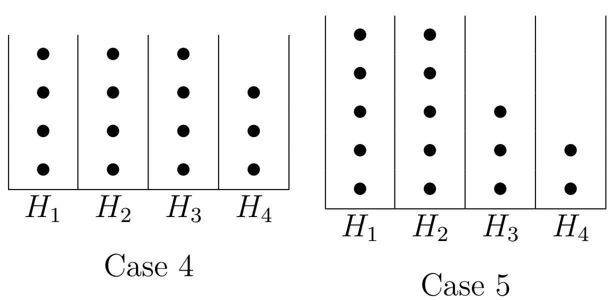


Figure 4.3: The configurations of two distributions of the 15 vertices into $H_1, \ldots, H_4$.

Observe from Cases 1, 2 and 3 in Example 4.3.17 that $c_{\max}(G)$ should be minimized in order to maximize $q(G)$ so that $p_{\ell,k}$ can be attained. So, we shall consider graphs $G \in \mathcal{A}_{\ell,k}$ such that $0 \le \ell - k - c_{\max}(G)q(G) \le c_{\max}(G) - 1$, and then investigate the minimum of $c_{\max}(G)$ among the graphs G. However, Cases 4 and 5 in Example 4.3.17 show that the minimum of $c_{\max}(G)$ being attained at $\hat{G}$ does not guarantee attaining $p_{\ell,k}$ if $\ell - k = c_{\max}(\hat{G})q(\hat{G}) - 1$.

Lemma 4.3.18 (Case (iii))**.** *Let $G \in \mathcal{A}_{\ell,k}$ where $k \nmid \ell$ and $2 \le k \le \ell - 2$. Let $\tilde{c} = \max\{\lceil \frac{\ell-k}{k} \rceil, 2\}$. Then,*

$$m_{\ell,k} = \begin{cases} \ell - \lfloor \frac{\ell-k}{3} \rfloor, & \text{if } \ell - k \text{ is odd, and } \lfloor \frac{\ell-k}{2} \rfloor \le k-1, \\ \ell - \lfloor \frac{k(\ell-k)}{\ell+1} \rfloor, & \text{if } k \mid (\ell+1), \text{ and } \ell + 1 \ge 4k, \\ \ell - \lfloor \frac{\ell-k}{\tilde{c}} \rfloor, & \text{otherwise.} \end{cases}$$

Proof. Let us consider a graph $G \in \mathcal{A}_{\ell,k}$. Then, there exist the elementary graphs $G_1, \dots, G_k$ of G. Suppose that $0 \le \ell - k - c_{\max}(G)q(G) \le c_{\max}(G) - 1$ where $k \nmid \ell$ and $2 \le k \le \ell - 2$. We may assume that $c_1 = \cdots = c_{q(G)} = c_{\max}(G)$ and $c_{q(G)+1} = r(G)$ where $r(G) = \ell - k - c_{\max}(G)q(G)$. Note that if $0 \le r(G) \le c_{\max}(G) - 2$, then $G \in \mathcal{G}_{\ell,k}$.

Let $c_0 = \min\{c \ge 2 | \lfloor \frac{\ell-k}{c} \rfloor \le k-1\}$ and $r_0 = \ell - k - c_0 \lfloor \frac{\ell-k}{c_0} \rfloor$. We shall consider 3 cases: (a) $c_0 = 2$ and $r_0 = 1$, (b) $\lfloor \frac{\ell-k}{c_0} \rfloor = k-1$ and $r_0 = c_0 - 1$ where $c_0 \ge 3$, (c) neither (a) nor (b) holds.

- (case (a)) If $c_{\max}(G) = 2$ and $r(G) = 1$, then $c_{\max}(G) - c_{q(G)+1} = 1$ so that $p(G) \ge k$. Suppose that $c_{\max}(G) = 3$. Since $c_0 = 2$ and $r_0 = 1$, $\lfloor \frac{\ell-k}{2} \rfloor \le k-1$ implies that $\lfloor \frac{\ell-k}{3} \rfloor \le k-2$. If $r(G) = 0$ or $r(G) = 1$, then $G \in \mathcal{G}_{\ell,k}$ and by Proposition 4.3.15, $p_{\ell,k} = k - \lfloor \frac{\ell-k}{3} \rfloor$. Assume that $r(G) = 2$. Since $\lfloor \frac{\ell-k}{3} \rfloor \le k-2$, there exists a graph $\hat{G} \in \mathcal{G}_{\ell,k}$ such that $c_1(\hat{G}) = \cdots = c_{q(G)}(\hat{G}) = 3$ and $c_{k-1}(\hat{G}) = c_k(\hat{G}) = 1$. By Proposition 4.3.15, we find that $m_{\ell,k} = \ell - \lfloor \frac{\ell-k}{3} \rfloor$. Furthermore, considering $c_0 = 2$, the condition $r_0 = 1$ is equivalent for $\ell - k$ to be odd.

- (case (b)) If $c_{\max}(G) = c_0 \ge 3$, $q(G) = k-1$ and $r(G) = c_0 - 1$, then $c_{\max} - c_k = 1$ so that $G \notin \mathcal{G}_{\ell,k}$. Note that $\ell - k = c_0(k-1) + c_0 - 1$ can be expressed as $c_0 = \frac{\ell+1}{k} - 1 \ge 3$, *i.e.*, $\ell + 1$ is divisible by k and $\ell + 1 \ge 4k$. Suppose that $c_{\max}(G) = c_0 + 1$. We have $q(G) = \lfloor \frac{\ell-k}{c_0+1} \rfloor = \lfloor \frac{k(\ell-k)}{\ell+1} \rfloor$. Since $\lfloor \frac{\ell-k}{c_0} \rfloor = k-1$, we have $q(G) \le k-2$. If $r(G) = 0$, there exists $\hat{G} \in \mathcal{G}_{\ell,k}$ such that $c_1(\hat{G}) = \cdots = c_{q(G)}(\hat{G}) = c_0 + 1$. If $r(G) \ge 1$, choose a graph $\hat{G} \in \mathcal{G}_{\ell,k}$ such that $c_1(\hat{G}) = \cdots = c_{q(G)}(\hat{G}) = c_0 + 1$, $c_{k-1}(\hat{G}) = r(G) - 1$ and $c_k(\hat{G}) = 1$. Hence, by Proposition 4.3.15, $m_{\ell,k} = \ell - \lfloor \frac{k(\ell-k)}{\ell+1} \rfloor$.

- (case (c)) Considering the cases (a) and (b), if $c_0 = 2$, then $r_0 = 0$; if $r_0 = c_0 - 1$, then $\lfloor \frac{\ell-k}{c_0} \rfloor \leq k-2$. Let $c_{\max}(G) = c_0$ and $q(G) = \lfloor \frac{\ell-k}{c_0} \rfloor$. It is readily checked that for $c_0 = 2$ we can obtain our desired result. If $r(G) = c_0 - 1 \geq 2$, then $q(G) \leq k-2$. Then, there exists a graph $\hat{G} \in \mathcal{G}_{\ell,k}$ such that $c_1(\hat{G}) = \cdots = c_{q(G)}(\hat{G}) = c_0$, $c_{k-1}(\hat{G}) = r(G) - 1$ and $c_k(\hat{G}) = 1$. If $r(G) < c_0 - 1$, it is straightforward that $G \in \mathcal{G}_{\ell,k}$. Therefore, $m_{\ell,k} = \ell - \lfloor \frac{\ell-k}{c_0} \rfloor$. Consider $c_0 = \min\{c \geq 2 | \lfloor \frac{\ell-k}{c} \rfloor \leq k-1\}$. Since $\left\lfloor \frac{\ell-k}{c} \right\rfloor \leq k-1 \Leftrightarrow \frac{\ell-k}{c} < k \Leftrightarrow \frac{\ell-k}{k} < c$, we have $c_0 = \max\{\left\lceil \frac{\ell-k}{k} \right\rceil, 2\}$.

$\square$

Summarizing Lemmas 4.3.13, 4.3.16 and 4.3.18, we have the following theorem.

Theorem 4.3.19. *Let $G \in \mathcal{A}_{\ell,k}$ where $1 \leq k \leq \ell$. Then,*

$$m_{\ell,k} = \begin{cases} \ell, & \text{if } k = \ell - 1 \geq 2 \text{ or } k = \ell, & (4.3.2) \\ \ell - k, & \text{if } k \mid \ell \text{ and } 1 \leq k < \ell, & (4.3.3) \\ \ell - \left\lfloor \dfrac{k(\ell-k)}{\ell+1} \right\rfloor, & \text{if } k \mid (\ell+1),\ \ell+1 \geq 4k,\ 2 \leq k \leq \ell-2, & (4.3.4) \\ \ell - \left\lfloor \dfrac{\ell-k}{3} \right\rfloor, & \text{if } k \nmid \ell,\ 2 \nmid (\ell-k),\ \lfloor \frac{\ell-k}{2} \rfloor \leq k-1 \leq \ell-3, & (4.3.5) \\ \ell - \left\lfloor \dfrac{\ell-k}{\tilde{c}} \right\rfloor, & \text{otherwise}, & (4.3.6) \end{cases}$$

where $\tilde{c} = \max\{\left\lceil \frac{\ell-k}{k} \right\rceil, 2\}$.

Corollary 4.3.20. *Let G be a non-complete connected graph of order n with $i(G) = 1$ and $\ell \geq 1$ vertices of $\delta(G)$. Then,*

$$am(\alpha(G)) \geq \begin{cases} \frac{\ell}{2}, & \ell \text{ is even}, \\ \ell - \lfloor \frac{\ell}{3} \rfloor, & \ell \text{ is odd}. \end{cases}$$

with equality for even ℓ if and only if $G = \vee_{i=1}^{\frac{\ell}{2}} N_2$ ($\ell \geq 4$) or $G = (\vee_{i=1}^{\frac{\ell}{2}} N_2) \vee K_{n-\ell}$. In particular, $G = N_2 \vee K_{n-2}$ for $\ell = 2$.

Proof. Let $m_\ell := \min\{am(\alpha(G)) | G \in \mathcal{A}_\ell\}$. We need only find m_ℓ for even ℓ and odd ℓ, respectively, to complete the proof. Continuing the notation of Theorem 4.3.19, for the case (4.3.4), there exists $a \geq 4$ such that $\ell + 1 = ak$. So, $\ell - \lfloor \frac{k(\ell-k)}{\ell+1} \rfloor$ can be recast as $\ell - \lfloor \frac{(\ell-k)}{a} \rfloor \geq \ell - \lfloor \frac{(\ell-k)}{3} \rfloor$, *i.e.*, $\lfloor \frac{(\ell-k)}{a} \rfloor \leq \lfloor \frac{(\ell-k)}{3} \rfloor$.

Suppose that ℓ is even. Then, $\frac{\ell}{2} \mid \ell$. From (4.3.3), we have $m_{\ell,\frac{\ell}{2}} = \ell - \frac{\ell}{2}$ with $k = \frac{\ell}{2}$. Note that $\tilde{c} \geq 2$. So, we have $\lfloor \frac{(\ell-k)}{3} \rfloor < \frac{\ell}{2}$ and $\lfloor \frac{(\ell-k)}{\tilde{c}} \rfloor < \frac{\ell}{2}$ for $1 \leq k \leq \ell$. Hence, $m_\ell = \ell - \frac{\ell}{2}$, which is only attained from (4.3.3). Furthermore, we find from Lemma 4.3.13 that $am(\alpha(G)) = \frac{\ell}{2}$ for $G \in \mathcal{A}_\ell$ if and only if $G = \vee_{i=1}^{\frac{\ell}{2}} N_2$ ($\ell \geq 4$) or $G = (\vee_{i=1}^{\frac{\ell}{2}} N_2) \vee G'$ where $\alpha(G') > |V(G')| - 2$. It follows from $\delta(G') \leq |V(G')| - 1$ that G' is the complete graph.

It is straightforward that $m_1 = 1$. Assume that ℓ is odd and $3 \mid \ell$. Applying (4.3.3), $m_{\ell,\frac{\ell}{3}} = \ell - \frac{\ell}{3}$. Suppose that for (4.3.6), there are $\tilde{c} \geq 2$ and $k_0 \geq 1$ such that $\ell \neq 3k_0$ and $\left\lfloor \frac{\ell-k_0}{\tilde{c}} \right\rfloor \geq \frac{\ell}{3}$. Since $k_0 \geq 1$, we must have $\tilde{c} = 2$. This implies that $\ell > 3k_0$. So, $\left\lceil \frac{\ell-k_0}{k_0} \right\rceil > 2$, which is a contradiction to $\tilde{c} = \max\{\left\lceil \frac{\ell-k_0}{k_0} \right\rceil, 2\} = 2$. Hence, $\left\lfloor \frac{\ell-k}{\tilde{c}} \right\rfloor < \frac{\ell}{3}$. Furthermore, since $\lfloor \frac{(\ell-k)}{3} \rfloor < \frac{\ell}{3}$ for $1 \leq k \leq \ell$, we have $m_\ell = \ell - \frac{\ell}{3}$.

Suppose that ℓ is odd and $\ell = 3b + 1$ for some $b \geq 2$. In order to consider the minimum in the case (4.3.6), we choose $k = b+1$ so that $\ell - k = 2b$. Then, it follows from $\lfloor \frac{\ell-k}{2} \rfloor = b$ that $m_{\ell,b+1} = \ell - \lfloor \frac{\ell}{3} \rfloor$. If k is in the case of (4.3.3), then k ($\neq \ell$) is a divisor of ℓ. Then, $k = 1$ or $k \geq 5$. Note that ℓ is odd and $\ell \geq 7$. It follows that $k < \left\lfloor \frac{\ell}{3} \right\rfloor$ for all divisors k ($\neq \ell$) of ℓ. Moreover, since we have $\lfloor \frac{(\ell-k)}{3} \rfloor < \lfloor \frac{\ell}{3} \rfloor$ for $k \geq 2$, $m_{\ell,b+1} < m_{\ell,k}$ for any k corresponding to (4.3.4) or (4.3.5). Therefore, $m_\ell = \ell - \lfloor \frac{\ell}{3} \rfloor$.

Similarly, assume that ℓ is odd and $\ell = 3d + 2$ for some $d \geq 1$. In order to consider the minimum in the case (4.3.6), we choose $k = d+2$. Then, it follows from $\ell - k = 2d$ that $m_{\ell,d+2} = \ell - \lfloor \frac{\ell}{3} \rfloor$. Note that $\ell \geq 5$. For (4.3.3), let k ($\neq \ell$) be a divisor of ℓ. Then, $k \leq \lfloor \frac{\ell}{3} \rfloor$ with equality if and only if $k = 1$ and $\ell = 5$. Furthermore, $\lfloor \frac{(\ell-k)}{3} \rfloor \leq \lfloor \frac{\ell}{3} \rfloor$ for $k \geq 2$ with equality if and only if $k = 2$. In particular, one can verify that if $k = 2$, then k falls under (4.3.4), and $\left\lfloor \frac{k(\ell-k)}{\ell+1} \right\rfloor = \lfloor \frac{\ell}{3} \rfloor$ if and only if $\ell = 5$. Hence, $m_{\ell,d+2} \leq m_{\ell,k}$ for any k corresponding to (4.3.4) or (4.3.5) with equality if and only if $k = 2$ and $\ell = 5$. $\square$

Remark 4.3.21. Continuing the notation of Corollary 4.3.20, graphs attaining the equality for odd ℓ can be classified by the proof in Corollary 4.3.20. Suppose that $3 \mid \ell$. By Lemma 4.3.13, $G = \vee_{i=1}^{\frac{\ell}{3}} N_3$ for $\ell \geq 6$ or $G = (\vee_{i=1}^{\frac{\ell}{3}} N_3) \vee G'$ where $\alpha(G') > |V(G')| - 3$. Assume that ℓ is odd and $\ell = 3b+1$ for some $b \geq 2$. Since $\ell \geq 7$, the equality is only attained by the case (4.3.6). Hence, $G = (\vee_{i=1}^{b} N_3) \vee (N_1 + K_2)$ or $G = (\vee_{i=1}^{b} N_3) \vee (N_1 + K_2) \vee G'$ where $\alpha(G') > |V(G')| - 3$. Suppose that $\ell = 3d+2$ for some $d \geq 1$. For $\ell = 5$, we have following cases: for $k = 1$, $G = N_5 \vee G'$ where $\alpha(G') > |V(G')| - 5$; for $k = 2$, $G = N_4 \vee (N_1 + K_3)$, $G = N_4 \vee (N_1 + (N_1 \vee K_2))$, $G = N_4 \vee (N_1 + K_3) \vee G'$ or $G = N_4 \vee (N_1 + (N_1 \vee K_2)) \vee G'$ where $\alpha(G') > |V(G')| - 4$; for $k = 3$, $G = N_3 \vee (N_1 + K_2) \vee (N_1 + K_2)$ or $G = N_3 \vee (N_1 + K_2) \vee (N_1 + K_2) \vee G'$

where $\alpha(G') > |V(G')| - 3$. For $\ell \geq 11$, it can be checked that m_ℓ is only attained by $G = (\vee_{i=1}^{d} N_3) \vee (N_1 + K_2) \vee (N_1 + K_2)$ or $G = (\vee_{i=1}^{d} N_3) \vee (N_1 + K_2) \vee (N_1 + K_2) \vee G'$ where $\alpha(G') > |V(G')| - 3$.

The following theorem is our main result in this section for classifying graphs G with $i(G) = 1$ and $am(\alpha(G)) = 1$.

Theorem 4.3.22. *Let G be a non-complete connected graph of order n. Then, $i(G) = 1$ and $am(\alpha(G)) = 1$ if and only if either $G = N_2 \vee K_{n-2}$ or $G = G_1 \vee G'$ where G_1 is a graph of order $n - \delta(G)$ with exactly one isolated vertex, and G' is a graph on $\delta(G)$ vertices with $\alpha(G') > 2\delta(G) - n$ and $\delta(G') > 2\delta(G) - n$.*

Proof. Suppose that $i(G) = 1$ and $am(\alpha(G)) = 1$. Let ℓ be the number of vertices of the minimum degree in G. By Corollary 4.3.20, $\ell = 1$ or $\ell = 2$. For $\ell = 1$, since G is connected, G is a 1-join with G'. Since $\deg_G(v) > \delta(G)$ for all $v \in V(G')$, we have $\delta(G') > 2\delta(G) - n$. The hypothesis that $am(\alpha(G)) = 1$ implies that $\alpha(G') > 2\delta(G) - n$. For $\ell = 2$, the conclusion is clear from Corollary 4.3.20.

It is straightforward to prove the converse. □

Example 4.3.23. Suppose that $G_1 = K_{n_1} + N_1$ and $G' = K_{n_2}$ where $n_1, n_2 > 0$. Consider $G = G_1 \vee G'$. Then, $\alpha(G') = n_2$, $\delta(G') = n_2 - 1$ and $2\delta(G) - |V(G)| = n_2 - n_1 - 1$. By Theorem 4.3.22, we have $i(G) = 1$ and $am(\alpha(G)) = 1$.

4.3.1 Pathological graphs with respect to applying spectral bisection

Now, we shall introduce a result without proof, as well as some notation in [67], to find pathological graphs with respect to applying spectral bisection for the graph partitioning problem. Let G be a connected graph of order n, and let X be the eigenspace corresponding to $\alpha(G)$, and denote

$$\begin{aligned}
i_+(\mathbf{x}) &:= \{j | 1 \leq j \leq n, x_j > 0\}, \\
i_-(\mathbf{x}) &:= \{j | 1 \leq j \leq n, x_j < 0\}, \\
i_0(\mathbf{x}) &:= \{j | 1 \leq j \leq n, x_j = 0\}, \\
i_0(X) &:= \bigcap_{\mathbf{x} \in X} i_0(\mathbf{x}).
\end{aligned}$$

Theorem 4.3.24 ([67])**.** *Let G be a connected graph. Then, there exists a Fiedler vector $\mathbf{x}$ such that the subgraphs of G induced by $i_+(\mathbf{x}) \cup i_0(\mathbf{x})$ and $i_-(\mathbf{x})$ are connected.*

Proposition 4.3.25. *Let G be a connected graph of order n, and X be the eigenspace corresponding to $\alpha(G)$. Suppose that there exists an induced subgraph G_2 of G such that $G = G_1 \vee G_2$ and $\alpha(G_2) > \alpha(G) - |V(G_1)|$. Then, $V(G_2) \subseteq i_0(X)$.*

Proof. Considering eigenvectors of the join of graphs and the condition that $\alpha(G_2) > \alpha(G) - |V(G_1)|$, it implies that for any Fiedler vector, vertices of $V(G_2)$ are valuated by 0. Hence, $V(G_2) \subseteq i_0(X)$. $\square$

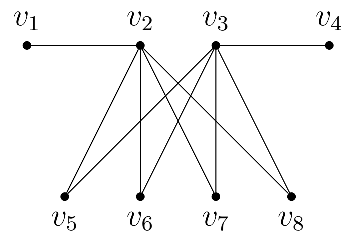


Figure 4.4: A graph G considered in Example 4.3.26.

Example 4.3.26. The converse of Proposition 4.3.25 does not hold for the graph G in Figure 4.4. Let X be the eigenspace corresponding to $\alpha(G)$. It follows from computations that $\lambda_1(G) < |V(G)| = 8$, $am(\alpha(G)) = 1$ and $i_0(X) = \{v_5, v_6, v_7, v_8\}$. Since $\lambda_1(G) < 8$, G cannot be expressed as a join.

Theorem 4.3.24 provides the existence of a Fiedler vector preserving connectedness of the two subgraphs for any connected graph. However, this does not guarantee that such a Fiedler vector gives a partition into two subgraphs such that they are similar in size. Next, we will show a family of graphs such that sign patterns of all Fiedler vectors are extremely unbalanced. In Theorem 4.3.24, we may slightly change the condition for the result as follows: the subgraphs of G induced by $i_-(\mathbf{x}) \cup i_0(\mathbf{x})$ and $i_+(\mathbf{x})$ are connected.

Example 4.3.27. Suppose that G is a non-complete connected graph of order n with $i(G) = 1$ and $am(\alpha(G)) = 1$. Then, by Theorem 4.3.22, either $G = N_2 \vee K_{n-2}$ or $G = G_1 \vee G'$ where G_1 is a graph of order $n - \delta(G)$ with exactly one isolated vertex, and G' is a graph on $\delta(G)$ vertices with $\alpha(G') > 2\delta(G) - n$ and $\delta(G') > 2\delta(G) - n$. For a Fiedler vector $\mathbf{x}$ of $G = N_2 \vee K_{n-2}$, without loss of generality, two subgraphs of G induced by $i_-(\mathbf{x}) \cup i_0(\mathbf{x})$ and $i_+(\mathbf{x})$ are K_{n-1} and N_1, respectively.

For the latter case $G = G_1 \vee G'$, let us revisit Example 4.3.23. Suppose that X is the eigenspace corresponding to $\alpha(G)$ where $G = (K_{n_1} + N_1) \vee K_{n_2}$. By Proposition

4.3.25, we have $K_{n_2} \subseteq i_0(X)$. Since $am(\alpha(G)) = 1$, $i_0(X) = K_{n_2}$. From Theorem 4.3.24, we may have that $i_-(\mathbf{x}) \cup i_0(\mathbf{x})$ and $i_+(\mathbf{x})$ are K_{n_2+1} and K_{n_1}, respectively. Therefore, for pairs (n_1, n_2) such that $\frac{n_1}{n_2} \to \infty$, the corresponding graph G will be pathological with respect to spectral bisection.

4.4 Some classes of graphs with $i(G) = 1$

In this section, we will consider threshold graphs and graphs with three distinct Laplacian eigenvalues in the context of $i(G) = 1$.

Definition 4.4.1. A *threshold graph* is a graph obtained from a single vertex by repeatedly performing one of the following operations:

(i) addition of a single isolated vertex to the graph,

(ii) addition of a dominating vertex.

Proposition 4.4.2. *Every connected threshold graph G of order n has $i(G) = 1$.*

Proof. We will use induction on the number of vertices to complete the proof. If G is a complete graph, we are done. Let G be a non-complete connected threshold graph of order n. For order 3, $N_2 \vee N_1$ is the only such graph, and $i(N_2 \vee N_1) = 1$. Let $n > 3$. Suppose that any non-complete connected threshold graph H of order $k < n$ satisfies $i(H) = 1$. Since G is a connected threshold graph, there exists a vertex v with $\deg(v) = n - 1$. Let $G' = G - \{v\}$. Suppose that G' is connected. Then, G' is not complete, otherwise, G would be complete. By induction, $i(G') = 1$, and so $\delta(G') = \alpha(G')$. Considering the spectrum of $G' \vee \{v\}$, we have

$$\alpha(G) = \alpha(G') + 1 = \delta(G') + 1 = \delta(G).$$

Therefore, $i(G) = 1$. If G' is disconnected, then G' has an isolated vertex. By Theorem 4.2.8, $i(G) = 1$. $\square$

The spectrum of a threshold graph appears in [52]. In the paper [52], a connected threshold graph is called a *maximal graph* since it is proved there that the degree sequence of a connected threshold graph of size m is not majorized by any other degree sequences of graphs of size m. In particular, we will introduce the following results used for seeing how $am(\alpha(G))$ plays a role.

Theorem 4.4.3 ([52]). *If G is a connected threshold graph, then $S(L(G)) = \mathbf{d}^*$ where $\mathbf{d}^*$ is the conjugate of the degree sequence of G.*

Theorem 4.4.4 ([52])**.** *Let G be a threshold graph. Suppose that G is disconnected so that there are $\ell+1$ connected components. Then, ℓ components consist of isolated vertices.*

Proposition 4.4.5. *Suppose that G is a non-complete connected threshold graph of order n. Then, $\alpha(G) = k$ and $am(\alpha(G)) = \ell$ if and only if there are exactly k vertices $v_1. \dots, v_k$ so that $\deg_G(v_i) = n-1$ for $i = 1, \dots, k$ and the subgraph G_1 of G induced by $V(G) - \{v_1, \dots, v_k\}$ consists of $\ell+1$ components, ℓ components of which consist of a single vertex, respectively.*

Proof. Suppose that $\alpha(G) = k$ and $am(\alpha(G)) = \ell$. By Theorem 4.4.3, the number of vertices of degree $n-1$ is $\alpha(G)$. There are exactly k vertices $v_1, \dots, v_k$ such that $\deg_G(v_i) = n-1$ for $i = 1, \dots, k$. Suppose that G_1 is the subgraph of G induced by $V(G) - \{v_1, \dots, v_k\}$. Since there are only k vertices of degree $n-1$ in G, the graph G_1 is disconnected. Moreover, $G = G_1 \vee K_k$. Since $am(\alpha(G)) = \ell$, from Theorem 4.4.4, we obtain the desired result.

For the converse, evidently we have $G = G_1 \vee K_k$. Since G_1 has exactly ℓ isolated vertices, $\alpha(G) = k$ and $am(\alpha(G)) = \ell$. □

Now, we will investigate an equivalent condition for a graph G that is a join having three distinct Laplacian eigenvalues to have $i(G) = 1$.

Proposition 4.4.6. *Let G be a non-complete, connected graph of order n. The graph G has three distinct Laplacian eigenvalues $0, \alpha(G)$ and n where $am(\alpha(G)) = k$ if and only if there exist integers $p \geq 0$, $q \geq 1$ and $r \geq 2$ such that $p+q \geq 2$ and $G = K_p \vee (\vee_{i=1}^{q} N_r)$ where $n = qr+p$, $\alpha(G) = r(q-1)+p$ and $k = q(r-1)$.*

Proof. Suppose that G has 3 distinct Laplacian eigenvalues $0, \alpha(G)$ and n. Then, the complement $\bar{G}$ of G has $n-k$ connected components since $\bar{G}$ has 0 as an eigenvalue with multiplicity $n-k$. Hence, there are graphs $G_1, \dots, G_{n-k}$ such that $G = G_1 \vee \cdots \vee G_{n-k}$ where $n-k \geq 2$. Note that for $i = 1, \dots, n-k$, $L(G_i)$ does not have $|V(G_i)|$ as an eigenvalue. If there is a G_j with three distinct eigenvalues, then from the spectrum of a join of graphs, we find that G has more than three distinct eigenvalues, a contradiction. So, each G_i has either one or two distinct eigenvalues. The only graphs with one eigenvalue are empty graphs, and the only graphs with two distinct eigenvalues are complete graphs. So, each G_i is either N_{r_i} or K_{p_i} for some r_i or p_i. Consider N_{r_i} and N_{r_j} for $r_i, r_j \geq 2$ and $r_i \neq r_j$. Then, $L(N_{r_i} \vee N_{r_j})$ has 4 distinct eigenvalues $0, r_i, r_j$ and $r_i + r_j$. Hence, all empty graphs as factors in $G_1 \vee \cdots \vee G_{n-k}$ must have the same order. Evidently, $K_{p_i} \vee K_{p_j} = K_{p_i+p_j}$ for

$p_i, p_j \geq 1$. If G_i is a complete graph, then $G_i = K_1$. Let p be the number of isolated vertices in $\bar{G}$, let q be the number of the complete graphs of order $r \geq 2$ in $\bar{G}$. If $q = 0$, then G is a complete graph. So, $q \geq 1$. If $p + q = 1$, then G is disconnected and so $p+q \geq 2$. Therefore, we have the desired graph G. Considering the spectrum of a join of graphs, the remaining conditions for n, $\alpha(G)$ and k can be checked.

By the spectrum of a join, the proof of the converse is straightforward. $\square$

Corollary 4.4.7. *Let G be a non-complete, connected graph of order n with three distinct Laplacian eigenvalues. The largest Laplacian eigenvalue is n if and only if $i(G) = 1$.*

Proof. Suppose that the largest Laplacian eigenvalue is n. From Proposition 4.4.6, there exist $p \geq 0$, $q \geq 1$ and $r \geq 2$ such that $p + q \geq 2$ and $G = K_p \vee (\vee_{i=1}^{q} N_r)$. Since $G = N_r \vee (K_p \vee (\vee_{i=1}^{q-1} N_r))$, we obtain $i(G) = 1$ by Theorem 4.2.8. Conversely, $i(G) = 1$ implies that G is a join of some graphs. So, the largest eigenvalue is n. $\square$

Corollary 4.4.8. *Let G be a non-complete, connected graph of order n with three distinct Laplacian eigenvalues 0, $\alpha(G)$ and n where $k = am(\alpha(G))$. Then, the clique number of G is*

$$\omega(G) = n - k.$$

Proof. It follows from Proposition 4.4.6 that there exist $p \geq 0$, $q \geq 1$ and $r \geq 2$ such that $p + q \geq 2$ and $G = K_p \vee (\vee_{i=1}^{q} N_r)$. So, $\omega(G) = p + q$. Since $n = qr + p$ and $k = qr - q$, we have $\omega(G) = n - k$. $\square$

Problem 4.4.9. *As done in this section, find more classes of graphs G with $i(G) = 1$, and investigate $am(\alpha(G))$. One could consider cographs, split graphs, Laplacian integral graphs, and so on.*

4.5 Characterization of regular graphs with $i(G) = 2$

In this section, we shall consider $i(G) = 2$. It turns out that $i(K_n) = 1$. So, if $i(G) = 2$, then G is non-complete and connected.

Proposition 4.5.1. *Let G be a connected graph of order n with $i(G) = 2$, and $\mathbf{x}$ be a Fiedler vector with $i(\mathbf{x}) = 2$. Then, two vertices valuated by negative numbers of $\mathbf{x}$ are adjacent and $0 < \delta(G) - \alpha(G) \leq 1$. Moreover, one of the two vertices has degree $\delta(G)$.*

Proof. Since $i(G) = 2$, there exists $\mathbf{x} = (x_1 \dots, x_n)^T \in \mathbb{R}^n$ such that $x_1, x_2 < 0$, $x_j \geq 0$ for $j = 3, \dots, n$ and $(L(G) - \alpha(G)I)\mathbf{x} = 0$. We have

$$(\ell_{11} - \alpha(G))x_1 + \ell_{12}x_2 + \ell_{13}x_3 + \cdots + \ell_{1n}x_n = 0, \tag{4.5.1}$$

$$\ell_{21}x_1 + (\ell_{22} - \alpha(G))x_2 + \ell_{23}x_3 + \cdots + \ell_{2n}x_n = 0. \tag{4.5.2}$$

Since $i(G) > 1$, it follows that

$$\ell_{ii} - \alpha(G) \geq \delta(G) - \alpha(G) > 0 \tag{4.5.3}$$

for $i = 1, \dots, n$. Assume that $\ell_{12} = \ell_{21} = 0$. Thus, $(\ell_{11} - \alpha(G))x_1 < 0$ and $\sum_{j=3}^{n} \ell_{1j}x_j \leq 0$, which leads to having the left side of (4.5.1) negative. Therefore, $\ell_{12} = \ell_{21} = -1$.

Adding (4.5.1) and (4.5.2), we have

$$(\ell_{11} - \alpha(G) - 1)x_1 + (\ell_{22} - \alpha(G) - 1)x_2 + \sum_{j=3}^{n}(\ell_{1j} + \ell_{2j})x_j = 0. \tag{4.5.4}$$

Without loss of generality, suppose that $\ell_{11} \leq \ell_{22}$. If $\ell_{11} - \alpha(G) > 1$, then the left side of the equation (4.5.4) is negative. Therefore, $\ell_{11} - \alpha(G) \leq 1$ and by (4.5.3), $0 < \delta(G) - \alpha(G) \leq 1$. Furthermore, suppose that $\ell_{11} > \delta(G)$, that is, $\ell_{11} \geq \delta(G) + 1$. Using $\ell_{11} - \alpha(G) \leq 1$, we deduce $\alpha(G) = \delta(G)$, which is a contradiction to $i(G) = 2$. Thus, $\ell_{11} = \delta(G)$. $\square$

Remark 4.5.2. Proposition 4.5.1 provides two cases: $0 < \delta(G) - \alpha(G) < 1$ and $\delta(G) - \alpha(G) = 1$. Note that $\delta(G) \geq v(G) \geq \alpha(G)$. Consider the case $0 < \delta(G) - \alpha(G) < 1$. Since $\alpha(G)$ is not an integer, we have $\delta(G) = v(G) > \alpha(G)$.

Suppose that $\delta(G) - \alpha(G) = 1$. Then, continuing the notation and hypothesis in the proof of Proposition 4.5.1, it follows from (4.5.4) that $\ell_{22} \leq \alpha(G) + 1 = \delta(G)$; by $\ell_{22} \geq \delta(G)$, we have $\ell_{22} = \delta(G)$. Hence, the two vertices valuated by negative signs of a Fiedler vector $\mathbf{x}$ in Proposition 4.5.1 have degree $\delta(G)$. Furthermore, we have either $\delta(G) - v(G) = 0$ or $\delta(G) - v(G) = 1$. For the latter case, since $\delta(G) - \alpha(G) = 1$, we have $v(G) = \alpha(G)$. It follows from [45] that G can be written as a join of two graphs G_1 and G_2 such that G_1 is a disconnected graph of order $n - v(G)$ and G_2 is a graph on $v(G)$ vertices with $\alpha(G_2) \geq 2v(G) - n$.

Recall that given the sequences of eigenvalues $S(A(G)) = (\mu_1(G), \dots, \mu_n(G))$ and $S(L(G)) = (\lambda_1(G), \dots, \lambda_n(G))$ in non-increasing order for a graph G, the $\mu_k(G)$ and $\lambda_k(G)$ are k^{th}-Laplacian and k^{th}-adjacency eigenvalues, respectively. We shall consider a connected r-regular graph G of order n with $i(G) = 2$. Note that $L(G) = rI - A(G)$. So, $\alpha(G) = r - \mu_2(G)$ where $\mu_2 < r$, and any Fiedler vector of G is an eigenvector of $A(G)$ associated to μ_2. Therefore, we also use eigenvectors associated to the second largest eigenvalue of $A(G)$ as Fiedler vectors without distinction.

A matching in a graph G is a set of edges in G such that no two edges in the set share a common vertex.

Proposition 4.5.3. *Let G be a connected r-regular graph G of order n with $i(G) = 2$. Then,*

$$0 < \mu_2(G) \leq 1.$$

In particular, if $\mu_2(G) = 1$, then there is a matching of size at least 2 in G.

Proof. Consider $\alpha(G) = r - \mu_2(G)$ and $\delta(G) = r$. It is straightforward from Proposition 4.5.1 that $0 < \mu_2(G) \leq 1$.

Suppose that $\mu_2(G) = 1$. Since $i(G) = 2$, there exists $\mathbf{x} \in \mathbb{R}^n$ such that $(A(G) - \mu_2(G)I)\mathbf{x} = \mathbf{0}$ and $i(\mathbf{x}) = 2$. We may assume that $\mathbf{x} = (x_1, \ldots, x_n)^T \in \mathbb{R}^n$ such that $x_1, x_2 < 0$, $x_j \geq 0$ for $j = 3, \ldots, n$. Let $A(G) = [a_{ij}]_{n \times n}$. By Proposition 4.5.1, we have $a_{12} = a_{21} = 1$. From the equations in the first and second rows of $(A(G) - \mu_2(G)I)\mathbf{x} = \mathbf{0}$,

$$-x_1 + x_2 + \sum_{j=3}^{n} a_{1j} x_j = 0 \text{ and } \ x_1 - x_2 + \sum_{j=3}^{n} a_{2j} x_j = 0.$$

Adding the two equations, we obtain

$$\sum_{j=3}^{n} a_{1j} x_j + \sum_{j=3}^{n} a_{2j} x_j = 0.$$

Since $x_j \geq 0$ for $j = 3, \ldots, n$ and $A(G) \geq 0$, it follows that $\sum_{j=3}^{n} a_{1j} x_j = \sum_{j=3}^{n} a_{2j} x_j = 0$ and $x_k = 0$ for any vertex v_k adjacent to v_1 or v_2. Furthermore, $x_1 = x_2$. Let $I = \{k \in [n] | x_k > 0\}$ where $[n] = \{1, \ldots, n\}$, and let $\widetilde{A}$ be the corresponding principal submatrix $A[I]$ and $\tilde{\mathbf{x}}$ be the corresponding subvector $\mathbf{x}[I]$. Then, $\widetilde{A}\tilde{\mathbf{x}} = \tilde{\mathbf{x}}$ where $\tilde{\mathbf{x}} > 0$. Suppose that a subgraph H associated with $\widetilde{A}$ is connected. By the Perron–Frobenius theorem, the eigenvalue 1 is the spectral radius of $\widetilde{A}$ and is simple. It implies that $H = K_2$. Since any vertex v_k for $k \in I$ is not adjacent to v_1 and v_2, there are two edges, namely $v_1 \sim v_2$ and the edge in H, such that they do not share any vertex in common. Next, assume that H is disconnected. Since each component of H is connected, H consists of pairwise non-adjacent edges. Therefore, G contains at least 2 pairwise non-adjacent edges. $\square$

It can be found in [26] that $\mu_2(K_{n_1,n_2,\ldots,n_k}) = 0$, where $\max(n_1, n_2, \ldots, n_k) \geq 2$, $\mu_2(K_n) = -1$, and $\mu_2(G) > 0$ for all other connected graphs G. It is clear that $i(K_n) = i(K_{n_1,n_2,\ldots,n_k}) = 1$. Motivated by Proposition 4.5.3, we will consider all regular graphs G with $0 < \mu_2(G) \leq 1$ and $i(G) = 2$. Since $A(G) + A(\bar{G}) = J - I$, it follows that $0 < \mu_2(G) \leq 1$ is equivalent to $-2 \leq \mu_n(\bar{G}) < -1$. Moreover, any eigenvector of $A(\bar{G})$ associated to $\mu_n(\bar{G})$ is an eigenvector of $A(G)$ associated to $\mu_2(G)$, vice versa. It follows that the eigenspace associated to $\alpha(G)$ coincides with the eigenspace associated to $\mu_n(\bar{G})$, which is the least adjacency eigenvalue of $\bar{G}$. Furthermore, the eigenspace corresponding to $\mu_n(\bar{G})$ is the same as the eigenspace corresponding to $\lambda_1(\bar{G})$. Recall that $i^*_\lambda(G) := \min\{i_\lambda(\mathbf{x}) | A(G)\mathbf{x} = \lambda\mathbf{x}\}$. Therefore, for a regular graph G,

$$i(G) = i^*_{\mu_2}(G) = i^*_{\mu_n}(\bar{G}) = i_{\lambda_1}(\bar{G}).$$

Let G be a connected regular graph of order n with $i(G) = 2$. Then $i^*_{\mu_n}(\bar{G}) = 2$. It can be easily checked that G is connected if and only if $\bar{G}$ is not expressed as a join of graphs. Hence, the difference between the degree in $\bar{G}$ and $\mu_n(\bar{G})$, which is the largest Laplacian eigenvalue of $\bar{G}$, is less than n. Suppose that $\bar{G}$ is disconnected and H_j is a component on m_j vertices in $\bar{G}$ for $j = 1, \ldots, k$ for some $k \geq 2$. Then there exist components $H_{j_1}, \ldots, H_{j_q}$ for some $1 \leq q \leq k$ such that $\mu_n(\bar{G}) = \mu_{m_{j_i}}(H_{j_i})$ for $i = 1, \ldots, q$. It follows that

$$i^*_{\mu_{m_{j_i}}}(H_{j_i}) \geq i^*_{\mu_n}(\bar{G})$$

for $i = 1, \ldots, q$. Since the eigenspace of $\bar{G}$ corresponding to μ_n is the direct sum of the eigenspaces associated to $\mu_{m_{j_i}}$ of H_{j_i} for $i = 1, \ldots, q$, the condition $i^*_{\mu_n}(\bar{G}) = 2$ implies that there exists an $i \in \{1, \ldots, q\}$ such that $i^*_{\mu_{m_{j_i}}}(H_{j_i}) = 2$. Thus, we have the following result.

Lemma 4.5.4. *Let G be a connected regular graph of order n. Suppose that H_j is a component on m_j vertices in $\bar{G}$ for $j = 1, \ldots, k$ for some $k \geq 1$. We have $i(G) = 2$ if and only if there exists a component H_j for $j \in \{1, \ldots, k\}$ such that $\mu_{m_i}(H_i) \geq \mu_{m_j}(H_j)$ for all $1 \leq i \leq k$ and $i^*_{\mu_{m_j}}(H_j) = 2$.*

Lemma 4.5.4 tells us that to understand a regular graph G with $i(G) = 2$, we should investigate the components of the complement of G. Specifically, we may narrow our focus to eigenvectors of the least adjacency eigenvalue $-2 \leq \mu_n < -1$ of a connected r-regular graph H of order n where $r - \mu_n < n$, that is, H can not be written as a join of graphs.

It appears in [25] that an r-regular graph H of order n with $\mu_n(H) \geq -2$ is either a line graph, a cocktail party graph or a regular exceptional graph. It is known that every cocktail party graph is written as a join of graphs. So, all cocktail party graphs are excluded.

Proposition 4.5.5. *[25] A connected regular graph with least adjacency eigenvalue greater than -2 is either a complete graph or an odd cycle.*

Since $i(K_n) = 1$, K_n is ruled out. We will consider eigenvectors of the least adjacency eigenvalue of a cycle C_n of length n. As stated in [11], for $\ell = 0, \ldots, n-1$, $2\cos\left(\frac{2\pi\ell}{n}\right)$ is an eigenvalue of $A(C_n)$ associated to $\mathbf{x}_\ell = \left(1, \epsilon^\ell, \ldots, \epsilon^{(n-1)\ell}\right)^T$ where $\epsilon = e^{\frac{2\pi i}{n}}$. If n is even, then $\mu_n(C_n)$ is simple and $\mathbf{x}_{\frac{n}{2}} = (1, -1, 1, \ldots, 1, -1)^T$ is a corresponding eigenvector. So, we have $i^*_{\mu_n}(C_n) = \frac{n}{2}$ for even n. Suppose that n is odd. Then, the algebraic multiplicity of μ_n is 2, and corresponding linearly independent eigenvectors are $\mathbf{x}_{\frac{n-1}{2}}$ and $\mathbf{x}_{\frac{n+1}{2}}$. Let $\mathbf{v} = (v_0, \ldots, v_{n-1})^T$ and $\mathbf{w} = (w_0, \ldots, w_{n-1})^T$ where $v_j = (-1)^j\cos\left(\frac{\pi}{n}j\right)$ and $w_j = (-1)^j\sin\left(\frac{\pi}{n}j\right)$ for $j = 0, \ldots, n-1$, respectively. One can verify that $\mathbf{v} = \frac{\mathbf{x}_{\frac{n-1}{2}} + \mathbf{x}_{\frac{n+1}{2}}}{2}$ and $\mathbf{w} = \frac{-\mathbf{x}_{\frac{n-1}{2}} + \mathbf{x}_{\frac{n+1}{2}}}{2i}$. Hence, in order to find $i^*_{\mu_n}(C_n)$ for odd n, we need to consider all possible linear combinations of $\mathbf{v}$ and $\mathbf{w}$.

Proposition 4.5.6. *Let C_n be a cycle of length n. Then, $i^*_{\mu_n}(C_n) = \lfloor \frac{n}{2} \rfloor$.*

Proof. For an even cycle, it is clear that $i^*_{\mu_n}(C_n) = \frac{n}{2}$. Suppose that n is odd. Since every Fiedler vector of C_n is a linear combination of $\mathbf{v}$ and $\mathbf{w}$,

$$i^*_{\mu_n}(C_n) = \min\{i_{\mu_n}(c_1\mathbf{v} + c_2\mathbf{w}) | c_1, c_2 \in \mathbb{R},\ (c_1, c_2) \neq (0, 0)\}.$$

Let $\mathbf{u} = c_1\mathbf{v} + c_2\mathbf{w}$ where $\mathbf{u} = (u_0, \ldots, u_{n-1})^T$. If $c_1 = 0$ and $c_2 \neq 0$, then $i^*_{\mu_n}(\mathbf{u}) = \frac{n-1}{2}$. Assume that $c_1 \neq 0$. Note that for $j = 0, \ldots, n-1$, $u_j = c_1v_j + c_2w_j = (-1)^j\sqrt{c_1^2 + c_2^2}\cos\left(\frac{\pi}{n}j - \theta\right)$ where $\tan(\theta) = \frac{c_2}{c_1}$. We have $u_ju_{j+1} = -(c_1^2 + c_2^2)\cos(\alpha_j)\cos\left(\alpha_j + \frac{\pi}{n}\right)$ where $\alpha_j = \frac{\pi}{n}j - \theta$. One can check that $u_ju_{j+1} > 0$ if and only if $\alpha_j \in (0, \frac{\pi}{2})$ and $\alpha_j + \frac{\pi}{n} \in (\frac{\pi}{2}, \pi)$, or $\alpha_j \in (\pi, \frac{3\pi}{2})$ and $\alpha_j + \frac{\pi}{n} \in (\frac{3\pi}{2}, 2\pi)$. Suppose that $u_j \neq 0$ for all $j = 0, \ldots, n-1$. Since $\alpha_0, \ldots, \alpha_{n-1} \in [-\theta, -\theta + \pi)$, there exists at most one index j in $\{0, \ldots, n-2\}$ such that $u_ju_{j+1} > 0$. Hence, since $u_ju_{j+1} > 0$ implies that u_j and u_{j+1} have the same sign, a change of signs between u_j and u_{j+1} for $j = 0, \ldots, n-2$ occurs at least $(n-2)$ times. It follows that there are either $\frac{n-1}{2}$ negative and $\frac{n+1}{2}$ positive signs in $\mathbf{u}$ or $\frac{n-1}{2}$ positive and $\frac{n+1}{2}$ negative signs in $\mathbf{u}$. Therefore, $i^*_{\mu_n}(\mathbf{u}) = \frac{n-1}{2}$. Assume that there exists $j_0 \in \{0, \ldots, n-1\}$ such that $u_j = 0$. Since $\alpha_0, \ldots, \alpha_{n-1} \in [-\theta, -\theta + \pi)$, the j_0 is the only solution to $u_j = 0$ for $j = 0, \ldots, n-1$. Consider $u_{j_0-1}u_{j_0+1} = (c_1^2 + c_2^2)\cos(\alpha_{j_0-1})\cos(\alpha_{j_0+1})$. Since $\alpha_{j_0-1} \in (0, \frac{\pi}{2})$ and $\alpha_{j_0+1} \in (\frac{\pi}{2}, \pi)$, or $\alpha_{j_0-1} \in (\pi, \frac{3\pi}{2})$ and $\alpha_{j_0+1} \in (\frac{3\pi}{2}, 2\pi)$, we obtain $u_{j_0-1}u_{j_0+1} < 0$. Furthermore, $u_j u_{j+1} < 0$ for $j \in \{0, \ldots, n-2\} \backslash \{j_0 - 1, j_0\}$. Then, there are $\frac{n-1}{2}$ positive and negative signs, respectively, and one 0 in $\mathbf{u}$. Hence, $i^*_{\mu_n}(\mathbf{u}) = \frac{n-1}{2}$. Therefore, we have the desired result. $\square$

Corollary 4.5.7. *Let C_n be a cycle of length n. Then, $i^*_{\mu_n}(C_n) = 2$ if and only if $n = 4, 5$.*

Lemma 4.5.8. *Suppose that a connected regular graph H of order n has $\mu_n(H) > -2$. Then, $i^*_{\mu_n}(H) = 2$ if and only if $H = C_5$.*

Proof. It is immediately proved by Proposition 4.5.5 and Corollary 4.5.7. $\square$

Problem 4.5.9. *Develop a systematic tool to find $i(G)$ where G is a connected graph. As seen in the proof of Proposition 4.5.6, we consider all possible linear combinations of Fiedler vectors of C_n in order to find $i(C_n)$. It can be seen that this work is related to polyhedra [33]. One could approach this question with oriented matroids.*

Recall that $\mathbf{e}_i$ is a vector whose i^{th} component is 1 and zeros elsewhere.

Definition 4.5.10. [25] For $n > 1$, let D_n be the set of vectors of the form $\pm\mathbf{e}_i \pm \mathbf{e}_j$ $(i < j)$.

Definition 4.5.11. [25] Let E_8 be the set of vectors in $\mathbb{R}^8$ consisting of the 112 vectors in D_8 together with the 128 vectors of the form $\pm\frac{1}{2}\mathbf{e}_1 \pm \frac{1}{2}\mathbf{e}_2 \pm \cdots \pm \frac{1}{2}\mathbf{e}_8$, where the number of positive coefficients is even.

Now, the regular line graphs and regular exceptional graphs with least adjacency eigenvalue -2 are left to consider. These graphs are studied in [25] using D_n and E_8, the so-called *root systems*. Let H be a graph on n vertices with least adjacency eigenvalue -2. The symmetric matrix $2I + A(H)$ is positive semi-definite of rank s, say. Since $2I + A(H)$ is orthogonally diagonalisable, it follows that $C^TC = 2I + A(H)$ where C is an $s \times n$ matrix of rank s. According to [25], the column vectors of C are determined by D_n or E_8.

Lemma 4.5.12. *Let H be a connected regular graph with the least adjacency eigenvalue -2. If H contains an induced 4-cycle, there exists an eigenvector $\mathbf{x}^T = (1, -1, 1, -1, 0, \ldots, 0)$ of $A(H)$ associated with -2.*

Proof. Considering the root systems, there exists a real matrix C such that $C^TC = 2I + A(H)$. Since H contains an induced 4-cycle, without loss of generality, the leading principal 4×4 submatrix of $A(H)$ is an adjacency matrix of C_4. Let the first four columns of C comprise the matrix $\widetilde{C}$. Then,

$$\widetilde{C}^T\widetilde{C} = 2I + A(C_4).$$

Since $\tilde{\mathbf{x}}^T = (1, -1, 1, -1)$ is an eigenvector of $A(C_4)$ associated to -2, we have that $(\widetilde{C}\tilde{\mathbf{x}})^T\widetilde{C}\tilde{\mathbf{x}} = 0$. C is real, so $\widetilde{C}\tilde{\mathbf{x}} = 0$. Suppose that $\mathbf{x}^T = (1, -1, 1, -1, 0, \dots, 0)$. Then, $C\mathbf{x} = 0$. Therefore, follows that $\mathbf{x}$ is an eigenvector of $A(H)$ associated to -2. $\square$

Lemma 4.5.13. *Let H be a connected r-regular graph of order n with $\mu_n(H) = -2$ where $r+2 < n$. Then, $i^*_{\mu_n}(H) = 2$ if and only if H contains a 4-cycle as an induced subgraph.*

Proof. Suppose that $i^*_{\mu_n}(H) = 2$. Since $r + 2 < n$, the complement $\bar{H}$ of H is connected and regular with $\mu_2(\bar{H}) = 1$. Moreover, $i_{\mu_2}(\bar{H}) = i(\bar{H}) = 2$. By Proposition 4.5.3, $\bar{H}$ contains two non-adjacent edges as an induced subgraph. Therefore, H has an induced subgraph C_4.

Let us consider the converse. By Lemma 4.5.12, there exists an eigenvector $\mathbf{x}^T = (1, -1, 1, -1, 0, \dots, 0)$ of $A(H)$ associated to -2. So, $i^*_{\mu_n}(H) \leq 2$. Since $\mu_n \neq r$, any eigenvector associated to μ_n must contain negative and positive components. So, $i^*_{\mu_n}(H) > 0$. Suppose that $i^*_{\mu_n}(H) = 1$. Since $\bar{H}$ is connected, it follows that $i^*_{\mu_n}(H) = i_{\mu_2}(\bar{H}) = i(\bar{H}) = 1$. So, $\bar{H}$ can be expressed as a join of two graphs by Theorem 4.2.8. This is a contradiction to being a connected graph. Therefore, $i^*_{\mu_n}(H) = 2$. $\square$

Here is the our main result in this section regarding the characterization of all connected regular graphs G with $i(G) = 2$.

Theorem 4.5.14. *Let G be a connected r-regular graph of order n. Then, $i(G) = 2$ if and only if there exists a component H of order m in $\bar{G}$ such that $\mu_n(\bar{G}) = \mu_m(H) = \alpha(G) - r - 1$ and H satisfies either*

(i) $r - 1 < \alpha(G) < r$ *and* $H = C_5$, *or*

(ii) $\alpha(G) = r - 1$, *H is not a cocktail party graph and H contains C_4 as an induced subgraph.*

Proof. Combining Lemmas 4.5.4, 4.5.8 and 4.5.13, we obtain the desired result. □

Example 4.5.15. Let H be a strongly regular graph with least adjacency eigenvalue -2. According to Seidel's classification [61], H is one of

(i) the complete n-partite graph $K_{2,\dots,2}$ for $n \geq 2$,

(ii) the Petersen graph,

(iii) the line graph of K_n for $n \geq 5$,

(iv) the Cartesian product of two K_ns for $n \geq 3$,

(v) the Shrikhande graph,

(vi) one of the three Chang graphs,

(vii) the Clebsch graph,

(viii) the Schläfli graph.

We refer the reader to [25] for details of graphs (v)–(viii). Note that $K_{2,\dots,2}$ is expressed as a join of graphs. The girth of the Petersen graph is 5. It can be checked that H has an induced 4-cycle if and only if the line graph of H contains C_4 as an induced graph. This implies that any line graph of a complete graph is C_4-free. For the other graphs from (4) to (8), it can be checked that they have C_4 as an induced subgraph. Therefore, if a connected regular graph G has one of graphs from (4) to (8) as a component in $\bar{G}$, then $i(G) = 2$.

Problem 4.5.16. *Completely characterize graphs with* $i(G) = 2$*.*

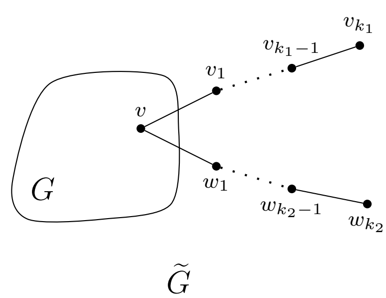
5

Families of graphs with the Braess edge on twin pendent paths

This chapter is essentially based on a study of Kemeny's constant from a combinatorial standpoint. Recall that for a connected graph G, Kemeny's constant $\kappa(G)$ for the transition matrix of the random walk on G is

$$\kappa(G) = \frac{\mathbf{d}_G^T F_G \mathbf{d}_G}{4 m_G \tau_G}.$$

We refer the reader to Sections 2.1 and 2.4 for the symbols in the formula of Kemeny's constant. We also recall that if, for a non-edge e of G, $\kappa(G) < \kappa(G \cup e)$, then e is said to be a Braess edge for G. Let us revisit Figure 2.1 for twin pendent paths:



Then, our main work is to study if the non-edge $v_{k_1} \sim w_{k_2}$ is a Braess edge for $\widetilde{G}$.

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5.1 Introduction

Kemeny's constant can be used to quantify the average time for travel of a Markov chain between randomly chosen states; related applications can be found in [70] for detecting potential super-spreaders of COVID-19, and in [22] for determining 'critical' roads in vehicle traffic networks based on Markov chains.

Intuitively, in the context of a random walk on a graph, 'well connected' graphs have 'low' Kemeny's constants. However, there are graphs such that the addition of an edge results in an increase of Kemeny's constant. The term Braess edge is introduced for such edges in [47], and acknowledges Dietrich Braess who studied the so-called Braess' paradox for traffic networks [9]. Kirkland and Zeng [47] provide a particular family of trees with twin pendent vertices such that the non-edge between the twin pendent vertices is a Braess edge. Furthermore, Ciardo [21] extends the result to all connected graphs with twin pendent vertices. Unlike the works [47] and [21], Hu and Kirkland [39] establish equivalent conditions for complete multipartite graphs and complete split graphs to have every non-edge as a Braess edge.

Our objective is to generalise the circumstances in [47, 21] where graphs have a pair of twin pendent vertices; so, we consider graphs that can be constructed from a connected graph and two paths by identifying a vertex of the graph and a pendent vertex of each path. We call the two paths *twin pendent paths* in the constructed graph. In Section 5.2, a formula is derived that identifies a graph with twin pendent paths in which the non-edge between the pendent vertices of the twin pendent paths in the graph is a Braess edge. In Sections 5.3 and 5.4, tools are provided in order to investigate the asymptotic behaviour of a family of graphs with twin pendent paths regarding the tendency to have a non-edge as a Braess edge. Furthermore, several families of graphs are discussed throughout Sections 5.2, 5.3, and 5.4. In particular, asymptotic behaviours of families of trees are characterized in Section 5.4.

5.2 Graphs with the Braess edge on twin pendent paths

Recall that given a graph G of order n with a labelling of $V(G)$, $\mathbf{d}_G$ denotes the column vector whose i^{th} component is $\deg_G(v_i)$ for $1 \leq i \leq n$, where v_i is the i^{th} vertex in $V(G)$.

Proposition 5.2.1. *Let H_1 and H_2 be connected graphs, and let $v_1 \in V(H_1)$ and $v_2 \in V(H_2)$. Assume that G is obtained from H_1 and H_2 by identifying v_1 and v_2*

as a vertex v. Suppose that $\widetilde{H}_1 = H_1 - v_1$ and $\widetilde{H}_2 = H_2 - v_2$. Then, labelling the vertices of G in order of $V(\widetilde{H}_1)$, v, and $V(\widetilde{H}_2)$, we have:

$$\begin{aligned}
\mathbf{d}_G^T &= \begin{bmatrix}\mathbf{d}_{\widetilde{H}_1}^T & \deg_{H_1}(v) & \mathbf{0}_{|V(\widetilde{H}_2)|}^T\end{bmatrix} + \begin{bmatrix}\mathbf{0}_{|V(\widetilde{H}_1)|}^T & \deg_{H_2}(v) & \mathbf{d}_{\widetilde{H}_2}^T\end{bmatrix},\\
m_G &= m_{H_1} + m_{H_2},\\
\tau_G &= \tau_{H_1}\tau_{H_2},\\
F_G &= \left[\begin{array}{c|c|c}
\tau_{H_2}F_{\widetilde{H}_1} & \tau_{H_2}\mathbf{f}_1 & \tau_{H_2}\mathbf{f}_1\mathbf{1}^T + \tau_{H_1}\mathbf{1}\mathbf{f}_2^T\\ \hline
\tau_{H_2}\mathbf{f}_1^T & 0 & \tau_{H_1}\mathbf{f}_2^T\\ \hline
\tau_{H_1}\mathbf{f}_2\mathbf{1}^T + \tau_{H_2}\mathbf{1}\mathbf{f}_2^T & \tau_{H_1}\mathbf{f}_2 & \tau_{H_1}F_{\widetilde{H}_2}
\end{array}\right],
\end{aligned}$$

where $\mathbf{f}_1$ and $\mathbf{f}_2$ are the column vectors obtained from $\mathbf{f}_{H_1}^v$ and $\mathbf{f}_{H_2}^v$ by deleting the v^{th} component (which is 0), respectively.

Proof. The conclusions for $\mathbf{d}_G$ and m_G are readily established. Since $f_{i,j}^G = f_{j,i}^G$ for all $i, j \in V(G)$, F_G is symmetric. Hence, we only need to verify the entries above the main diagonal. Note that v is a cut-vertex of G. Since all spanning trees of G can be obtained from spanning trees in H_1 and H_2 by identifying v_1 and v_2 as v, we have $\tau_G = \tau_{H_1}\tau_{H_2}$. Let $i, j \in V(H_1)$. For each spanning forest of H_1 in $\mathcal{F}_{H_1}(i;j)$, we can obtain τ_{H_2} spanning forests of G in $\mathcal{F}_G(i;j)$ from the forest of H_1 and each of τ_{H_2} spanning trees of H_2 by identifying v_1 and v_2. Therefore, $f_{i,j}^G = \tau_{H_2} f_{i,j}^{H_1}$ for $i, j \in V(H_1)$. Similarly, for $i, j \in V(H_2)$, we have $f_{i,j}^G = \tau_{H_1} f_{i,j}^{H_2}$. Let $i \in V(\widetilde{H}_1)$ and $j \in V(\widetilde{H}_2)$. The set $\mathcal{F}_G(i;j)$ is a disjoint union of A_i and A_j, where A_i is the set of spanning forests of G in $\mathcal{F}_G(i;j)$ such that the tree having the vertex i among the two trees contains v, and $A_j = \mathcal{F}_G(i;j)\backslash A_i$. Since for each spanning forest in A_i the tree with i has v, the tree contains a spanning tree of H_1 as a subtree. So, any forest in A_i can be constructed from a spanning tree of H_1 and a spanning forest in $\mathcal{F}_{H_2}(v_2;j)$ with v_1 and v_2 identified as v. Hence, we have $|A_i| = \tau_{H_1} f_{v_2,j}^{H_2}$. Note that $f_{i,v_1}^{H_1} = f_{v_1,i}^{H_1}$. Applying an analogous argument to the case $|A_j|$, we have $|A_j| = \tau_{H_2} f_{i,v_1}^{H_1}$. Therefore, $f_{i,j}^G = \tau_{H_2} f_{i,v}^{H_1} + \tau_{H_1} f_{v,j}^{H_2}$ for $i \in V(\widetilde{H}_1)$ and $j \in V(\widetilde{H}_2)$. $\square$

Continuing with the hypotheses and notation of Proposition 5.2.1, we have

$$\tau_{H_2}F_{H_1} = \begin{bmatrix}\tau_{H_2}F_{\widetilde{H}_1} & \tau_{H_2}\mathbf{f}_1\\ \tau_{H_2}\mathbf{f}_1^T & 0\end{bmatrix},\ \tau_{H_1}F_{H_2} = \begin{bmatrix}0 & \tau_{H_1}\mathbf{f}_2^T\\ \tau_{H_1}\mathbf{f}_2 & \tau_{H_1}F_{\widetilde{H}_2}\end{bmatrix}.$$

Note that $(\mathbf{f}^v_{H_1})^T = \begin{bmatrix}\mathbf{f}_1^T & 0\end{bmatrix}$ and $(\mathbf{f}^v_{H_2})^T = \begin{bmatrix}0 & \mathbf{f}_2^T\end{bmatrix}$. Then,

$$\begin{bmatrix}\tau_{H_2}\mathbf{f}_1 & \tau_{H_2}\mathbf{f}_1\mathbf{1}^T_{|V(\widetilde{H}_2)|} + \tau_{H_1}\mathbf{1}_{|V(\widetilde{H}_1)|}\mathbf{f}_2^T \\ 0 & \tau_{H_1}\mathbf{f}_2^T\end{bmatrix} = \tau_{H_2}\mathbf{f}^v_{H_1}\mathbf{1}^T_{|V(H_2)|} + \tau_{H_1}\mathbf{1}_{|V(H_1)|}(\mathbf{f}^v_{H_2})^T.$$

Considering $\mathbf{d}_G^T = [\mathbf{d}_{H_1}^T \ \mathbf{0}^T_{|V(\widetilde{H}_2)|}] + [\mathbf{0}^T_{|V(\widetilde{H}_1)|} \ \mathbf{d}^T_{H_2}]$, we have

$$\begin{aligned}
&\mathbf{d}_G^T F_G \mathbf{d}_G \\
=&\tau_{H_2}\mathbf{d}^T_{H_1}F_{H_1}\mathbf{d}_{H_1} + \tau_{H_1}\mathbf{d}^T_{H_2}F_{H_2}\mathbf{d}_{H_2} + 2\mathbf{d}^T_{H_1}\begin{bmatrix}\tau_{H_2}\mathbf{f}_1 & \tau_{H_2}\mathbf{f}_1\mathbf{1}^T + \tau_{H_1}\mathbf{1}\mathbf{f}_2^T \\ 0 & \tau_{H_1}\mathbf{f}_2^T\end{bmatrix}\mathbf{d}_{H_2} \\
=&\tau_{H_2}\mathbf{d}^T_{H_1}F_{H_1}\mathbf{d}_{H_1} + \tau_{H_1}\mathbf{d}^T_{H_2}F_{H_2}\mathbf{d}_{H_2} + 2\mathbf{d}^T_{H_1}\left(\tau_{H_2}\mathbf{f}^v_{H_1}\mathbf{1}^T_{|V(H_2)|} + \tau_{H_1}\mathbf{1}_{|V(H_1)|}(\mathbf{f}^v_{H_2})^T\right)\mathbf{d}_{H_2} \\
=&\tau_{H_2}\mathbf{d}^T_{H_1}F_{H_1}\mathbf{d}_{H_1} + \tau_{H_1}\mathbf{d}^T_{H_2}F_{H_2}\mathbf{d}_{H_2} + 4\tau_{H_2}m_{H_2}\mathbf{d}^T_{H_1}\mathbf{f}^v_{H_1} + 4\tau_{H_1}m_{H_1}\mathbf{d}^T_{H_2}\mathbf{f}^v_{H_2}. \qquad (5.2.1)
\end{aligned}$$

Hence, given m_{H_i} and τ_{H_i} for $i = 1, 2$, $\mathbf{d}_G^T F_G \mathbf{d}_G$ can be computed from $\mathbf{d}^T_{H_i}F_{H_i}\mathbf{d}_{H_i}$ and $\mathbf{d}^T_{H_i}\mathbf{f}^v_{H_i}$ for $i = 1, 2$. The following examples regarding K_n, C_n, P_n and S_n present the corresponding quantities $\mathbf{d}^T F\mathbf{d}$ and $\mathbf{d}^T\mathbf{f}^v$, and will assist us later to obtain several results and related examples.

Example 5.2.2. Consider a complete graph K_n. Then, $m = \binom{n}{2}$ and $\tau = n^{n-2}$ by Cayley's formula (see [17]). Note that K_n is edge-transitive (see [35]), *i.e.,* for any pair of edges of K_n, there is an automorphism that maps one edge to the other. So, $F_{K_n} = \alpha(J - I)$ where $\alpha = f^{K_n}_{i,j}$ for all $i, j \in V(K_n)$. Then, α is the determinant of a submatrix obtained from the Laplacian matrix of K_n by deleting i^{th} and j^{th} rows and columns where $i \neq j$ (see [15]). It can be seen that $\alpha = 2n^{n-3}$. Therefore, for any vertex v in K_n, we have

$$\begin{aligned}
\mathbf{d}^T F\mathbf{d} &= \alpha(n-1)^2\mathbf{1}^T(J - I)\mathbf{1} = 2n^{n-2}(n-1)^3, \\
\mathbf{d}^T\mathbf{f}^v &= \alpha(n-1)\mathbf{1}^T(\mathbf{1} - \mathbf{e}_v) = 2n^{n-3}(n-1)^2.
\end{aligned}$$

Example 5.2.3. Consider the cycle $C_n = (1, 2, \ldots, n, 1)$ where $n \geq 3$. For $1 \leq v \leq n$, we obtain

$$\begin{aligned}
&F_{C_n} = \Big[d(i,j)(n - d(i,j))\Big]_{1\leq i,j\leq n}, \ \mathbf{d} = 2\mathbf{1}, \\
&(\mathbf{f}^v)^T = \Big[(v-1)(n-(v-1)) \ \ \cdots \ \ 1\cdot(n-1) \ \ 0 \ \ 1\cdot(n-1) \ \ \cdots \ \ (n-v)v\Big].
\end{aligned}$$

It can be checked that

$$\mathbf{d}^T F \mathbf{d} = \frac{2}{3}(n-1)n^2(n+1),$$
$$\mathbf{d}^T \mathbf{f}^v = \frac{1}{3}(n-1)n(n+1) \text{ for } v = 1, \ldots, n.$$

Note that for any tree $\mathcal{T}$, $F_{\mathcal{T}}$ is the distance matrix of $\mathcal{T}$ (see [47]), which is the matrix whose (i,j)-entry is the distance between i and j.

Example 5.2.4. Consider the path $P_n = (1, 2, \ldots, n)$ where $n \geq 2$. Let v be a vertex of P_n. For $1 \leq v \leq n$, we have

$$F_{P_n} = \Big[|i-j|\Big]_{1 \leq i,j \leq n}, \ \mathbf{d} = 2\mathbf{1}_n - \mathbf{e}_1 - \mathbf{e}_n,$$
$$(\mathbf{f}^v)^T = \begin{bmatrix} v-1 & \cdots & 1 & 0 & 1 & \cdots & n-v \end{bmatrix}.$$

One can verify that

$$\mathbf{d}^T F \mathbf{d} = 4\mathbf{1}^T F \mathbf{1} - 4\mathbf{1}^T F \mathbf{e}_1 - 4\mathbf{1}^T F \mathbf{e}_n + 2\mathbf{e}_1^T F \mathbf{e}_n = \frac{4}{3}(n-1)^3 + \frac{2}{3}(n-1),$$
$$\mathbf{d}^T \mathbf{f}^v = (v-1)^2 + (n-v)^2 \text{ for } v = 1, \ldots, n.$$

Example 5.2.5. Consider a star S_n where $n \geq 3$. Suppose that n is the centre vertex. Then, we have

$$\mathbf{d}^T = \begin{bmatrix} \mathbf{1}_{n-1}^T & 0 \end{bmatrix} + (n-1)\mathbf{e}_n, \ F_{S_n} = \begin{bmatrix} 2(J-I) & \mathbf{1}_{n-1} \\ \mathbf{1}_{n-1}^T & 0 \end{bmatrix}.$$

Hence, for a vertex $1 \leq v \leq n$,

$$\mathbf{d}^T F \mathbf{d} = 2\mathbf{1}_{n-1}^T (J-I)\mathbf{1}_{n-1} + 2(n-1)^2 = 2(n-1)(2n-3),$$
$$\mathbf{d}^T \mathbf{f}^v = \begin{cases} n-1, & \text{if } v = n \\ 3n-5, & \text{if } v \neq n. \end{cases}$$

Lemma 5.2.6. *Let P_k be a path with two pendent vertices x and y where $k \geq 2$, and H be a connected graph. Suppose that G is the graph obtained from P_k and H by identifying a vertex of P_k and a vertex of H, say v. Suppose that $d_G(v,x) = k_1$ and $d_G(v,y) = k_2$. Then,*

$$\mathbf{d}_G^T F_G \mathbf{d}_G = \mathbf{d}_H^T F_H \mathbf{d}_H + 4(k-1)\mathbf{d}_H^T \mathbf{f}_H^v + \tau_H \left(\frac{4}{3}(k-1)^3 + \frac{2}{3}(k-1) + 4m_H(k_1^2 + k_2^2) \right).$$

Proof. The conclusion is straightforward from (5.2.1) and Example 5.2.4. $\square$

Lemma 5.2.7. *Let C_k be a cycle where $k \geq 3$, and H be a connected graph. Suppose that G is the graph obtained from C_k and H by identifying a vertex of C_k and a vertex of H, say v. Then,*

$$\mathbf{d}_G^T F_G \mathbf{d}_G = k\mathbf{d}_H^T F_H \mathbf{d}_H + 4k^2 \mathbf{d}_H^T \mathbf{f}_H^v + \frac{2\tau_H}{3}(k + 2m_H)(k-1)k(k+1).$$

Proof. The conclusion is readily established from (5.2.1) and Example 5.2.3. $\square$

We shall investigate paradoxical graphs under certain circumstances. Let G be a connected graph on n vertices, and $v \in V(G)$. Fix two non-negative integers k_1, k_2 with $k_1 + k_2 \geq 2$. Let $\widetilde{G}(v, k_1, k_2)$ denote the graph obtained from G, $P_{k_1} = (v_0, \ldots, v_{k_1})$ and $P_{k_2} = (w_0, \ldots, w_{k_2})$ by identifying the vertices v, v_0 and w_0. Also, we denote by $\widehat{G}(v, k_1, k_2)$ the graph obtained from $\widetilde{G}(v, k_1, k_2)$ by inserting the edge $v_{k_1} \sim w_{k_2}$. We say that G is (v, k_1, k_2)-*paradoxical* if $\kappa(\widehat{G}(v, k_1, k_2)) > \kappa(\widetilde{G}(v, k_1, k_2))$. If G is (v, k_1, k_2)-paradoxical for every $v \in V(G)$, then we say that G is (k_1, k_2)-*paradoxical*.

Theorem 5.2.8. *Let G be a connected graph with a vertex v. Suppose that $k_1, k_2 \geq 0$, $k_1 + k_2 \geq 2$ and $k - 1 = k_1 + k_2$. Then, G is (v, k_1, k_2)-paradoxical if and only if*

$$\begin{aligned}
&k\mathbf{d}_G^T(2\mathbf{f}_G^v \mathbf{1}^T - F_G)\mathbf{d}_G + 4m_G^2 \tau_G k \left(-\frac{2}{3}(k_1 + k_2)(k_1 + k_2 - 1) + 2k_1 k_2\right) \\
&+ \frac{2m_G \tau_G k}{3}\left(-5(k_1 + k_2)^3 + (k_1 + k_2)^2 + (k_1 + k_2) + 12k_1 k_2(k_1 + k_2 + 1)\right) \\
&- \frac{2\tau_G k}{3}(k_1 + k_2 + 1)(k_1 + k_2)(k_1 + k_2 - 1)^2 > 0.
\end{aligned} \tag{5.2.2}$$

Proof. Evidently, $m_{\widetilde{G}} = m_G + k - 1$, $m_{\widehat{G}} = m_G + k$ and $\tau_{\widetilde{G}} = \tau_G$. Since v is a cut-vertex in $\widehat{G}$, we have $\tau_{\widehat{G}} = k\tau_G$. Then,

$$\begin{aligned}
\kappa(\widehat{G}(v, k_1, k_2)) - \kappa(\widetilde{G}(v, k_1, k_2)) &= \frac{\mathbf{d}_{\widehat{G}}^T F_{\widehat{G}} \mathbf{d}_{\widehat{G}}}{4m_{\widehat{G}} \tau_{\widehat{G}}} - \frac{\mathbf{d}_{\widetilde{G}}^T F_{\widetilde{G}} \mathbf{d}_{\widetilde{G}}}{4m_{\widetilde{G}} \tau_{\widetilde{G}}} \\
&= \frac{(m_G + k - 1)\mathbf{d}_{\widehat{G}}^T F_{\widehat{G}} \mathbf{d}_{\widehat{G}} - k(m_G + k)\mathbf{d}_{\widetilde{G}}^T F_{\widetilde{G}} \mathbf{d}_{\widetilde{G}}}{4k(m_G + k)(m_G + k - 1)\tau_G}.
\end{aligned} \tag{5.2.3}$$

Then, G is (v, k_1, k_2)-paradoxical if and only if

$$(m_G + k - 1)\mathbf{d}_{\widehat{G}}^T F_{\widehat{G}} \mathbf{d}_{\widehat{G}} - k(m_G + k)\mathbf{d}_{\widetilde{G}}^T F_{\widetilde{G}} \mathbf{d}_{\widetilde{G}} > 0.$$

For simplicity, let $\mathbf{d} = \mathbf{d}_G$, $\mathbf{f}^v = \mathbf{f}^v_G$, $F = F_G$, $m = m_G$ and $\tau = \tau_G$. Using Lemmas 5.2.6 and 5.2.7, we have

$$\begin{aligned}
&(m+k-1)\mathbf{d}^T_{\widehat{G}}F_{\widehat{G}}\mathbf{d}_{\widehat{G}} - k(m+k)\mathbf{d}^T_{\widetilde{G}}F_{\widetilde{G}}\mathbf{d}_{\widetilde{G}} \\
=&(m+k-1)\left(k\mathbf{d}^TF\mathbf{d} + 4k^2\mathbf{d}^T\mathbf{f}^v + \frac{2\tau}{3}(k+2m)(k-1)k(k+1)\right) \\
&- k(m+k)\left(\mathbf{d}^TF\mathbf{d} + 4(k-1)\mathbf{d}^T\mathbf{f}^v + \frac{4}{3}\tau(k-1)^3 + \frac{2}{3}\tau(k-1) + 4m\tau(k_1^2+k_2^2)\right) \\
=&-k\mathbf{d}^TF\mathbf{d} + 4mk\mathbf{d}^T\mathbf{f}^v + 4m^2\tau k\left(\frac{1}{3}(k-1)(k+1) - k_1^2 - k_2^2\right) \\
&+\frac{2m\tau k}{3}\left((k-1)k(k+1) + 2(k-1)^2(k+1) - 2(k-1)^3 - (k-1) - 6k(k_1^2+k_2^2)\right) \\
&+\frac{2\tau k}{3}\left((k-1)^2k(k+1) - 2k(k-1)^3 - k(k-1)\right).
\end{aligned} \tag{5.2.4}$$

Since $\mathbf{1}^T\mathbf{d} = 2m$, we have $4mk\mathbf{d}^T\mathbf{f}^v = 2k\mathbf{d}^T\mathbf{f}^v\mathbf{1}^T\mathbf{d}$. Then, one can check from $k-1 = k_1 + k_2$ that the last expression in (5.2.4) can be recast as the left side of the inequality (5.2.2). □

Problem 5.2.9. *Generalise Theorem 5.2.8 as follows. Let G be a connected graph with a vertex v, and let $P_{k_1} = (v_0, \ldots, v_{k_1})$ and $P_{k_2} = (w_0, \ldots, w_{k_2})$ where $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$. Suppose that H is the graph obtained from $\widetilde{G}(v, k_1, k_2)$ by adding an edge $v_i \sim w_j$ for some $1 \leq i \leq k_1$ and $1 \leq j \leq k_2$. Establish an equivalent condition for $\kappa(H) > \kappa(\widetilde{G}(v, k_1, k_2))$ as in that theorem.*

Let G be a connected graph of order n with $V(G) = \{1, \ldots, n\}$. Let

$$\begin{aligned}
\phi_G(v) &:= \mathbf{d}^T_G(2\mathbf{f}^v_G\mathbf{1}^T - F_G)\mathbf{d}_G, \\
\phi_1(k_1, k_2) &:= -\frac{2}{3}(k_1+k_2)(k_1+k_2-1) + 2k_1k_2, \\
\phi_2(k_1, k_2) &:= -(k_1+k_2)(5(k_1+k_2)^2 - (k_1+k_2) - 1) + 12k_1k_2(k_1+k_2+1), \\
\phi_3(k_1, k_2) &:= -(k_1+k_2+1)(k_1+k_2)(k_1+k_2-1)^2,
\end{aligned}$$

where v, k_1 and k_2 are integers such that $1 \leq v \leq n$, $k_1, k_2 \geq 0$ and $k_1 + k_2 \geq 2$. Furthermore, let

$$\Phi_G(v, k_1, k_2) := k\phi_G(v) + 4m_G^2\tau_G k\phi_1(k_1, k_2) + \frac{2m_G\tau_G k}{3}\phi_2(k_1, k_2) + \frac{2\tau_G k}{3}\phi_3(k_1, k_2). \tag{5.2.5}$$

By Theorem 5.2.8, G is (v, k_1, k_2)-paradoxical if and only if $\Phi_G(v, k_1, k_2) > 0$. We simply write $\Phi_G(v,k_1,k_2)$ and $\phi_G(v)$ as $\Phi(v,k_1,k_2)$ and $\phi(v)$, respectively, if G is clear from the context. Note that $\phi_i(k_1,k_2)=\phi_i(k_2,k_1)$ for $i=1,2,3$. So, $\Phi_G(v,k_1,k_2)=\Phi_G(v,k_2,k_1)$.

Remark 5.2.10. A connected graph G is (v,k_1,k_2)-paradoxical if and only if G is (v,k_2,k_1)-paradoxical. Furthermore, G is (k_1,k_2)-paradoxical if and only if G is (k_2,k_1)-paradoxical.

We shall consider the signs of $\phi_i(k_1,k_2)$ for $i=1,2,3$ in terms of k_1 and k_2. Evidently, $\phi_3(k_1,k_2)$ decreases as k_1+k_2 increases, and so

$$\phi_3(k_1,k_2)\le -6 \text{ for any } k_1,k_2\ge 0 \text{ where } k_1+k_2\ge 2 \tag{5.2.6}$$

with equality if and only if $k_1+k_2=2$. Next, $\phi_1(k_1,k_2)$ can be written as

$$\phi_1(k_1,k_2)=-\frac{2}{3}(k_1^2-(k_2+1)k_1+k_2^2-k_2).$$

Setting $\phi_1(k_1,k_2)=0$, we have

$$k_1=\frac{1}{2}\left((k_2+1)\pm\sqrt{-3k_2^2+6k_2+1}\right).$$

Since $\phi_1(k_1,k_2)$ is symmetric, without loss of generality, we shall fix k_2 first. It follows from $-3k_2^2+6k_2+1<0$ that if $k_2<1-\frac{2\sqrt{3}}{3}<0$ or $k_2>1+\frac{2\sqrt{3}}{3}>2$, then $\phi_1(k_1,k_2)<0$ for any $k_1\ge 0$. Furthermore, if $k_2=1$, then $\phi_1(1,1)=\frac{2}{3}$, $\phi_1(2,1)=0$ and $\phi_1(k_1,1)<0$ for $k_1>2$. Finally, for $k_2=2$, we have $\phi_1(0,2)=-\frac{4}{3}$, $\phi_1(1,2)=\phi_1(2,2)=0$ and $\phi_1(k_1,2)<0$ for $k_1>2$. Therefore, $\phi_1(k_1,k_2)>0$ if and only if $(k_1,k_2)=(1,1)$; $\phi_1(k_1,k_2)=0$ if and only if $(k_1,k_2)\in\{(1,2),(2,1),(2,2)\}$; and $\phi_1(k_1,k_2)<0$ for any $k_1,k_2\ge 0$ with $k_1+k_2\ge 2$ and $(k_1,k_2)\notin\{(1,1),(1,2),(2,1),(2,2)\}$.

Remark 5.2.11. We have $\frac{\partial\phi_1}{\partial k_1}=-\frac{4}{3}k_1+\frac{2}{3}(k_2+1)$. Then, $\phi_1(2,0)=-\frac{4}{3}$ and $\left.\frac{\partial\phi_1}{\partial k_1}\right|_{k_2=0}<0$ for $k_1\ge 2$; $\phi_1(3,1)=-2$ and $\left.\frac{\partial\phi_1}{\partial k_1}\right|_{k_2=1}<0$ for $k_1\ge 3$; $\phi_1(3,2)=-\frac{4}{3}$ and $\left.\frac{\partial\phi_1}{\partial k_1}\right|_{k_2=2}<0$ for $k_1\ge 3$; finally, $\phi_1(k_2,k_2)=-\frac{2}{3}(k_2^2-2k_2)\le -2$ for $k_2\ge 3$ and $\frac{\partial\phi_1}{\partial k_1}<0$ for $k_1\ge k_2\ge 3$. Hence, since $\phi_1(k_1,k_2)$ is symmetric, $\phi_1(k_1,k_2)\le -\frac{4}{3}$ for integers $k_1,k_2\ge 0$ with $k_1+k_2\ge 2$ and $(k_1,k_2)\notin\{(1,1),(1,2),(2,1),(2,2)\}$. Furthermore, by computation, we have $\phi_1(3,0)=\phi_1(4,2)=-4$. Therefore, $\phi_1(k_1,k_2)\le -2$ for integers $k_1,k_2\ge 0$ with $k_1+k_2\ge 2$ and

$$(k_1,k_2)\notin\{(0,2),(2,0),(1,1),(1,2),(2,1),(2,2),(2,3),(3,2)\}.$$

Putting $k-1 = k_1 + k_2 \geq 2$, $\phi_2(k_1, k_2)$ can be written as

$$\phi_2(k_1, k_2) = -12kk_1^2 + 12k(k-1)k_1 - (k-1)(5k^2 - 11k + 5).$$

Setting $\phi_2(k_1, k_2) = 0$, we have

$$k_1 = \frac{1}{12k}\left(6k(k-1) \pm \sqrt{-12k(k-1)(2k^2 - 8k + 5)}\right).$$

Since $2k^2 - 8k + 5 > 0$ for all $k \geq 4$, $\phi_2(k_1, k_2) < 0$ for any $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 3$. For $k = 3$, we have $\phi_2(1, 1) = 2 > 0$ and $\phi_2(2, 0) = -34 < 0$. Let $f(t) = -(t-1)(2t^2 - 8t + 5)$ where t is real number. Then, for fixed $t \geq 3$, the maximum of $\phi_2(t_1, t_2)$ for nonnegative numbers t_1 and t_2 with $t_1 + t_2 = t - 1$ is attained as $f(t)$ at $t_1 = \frac{t-1}{2}$. We can find that $f(3) > 0$, $f(4) = -15$ and $f'(t) < 0$ for $t \geq 4$. From computation, we have $\phi_2(0, 3) = -123$ and $\phi_2(1, 2) = -27$. Hence,

$$\phi_2(k_1, k_2) < -15 \text{ for any } k_1, k_2 \geq 0 \text{ with } k_1 + k_2 \geq 2 \text{ and } (k_1, k_2) \neq (1, 1). \quad (5.2.7)$$

We claim that for a non-trivial connected graph G, $\phi(v) = \mathbf{d}^T(2\mathbf{f}^v\mathbf{1}^T - F)\mathbf{d} > 0$ for $v = 1, \ldots, n$. In order to establish our claim, we first show that $f_{i,j}^G$ is a metric on the vertex set of G by using the resistance distance (see [49] for an introduction). Let L be the Laplacian matrix of G, and let $L^\dagger = [\ell_{i,j}^\dagger]_{n\times n}$ be the Moore–Penrose inverse of L [56]. Then, the resistance distance $\Omega_{i,j}$ between vertices i and j of G is represented (see [48]) as:

$$\Omega_{i,j} = \ell_{i,i}^\dagger + \ell_{j,j}^\dagger - \ell_{i,j}^\dagger - \ell_{j,i}^\dagger.$$

Moreover, the resistance distance is a metric on $V(G)$ (see [6]). As proved in [18], the number $f_{i,j}^G$ of 2-tree spanning forests of G having i and j in different trees is

$$f_{i,j}^G = \tau_G \Omega_{i,j}.$$

Therefore, we have the following properties endowed by the metric $\Omega_{i,j}$:

(i) $f_{i,j}^G \geq 0$, with equality if and only if $i = j$;

(ii) $f_{i,j}^G = f_{j,i}^G$ for all i, j;

(iii) for any i, j, k, $f_{i,j}^G \leq f_{i,k}^G + f_{k,j}^G$, with equality [13] if and only if either all paths in G from i to j pass through k or k is one of i and j.

Let $X = 2\mathbf{f}^v\mathbf{1}^T - F$, and $R = [r_{i,j}] = \frac{X+X^T}{4}$. Then,

$$\mathbf{d}^T X\mathbf{d} = \frac{1}{2}(\mathbf{d}^T X\mathbf{d} + \mathbf{d}^T X^T\mathbf{d}) = 2\mathbf{d}^T R\mathbf{d}.$$

Since $2R = \mathbf{f}^v\mathbf{1}^T + \mathbf{1}(\mathbf{f}^v)^T - F$, we have $2r_{i,j} = f_{i,v} + f_{v,j} - f_{i,j} \geq 0$. Since G is connected, if $i \neq v$, then there exists a 2-tree spanning forest having i and v in different trees, *i.e.*, $f_{i,v} > 0$. For a non-trivial connected graph G, there exists a vertex i with $i \neq v$ such that $2r_{i,i} = f_{i,v} + f_{v,i} > 0$. Hence, R is a non-negative symmetric matrix with $R \neq 0$. Since $\mathbf{d} > 0$, we have $\mathbf{d}^T R\mathbf{d} > 0$. Therefore, $\mathbf{d}^T(2\mathbf{f}^v\mathbf{1}^T - F)\mathbf{d} > 0$.

We now discuss a combinatorial interpretation for $r_{i,j}$. Denote by $\mathcal{F}_G(i,j;v)$ (or equivalently $\mathcal{F}_G(v;i,j)$) the set of all spanning forests consisting of two trees in G, one of which contains vertices i and j and the other of which contains a vertex v. Then, we have

$$\begin{aligned}
|\mathcal{F}_G(i;j)| &= |\mathcal{F}_G(i;v,j)| + |\mathcal{F}_G(i,v;j)|,\\
|\mathcal{F}_G(i;v)| &= |\mathcal{F}_G(i,j;v)| + |\mathcal{F}_G(i;v,j)|,\\
|\mathcal{F}_G(v;j)| &= |\mathcal{F}_G(i,v;j)| + |\mathcal{F}_G(v;i,j)|.
\end{aligned}$$

It follows that $2r_{i,j} = f_{i,v} + f_{v,j} - f_{i,j} = 2|\mathcal{F}_G(i,j;v)|$, that is, $r_{i,j}$ is the number of 2-tree spanning forests of G having i, j in one tree and v in the other. Thus, we define $R_{G,v}$ as the matrix $R_{G,v} = [r_{i,j}]$ associated to G and v where $r_{i,j} = \frac{1}{2}(f_{i,v} + f_{v,j} - f_{i,j})$. The matrix $R_{G,v}$ is written as R if no confusion arises from the context.

Remark 5.2.12. Let G be a connected graph with a vertex v. Let $R_{G,v} = [r_{i,j}]$. Since $2r_{i,j} = f_{i,v} + f_{v,j} - f_{i,j}$, we have $r_{i,j} = 0$ whenever $v = i$ or $v = j$. Suppose that v is a cut-vertex. If there is no path from i to j with $i \neq v$ and $j \neq v$ in $G - v$, then by the combinatorial interpretation for $r_{i,j}$, we obtain $r_{i,j} = 0$. Consider a branch B of G at v. Let $i, j \in V(B)$. For each forest in $\mathcal{F}_G(i,j;v)$, the subtree with the vertex v in the forest must contain all vertices of $V(G)\backslash V(B)$. Thus, we have $|\mathcal{F}_G(i,j;v)| = |\mathcal{F}_B(i,j;v)|$.

Given a tree $\mathcal{T}$ with a vertex v, let $R_{\mathcal{T},v} = [r_{i,j}]$. Consider two vertices i and j in $\mathcal{T}$ with $i \neq v$ and $j \neq v$. For each forest in $\mathcal{F}_{\mathcal{T}}(i,j;v)$, there is a subtree of the forest having i and j. Then, all vertices $w_0, w_1, \ldots, w_{d(i,j)}$ on the subpath with pendent vertices i and j must be contained in the subtree. Therefore, $r_{i,j} = \min\{d(v, w_p) | p = 0, \ldots, d(i,j)\}$. In particular, if $i = j$ then $r_{i,j} = d(i,v)$.

Example 5.2.13. Consider the path $P_6 = (1, \ldots, 6)$. Let $R_{P_n,v} = [r_{i,j}]$ where $v = 3$. Remark 5.2.12 can be used for finding $R_{P_n,v}$ as follows. Evidently, $r_{3,i} = r_{i,3} = 0$ for $1 \le i \le 6$. Since v is a cut vertex, we have $r_{i,j} = 0$ for $i \in \{1, 2\}$ and $j \in \{4, 5, 6\}$. Finally, using the argument in the last paragraph in Remark 5.2.12, we have

$$R_{P_n,v} = \begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 2 & 2 \\ 0 & 0 & 0 & 1 & 3 & 3 \end{bmatrix}.$$

We now compute $\mathbf{d}^T R\mathbf{d}$ for K_n, C_n, P_n, and S_n.

Example 5.2.14. Given a complete graph K_n and a vertex v of K_n, from $2\mathbf{d}^T R\mathbf{d} = \mathbf{d}^T(2\mathbf{f}^v\mathbf{1}^T - F_{K_n})\mathbf{d}$ and Example 5.2.2, it is readily seen that

$$\mathbf{d}^T R\mathbf{d} = n^{n-2}(n-1)^3.$$

Example 5.2.15. Given a cycle C_n with a vertex v, from $2\mathbf{d}^T R_{C_n,v}\mathbf{d} = \mathbf{d}^T(2\mathbf{f}^v\mathbf{1}^T - F_{C_n})\mathbf{d}$ and Example 5.2.3, we have

$$\mathbf{d}^T R\mathbf{d} = \frac{1}{3}(n-1)n^2(n+1).$$

Let us compute $\mathbf{d}^T R\mathbf{d}$ for P_n and S_n by finding R instead of using F and $\mathbf{f}^v$.

Example 5.2.16. Given the path $P_n = (1, 2, \ldots, n)$ and a vertex v for $1 \le v \le n$, considering Remark 5.2.12 and Example 5.2.13, we have

$$R_{P_n,v} = \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix}$$

where $M_1 = \Big[\min\{v-i, v-j\}\Big]_{1 \le i,j \le v}$ and $M_2 = \Big[\min\{i, j\}\Big]_{1 \le i,j \le n-v}$. We have

$\mathbf{d}_{P_n} = 2\mathbf{1}_n - \mathbf{e}_1 - \mathbf{e}_n$. Then,

$$\begin{aligned}\mathbf{d}^T R\mathbf{d} &= 4\mathbf{1}^T R_{P_n,v}\mathbf{1} + (M_1)_{1,1} + (M_2)_{n-v,n-v} - 4\mathbf{1}^T R\mathbf{e}_1 - 4\mathbf{1}^T R\mathbf{e}_n \\ &= 4\left(\sum_{k=1}^{v-1} k^2 + \sum_{k=1}^{n-v} k^2\right) + n - 1 - 2v(v-1) - 2(n-v)(n-v+1) \\ &= 4(n-1)v^2 - 4(n^2-1)v + \frac{4}{3}n^3 - \frac{1}{3}n - 1.\end{aligned}$$

The minimum of $\mathbf{d}^T R\mathbf{d}$ is attained as $\frac{1}{3}n(n-1)(n-2)$ if n is odd, and as $\frac{1}{3}n^3 - n^2 + \frac{5}{3}n - 1$ if n is even. The maximum of $\mathbf{d}^T R\mathbf{d}$ is $\frac{1}{3}(n-1)(2n-1)(2n-3)$ at $v = 1$ or $v = n$.

Example 5.2.17. Consider a star S_n. Suppose that n is the centre vertex. Using Remark 5.2.12, it can be checked that

$$R_{S_n,v} = \begin{cases} J + \begin{bmatrix} I_{n-1} & 0 \\ 0 & 0 \end{bmatrix} - \mathbf{e}_v\mathbf{1}^T - \mathbf{1}\mathbf{e}_v^T, & \text{if } \deg(v) = 1, \\ \begin{bmatrix} I_{n-1} & 0 \\ 0 & 0 \end{bmatrix}, & \text{if } \deg(v) = n-1. \end{cases}$$

Hence,

$$\mathbf{d}^T R\mathbf{d} = \begin{cases} (n-1)(4n-7), & \text{if } \deg(v) = 1, \\ n-1, & \text{if } \deg(v) = n-1. \end{cases}$$

Recall that given a connected graph G of order n where $n \geq 2$, G is (v, k_1, k_2)-paradoxical if and only if $\Phi(v, k_1, k_2) > 0$, where $1 \leq v \leq n$ and integers $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$. We have seen that $\phi(v) > 0$ for any $1 \leq v \leq n$ regardless of k_1 and k_2; $\phi_1(k_1, k_2) \geq 0$ if and only if $(k_1, k_2) \in \{(1,1), (1,2), (2,1), (2,2)\}$; $\phi_2(k_1, k_2) < 0$ for any k_1, k_2 with $(k_1, k_2) \neq (1,1)$; and $\phi_3(k_1, k_2) < 0$ for any k_1, k_2. Hence, $\phi(v)$ must have a relatively larger quantity in order for G to be (v, k_1, k_2)-paradoxical.

Consider the case $k_1 = k_2 = 1$. Then, $\Phi(v, 1, 1) = 3\phi(v) + 8m_G^2\tau_G + 4m_G\tau_G - 12\tau_G$. Clearly, $\Phi(v, 1, 1) > 0$ for any non-trivial connected graph G and any vertex v of G. Hence, we have the following result.

Theorem 5.2.18. *[21] Let G be a connected graph of order n where $n \geq 2$. Then, G is $(1,1)$-paradoxical.*

We now find conditions for K_n, C_n, P_n or S_n to be (v, k_1, k_2)-paradoxical or (k_1, k_2)-paradoxical. For simplicity, set $k - 1 = k_1 + k_2$ and $\phi_i = \phi_i(k_1, k_2)$ for $i = 1, 2, 3$. Note that $\phi_G(v) = 2\mathbf{d}_G^T R_{G,v}\mathbf{d}_G$ and $\phi_i(k_1, k_2) = \phi_i(k_2, k_1)$ for $i = 1, 2, 3$.

For convenience, the following quantities are computed in advance: $\phi_2(1,2) = -27$, $\phi_3(1,2) = -48$, $\phi_2(2,2) = -60$ and $\phi_3(2,2) = -180$.

Example 5.2.19. Consider a complete graph K_n. Let v be a vertex of K_n. From Example 5.2.14, $\phi(v) = 2n^{n-2}(n-1)^3 = 2\tau(n-1)^3$. Using (5.2.5) with $m = \frac{n(n-1)}{2}$, we obtain

$$\Phi_{K_n}(v, k_1, k_2) = \tau k \left(2(n-1)^3 + n^2(n-1)^2\phi_1 + \frac{1}{3}n(n-1)\phi_2 + \frac{2}{3}\phi_3\right).$$

Suppose that $(k_1, k_2) \notin \{(1,1),(1,2),(2,1),(2,2)\}$. By Remark 5.2.11, $\phi_1 \leq -\frac{4}{3}$. From (5.2.7), we have $\phi_2 < -15$. By (5.2.6), $\phi_3 \leq -6$. Hence,

$$\Phi(v, k_1, k_2) < \tau k \left(-\frac{4}{3}n^4 + \frac{14}{3}n^3 - \frac{37}{3}n^2 + 11n - 6\right).$$

One can verify that $-\frac{4}{3}n^4 + \frac{14}{3}n^3 - \frac{37}{3}n^2 + 11n - 6 < 0$ for $n \geq 1$. Therefore, if $(k_1, k_2) \notin \{(1,1),(1,2),(2,1),(2,2)\}$, then K_n is not (v, k_1, k_2)-paradoxical for any $n \geq 1$.

Consider $(k_1, k_2) = (1,2)$ and $(k_1, k_2) = (2,2)$. Then,

$$\begin{aligned}
\Phi(v, 1, 2) &= 4\tau \left(2(n-1)^3 - 9n(n-1) - 32\right),\\
\Phi(v, 2, 2) &= 5\tau \left(2(n-1)^3 - 20n(n-1) - 120\right).
\end{aligned}$$

Using the derivatives of $\frac{\Phi(v,1,2)}{4\tau}$ and $\frac{\Phi(v,2,2)}{10\tau}$ with respect to n, it can be checked that $\Phi(v,1,2) > 0$ if and only if $n \geq 7$; $\Phi(v,2,2) > 0$ if and only if $n \geq 13$. Hence, K_n is $(1,2)$-paradoxical for $n \geq 7$, and $(2,2)$-paradoxical for $n \geq 13$.

Example 5.2.20. Given a cycle C_n with a vertex v, by Example 5.2.15, we have $\phi(v) = \frac{2}{3}(n-1)n^2(n+1) = \frac{2\tau}{3}(n-1)n(n+1)$. Using (5.2.5), we find

$$\Phi_{C_n}(v, k_1, k_2) = \tau k \left(\frac{2}{3}(n-1)n(n+1) + 4n^2\phi_1 + \frac{2}{3}n\phi_2 + \frac{2}{3}\phi_3\right).$$

We observe that the term with the highest degree in $\frac{\Phi(v,k_1,k_2)}{\tau k}$ as a polynomial of n has a positive coefficient. This implies that given $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$, C_n is (k_1, k_2)-paradoxical for sufficiently large n. Consider $(k_1, k_2) = (1,2)$ and

$(k_1, k_2) = (2, 2)$. Then,

$$\Phi(v, 1, 2) = 4\tau \left(\frac{2}{3}(n-1)n(n+1) - 18n - 32 \right),$$
$$\Phi(v, 2, 2) = 5\tau \left(\frac{2}{3}(n-1)n(n+1) - 40n - 120 \right).$$

One can verify that $\Phi(v, 1, 2) \geq 0$ for $n \geq 6$ with equality if and only if $n = 6$; $\Phi(v, 2, 2) \geq 0$ for $n \geq 9$ with equality if and only if $n = 9$. Hence, C_n is $(1, 2)$-paradoxical for $n \geq 7$, and $(2, 2)$-paradoxical for $n \geq 10$.

Example 5.2.21. Consider the path $P_n = (1, \ldots, n)$ with a vertex v. By (5.2.5) and the minimum of $\phi(v) = 2\mathbf{d}^T R\mathbf{d}$ in Example 5.2.16, we have

$$\Phi_{P_n}(v, k_1, k_2) \geq k \left(\frac{2}{3}n(n-1)(n-2) + 4(n-1)^2\phi_1 + \frac{2}{3}(n-1)\phi_2 + \frac{2}{3}\phi_3 \right).$$

Hence, given $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$, P_n is (k_1, k_2)-paradoxical for sufficiently large n.

Example 5.2.22. Consider a star S_n with a vertex v. Suppose that v is the centre vertex. Then, $n \geq 3$. By Example 5.2.17,

$$\Phi_{S_n}(v, k_1, k_2) = k \left(2(n-1) + 4(n-1)^2\phi_1 + \frac{2}{3}(n-1)\phi_2 + \frac{2}{3}\phi_3 \right).$$

Let $(k_1, k_2) \neq (1, 1)$. Clearly, $\phi_1 \leq 0$. By (5.2.7) and (5.2.6), we have $\phi_2 < -15$ and $\phi_3 \leq -6$, respectively. So, $\Phi(v, k_1, k_2) < -4k(2n-1)$. Hence, if S_n is (v, k_1, k_2)-paradoxical where v is the centre vertex of S_n, then $(k_1, k_2) = (1, 1)$ and $n \geq 3$.

Suppose that v is a pendent vertex. From Example 5.2.17,

$$\Phi_{S_n}(v, k_1, k_2) = k \left(2(n-1)(4n-7) + 4(n-1)^2\phi_1 + \frac{2}{3}(n-1)\phi_2 + \frac{2}{3}\phi_3 \right).$$

We have $\phi_1(2, 0) = -\frac{4}{3}$, $\phi_2(2, 0) = -34$ and $\phi_3(2, 0) = -6$; $\phi_1(3, 2) = -\frac{4}{3}$, $\phi_2(3, 2) = -163$ and $\phi_3(3, 2) = -480$. One can check that $\Phi(v, 2, 0) = 8n^2 - 102n + 82 > 0$ for $n \geq 12$; $\Phi(v, 2, 1) = 32n^2 - 160n > 0$ for $n \geq 6$; $\Phi(v, 2, 2) = 40n^2 - 310n - 330 > 0$ for $n \geq 9$; and $\Phi(v, 3, 2) = 16n^2 - 720n - 1216 > 0$ for $n \geq 47$. Let

$$A = \{(0, 2), (2, 0), (1, 1), (1, 2), (2, 1), (2, 2), (2, 3), (3, 2)\}.$$

Suppose that $(k_1, k_2) \notin A$. By Remark 5.2.11, we have $\phi_1(k_1, k_2) \leq -2$. From (5.2.7) and (5.2.6), $\phi_2 < -15$ and $\phi_3 \leq -6$, respectively. Hence, $\Phi(v, k_1, k_2) < -k(16n-12)$.

Therefore, if S_n is (v, k_1, k_2)-paradoxical for a pendent vertex v, then k_1, k_2 and n satisfy one of the following: (i) $(k_1, k_2) = (1, 1)$, $n \geq 2$; (ii) $(k_1, k_2) \in \{(0, 2), (2, 0)\}$, $n \geq 12$; (iii) $(k_1, k_2) \in \{(1, 2), (2, 1)\}$, $n \geq 6$; (iv) $(k_1, k_2) = (2, 2)$, $n \geq 9$; and (v) $(k_1, k_2) \in \{(2, 3), (3, 2)\}$, $n \geq 47$.

Problem 5.2.23. *If Problem 5.2.9 is resolved, then apply the result to the graphs K_n, C_n, P_n, and S_n as done in this section.*

5.3 Asymptotic behaviour of a sequence of graphs with twin pendent paths regarding the Braess edge

We have seen the families of complete graphs, cycles, stars, and paths in the previous section, and we have observed their asymptotic behaviours with respect to the property of being (v, k_1, k_2)-paradoxical as the orders of graphs increase. In particular, except for complete graphs and stars, any graph with sufficiently large order n relative to k_1 and k_2 in a family of cycles or paths is (k_1, k_2)-paradoxical. This idea is formalized and a tool for finding such families is described in this section.

Definition 5.3.1. Let $\mathcal{G}^v$ be a sequence of graphs $G_1, G_2, \dots$ where for each $n \geq 1$, G_n is a connected graph of order n with a vertex v. Fix integers $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$. The sequence $\mathcal{G}^v$ is *asymptotically* (k_1, k_2)*-paradoxical* if there exists $N > 0$ such that G_n is (v, k_1, k_2)-paradoxical for all $n \geq N$. The sequence $\mathcal{G}^v$ is *asymptotically paradoxical* if for any integers $l_1, l_2 \geq 0$ with $l_1 + l_2 \geq 2$, $\mathcal{G}^v$ is asymptotically (l_1, l_2)-paradoxical.

In what follows, $\mathcal{G}^v = (G_n)^v$ denotes a sequence of connected graphs $G_1, G_2, \dots$ where for each $n \geq 1$, $|V(G_n)| = n$ and $v \in V(G_n)$.

Example 5.3.2. From Theorem 5.2.18, any sequence $\mathcal{G}^v = (G_n)^v$ is asymptotically $(1, 1)$-paradoxical.

Example 5.3.3. Let $\mathcal{G}_1^v = (K_n)^v$, $\mathcal{G}_2^v = (C_n)^v$, $\mathcal{G}_3^v = (P_n)^v$ and $\mathcal{G}_4^v = (S_n)^v$. From Examples 5.2.19–5.2.22, $\mathcal{G}_2^v$ and $\mathcal{G}_3^v$ are asymptotically paradoxical, but $\mathcal{G}_1^v$ and $\mathcal{G}_4^v$ are not. In particular, $\mathcal{G}_1^v$ is asymptotically (k_1, k_2)-paradoxical if and only if $(k_1, k_2) \in \{(1, 1), (1, 2), (2, 1), (2, 2)\}$. Consider $\mathcal{G}_4^v = (S_n)^v$. Suppose that there exists $N > 0$ such that v is a pendent vertex of S_n for all $n \geq N$. Then, $\mathcal{G}_4^v$ is asymptotically (k_1, k_2)-paradoxical if and only if (k_1, k_2) is in the set A described in Example 5.2.22.

If there exists $N > 0$ such that v is the centre vertex of S_n for all $n \geq N$, then $\mathcal{G}_4^v$ is asymptotically (k_1, k_2)-paradoxical if and only if $(k_1, k_2) = (1, 1)$.

Consider a sequence $\mathcal{G}^v = (G_n)^v$. Examining the proof of Theorem 5.2.8 with (5.2.3), we find from (5.2.5) that

$$\begin{aligned}
&\kappa(\widehat{G}_n(v,k_1,k_2)) - \kappa(\widetilde{G}_n(v,k_1,k_2)) \\
=&\frac{\Phi_{G_n}(v,k_1,k_2)}{4k(m_{G_n}+k)(m_{G_n}+k-1)\tau_{G_n}} \\
=&\frac{\phi_{G_n}(v) + 4m_{G_n}^2\tau_{G_n}\phi_1(k_1,k_2) + \frac{2m_{G_n}\tau_{G_n}}{3}\phi_2(k_1,k_2) + \frac{2\tau_{G_n}}{3}\phi_3(k_1,k_2)}{4(m_{G_n}+k)(m_{G_n}+k-1)\tau_{G_n}}.
\end{aligned}$$

Note that since $\phi_{G_n}(v) > 0$ for all $n \geq 2$, we have $\frac{\phi_{G_n}(v)}{4m_{G_n}^2\tau_{G_n}} > 0$.

Suppose that $\frac{\phi_{G_n}(v)}{4m_{G_n}^2\tau_{G_n}}$ is bounded, say $0 < \frac{\phi_{G_n}(v)}{4m_{G_n}^2\tau_{G_n}} \leq L$ for any $n \geq 2$ where $L > 0$. Then,

$$\begin{aligned}
&\kappa(\widehat{G}_n(v,k_1,k_2)) - \kappa(\widetilde{G}_n(v,k_1,k_2)) \\
<&\frac{\phi_{G_n}(v) + 4m_{G_n}^2\tau_{G_n}\phi_1(k_1,k_2) + \frac{2m_{G_n}\tau_{G_n}}{3}\phi_2(k_1,k_2) + \frac{2\tau_{G_n}}{3}\phi_3(k_1,k_2)}{4m_{G_n}^2\tau_{G_n}} \\
\leq&L + \phi_1(k_1,k_2) + \frac{\phi_2(k_1,k_2)}{6m_{G_n}} + \frac{\phi_3(k_1,k_2)}{6m_{G_n}^2}.
\end{aligned}$$

Considering Remark 5.2.11, there exist integers $K_1 \geq 0$ and $K_2 \geq 0$ with $K_1 + K_2 \geq 2$ such that $\kappa(\widehat{G}_n(v,K_1,K_2)) - \kappa(\widetilde{G}_n(v,K_1,K_2)) < 0$ for all $n \geq 2$.

Suppose that $\frac{\phi_{G_n}(v)}{4m_{G_n}^2\tau_{G_n}}$ diverges to infinity. Fix $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$. Since G_n is connected for all $n \geq 1$, m_{G_n} approaches infinity as $n \to \infty$. Then,

$$\lim_{n\to\infty}\Big(\kappa(\widehat{G}_n(v,k_1,k_2)) - \kappa(\widetilde{G}_n(v,k_1,k_2))\Big) = \infty$$

Therefore, we have the following theorem.

Theorem 5.3.4. *Given a sequence $\mathcal{G}^v = (G_n)^v$, $\mathcal{G}^v$ is asymptotically paradoxical if and only if $\frac{\phi_{G_n}(v)}{4m_{G_n}^2\tau_{G_n}} \to \infty$ as $n \to \infty$.*

Example 5.3.5. Here we revisit Examples 5.2.14–5.2.17. Note that $\phi_{G_n}(v) = 2\mathbf{d}^T R_{G_n,v}\mathbf{d}$. One can verify that as $n \to \infty$, $\frac{\phi_{K_n}(v)}{4m_{K_n}^2\tau_{K_n}} = 0$; $\frac{\phi_{C_n}(v)}{4m_{C_n}^2\tau_{C_n}} \to \infty$; $\frac{\phi_{P_n}(v)}{4m_{P_n}^2\tau_{P_n}} \to \infty$; $\frac{\phi_{S_n}(v)}{4m_{S_n}^2\tau_{S_n}} = 2$ where v is a pendent vertex of S_n; and $\frac{\phi_{S_n}(v)}{4m_{S_n}^2\tau_{S_n}} = 0$ where v is the centre vertex of S_n. By Theorem 5.3.4, the sequences $(C_n)^v$ and $(P_n)^v$ are asymptotically paradoxical.

Proposition 5.3.6. *Let G be a connected graph, and v be a cut-vertex. Suppose that there are ℓ branches $B_1, \ldots, B_\ell$ of G at v. Then,*

$$\mathbf{d}_G^T R_{G,v} \mathbf{d}_G = \sum_{k=1}^{\ell} \mathbf{d}_{B_k}^T R_{B_k,v} \mathbf{d}_{B_k}. \tag{5.3.1}$$

This implies that $\phi_G(v) = \sum_{k=1}^{\ell} \phi_{B_k}(v)$.

Proof. Let $R_{G,v} = [r_{i,j}]$. By Remark 5.2.12, if $i = v$ or $j = v$, then $r_{i,j} = 0$. Consider $i \neq v$ and $j \neq v$. Suppose that $i \in V(B_{k_1})$ and $j \in V(B_{k_2})$ for $k_1 \neq k_2$. Since v is a cut-vertex of G, we find from Remark 5.2.12 that $r_{i,j} = 0$. Hence, for $k = 1, \ldots, \ell$, the submatrix of $R_{G,v}$ whose rows and columns are indexed by $V(B_k)$ and $V(G)\backslash V(B_k)$, respectively, is the zero matrix. For $k = 1, \ldots, \ell$, assume $i, j \in V(B_k)$. Since v is a cut-vertex, by Remark 5.2.12, $|\mathcal{F}_G(i,j;v)| = |\mathcal{F}_{B_k}(i,j;v)|$. Therefore, the submatrix of $R_{G,v}$ whose rows and columns are indexed by the vertex set $V(B_k)$ is $R_{B_k,v}$.

Let $1 \leq k \leq \ell$. For $\mathbf{d}_{B_k} = (d_i)_{i \in V(B_k)}$, let $\widehat{\mathbf{d}}_{B_k} = (\hat{d}_i)_{i \in V(G)}$ where $\hat{d}_i = d_i$ if $i \in V(B_k)$, and $\hat{d}_i = 0$ if $i \in V(G)\backslash V(B_k)$. Then, for $1 \leq k_1, k_2 \leq \ell$,

$$\widehat{\mathbf{d}}_{B_{k_1}}^T R_{G,v} \widehat{\mathbf{d}}_{B_{k_2}} = \mathbf{d}_{B_{k_1}}^T \widetilde{R}_{G,v} \mathbf{d}_{B_{k_2}}$$

where $\widetilde{R}_{G,v}$ is the submatrix of $R_{G,v}$ whose rows and columns are indexed by $V(B_{k_1})$ and $V(B_{k_2})$, respectively. Hence, it follows that $\mathbf{d}_{B_{k_1}}^T \widetilde{R}_{G,v} \mathbf{d}_{B_{k_2}} = \mathbf{d}_{B_{k_1}}^T R_{B_{k_1},v} \mathbf{d}_{B_{k_1}}$ if $k_1 = k_2$, and $\mathbf{d}_{B_{k_1}}^T \widetilde{R}_{G,v} \mathbf{d}_{B_{k_2}} = 0$ otherwise. Evidently, $\mathbf{d}_G = \sum_{k=1}^{\ell} \widehat{\mathbf{d}}_{B_k}$. Therefore, the desired result follows. $\square$

Proposition 5.3.7. *Let H_i be a connected graph with a vertex v_i for $i = 1, \ldots, \ell$. Suppose that a sequence $\mathcal{G}^v = (G_n)^v$ is asymptotically paradoxical. Consider a sequence $(\mathcal{G}')^v = (G'_n)^v$ where for $1 \leq n \leq \sum_{i=1}^{\ell} |V(H_i)|$, $G'_n = G_n$, and for $n > \sum_{i=1}^{\ell} |V(H_i)|$, G'_n is the graph obtained from $H_1, \ldots, H_\ell$ and $G_{n - \sum_{i=1}^{\ell} |V(H_i)|}$ by identifying the vertices $v_1, \ldots, v_\ell, v$. Then, $(\mathcal{G}')^v$ is asymptotically paradoxical.*

Proof. Suppose that $n > \sum_{i=1}^{\ell} |V(H_i)|$. Let $n_0 = n - \sum_{i=1}^{\ell} |V(H_i)|$. Since v is a cut-vertex in G'_n, we have $\tau_{G'_n} = \tau_{G_{n_0}} \tau_{H_1} \cdots \tau_{H_\ell}$. Using Proposition 5.3.6,

$$\frac{\phi_{G'_n}(v)}{4m_{G'_n}^2 \tau_{G'_n}} = \frac{\phi_{G_{n_0}}(v) + \sum_{i=1}^{\ell} \phi_{H_i}(v_i)}{4(m_{G_{n_0}} + \sum_{i=1}^{\ell} m_{H_i})^2 \tau_{G_{n_0}} \tau_{H_1} \cdots \tau_{H_\ell}}.$$

As $n \to \infty$, we have $n_0 \to \infty$. Since $(\mathcal{G})^v$ is asymptotically paradoxical, by Theorem 5.3.4 we obtain $\frac{\phi_{G_{n_0}}(v)}{4m_{G_{n_0}}^2 \tau_{G_{n_0}}} \to \infty$ as $n \to \infty$. It follows that $\frac{\phi_{G'_n}(v)}{4m_{G'_n}^2 \tau_{G'_n}} \to \infty$ as $n \to \infty$. Therefore, $(\mathcal{G}')^v$ is asymptotically paradoxical. $\square$

Example 5.3.8. Suppose that for a connected graph G with a vertex v, G is not (v, k_1, k_2)-paradoxical for some integers k_1 and k_2 with $k_1 + k_2 \geq 2$. By Example 5.3.5 and Proposition 5.3.7, we can obtain a (v, k_1, k_2)-paradoxical graph G' from G by identifying v and a vertex of a cycle C_n (or a vertex of a path P_n) for sufficiently large order n.

5.4 Asymptotically paradoxical sequences of trees

In order to examine the asymptotic behaviour of a sequence of trees, we shall find the minimum of $\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v} \mathbf{d}_{\mathcal{T}}$ for trees $\mathcal{T}$ with a vertex v provided the number of branches of $\mathcal{T}$ at v and the eccentricity of v in each branch are given. We first consider the minimum of $\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v} \mathbf{d}_{\mathcal{T}}$ when v is a pendent vertex.

Let $\mathcal{T}$ be a tree of order n, and v be a pendent vertex in $\mathcal{T}$. Consider $R_{\mathcal{T},v} = [r_{i,j}]$. Suppose that α is the eccentricity $e_{\mathcal{T}}(v)$ of v in $\mathcal{T}$. Then, there exists a path $P = (v_0, v_1, \ldots, v_\alpha)$ of length α in $\mathcal{T}$ with $v_0 = v$. Evidently, v_0 and v_α are pendent vertices in $\mathcal{T}$. Let $\mathcal{T}_0$ and $\mathcal{T}_\alpha$ be the trees where $V(\mathcal{T}_0) = \{v_0\}$ and $V(\mathcal{T}_\alpha) = \{v_\alpha\}$. For $k = 1, \ldots, \alpha - 1$, if there are more than two branches of $\mathcal{T}$ at v_k, then we define $\mathcal{T}_k$ to be the tree obtained from $\mathcal{T}$ by deleting the two branches except v_k where one contains v_{k-1} and the other v_{k+1}; if there are exactly two branches of $\mathcal{T}$ at v_k, then we define $\mathcal{T}_k$ to be the tree with $V(\mathcal{T}_k) = \{v_k\}$. Then, $V(\mathcal{T}_0), \ldots, V(\mathcal{T}_\alpha)$ are mutually disjoint sets. Moreover, for each $k = 0, \ldots, \alpha$, we have $e_{\mathcal{T}_k}(v_k) \leq \alpha - k$.

Recall that $r_{i,j} = |\mathcal{F}_{\mathcal{T}}(i, j; v)|$ is the number of 2-tree spanning forests of $\mathcal{T}$ having i, j in one tree and v in the other. Note that $v = v_0$. Suppose that $i \in V(\mathcal{T}_{k_1})$ and $j \in V(\mathcal{T}_{k_2})$ where $0 \leq k_1 < k_2 \leq \alpha$. For each forest in $\mathcal{F}_{\mathcal{T}}(i, j; v)$, since i and j belong to the same subtree in the forest, the subtree must contain v_{k_1} and v_{k_2}. For any vertex w on the subpath of $\mathcal{T}$ with i and j as the pendent vertices, we have $d_{\mathcal{T}}(v, v_{k_1}) \leq d_{\mathcal{T}}(v, w)$. Hence, by Remark 5.2.12, $r_{i,j} = k_1$ for $i \in V(\mathcal{T}_{k_1})$ and $j \in V(\mathcal{T}_{k_2})$ with $0 \leq k_1 < k_2 \leq \alpha$.

Assume that i, j are in $V(\mathcal{T}_k)$ for some $1 \leq k \leq \alpha$. Consider the subpath P' of $\mathcal{T}_k$ with i and j as the pendent vertices. Suppose that w_0 is the vertex on P' such that $d_{\mathcal{T}_k}(v_k, w_0) \leq d_{\mathcal{T}_k}(v_k, w)$ for $w \in V(P')$. Then, $d_{\mathcal{T}}(v, w_0) = k + d_{\mathcal{T}_k}(v_k, w_0)$. Let $R_{\mathcal{T}_k, v_k} = [\tilde{r}_{i,j}]$. By Remark 5.2.12, we have $r_{i,j} = k + \tilde{r}_{i,j}$.

Labelling the rows and columns of $R_{\mathcal{T},v}$ in order of $v, V(\mathcal{T}_1), \ldots, V(\mathcal{T}_\alpha)$, we obtain the following structure:

$$R_{\mathcal{T},v} = \left[\begin{array}{c|c|c|c|c|c} 0 & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & J + R_{\mathcal{T}_1,v_1} & J & J & \cdots & J \\ \hline 0 & J & 2J + R_{\mathcal{T}_2,v_2} & 2J & \cdots & 2J \\ \hline 0 & J & 2J & 3J + R_{\mathcal{T}_3,v_3} & \cdots & \vdots \\ \hline \vdots & \vdots & \vdots & \vdots & \ddots & (\alpha-1)J \\ \hline 0 & J & 2J & 3J & \cdots & \alpha J + R_{\mathcal{T}_\alpha,v_\alpha} \end{array}\right]$$

where the Js in the blocks of $R_{\mathcal{T},v}$ are appropriately sized. Let $n_k = |V(\mathcal{T}_k)|$ for $k = 0, \ldots, \alpha$. Note that $n_0 = n_\alpha = 1$. Then, $R_{\mathcal{T},v}$ can be recast as

$$\begin{aligned} R_{\mathcal{T},v} &= \sum_{i=0}^{\alpha-1} \begin{bmatrix} 0 & 0 \\ 0 & J_{n-(n_0+\cdots+n_i)} \end{bmatrix} + \operatorname{diag}(0, R_{\mathcal{T}_1,v_1}, \ldots, R_{\mathcal{T}_\alpha,v_\alpha}) \\ &= \sum_{i=0}^{\alpha-1} \begin{bmatrix} \mathbf{0}_{n_0+\cdots+n_i} \\ \mathbf{1}_{n-(n_0+\cdots+n_i)} \end{bmatrix} \begin{bmatrix} \mathbf{0}^T_{n_0+\cdots+n_i} & \mathbf{1}^T_{n-(n_0+\cdots+n_i)} \end{bmatrix} + \operatorname{diag}(0, R_{\mathcal{T}_1,v_1}, \ldots, R_{\mathcal{T}_\alpha,v_\alpha}) \end{aligned}$$

where $n = n_0 + n_1 + \cdots + n_\alpha$.

Now, we shall compute $\mathbf{d}^T_{\mathcal{T}} R_{\mathcal{T},v} \mathbf{d}_{\mathcal{T}}$. Let $\mathbf{x}^T = \begin{bmatrix} 0 & \mathbf{d}^T_{\mathcal{T}_1} & \cdots & \mathbf{d}^T_{\mathcal{T}_{\alpha-1}} & 0 \end{bmatrix}$ and $\mathbf{y} = \mathbf{e}_v + \sum_{i=1}^{\alpha-1} 2\mathbf{e}_{v_i} + \mathbf{e}_{v_\alpha}$. Then,

$$\begin{aligned} \mathbf{x}^T R_{\mathcal{T},v} \mathbf{x} &= \sum_{i=0}^{\alpha-2} \left(\mathbf{d}^T_{\mathcal{T}_{i+1}} \mathbf{1} + \cdots + \mathbf{d}^T_{\mathcal{T}_{\alpha-1}} \mathbf{1} \right)^2 + \sum_{i=1}^{\alpha-1} \mathbf{d}^T_{\mathcal{T}_i} R_{\mathcal{T}_i,v_i} \mathbf{d}_{\mathcal{T}_i} \\ &= 4 \sum_{i=0}^{\alpha-2} \left(\sum_{j=i+1}^{\alpha-1} (n_j - 1) \right)^2 + \sum_{i=1}^{\alpha-1} \mathbf{d}^T_{\mathcal{T}_i} R_{\mathcal{T}_i,v_i} \mathbf{d}_{\mathcal{T}_i} \\ &= 4 \sum_{i=1}^{\alpha-1} \left(\sum_{j=i}^{\alpha-1} (n_j - 1) \right)^2 + \sum_{i=1}^{\alpha-1} \mathbf{d}^T_{\mathcal{T}_i} R_{\mathcal{T}_i,v_i} \mathbf{d}_{\mathcal{T}_i}. \end{aligned}$$

We can find that the submatrix of $R_{\mathcal{T},v}$ whose rows and columns are indexed by $\{v_0, \ldots, v_\alpha\}$ is the matrix $[\min(i,j)]_{0 \le i,j \le \alpha}$. So, $\left(\sum_{k=0}^{\alpha} \mathbf{e}_{v_k}\right)^T R_{\mathcal{T},v} \left(\sum_{k=0}^{\alpha} \mathbf{e}_{v_k}\right)$ is the sum of all entries in $[\min(i,j)]_{0 \le i,j \le \alpha}$. Thus, from $\mathbf{y} = 2\left(\sum_{k=0}^{\alpha} \mathbf{e}_{v_k}\right) - (\mathbf{e}_v + \mathbf{e}_\alpha)$, we

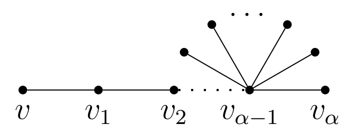


Figure 5.1: An illustration of a broom on n vertices considered in Example 5.4.1.

have

$$\begin{aligned}
&\mathbf{y}^T R_{\mathcal{T},v}\mathbf{y}\\
&= 4\mathbf{1}^T[\min(i,j)]_{0\le i,j\le \alpha}\mathbf{1} - 4(\mathbf{e}_v+\mathbf{e}_\alpha)^T R_{\mathcal{T},v}\left(\sum_{k=0}^{\alpha}\mathbf{e}_{v_k}\right) + (\mathbf{e}_v+\mathbf{e}_\alpha)^T R_{\mathcal{T},v}(\mathbf{e}_v+\mathbf{e}_\alpha)\\
&= \frac{2}{3}\alpha(\alpha+1)(2\alpha+1) - 2\alpha(\alpha+1) + \alpha = \frac{1}{3}\alpha(2\alpha-1)(2\alpha+1).
\end{aligned}$$

Finally, we find

$$\begin{aligned}
&\sum_{i=0}^{\alpha-1}\mathbf{x}\begin{bmatrix}0 & 0\\ 0 & J_{n-(n_0+\cdots+n_i)}\end{bmatrix}\mathbf{y}\\
&=\sum_{i=0}^{\alpha-2}\left(\mathbf{d}_{\mathcal{T}_{i+1}}^T\mathbf{1}+\cdots+\mathbf{d}_{\mathcal{T}_{\alpha-1}}^T\mathbf{1}\right)(2(\alpha-i)-1)\\
&=2\sum_{i=0}^{\alpha-2}\left(\sum_{j=i+1}^{\alpha-1}(n_j-1)\right)(2(\alpha-i)-1) = 2\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)(2(\alpha-i)+1).
\end{aligned}$$

From Remark 5.2.12, for each $k=0,\dots,\alpha$, we have $|\mathcal{F}_{\mathcal{T}_k}(l,v_k;v_k)|=0$ for $l\in V(\mathcal{T}_k)$. So, the v_k^{th} column of $\operatorname{diag}(0,R_{\mathcal{T}_1,v_1},\dots,R_{\mathcal{T}_\alpha,v_\alpha})$ is the zero vector. This implies $\mathbf{x}^T\operatorname{diag}(0,R_{\mathcal{T}_1,v_1},\dots,R_{\mathcal{T}_\alpha,v_\alpha})\mathbf{y}=0$. Hence,

$$2\mathbf{x}^T R_{\mathcal{T},v}\mathbf{y} = 4\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)(2(\alpha-i)+1).$$

Note that $\mathbf{d}_{\mathcal{T}}=\mathbf{x}+\mathbf{y}$. Therefore, for a tree $\mathcal{T}$ with a pendent vertex v,

$$\begin{aligned}
\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}} &= \mathbf{x}^T R_{\mathcal{T},v}\mathbf{x} + 2\mathbf{x}^T R_{\mathcal{T},v}\mathbf{y} + \mathbf{y}^T R_{\mathcal{T},v}\mathbf{y}\\
&= 4\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)^2 + \sum_{i=1}^{\alpha-1}\mathbf{d}_{\mathcal{T}_i}^T R_{\mathcal{T}_i,v_i}\mathbf{d}_{\mathcal{T}_i}\\
&+4\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)(2(\alpha-i)+1) + \frac{1}{3}\alpha(2\alpha-1)(2\alpha+1).
\end{aligned} \tag{5.4.1}$$

Example 5.4.1. Let $n \geq \alpha \geq 1$, and $\mathcal{B}_{n,\alpha}$ be the broom with vertices $v, v_1, \ldots, v_\alpha$ in Figure 5.1. Let $v_0 = v$, and $X = \{0, \ldots, \alpha\}\backslash\{\alpha-1\}$. Suppose that for $i \in X$, $\mathcal{T}_i$ is the tree with $V(\mathcal{T}_i) = \{v_i\}$, and $\mathcal{T}_{\alpha-1}$ is the subtree induced by $V(\mathcal{B}_{n,\alpha})\backslash\{v_1, \ldots, v_{\alpha-2}, v_\alpha\}$. Then, $\mathcal{T}_{\alpha-1}$ is a star of order $n-\alpha$ with the centre vertex $v_{\alpha-1}$. Let $n_i = |V(\mathcal{T}_i)|$ for $i = 0, \ldots, \alpha$. By (5.4.1) and Example 5.2.17, we obtain

$$\begin{aligned}
\mathbf{d}^T R_{\mathcal{B}_{n,\alpha},v}\mathbf{d} &= 4\sum_{i=1}^{\alpha-1}(n-\alpha-1)^2 + \mathbf{d}_{S_{n-\alpha}}^T R_{S_{n-\alpha},v_{\alpha-1}}\mathbf{d}_{S_{n-\alpha}} \\
&\quad + 4\sum_{i=1}^{\alpha-1}(n-\alpha-1)(2(\alpha-i)+1) + \frac{1}{3}\alpha(2\alpha-1)(2\alpha+1) \\
&= 4(\alpha-1)(n-\alpha-1)^2 + (n-\alpha-1)(4\alpha^2-3) + \frac{1}{3}\alpha(2\alpha-1)(2\alpha+1).
\end{aligned}$$

We now consider the minimum of $\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}}$ for trees $\mathcal{T}$ and a pendent vertex v in $\mathcal{T}$. We adopt the same hypotheses and notation used to derive (5.4.1). Note that for $i = 0, \ldots, \alpha$, v_i is not necessarily a pendent vertex in $\mathcal{T}_{v_i}$. The result for the minimum of $\mathbf{d}_{\mathcal{T}_i}^T R_{\mathcal{T}_i,v_i}\mathbf{d}_{\mathcal{T}_i}$ for $i = 1, \ldots, \alpha-1$ in (5.4.1) appears in the paper [47] as the minimum of $\mathbf{d}_{\mathcal{T}_i}^T(2\mathbf{f}_{\mathcal{T}_i}^v\mathbf{1}^T - F_{\mathcal{T}_i})\mathbf{d}_{\mathcal{T}_i}$. We shall introduce the result, which is proved by induction in [47], with a different proof by using the combinatorial interpretation for entries in $R_{\mathcal{T}_i,v_i}$.

Lemma 5.4.2. *[47] Let $\mathcal{T}$ be a tree of order $n \geq 2$ with a vertex v. Then,*

$$\mathbf{d}^T R_{\mathcal{T},v}\mathbf{d} \geq n-1$$

with equality if and only if one of the following holds: (i) for $n = 2$, $\mathcal{T} = P_2$; (ii) for $n \geq 3$, $\mathcal{T} = S_n$ and v is the centre vertex.

Proof. Let $R_{\mathcal{T},v} = [r_{i,j}]$. By Remark 5.2.12, we have $r_{ii} = d(i,v) \geq 1$ whenever $i \neq v$. The degree of each vertex is at least 1. So, we have $\mathbf{d}^T R_{\mathcal{T},v}\mathbf{d} \geq (n-1)$. To attain the equality, $r_{i,j} = 0$ if $i \neq j$. From Remark 5.2.12, we find that v is a cut-vertex so that $\mathcal{T} - v$ consists of $n-1$ isolated vertices. Therefore, our desired result is obtained. $\square$

Applying Lemma 5.4.2 to $\mathbf{d}_{\mathcal{T}_i}^T R_{\mathcal{T}_i,v_i}\mathbf{d}_{\mathcal{T}_i}$ in (5.4.1) for each $i = 1, \ldots, \alpha-1$, we obtain $\sum_{i=1}^{\alpha-1}\mathbf{d}_{\mathcal{T}_i}^T R_{\mathcal{T}_i,v_i}\mathbf{d}_{\mathcal{T}_i} \geq n-\alpha-1$. Thus, $\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}}$ in (5.4.1) is bounded below as follows:

$$\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}} \geq 4\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)^2 + 4\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)(2(\alpha-i)+1)$$
$$+ (n-\alpha-1) + \frac{1}{3}\alpha(2\alpha-1)(2\alpha+1).$$

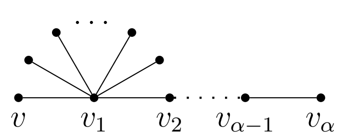
Consider

$$\begin{aligned}
&\sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)^2 + \sum_{i=1}^{\alpha-1}\left(\sum_{j=i}^{\alpha-1}(n_j-1)\right)(2(\alpha-i)+1) \qquad (5.4.2)\\
&= \Big[(n_1+\cdots+n_{\alpha-1}-(\alpha-1))^2 + (n_1+\cdots+n_{\alpha-1}-(\alpha-1))(2\alpha-1)\Big]\\
&\quad + \Big[(n_2+\cdots+n_{\alpha-1}-(\alpha-2))^2 + (n_2+\cdots+n_{\alpha-1}-(\alpha-2))(2\alpha-3)\Big]\\
&\quad + \cdots + \Big[(n_{\alpha-1}-1)^2 + (n_{\alpha-1}-1)3\Big].
\end{aligned}$$

Since $n_1+\cdots+n_{\alpha-1}$ is constant, we find that the minimum of (5.4.2) can be attained as $(n-\alpha-1)(n+\alpha-2)$ at $n_1 = n-\alpha$ and $n_2 = \cdots = n_{\alpha-1} = 1$. Therefore, when v is a pendent vertex, we have

$$\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}} \geq (n-\alpha-1)(4n+4\alpha-7) + \frac{1}{3}\alpha(2\alpha-1)(2\alpha+1) \qquad (5.4.3)$$

where equality holds if and only if $\mathcal{T}$ is a broom $\mathcal{B}_{n,\alpha}$ with $v, v_1, \ldots, v_\alpha$ described below:



Here is the result for the minimum of $\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}}$ mentioned at the beginning of this section.

Proposition 5.4.3. *Let $\mathcal{T}$ be a tree with a vertex v. Suppose that $B_1, \ldots, B_\ell$ are the branches of $\mathcal{T}$ at v for some $\ell \geq 1$. Let $n_i = |V(B_i)|$, and let $e_i = e_{B_i}(v)$ for $i = 1, \ldots, \ell$. Then,*

$$\mathbf{d}_{\mathcal{T}}^T R_{\mathcal{T},v}\mathbf{d}_{\mathcal{T}} \geq \sum_{i=1}^{\ell}\left[(n_i-e_i-1)(4n_i+4e_i-7) + \frac{1}{3}e_i(2e_i-1)(2e_i+1)\right]$$

where equality holds if and only if for $i = 1, \ldots, \ell$, each branch B_i is a broom $\mathcal{B}_{n_i,e_i}$ such that if $n_i > e_i + 1$, then v is one of the $(n_i - e_i)$ pendent vertices having a *common neighbour; if $n_i = e_i + 1$, then v is a pendent vertex in $\mathcal{B}_{n_i,e_i}$ (which is a path).*

Proof. The conclusions can be readily established by Proposition 5.3.6 and (5.4.3). $\square$

Hereafter, the symbols ω, $\mathcal{O}$ and Θ stand for the small Omega notation, the big O notation and the big Theta notation, respectively (see [4] for an introduction).

Now, we consider the following sequence of trees. We assume, in what follows, that for any sequence $\mathcal{G}^v = (\mathcal{T}_n)^v$ of trees, $V(\mathcal{T}_1) = \{v\}$ and for each $n \geq 2$, $\mathcal{T}_n$ is obtained from $\mathcal{T}_{n-1}$ by adding a new pendent vertex to a vertex of $\mathcal{T}_{n-1}$, or by subdividing an edge in $\mathcal{T}_{n-1}$ into two edges connecting to a new vertex. We denote by α_n and ℓ_n the eccentricity of v in $\mathcal{T}_n$ and the number of branches of $\mathcal{T}_n$ at v, respectively. Define $B_1^{(1)} = \mathcal{T}_1$ and $\ell_1 = 1$. Assume that for $n \geq 2$, $B_1^{(n-1)}, \ldots, B_{\ell_{n-1}}^{(n-1)}$ are the branches of $\mathcal{T}_{n-1}$ at v. Let $\{w\} = V(\mathcal{T}_n)\backslash V(\mathcal{T}_{n-1})$. Consider the case $\ell_n - \ell_{n-1} = 1$. Then, w must be added to the vertex v in $\mathcal{T}_{n-1}$ to form $\mathcal{T}_n$. For this case, we define $B_i^{(n)}$ as $B_i^{(n-1)}$ for $i = 1, \ldots, \ell_n - 1$, and define $B_{\ell_n}^{(n)}$ as the path (v, w). Suppose $\ell_n = \ell_{n-1}$. Then, there exists exactly one branch $B_k^{(n-1)}$ for some $k \in \{1, \ldots, \ell_{n-1}\}$ such that w is adjacent to at least a vertex of $B_k^{(n-1)}$ in $\mathcal{T}_n$. We define $B_i^{(n)}$ as $B_i^{(n-1)}$ for $1 \leq i \leq \ell_{n-1}$ with $i \neq k$, and define $B_k^{(n)}$ as the induced subtree of $\mathcal{T}_n$ by $V\left(B_k^{(n-1)}\right) \cup \{w\}$. Hence, we define

$$\beta_n = |\{i | e_{B_i^{(n)}}(v) = \Theta(\alpha_n), i = 1, \ldots, \ell_n\}|.$$

Remark 5.4.4. Consider a sequence $\mathcal{G}^v = (\mathcal{T}_n)^v$ of trees. Evidently, $\beta_n \leq \ell_n = \mathcal{O}(n)$ and $\alpha_n = \mathcal{O}(n)$. Since $\alpha_n = \max\{e_{B_i^{(n)}}(v) | 1 \leq i \leq \ell_n\}$, we have $\beta_n \geq 1$.

Here is the main result in this section.

Theorem 5.4.5. *Let $\mathcal{G}^v = (\mathcal{T}_n)^v$ be a sequence of trees. If $\beta_n \alpha_n^3 = \omega(n^2)$, then $\mathcal{G}^v$ is asymptotically paradoxical.*

Proof. Suppose that $\beta_n \alpha_n^3 = \omega(n^2)$. For $n \geq 2$, suppose that $B_1^{(n)}, \ldots, B_{\ell_n}^{(n)}$ are the branches of $\mathcal{T}_n$ at v. Let $e_i^{(n)} = e_{B_i^{(n)}}(v)$ and $k_i^{(n)} = \left|V\left(B_i^{(n)}\right)\right|$ for $i = 1, \ldots, \ell_n$. We may assume that $e_j^{(n)} = \Theta(\alpha_n)$ for $j = 1, \ldots, \beta_n$. Then, for each $j = 1, \ldots, \beta_n$, there exist $C_j > 0$ and $N_j > 0$ such that $e_j^{(n)} \geq C_j \alpha_n$ for all $n \geq N_j$. Choose $C_0 = \min\{C_j | j = 1, \ldots, \beta_n\}$ and $N_0 = \max\{N_j | j = 1, \ldots, \beta_n\}$. Then, $e_j^{(n)} \geq C_0 \alpha_n$

for all $n \geq N_0$ and $1 \leq j \leq \beta_n$. By Proposition 5.4.3, for $n \geq N_0$, we have

$$\begin{aligned}
\frac{\phi_{\mathcal{T}_n}(v)}{4m_{\mathcal{T}_n}^2 \tau_{\mathcal{T}_n}} &= \frac{2\mathbf{d}_{\mathcal{T}_n}^T R_{\mathcal{T}_n,v} \mathbf{d}_{\mathcal{T}_n}}{4(n-1)^2} \\
&\geq \frac{\sum_{i=1}^{\ell_n} \left[(k_i^{(n)} - e_i^{(n)} - 1)(4k_i^{(n)} + 4e_i^{(n)} - 7) + \frac{1}{3} e_i^{(n)} (2e_i^{(n)} - 1)(2e_i^{(n)} + 1) \right]}{2(n-1)^2} \\
&\geq \frac{\beta_n C_0 \alpha_n (2C_0\alpha_n - 1)(2C_0\alpha_n + 1)}{6(n-1)^2}.
\end{aligned}$$

Since $\beta_n \alpha_n^3 = \omega(n^2)$, we have $\frac{\phi_{\mathcal{T}_n}(v)}{4m_{\mathcal{T}_n}^2 \tau_{\mathcal{T}_n}} \to \infty$ as n approaches infinity. Therefore, the conclusion follows. $\square$

Corollary 5.4.6. *Suppose that $\mathcal{G}^v = (\mathcal{T}_n)^v$ is a sequence of trees such that $\alpha_n = \omega(n^{\frac{2}{3}})$. Then, $\mathcal{G}^v$ is asymptotically paradoxical.*

Proof. It is straightforward from Theorem 5.4.5. $\square$

Corollary 5.4.7. *Suppose that $\mathcal{G}^v = (\mathcal{T}_n)^v$ is a sequence of trees such that $\mathrm{diam}(\mathcal{T}_n) = \omega(n^{\frac{2}{3}})$. Then, $\mathcal{G}^v$ is asymptotically paradoxical.*

Proof. Let P be a longest path in $\mathcal{T}_n$. Suppose that w_0 is the vertex on P such that $d(v, w_0) \leq d(v, w)$ for all vertices w on P. Then, $\alpha_n \geq d(v, w_0) + \frac{1}{2}\mathrm{diam}(\mathcal{T}_n)$. By Corollary 5.4.6, our desired result follows. $\square$

A *rooted* tree, or a tree *rooted at* v, is a tree in which a vertex v is designated as the root vertex. Conventionally, we place the root vertex on top, and every edge is directed away from the root. A *leaf* in a rooted tree is a vertex of degree 1 which is not the root vertex. The *depth* of a vertex v in a rooted tree is the distance between v and the root. The *height* of a rooted tree is the maximum distance from the root to all leaves.

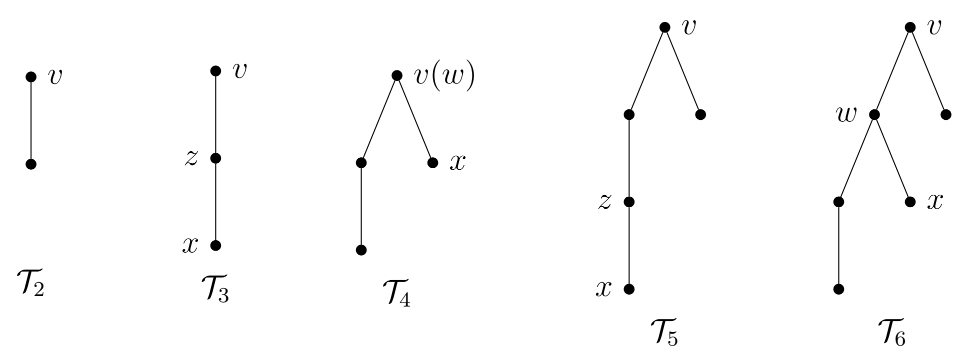


Figure 5.2: A sequence of rooted trees considered in Example 5.4.8.

Example 5.4.8. Let $\mathcal{G}^v = (\mathcal{T}_n)^v$ be a sequence of trees. For each $n \geq 1$, $\mathcal{T}_n$ can be considered as a tree rooted at v. We may also regard branches $B_1^{(n)}, \ldots, B_{\ell_n}^{(n)}$ of $\mathcal{T}_n$ at v as trees rooted at v. For each $n \geq 3$, let $\mathcal{T}_n$ be obtained from $\mathcal{T}_{n-1}$ as follows: if $e_{B_1^{(n-1)}}(v) = \lfloor n^{c_0} \rfloor - 1$, then a new vertex x is added to a leaf z of $B_1^{(n-1)}$ such that the depth of z is the height of $B_1^{(n-1)}$; if $e_{B_1^{(n-1)}}(v) = \lfloor n^{c_0} \rfloor$, then a new vertex x is added to a vertex w in $\mathcal{T}_{n-1}$ such that $d(v, w) < e_{B_1^{(n-1)}}(v)$. Assume that $c_0 = 0.7$. Considering $\lfloor 3^{c_0} \rfloor = \lfloor 4^{c_0} \rfloor = 2$ and $\lfloor 5^{c_0} \rfloor = \lfloor 6^{c_0} \rfloor = 3$, one of all possible sequences can be obtained as in Figure 5.2. Note that the very left branch of each tree rooted at v in that figure is $B_1^{(n)}$ for $n = 2, \ldots, 6$. Then, $e_{B_1^{(n)}}(v) \geq e_{B_k^{(n)}}(v)$ for all $n \geq 2$ and $2 \leq k \leq \ell_n$. Moreover, $e_{B_1^{(n)}}(v) \geq n^{c_0} - 1$ for all $n \geq 2$. By Corollary 5.4.6, $\mathcal{G}^v$ is asymptotically paradoxical—that is, for integers $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$, $\mathcal{T}_n$ is (v, k_1, k_2)-paradoxical for sufficiently large n.

From the following example, the converses of Theorem 5.4.5, Corollaries 5.4.6 and 5.4.7 do not hold.

Example 5.4.9. Consider a sequence $\mathcal{G}^v = (\mathcal{T}_n)^v$ where for $n \geq 4$, $\mathcal{T}_n$ is a broom $\mathcal{B}_{n,\alpha_n}$ with $\alpha_n \geq 3$. Suppose that for each $n \geq 4$, v is the pendent vertex of $\mathcal{B}_{n,\alpha_n}$ that does not have any common neighbour with other pendent vertices in $\mathcal{B}_{n,\alpha_n}$. Clearly, $\beta_n = 1$. Suppose that $\alpha_n = \omega(1)$. By Example 5.4.1, we obtain

$$\begin{aligned}
&\frac{\phi_{\mathcal{B}_{n,\alpha_n}}(v)}{4m^2_{\mathcal{B}_{n,\alpha_n}} \tau_{\mathcal{B}_{n,\alpha_n}}} \\
=&\frac{4(\alpha_n - 1)(n - \alpha_n - 1)^2 + (n - \alpha_n - 1)(4\alpha_n^2 - 3) + \frac{1}{3}\alpha_n(2\alpha_n - 1)(2\alpha_n + 1)}{2(n-1)^2} \\
\geq&\frac{2(\alpha_n - 1)(n - \alpha_n - 1)^2}{(n-1)^2}
\end{aligned}$$

for $n \geq 4$. Since $n^2\alpha_n = \omega(n^2)$, we have $\frac{\phi_{\mathcal{T}_n}(v)}{4m^2_{\mathcal{T}_n}\tau_{\mathcal{T}_n}} \to \infty$ as n approaches infinity. Therefore, $\mathcal{G}^v$ is asymptotically paradoxical. Moreover, we have $\beta_n \alpha_n^3 = \omega(1)$.

Problem 5.4.10. *If Problem 5.2.9 is solved, then with the result from that problem, establish analogous results as done in Sections 5.3 and 5.4.*

6

Equidistant switched hypercubes: their properties and sensitivity analysis under PST

This chapter is a study of graph properties and spectral properties of hypercubes and graphs resulting from switching edges on hypercubes. Using those properties, we conduct sensitivity analysis under perfect state transfer (PST) with respect to readout time and edge weight.

Before we begin this chapter, let us recall the definition of PST for the hypercube Q_n and a related property. Consider the adjacency matrix $A(Q_n)$ of the hypercube Q_n. The fidelity of state transfer between vertices v and w at time t in Q_n is $p_{Q_n}(t) = |(U(t))_{v,w}|^2$ where $U(t) = e^{itA(Q_n)}$; and if $p_{Q_n}(t_0) = 1$, then we say that there is PST between v and w at time t_0. By Proposition 2.5.2, for any vertex x in $V(Q_n)$, x and the antipodal vertex of x pair up to exhibit PST at time $\frac{\pi}{2}$.

6.1 Introduction

An important task within a quantum computer is to transfer a quantum state from one place to another. To realize the task, a quantum spin network, represented by a graph, is used as a channel for quantum communication within a quantum computer [8]. While a collection of qubits (vertices) allows quantum states to be transferred from one location to another by continuous time quantum walks, we consider the amount of similarity between the transmitted state and the received state. The fidelity of state transfer, as a measure of the closeness between two quantum states, is the probability of a quantum state placed at a vertex to be transmitted to another vertex at a given time. Although graphs exhibiting perfect state transfer (PST)—the fidelity of transfer is 1—have been extensively researched, *e.g.,* [3, 34], practical benefits from the discovery of such graphs need to be discussed further.

In order to control qubits within a quantum computer, they need to be isolated completely from external environments, a crucial and challenging task. This brings our attention to researching PST under perturbation of readout time or the weight of an edge [40]. Sensitivity of the fidelity of state transfer with respect to readout time or the weight of an edge is analysed in [43]. Recent work [46] explores graphs constructed from hypercubes by Godsil-MaKay switching so that they are not isomorphic, but maintain PST and preserve the same sensitivity (of the fidelity of state transfer) with respect to readout time under PST. Regarding switching edges on hypercubes and the structure of resulting graphs, there are further works: the twisted n-cube in [29], the Möbius cubes in [23], and the generalized twisted cubes in [19].

The direction of our work is parallel to that of the work [46], but our ultimate goal is to furnish graphs obtained from hypercubes by certain types of switches that are less sensitive to changes in the weight of an edge under PST. In Section 6.2, we define particular matchings in graphs through distances among vertices, and study them in a family of bipartite graphs. In Section 6.3, those matchings are used to define the so-called *equidistant switches*, and in particular, the so-called *equidistant switched hypercubes* obtained from hypercubes by equidistant switches are investigated. We show that the switched graph is not isomorphic to the original one (Theorem 6.3.8), and we provide a sufficient condition for equidistant switched hypercubes to maintain PST (Theorem 6.3.12). Furthermore, we analyse the number of pairs of vertices exhibiting PST in equidistant switched hypercubes with extra conditions. In Section 6.4, we first provide a result that the sensitivity to readout time errors under PST between particular vertices in hypercubes is invariant under equidistant switches (Theorem 6.4.2). Moreover we produce explicit expressions for the sensitivity under PST in hypercubes with respect to the weights of two types of edges (Theorems 6.4.20 and 6.4.22 for the one, and Theorems 6.4.23 and 6.4.24 for the other). In Section 6.5, we present spectral properties of particular equidistant switched hypercubes (Theorem 6.5.14), and provide all necessary interim results (introduced by Remark 6.5.19) required to reach the expressions for the sensitivity to the edge-weight errors in the equidistant switched hypercubes. Finally, we conclude Section 6.5 by providing numerical results about our ultimate goal and a related conjecture (Conjecture 6.5.24).

6.2 Equidistant matchings in bipartite graphs

We shall define matchings with a certain restriction regarding distance in graphs in order to describe a particular type of switch on hypercubes in Section 6.3.

Definition 6.2.1. A matching M in a graph G is said to be *equidistant* if there exist subsets $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$ of $V(G)$ for $k \geq 2$ such that $M = \{v_i \sim w_i | i = 1, \ldots, k\}$, the distances between v_i's are the same constant, and the distances between w_i's are also the same constant (the two constants are not necessarily equal). The subsets $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$ are called *distance-partite sets* of M.

A matching M in a graph G is said to be a $(k, a, b; \Gamma)$-*matching* if M is equidistant so that for distance-partite sets $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$ with $k \geq 2$, we have

(i) $d(v_i, v_j) = a$ for $i, j \in \{1, \ldots, k\}$ with $i \neq j$;

(ii) $d(w_i, w_j) = b$ for $i, j \in \{1, \ldots, k\}$ with $i \neq j$; and

(iii) Γ is the multi-set of distances $d(v_i, w_j)$ for $i, j \in \{1, \ldots, k\}$ with $i \neq j$.

When the distances a and b are specified, we use M^a and M_b to denote $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$, respectively.

Remark 6.2.2. Let M be a $(k, a, b; \Gamma)$-matching in a graph G. Since M consists of non-incident edges, we have $a, b \geq 2$.

Example 6.2.3. Let $v_1 = 0000$, $v_2 = 0111$, $w_1 = 1000$, and $w_2 = 1111$ in Q_4. Let $M = \{v_1 \sim w_1, v_2 \sim w_2\}$. Since $d_{Q_4}(v_1, v_2) = d_{Q_4}(w_1, w_2) = 3$, M is equidistant. Furthermore, M is a $(2, 3, 3; \{4, 4\})$-matching in Q_4.

Let G be a bipartite graph. Suppose that $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ is a $(k, a, b; \Gamma)$-matching in G with distance-partite sets $M^a = \{v_1, \ldots, v_k\}$ and $M_b = \{w_1, \ldots, w_k\}$. For $i, j \in \{1, \ldots, k\}$ with $i \neq j$, consider $v_i, v_j \in M^a$ and $w_i, w_j \in M_b$. By the triangle inequality, we have

$$d(v_i, v_j) \leq d(v_i, w_j) + d(w_j, v_j) \text{ and } d(v_i, w_j) \leq d(v_i, v_j) + d(v_j, w_j).$$

Since $d(v_i, v_j) = a$ and $d(w_j, v_j) = 1$, we obtain $a - 1 \leq d(v_i, w_j) \leq a + 1$. Since G is a bipartite graph and $v_i \sim w_i \in E(G)$, v_i and w_i are in the different partite sets of G. Similarly, v_j and w_j are in the different partite sets. It follows that $d(v_i, v_j)$ and $d(w_i, w_j)$ have the same parity. Furthermore, $d(v_i, w_j)$ has the opposite parity from that of $d(v_i, v_j)$ and $d(w_i, w_j)$. Thus, from $d(v_i, v_j) = a$, we have either $d(v_i, w_j) = a - 1$ or $d(v_i, w_j) = a + 1$.

Applying the triangle inequality twice, we have $d(w_i, w_j) \leq d(w_i, v_i) + d(v_i, v_j) + d(v_j, w_j) = a + 2$. So, $b \leq a + 2$. Similarly, one can find that $a \leq b + 2$. Without loss of generality, $a \leq b$. Since $d(v_i, v_j)$ and $d(w_i, w_j)$ have the same parity, we have either $b = a$ or $b = a + 2$. In particular, if $b = a + 2$, then we find from $d(w_i, w_j) \leq d(w_i, v_j) + d(v_j, w_j)$ that $d(w_i, v_j) \geq a + 1$; and from the fact above that either $d(v_i, w_j) = a - 1$ or $d(v_i, w_j) = a + 1$, we must have $d(w_i, v_j) = a + 1$. Therefore, we have the following.

Proposition 6.2.4. *Let G be a bipartite graph. Suppose that M is an equidistant matching in G. Then, M is one of the following cases: for $k \geq 2$ and $a \geq 2$,*

(M1) M is a $(k, a, a; \{(a+1)^m\}$-matching;

(M2) M is a $(k, a, a+2; \{(a+1)^m\})$-matching;

(M3) M is a $(k, a, a; \{(a-1)^m\})$-matching;

(M4) M is a $(k, a, a; \{(a-1)^s, (a+1)^{m-s}\})$-matching for some $0 < s < m$,

where $m = k(k-1)$ in (M1)–(M4).

Remark 6.2.5. Let G be a bipartite graph with partite sets U and W. Let M be a $(k, a, b; \Gamma)$-matching in G with distance-partite sets M^a and M_b. Suppose $k \geq 3$. Then, for vertices x and y of G, $d(x, y)$ is odd if and only if x is in one of U and W, and y is in the other. So, if $d(x, y)$ and $d(y, z)$ both are odd, then $d(x, z)$ must be even. This implies that a and b must be even. Hence, M is one of the following cases: for $k \geq 3$ and $\alpha \geq 1$, (i) M is a $(k, 2\alpha, 2\alpha; \{(2\alpha+1)^m\})$-matching; (ii) M is a $(k, 2\alpha, 2\alpha+2; \{(2\alpha+1)^m\})$-matching; (iii) M is a $(k, 2\alpha, 2\alpha; \{(2\alpha-1)^m\})$-matching; and (iv) M is a $(k, 2\alpha, 2\alpha; \{(2\alpha-1)^s, (2\alpha+1)^{m-s}\})$-matching for some $0 < s < m$, where $m = k(k-1)$.

As seen in Example 6.2.3, if $k = 2$, then a and b need not be even.

Problem 6.2.6. *Given a bipartite graph G, investigate quadruples (k, a, b, Γ) that guarantee the existence of a $(k, a, b; \Gamma)$-matching in G. One might explore, using Menger's theorem, the range of k by considering graph parameters such as vertex-connectivity.*

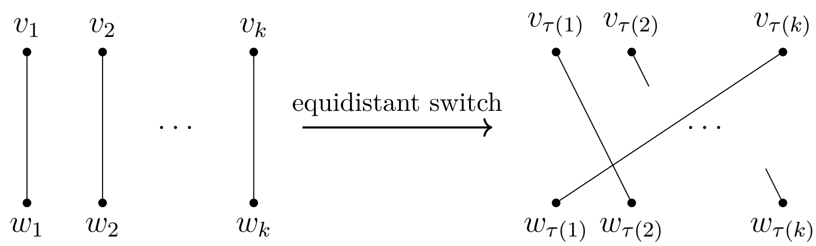


Figure 6.1: An illustration of the equidistant switch via M_τ in Definition 6.3.1.

6.3 Properties of equidistant switched hypercubes and PST

In this section, we discuss a difference and a similarity between Q_n and the graph obtained from Q_n by a switch related to an equidistant matching. Furthermore, we investigate pairs of vertices exhibiting PST in the resulting graph.

Recall that $\mathcal{S}_k$ is the symmetric group on $\{1, \ldots, k\}$.

Definition 6.3.1. Let $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ be an equidistant matching in a graph G with distance-partite sets $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$ where $k \geq 2$. Given $\tau \in \mathcal{S}_k$, M_τ denotes the set $\{v_{\tau(i)} \sim w_{\tau(i)} | i = 1, \ldots, k\}$. ($M_\tau$ may be regarded as an ordered set of edges in M.) The process of deleting edges $v_i \sim w_i$ for $i = 1, \ldots, k$ from G and adding edges $v_{\tau(k)} \sim w_{\tau(1)}$ and $v_{\tau(j)} \sim w_{\tau(j+1)}$ for $j = 1, \ldots k-1$ to G is referred to as the *equidistant switch* via M_τ in G. The equidistant switch via M_τ in G is said to be the $(k, a, b; \Gamma)$*-switch* via M_τ if M is a $(k, a, b; \Gamma)$-matching in G. The graph, denoted $\widetilde{G}^{(M_\tau)}$, obtained from G by the equidistant switch via M_τ (resp. the $(k, a, b; \Gamma)$-switch via M_τ) is said to be the *equidistant switched* graph via M_τ (resp. the $(k, a, b; \Gamma)$*-switched* graph via M_τ). If $\widetilde{G}^{(M_\tau)}$ is isomorphic to $\widetilde{G}^{(M_\sigma)}$ for all $\sigma \in \mathcal{S}_k$, then we use $\widetilde{G}^{(M)}$ to denote a representative $\widetilde{G}^{(M_\tau)}$.

Remark 6.3.2. For clarity we discuss Definition 6.3.1. Given an equidistant matching M of size k in a graph G, we have k edges for performing an equidistant switch on G. Considering orderings of the edges, we have $k!$ choices for an equidistant switch. (Note that we permute the edges, not vertices of a distance-partite set.) So, if M_τ is specified in the context, *i.e.* an ordered set of edges in M is given, then we use 'the' before each related terminology in Definition 6.3.1; unless M_τ is given, we shall use indefinite articles.

Example 6.3.3. Consider the graph G in Figure 6.2. Then, $M = \{v_i \sim w_i | 1 \leq i \leq 4\}$ is a $(4, 2, 2, \{(3)^{12}\})$-matching. Let id be the identity permutation, and $\tau = (1\ 2)$

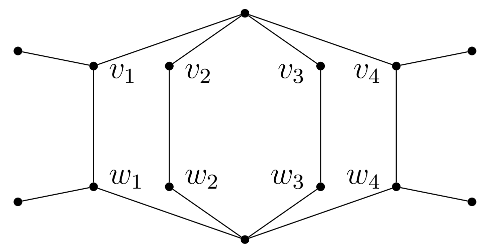


Figure 6.2: A graph G used in Example 6.3.3.

in the cyclic notation. One can verify that while $\widetilde{G}^{(M_{id})}$ has two adjacent vertices v_4 and w_1 of degree 3, $\widetilde{G}^{(M_\tau)}$ does not. Hence, $\widetilde{G}^{(M_{id})}$ and $\widetilde{G}^{(M_\tau)}$ are not isomorphic.

Problem 6.3.4. *Given an equidistant matching M of size $k \geq 3$ in a graph G, find conditions in order that an equidistant switched graph is uniquely determined up to permutations of the non-incident edges in M.*

Remark 6.3.5. Continuing with Problem 6.3.4, it is straightforward that if $k = 2$, then since M contains only two non-incident edges, we have $\widetilde{G}^{(M_{id})} = \widetilde{G}^{\left(M_{(1\ 2)}\right)}$. Hence, for the case $k = 2$, we may use $\widetilde{G}^{(M)}$ to indicate $\widetilde{G}^{(M_\tau)}$ for $\tau \in \mathcal{S}_2$.

We now turn our attention to hypercubes.

Problem 6.3.6. *Let $n \geq 4$ and $k \geq 3$. Let $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ be an equidistant matching in Q_n with distance-partite sets $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$. Prove or disprove that if there exists a vertex x in Q_n such that $d(x, v_1) = \cdots = d(x, v_k)$ and $d(x, w_1) = \cdots = d(x, w_k)$, then an equidistant switched n-cube is uniquely determined (up to permutations of the edges in M).*

We first consider whether there is an equidistant switched n-cube isomorphic to the n-cube.

Lemma 6.3.7. *[60] Let $n \geq 2$. A graph G is the n-cube if and only if (i) G is connected, (ii) every pair of incident edges lies in exactly one 4-cycle, and (iii) $|V(G)| = 2^n$.*

Theorem 6.3.8. *Let $n \geq 4$, and let M be a matching in Q_n where $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ for some $k \geq 2$. Suppose that H is the graph obtained from Q_n by deleting edges $v_i \sim w_i$ for $i = 1, \ldots, k$ from Q_n and adding edges $v_k \sim w_1$ and $v_j \sim w_{j+1}$ for $j = 1, \ldots k-1$ to Q_n. Then, H is not isomorphic to Q_n.*

Proof. It is clear that H is connected and $|V(H)| = 2^n$. Assume to the contrary that H and Q_n are isomorphic. Note that we use the condition (ii) in Lemma 6.3.7

without reference in this proof. Let $M_1 = \{v_1, \ldots, v_k\}$ and $M_2 = \{w_1, \ldots, w_k\}$. Consider v_1, w_1, v_k and w_k. Choose z in $N_{Q_n}(w_1)\backslash\{v_1\}$. Since M is a matching, $z \notin M_1$. For incident edges $v_1 \sim w_1$ and $w_1 \sim z$, there exists exactly one vertex z' such that (v_1, w_1, z, z', v_1) is a 4-cycle in Q_n. Since v_1 is not adjacent to any vertex in $M_2\backslash\{w_1\}$, we have $z' \notin M_2$. So, $w_1 \sim z, z \sim z', z' \sim v_1 \in E(H)$. Note that $v_1 \sim w_1 \notin E(H)$. Since Q_n and H are isomorphic, for incident edges $w_1 \sim z$ and $z \sim z'$ of H, there must be exactly one vertex v such that (w_1, z, z', v, w_1) is a 4-cycle in H. Clearly, $v \neq v_1$. Since $N_H(w_1) \cap M_1 = \{v_k\}$, the vertex v is either v_k or some vertex not in M_1. If $v \neq v_k$, then there are two 4-cycles (v_1, w_1, z, z', v_1) and (w_1, z, z', v, w_1) in Q_n for the incident edges $w_1 \sim z$ and $z \sim z'$ of Q_n, which is a contradiction. Hence, $v = v_k$. By $z' \notin M_2$, $z' \sim v_k \in E(Q_n)$. For incident edges $z \sim z'$ and $z' \sim v_k$ of Q_n, there is a unique vertex w such that (z, z', v_k, w, z) is a 4-cycle in Q_n. Evidently, $w \neq w_1$. Since $N_{Q_n}(v_k) \cap M_2 = \{w_k\}$, the vertex w is either w_k or some vertex not in M_2. Note that $z' \sim v_k \in E(H)$. If $w \neq w_k$, then for incident edges $z \sim z'$ and $z' \sim v_k$, there are two 4 cycles (z, z', v_k, w, z) and (z, z', v_k, w_1, z) in H, a contradiction. Thus, $w = w_k$ and $z \sim w_k \in E(Q_n)$. Hence, $d_{Q_n}(w_1, w_k) = 2$.

Consider w_1 and w_k. Since $d_{Q_n}(w_1, w_k) = 2$, w_1 and w_k have exactly two common neighbours that are neither v_1 nor v_k. Otherwise, it would contradict (ii) in Lemma 6.3.7. Since every vertex in Q_n is of degree $n \geq 4$, there exists a vertex y in Q_n such that $y \notin M_1$, $y \sim w_k \in E(Q_n)$ and $y \sim w_1 \notin E(Q_n)$. For incident edges $v_k \sim w_k$ and $w_k \sim y$ of Q_n, there exists a unique vertex y' such that (v_k, w_k, y, y', v_k) is a 4-cycle in Q_n. Since $N_{Q_n}(v_k) \cap M_2 = \{w_k\}$, we have $y' \notin M_2$. Then, $y \sim y', y' \sim v_k \in E(H)$. Since H is isomorphic to Q_n and $v_k \sim w_k \notin E(H)$, for two incident edges $v_k \sim y'$ and $y' \sim y$, there must be a unique vertex x such that $x \neq w_k$ and (v_k, y', y, x, v_k) is a 4-cycle in H. We have $N_H(v_k) \cap M_2 = \{w_1\}$, so x is either w_1 or some vertex not in M_2. Since $y \notin M_1$ and $y \sim w_1 \notin E(Q_n)$, we have $y \sim w_1 \notin E(H)$. So, $x \neq w_1$. Hence, for incident edges $v_k \sim y'$ and $y' \sim y$, there are two 4-cycles (v_k, w_k, y, y', v_k) and (v_k, y', y, x, v_k) in Q_n, a contradiction. Therefore, our desired result is obtained. $\square$

Corollary 6.3.9. *Let $n \geq 4$. Then, no equidistant switched n-cube is isomorphic to the n-cube.*

Remark 6.3.10. Any matching in Q_3 is equidistant and is a $(2, 2, 2; \{3, 3\})$-matching. It can be easily seen that any $(2, 2, 2; \{3, 3\})$-switched 3-cube is isomorphic to Q_3.

Even though for $n \geq 4$, any equidistant switched n-cube is not isomorphic to the n-cube, they share the following property—used in Section 6.4 for showing that under PST, they have the same sensitivity to readout time errors.

Proposition 6.3.11. *Let $M = \{v_i \sim w_i | i = 1, \dots, k\}$ be an equidistant matching in Q_n with distance-partite sets $\{v_1, \dots, v_k\}$ and $\{w_1, \dots, w_k\}$. Let x be a vertex of Q_n, and $\tau \in \mathcal{S}_k$. Suppose that $d_{Q_n}(x, v_1) = \cdots = d_{Q_n}(x, v_k)$ and $d_{Q_n}(x, w_1) = \cdots = d_{Q_n}(x, w_k)$. Then, for any integer $j \geq 1$, the number of walks of length j from x to x in Q_n is the same as that in $\widetilde{Q}_n^{(M_\tau)}$.*

Proof. Let $j \geq 1$ and $\tau \in \mathcal{S}_k$. Suppose that $\widetilde{M}_\tau = \{v_{\tau(1)} \sim w_{\tau(2)}, \dots, v_{\tau(k-1)} \sim w_{\tau(k)}, v_{\tau(k)} \sim w_{\tau(1)}\}$. Then, $\widetilde{M}_\tau$ is a matching in $\widetilde{Q}_n^{(M_\tau)}$. Define X_j (resp. Y_j) to be the set of walks of length j from x and back to itself in Q_n (resp. $\widetilde{Q}_n^{(M_\tau)}$) such that there appears at least one edge of M (resp. $\widetilde{M}_\tau$) in each walk (as a sequence of edges). Note that considering M as a subgraph in Q_n, the subgraph induced by the distance-partite sets is M. Since the equidistant switch via M_τ only changes adjacency of the induced subgraph M in Q_n, it suffices to show that $|X_j| = |Y_j|$ in order to obtain the desired conclusion.

We claim that there is a bijection between X_j and Y_j. Choose any walk ω in X_j. Regarding ω as a sequence of edges, we suppose that $(e_1, \dots, e_p)$ is the subsequence of ω such that $e_i \in M$ for $i = 1, \dots, p$. A walk ω' is constructed from ω as follows: for $i = 1, \dots, p$, if e_i is $v_\ell \sim w_\ell$ for some $1 \leq \ell \leq k-1$, then e_i is replaced by the edge $e_i' = v_{\tau(\ell)} \sim w_{\tau(\ell+1)}$; and if $e_i = v_k \sim w_k$, then $e_i' = v_{\tau(k)} \sim w_{\tau(1)}$ is substituted for e_i. Then, all the replaced edges in ω' are in $\widetilde{M}$. Thus, $\omega' \in Y_j$. Furthermore, ω' can be restored to ω by replacing e_i' by e_i for $1 \leq i \leq p$. This construction yields the desired bijection. Therefore, the conclusion follows. □

Now, we provide a sufficient condition for an equidistant switched n-cube to maintain PST. Recall that for a vertex v of a graph G and a subset X of $V(G)$, $N_X(v)$ is the set of neighbours of v that belong to X.

Theorem 6.3.12. *Let $M = \{v_i \sim w_i | i = 1, \dots, k\}$ be an equidistant matching in Q_n with distance-partite sets $M_1 = \{v_1, \dots, v_k\}$ and $M_2 = \{w_1, \dots, w_k\}$. Suppose that there exists a vertex $x \in V(Q_n)$ such that $d_{Q_n}(x, v_1) = \cdots = d_{Q_n}(x, v_k)$ and $d_{Q_n}(x, w_1) = \cdots = d_{Q_n}(x, w_k)$. Then, x and x^* pair up to exhibit PST at time $\frac{\pi}{2}$ in $\widetilde{Q}_n^{(M_\tau)}$ for any $\tau \in \mathcal{S}_k$.*

Proof. Let $\tau \in \mathcal{S}_k$. Suppose that $d_{Q_n}(x, v_i) = \ell$ and $d_{Q_n}(x, w_i) = \ell + 1$ for $1 \leq i \leq k$ where $\ell \geq 1$. Consider the distance partition $\pi = (S_0(x), \dots, S_n(x))$ of Q_n with respect to x. Then, $M_1 \subseteq S_\ell(x)$ and $M_2 \subseteq S_{\ell+1}(x)$. Since the equidistant switch via M_τ only changes adjacency of the subgraph of Q_n induced by $M_1 \cup M_2$, we can find from Proposition 2.5.6 that the distance partition $\tilde{\pi}$ of $\widetilde{Q}_n^{(M_\tau)}$ with respect to x is the same as π. By Theorem 2.5.5, π is equitable. So, $|N_{S_{l+1}(x)}(v_i)|$ and $|N_{S_l(x)}(w_i)|$ are constant for $1 \leq i \leq k$. Furthermore, we find that $|N_{S_{l+1}(x)}(v_i)|$ and $|N_{S_l(x)}(w_i)|$ are invariant under the equidistant switch. Hence, $\tilde{\pi}$ is equitable, and $\widehat{\widetilde{Q}_n^{(M_\tau)}/\tilde{\pi}}$ is the same as $\widehat{Q_n/\pi}$. Therefore, using Proposition 2.5.2 and Theorem 2.5.4, $\widetilde{Q}_n^{(M_\tau)}$ exhibits PST between x and x^* at time $\frac{\pi}{2}$. For $\ell > 1$, applying an analogous argument to the case that $d_{Q_n}(x, v_i) = \ell$ and $d_{Q_n}(x, w_i) = \ell - 1$ for $1 \leq i \leq k$, the desired conclusion is established. □

Remark 6.3.13. In this remark we maintain the hypotheses and notation of Theorem 6.3.12. Inspecting the proof of that theorem, we can see that $d_{Q_n}(x, v) = d_{\widetilde{Q}_n^{(M_\tau)}}(x, v)$ for $v \in V(Q_n)$. So, x^* is a unique antipodal vertex of x in $\widetilde{Q}_n^{(M_\tau)}$, and $d_{\widetilde{Q}_n^{(M_\tau)}}(x, x^*) = n$.

Example 6.3.14. Consider the hypercube Q_4, and antipodal vertices $x = 0000$ and $x^* = 1111$. Let $x = 0000$, $v_2 = 0011$, $w_1 = 1000$ and $w_2 = 1011$. Then, $M = \{x \sim w_1, v_2 \sim w_2\}$ is a $(2, 2, 2, \{3, 3\})$-matching in Q_4. We note Remark 6.3.5. Since $x \sim w_2 \in E\left(\widetilde{Q}_4^{(M)}\right)$, we have $d_{\widetilde{Q}_4^{(M)}}(x, x^*) = 2$. One can check that 1000, 1110, 1101 and 0111 are all at distance 3 from x, so they are all antipodal vertices of x in $\widetilde{Q}_4^{(M)}$. Therefore, x and x^* are not antipodal vertices in $\widetilde{Q}_4^{(M)}$.

Conjecture 6.3.15. *Prove the converse of Theorem 6.3.12. If this is proved, then for a $(2, a, b; \Gamma)$-matching M with a and b odd, $\widetilde{Q}_n^{(M)}$ does not exhibit PST between any pair of vertices at time $\frac{\pi}{2}$.*

We claim that a $(k, 2\alpha, 2\alpha; \{(2\alpha+1)^{k(k-1)}\})$-switched n-cube in type (M1) needs a weak condition relative to the hypothesis of Theorem 6.3.12 to exhibit PST.

Lemma 6.3.16. *Let $z = 0\ldots01\ldots1$ be a binary string of length n with p ones where p is even. Suppose that y is a binary string of length n with q ones and $d_{Q_n}(z, y) = q$. Then, y contains $\frac{2q-p}{2}$ ones among the first $n-p$ positions, and $\frac{p}{2}$ ones among the last p positions.*

Proof. Suppose that in y, 1 appears q_1 times for the first $n-p$ positions, and q_2 times for the last p positions. Then, $q = d_{Q_n}(z, y) = q_1 + (p - q_2)$. Since $q_1 + q_2 = q$, it follows that $q_1 = \frac{2q-p}{2}$ and $q_2 = \frac{p}{2}$. The conclusion follows. □

Lemma 6.3.17. *Let $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ be a $(k, 2\alpha, 2\alpha; \{(2\alpha+1)^{k(k-1)}\})$-matching in Q_n with distance-partite set $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$ where $n \geq 3$. Let $x \in V(Q_n)$. Then, $d(x, v_1) = \cdots = d(x, v_k)$ if and only if $d(x, w_1) = \cdots = d(x, w_k)$.*

Proof. It is enough to show that $d(x, v_1) = d(x, v_2)$ if and only if $d(x, w_1) = d(x, w_2)$. Let $d(x, v_1) = d(x, v_2) = \ell$. From $d(v_1, v_2) = 2\alpha$, we have $\ell \geq \alpha$. By (iii) of Proposition 2.5.1, we may assume that $v_1 = 0\ldots0$ and $v_2 = 0\ldots01\ldots1$ where 1 appears 2α times in v_2. By $d(x, v_1) = \ell$, x contains ℓ ones. Applying Lemma 6.3.16 to vertices v_2 and x, the vertex x must contain $\ell-\alpha$ ones among the first $n-2\alpha$ positions, and α ones among the last 2α positions. Let $w_1 = a_1 \ldots a_n$ and $w_2 = b_1 \ldots b_n$. From $v_1 \sim w_1 \in E(Q_n)$, w_1 has a single one. By $d(v_2, w_1) = 2\alpha + 1$, the single one appears among the first $n - 2\alpha$ positions of w_1, say $a_{i_0} = 1$ for some $i_0 \in \{1, \ldots, n - 2\alpha\}$. Since $d(v_1, w_2) = 2\alpha+1$, w_2 contains $2\alpha+1$ ones. Furthermore, by $v_2 \sim w_2 \in E(Q_n)$, $b_j = 1$ for $j = n - 2\alpha + 1, \ldots, n$, and $b_{j_0} = 1$ for some $j_0 \in \{1, \ldots, n - 2\alpha\}$. Since $d(w_1, w_2) = 2\alpha$, we must have $i_0 = j_0$. It follows that $d(x, w_1) = d(x, w_2)$. In a similar way, it is readily established that $d(x, w_1) = d(x, w_2)$ implies $d(x, v_1) = d(x, v_2)$. $\square$

Given an equidistant matching M in one of types (M2), (M3) and (M4) in Q_n, we can see from the following example that it does not hold for the property in Lemma 6.3.17 that if a vertex is at the same distance from all vertices in a distance-partite set of M, then so is it from all vertices in the other distance-partite set.

Example 6.3.18. Let $v_1 = 0000$, $v_2 = 0011$, $w_1 = 0100$, $w_2 = 1011$, and $x_1 = 1001$. Then, $M_1 = \{v_1 \sim w_1, v_2 \sim w_2\}$ is a $(2, 2, 4; \{3, 3\})$-matching of type (M2) in Q_4. But, $d(x_1, v_1) = d(x_1, v_2)$ and $d(x_1, w_1) \neq d(x_1, w_2)$.

Furthermore, let $v_3 = 0000$, $v_4 = 1111$, $w_3 = 0100$, $w_4 = 1011$ and $x_2 = 0011$. Then, $M_2 = \{v_3 \sim w_3, v_4 \sim w_4\}$ is a $(2, 4, 4; \{3, 3\})$-matching of type (M3) in Q_4. However, $d(x_2, v_3) = d(x_2, v_4)$ and $d(x_2, w_3) \neq d(x_2, w_4)$.

Finally, let $v_5 = 000\ 000$, $v_6 = 001\ 111$, $w_5 = 010\ 000$, $w_6 = 000\ 111$ and $x_3 = 000\ 011$. Then, $M_3 = \{v_5 \sim w_5, v_6 \sim w_6\}$ is a $(2, 4, 4; \{3, 5\})$-matching of type (M4) in Q_6. However, $d(x_3, v_5) = d(x_3, v_6)$ and $d(x_3, w_5) \neq d(x_3, w_6)$.

Proposition 6.3.19. *Let $n \geq 4$, and let M be a $(k, 2\alpha, 2\alpha; \{(2\alpha + 1)^k\})$-matching with distance-partite sets $M^{2\alpha}$ and $M_{2\alpha}$, where $k \geq 2$ and $\alpha \geq 1$. Suppose that a vertex x of Q_n satisfies either $d_{Q_n}(x, v) = \ell$ for all $v \in M^{2\alpha}$ or $d_{Q_n}(x, w) = \ell$ for all $w \in M_{2\alpha}$. Let $\tau \in \mathcal{S}_k$. Then, $\widetilde{Q}_n^{(M_\tau)}$ exhibits PST between x and x^* at time $\frac{\pi}{2}$. Furthermore, $\alpha \leq \ell \leq n - \alpha$ and at least $\sum_{i=\alpha}^{n-\alpha} |S_i(M^{2\alpha})|$ vertices pair up to exhibit PST at time $\frac{\pi}{2}$ in $\widetilde{Q}_n^{(M_\tau)}$.*

Proof. Let $\tau \in \mathcal{S}_k$. Without loss of generality, suppose that x is a vertex in Q_n such that $d_{Q_n}(x, v) = \ell$ for all $v \in M^{2\alpha}$. By Lemma 6.3.17, $d_{Q_n}(x, w)$ is constant for all $w \in M_{2\alpha}$. Hence, by Theorem 6.3.12, x and x^* pair up to exhibit PST at time $\frac{\pi}{2}$ in

$\widetilde{Q}_n^{(M_\tau)}$. Since pairwise distances among vertices in $M^{2\alpha}$ are constant as 2α, we have $\ell \geq \alpha$. Considering the distance partition of Q_n with respect to x with Proposition 2.5.6, we have $d_{Q_n}(x^*, v) = n - \ell$ for all $v \in M^{2\alpha}$. Moreover, $n - \ell \geq \alpha$. It follows that $x \in \bigcup_{i=\alpha}^{n-\alpha} S_i(M^{2\alpha})$ if and only if $x^* \in \bigcup_{i=\alpha}^{n-\alpha} S_i(M^{2\alpha})$. Therefore, our desired result is established. □

Conjecture 6.3.20. *If Conjecture 6.3.15 holds, we obtain the exact number of pairs exhibiting PST at time $\frac{\pi}{2}$ in Proposition 6.3.19.*

Now, we find $\sum_{i=\alpha}^{n-\alpha} |S_i(M^{2\alpha})|$ where M is a $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matching in Q_n.

Proposition 6.3.21. *Let $n \geq 4$, and M be a $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matching in Q_n for $\alpha \geq 1$. Then, at least $2^{n-2\alpha}\binom{2\alpha}{\alpha}$ vertices pair up to have PST at time $\frac{\pi}{2}$ in $\widetilde{Q}_n^{(M)}$.*

Proof. Let $M^{2\alpha} = \{v_1, v_2\}$ and $M_{2\alpha} = \{w_1, w_2\}$. Suppose that $v_1 \sim w_1$ and $v_2 \sim w_2$. By (iii) of Proposition 2.5.1, $v_1 = 0\ldots0$ and $v_2 = 0\ldots01\ldots1$ where 1 appears 2α times in v_2. Since $d(v_1, w_1) = 1$ and $d(v_2, w_1) = 2\alpha+1$, there is a single 1 in w_1, and it must be placed on a position among the first $n - 2\alpha$ positions of w_1. For $i \in \{\alpha, \ldots, n-\alpha\}$, consider $x \in S_i(\{v_1, v_2\})$. Applying Lemma 6.3.16 to v_2 and x, we see that x has exactly $i - \alpha$ ones among the first $n - 2\alpha$ positions, and α ones among the last 2α positions. Hence, $|S_i(\{v_1, v_2\})| = \binom{2\alpha}{\alpha}\binom{n-2\alpha}{i-\alpha}$. Therefore, by Proposition 6.3.19, our desired result follows. □

Proposition 6.3.22. *Let $n \geq 4$ and M be a $(k, 2\alpha, 2\beta; \Gamma)$-matching in Q_n where $k \geq 3$ and $\alpha, \beta \geq 1$. If $|S_\alpha(M^{2\alpha})| \neq 0$, then $k\alpha \leq n$ and $|S_\alpha(M^{2\alpha})| = 1$. Similarly, if $|S_\beta(M^{2\beta})| \neq 0$, then $k\beta \leq n$ and $|S_\beta(M_{2\beta})| = 1$.*

Proof. Let $M^{2\alpha} = \{v_1, \ldots, v_k\}$, and let x be a vertex such that $d(x, v_i) = \alpha$ for $i = 1, \ldots, k$. By (iii) of Proposition 2.5.1, we may assume that $v_1 = 0\ldots0$, and x contains exactly α ones in the last α positions. From $d(v_1, v_j) = 2\alpha$ for $j = 2, \ldots, k$, each vertex v_j contains exactly 2α ones. Since $d(x, v_j) = \alpha$ for each $j = 2, \ldots, k$, we find that v_j contains α ones in the last α positions. Moreover, since v_{i_1} and v_{i_2} for $i_1, i_2 \in \{2, \ldots, k\}$ with $i_1 \neq i_2$ differ in exactly 2α positions, the α ones of v_{i_1} that are not in the last α positions do not have any position in common with those of v_{i_2} not in the last α positions. Hence, $k\alpha \leq n$. Furthermore, since $v_2, \ldots, v_k$ share exactly α ones in the last α positions, there are no vertices y other than x such that y has precisely α ones and $d(y, v_i) = \alpha$ for $i = 2, \ldots, k$. Therefore, $|S_\alpha(M^{2\alpha})| = 1$.

An analogous argument establishes the remaining result. □

Example 6.3.23. Consider $v_1 = 0000\ 0000$, $v_2 = 0000\ 1111$, $v_3 = 0011\ 0011$ and $v_4 = 0101\ 0110$ in Q_8. Pairwise distances among v_1, v_2, v_3, and v_4 are constant as 4, but $S_2(\{v_1, v_2, v_3, v_4\})$ is empty; furthermore, 0100 0011 and 0010 0110 are in $S_3(\{v_1, v_2, v_3, v_4\})$.

Problem 6.3.24. *Given a $(k, 2\alpha, 2\alpha; \{(2\alpha+1)^k\})$-matching M where $k \geq 3$, find $|\bigcup_{i=\alpha}^{n-\alpha} S_i(M^{2\alpha})|$.*

We consider 'transitivity of a $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matching' in Q_n—used in Subsection 6.5.1 for $\alpha = 1$.

Proposition 6.3.25. *Let $n \geq 3$, and let $M = \{v_1 \sim w_1, v_2 \sim w_2\}$ and $N = \{v_3 \sim w_3, v_4 \sim w_4\}$ be $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matchings in Q_n. Suppose that $d(v_1, v_2) = d(w_1, w_2) = d(v_3, v_4) = d(w_3, w_4) = 2\alpha$. Then, there exists an automorphism f of Q_n such that $f(v_1) = v_3$, $f(v_2) = v_4$, $f(w_1) = w_3$, and $f(w_2) = w_4$.*

Proof. Let $y_1 = 0\ldots0$ and $y_2 = 0\ldots01\ldots1$ in $V(Q_n)$ where 1 appears 2α times in y_2. Let z_1 and z_2 be in $V(Q_n)$, where $d(y_1, z_1) = d(y_2, z_2) = 1$, a single one appears at the $(n-2\alpha)^{\text{th}}$ position in z_1, and $2\alpha+1$ ones appear in the last $2\alpha+1$ positions in z_2. Then, it suffices to show that all $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matchings in Q_n may be identified as the $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matching $\{y_1 \sim z_1, y_2 \sim z_2\}$.

Suppose that $M = \{v_1 \sim w_1, v_2 \sim w_2\}$ is a $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matching in Q_n with distance-partite sets $M^{2\alpha} = \{v_1, v_2\}$ and $M_{2\alpha} = \{w_1, w_2\}$. By (iii) of Proposition 2.5.1, there exists an automorphism f of Q_n such that $f(v_1) = y_1$ and $f(v_2) = y_2$. Considering the distances among vertices in $M^{2\alpha} \cup M_{2\alpha}$, we can find that $f(w_1) = a_1 \ldots a_n$ and $f(w_2) = b_1 \ldots b_n$ must contain a single one and $(2\alpha+1)$ ones, respectively, so that $a_{i_0} = b_{i_0} = 1$ for some $i_0 \in \{1, \ldots, n-2\alpha\}$, and $b_i = 1$ for $i \in \{n-2\alpha+1, \ldots, n\}$. Let σ be the permutation $(i_0, n-2\alpha)$ in the cyclic notation. Then, one can check that a bijection $g : V(Q_n) \to V(Q_n)$ defined by $g(x_1 \ldots x_n) = x_{\sigma(1)} \ldots x_{\sigma(n)}$ is an automorphism of Q_n. Hence, $g(f(v_1)) = y_1$, $g(f(v_2)) = y_2$, $g(f(w_1)) = z_1$, and $g(f(w_2)) = z_2$. The conclusion follows. $\square$

Remark 6.3.26. When we classify equidistant switched n-cubes up to isomorphism, we need to consider two factors: orderings of the edges in an equidistant matching M (discussed in Remark 6.3.2), and transitivity of M in Q_n.

Given $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-matchings M and N in Q_n, by Remark 6.3.5 $\widetilde{Q}_n^{(M)}$ and $\widetilde{Q}_n^{(N)}$ both are uniquely determined up to orderings of the edges in M and N, respectively. Furthermore, it follows from Proposition 6.3.25 that $\widetilde{Q}_n^{(M)}$ and $\widetilde{Q}_n^{(N)}$ are isomorphic. Therefore, we may study only $\widetilde{Q}_n^{(M)}$ in order to describe any properties of $(2, 2\alpha, 2\alpha; \{(2\alpha+1)^2\})$-switched n-cubes.

Problem 6.3.27. *Study quadruples $(k, \alpha, \beta, \Gamma)$ that allow attaining 'transitivity of a $(k, \alpha, \beta; \Gamma)$-matching' in Q_n. As discussed in Remark 6.3.26, this problem is related to classification of non-isomorphic equidistant switched n-cubes via $(k, \alpha, \beta; \Gamma)$-matchings.*

6.4 Sensitivity of the fidelity under PST in hypercubes

Kirkland [43] derives formulas to quantify sensitivity of the fidelity: derivatives of all orders of the fidelity of state transfer with respect to readout time, and the first and second partial derivatives of the fidelity of state transfer with respect to the weight of an edge. Throughout Sections 6.4 and 6.5, we shall ultimately compare sensitivity of the fidelity under PST—between the pair of vertices in Theorem 6.3.12—in Q_n and in an equidistant switched n-cube $\widetilde{Q}_n$. In Section 6.4, we first show that Q_n and $\widetilde{Q}_n$ have the same sensitivity under PST between that pair with respect to readout time, and we focus on sensitivity under PST to changes in the weight of an edge in Q_n. In Subsections 6.4.1 and 6.4.2, we provide necessary information to establish the desired first and second derivatives for Q_n. Through Subsections 6.4.3 and 6.4.4, we derive explicit expressions for the derivatives with respect to the weights of two types of edges.

We introduce the following theorem that can be readily deduced from the result (Theorem 2.2) in [43].

Theorem 6.4.1. *[43] Let G_1 and G_2 be weighted graphs with the same vertex set. Suppose that G_1 and G_2 both exhibit PST between s and r at time t_0. If for any positive integer j, the number of walks of length j from s to s in G_1 is the same as that in G_2, then the fidelity of state transfer from s to r has the same derivatives of all orders with respect to readout time in G_1 and G_2.*

Theorem 6.4.2. *Let M be an equidistant matching of size k in Q_n. Suppose that x is at the same distance from vertices in each distance-partite set of M. Then, for any $\tau \in \mathcal{S}_k$, Q_n and $\widetilde{Q}_n^{(M_\tau)}$ exhibit PST between x and x^* at time $\frac{\pi}{2}$, and the fidelity of state transfer between x and x^* have the same derivatives of all orders with respect to readout time in Q_n and $\widetilde{Q}_n^{(M_\tau)}$.*

Proof. It is straightforward from Proposition 6.3.11, Theorems 6.3.12 and 6.4.1. □

We briefly elaborate formulas in [43] for the first and second partial derivatives of the fidelity with respect to the weight of an edge in Q_n. Let k and l be vertices in Q_n. Let $A(Q_n)$ be the adjacency matrix of Q_n and $E = \begin{bmatrix}\mathbf{e}_k & \mathbf{e}_l\end{bmatrix}\begin{bmatrix}\mathbf{e}_l & \mathbf{e}_k\end{bmatrix}^T$. We shall adopt the notation used in Subsection 3.2 of the paper [43]. As stated in [43], there is an $\epsilon > 0$ such that for each $h \in (-\epsilon, \epsilon)$, $A(Q_n) + hE$ can be diagonalised as $A(Q_n) + hE = V_h\Lambda_h V_h^T$, where both V_h and Λ_h are analytic in h, V_h is orthogonal, and $\Lambda_h = \mathrm{diag}(\lambda_1(h), \dots, \lambda_n(h))$. Furthermore, it is found that

$$\left.\frac{d\lambda_i}{dh}\right|_{h=0} = \mathbf{e}_i^T V_0^T E V_0 \mathbf{e}_i. \tag{6.4.1}$$

for $i = 1, \dots, n$. Considering the dependence of V_h and Λ_h for $h \in (-\epsilon, \epsilon)$ on two particular vertices k and l among 2^n vertices, we use $\frac{\partial V}{\partial_{k,l}}$ and $\frac{\partial \Lambda}{\partial_{k,l}}$ to denote $\left.\frac{dV}{dh}\right|_{h=0}$ and $\left.\frac{d\Lambda}{dh}\right|_{h=0}$, respectively. For simplicity, let $V := V_0$ and $\Lambda := \Lambda_0$.

Let s and r be vertices of Q_n. For each $t \geq 0$, let $U(t) = e^{itA(Q_n)}$, and $p(t) = |(U(t))_{s,r}|^2$. Suppose that for some $t_0 > 0$, $p(t_0) = 1$ and denote $(U(t_0))_{s,r}$ by $\alpha + i\beta$. The first derivative $\frac{\partial p(t_0)}{\partial_{k,l}}$ (Theorem 3.3 in [43]) and the second derivative $\frac{\partial^2 p(t_0)}{\partial_{k,l}^2}$ (Theorem 3.10 in [43]) with respect to the weight of $k \sim l$ for Q_n are

$$\frac{\partial p(t_0)}{\partial_{k,l}} = 2t_0X_1 + 2X_2,\ \frac{\partial^2 p(t_0)}{\partial_{k,l}^2} = -2t_0^2Y_1 - 2Y_2, \tag{6.4.2}$$

where

$$\begin{aligned}
X_1 =& \mathbf{e}_s^T V \frac{\partial \Lambda}{\partial_{k,l}}(\beta\cos(t_0\Lambda) - \alpha\sin(t_0\Lambda))V^T\mathbf{e}_r,\\
X_2 =& \mathbf{e}_s^T \frac{\partial V}{\partial_{k,l}}(\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda))V^T\mathbf{e}_r + \mathbf{e}_s^T V(\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda))\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_r,\\
Y_1 =& \mathbf{e}_s^T V\left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 V^T\mathbf{e}_s - \left(\mathbf{e}_s^T V\frac{\partial \Lambda}{\partial_{k,l}}V^T\mathbf{e}_s\right)^2,\\
Y_2 =& \mathbf{e}_s^T\frac{\partial V}{\partial_{k,l}}\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_s + \mathbf{e}_r^T\frac{\partial V}{\partial_{k,l}}\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_r - 2\mathbf{e}_s^T\frac{\partial V}{\partial_{k,l}}(\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda))\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_r.
\end{aligned} \tag{6.4.3}$$

In order to compute the desired derivatives under PST between s and r in Q_n with less complexity of computation, we are to determine $\Lambda, V, \frac{\partial V}{\partial_{k,l}}$, and $\frac{\partial \Lambda}{\partial_{k,l}}$ under a specific condition that $t_0 = \frac{\pi}{2}$, $r = s^*$, $s \sim k$, and $k \sim l$. In Subsection 6.4.1, we investigate sign patterns of entries in $(1, -1)$ eigenvectors of $A(Q_n)$. In Subsection 6.4.2, by the sign patterns and the algorithms for computing V and $\frac{\partial V}{\partial_{k,l}}$ in [43], we obtain $\frac{\partial \Lambda}{\partial_{k,l}}$, the particular rows of V indexed by s, k, l, and r, and the s^{th} and r^{th} rows of $\frac{\partial V}{\partial_{k,l}}$. In Subsection 6.4.3, our desired derivatives with respect to the weight of the edge $k \sim l$ for Q_n are established. Finally, Subsection 6.4.4 exhibits the derivative with respect to the weight of the edge $s \sim k$.

6.4.1 Sign patterns of $(1, -1)$ eigenvectors for Q_n

In order to examine sign pattern of $(1, -1)$ eigenvectors, we shall define a particular total order on $V(Q_n)$, and find the corresponding adjacency matrix.

Given two disjoint (totally) ordered sets P and Q, the *linear sum* $P \cup_L Q$ of P and Q is defined as the union of P and Q such that elements of P (resp. Q) in the union are ordered as in P (resp. Q), and $x < y$ for each $x \in P$ and $y \in Q$.

Let $S_1 = \{0\}$ and $T_1 = \{1\}$. Suppose that for $i = 1, \ldots, n-1$, S_{i+1} (resp. T_{i+1}) is the ordered set of binary strings obtained from those in $S_i \cup_L T_i$ by attaching a 0 at the end of each string, *i.e.,* on the right (resp. by attaching a 1 at the end of each string).

Example 6.4.3. For $S_1 = \{0\}$ and $T_1 = \{1\}$, we can obtain ordered sets $S_2 = \{00, 10\}$ and $T_2 = \{01, 11\}$; $S_3 = \{000, 100, 010, 110\}$ and $T_3 = \{001, 101, 011, 111\}$.

Taking the vertex set of Q_n as the linear sum of S_n and T_n, the adjacency matrix A_n of Q_n can be recursively constructed:

$$A_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ A_{i+1} = \begin{bmatrix} A_i & I_{2^i} \\ I_{2^i} & A_i \end{bmatrix},\ i = 1, \ldots, n-1. \tag{6.4.4}$$

Throughout Subsections 6.4.1–6.4.4, we use A_n to denote the adjacency matrix of Q_n in form (6.4.4). Moreover, we consider the *standard (normalized) Hadamard matrix* H_n generated as follows:

$$H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},\ H_{i+1} = \begin{bmatrix} H_i & H_i \\ H_i & -H_i \end{bmatrix},\ i = 1, \ldots, n-1. \tag{6.4.5}$$

It is well-known that $H_n H_n^T = 2^n I$ (see [69]). Then, one can check, using induction, that the columns of $\frac{1}{\sqrt{2^n}} H_n$ form an orthonormal basis of eigenvectors for A_n. Furthermore, it can be found that eigenvalues of A_n are given by $n - 2j$ with respective multiplicity $\binom{n}{j}$ for $j = 0, \ldots, n$. Let $H_n(j)$ denote the submatrix of H_n that consists of all columns in H_n that are eigenvectors of A_n corresponding to the eigenvalue $n - 2j$. Evidently, there are $\binom{n}{j}$ columns in $H_n(j)$.

In what follows, we define $V(Q_n)$ as the set $\{1,\ldots,2^n\}$, and adjacency of vertices in Q_n is given by entries of the matrix A_n in form (6.4.4): vertices k and l are adjacent if and only if $(A_n)_{k,l}=1$.

Remark 6.4.4. From the recursive construction of Q_n through the linear sum of S_n and T_n, we can find that vertices 1 and 2^n of Q_n correspond to binary strings $0\ldots0$ and $1\ldots1$, respectively. Hence, $d_{Q_n}(1,2^n)=n$.

Before we characterize sign patterns of two entries in each column of $H_n(j)$ for $0\le j\le n$ that are indexed by distinct vertices l_1 and l_2, we first find the column $H_n(0)$ and the first row of H_n in Lemma 6.4.5, investigate each row of $H_n(i)$ for $1\le i\le n$ via H_{n-1} in Lemma 6.4.6, and obtain the last row of $H_n(i)$ for $0\le i\le n$ in Lemma 6.4.7.

Lemma 6.4.5. *Let $n\ge 1$. Then, for any $1\le l\le 2^n$, the l^{th} entry of the column $H_n(0)$ is 1, and $\mathbf{e}_1^T H_n(j)=\mathbf{1}^T_{\binom{n}{j}}$ for $j=0,\ldots,n$.*

Proof. Since $A_n\mathbf{1}=n\mathbf{1}$, we have $H_n(0)=\mathbf{1}$. We observe that the first row of the standard Hadamard matrix is the all ones vector. □

Lemma 6.4.6. *Let $n\ge 2$. Then, we have the following:*

(i) If $1\le l\le 2^{n-1}$, then the l^{th} row of $H_n(j)$ for $1\le j\le n-1$ is obtained from the l^{th} rows of $H_{n-1}(j-1)$ and $H_{n-1}(j)$ by appending one after the other, and permuting the entries of the resulting row appropriately.

(ii) If $2^{n-1}+1\le l\le 2^n$, then the l^{th} row of $H_n(j)$ for $1\le j\le n-1$ is obtained from the $(l-2^{n-1})^{th}$ row of $H_{n-1}(j-1)$ with change of the sign of the row and the $(l-2^{n-1})^{th}$ row of $H_{n-1}(j)$, by appending one after the other, and permuting the entries of the resulting row appropriately.

(iii) If $1\le l\le 2^{n-1}$, then the l^{th} entry of $H_n(n)$ equals that of $H_{n-1}(n-1)$.

(iv) If $2^{n-1}+1\le l\le 2^n$, then the l^{th} entry of $H_n(n)$ and the $(l-2^{n-1})^{th}$ entry $H_{n-1}(n-1)$ differ by sign.

Proof. Let $n\ge 2$. For $i=0,\ldots,n-1$, suppose that $\mathbf{x}$ is an eigenvector of A_{n-1} corresponding to the eigenvalue $(n-1)-2i$. Then,

$$A_n\begin{bmatrix}\mathbf{x}\\ \mathbf{x}\end{bmatrix}=\begin{bmatrix}A_{n-1} & I\\ I & A_{n-1}\end{bmatrix}\begin{bmatrix}\mathbf{x}\\ \mathbf{x}\end{bmatrix}=(n-2i)\begin{bmatrix}\mathbf{x}\\ \mathbf{x}\end{bmatrix},$$
$$A_n\begin{bmatrix}\mathbf{x}\\ -\mathbf{x}\end{bmatrix}=\begin{bmatrix}A_{n-1} & I\\ I & A_{n-1}\end{bmatrix}\begin{bmatrix}\mathbf{x}\\ -\mathbf{x}\end{bmatrix}=(n-2-2i)\begin{bmatrix}\mathbf{x}\\ -\mathbf{x}\end{bmatrix}.$$

Any eigenvector of A_{n-1} generates two linearly independent eigenvectors of A_n.

For $1 \leq j \leq n-1$, any eigenvector of A_n corresponding to the eigenvalue $n-2j$ can be expressed as either $\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_1 \end{bmatrix}$ or $\begin{bmatrix} \mathbf{x}_2 \\ -\mathbf{x}_2 \end{bmatrix}$, where $\mathbf{x}_1$ and $\mathbf{x}_2$ are eigenvectors of A_{n-1} corresponding to $(n-1)-2j$ and $(n-1)-2(j-1)$, respectively. Note that $H_{n-1}(j)$ consists of all eigenvectors of A_{n-1} associated to the eigenvalue $(n-1)-2j$. Hence, for $1 \leq j \leq n-1$, the statements (i) and (ii) follow. From $H_n(n) = \begin{bmatrix} H_{n-1}(n-1) \\ -H_{n-1}(n-1) \end{bmatrix}$, we obtain the results (iii) and (iv). $\square$

Lemma 6.4.7. *Let $n \geq 1$. Then, $\mathbf{e}_{2^n}^T H_n(j) = (-1)^j \mathbf{1}_{\binom{n}{j}}^T$ for $j = 0, \ldots, n$.*

Proof. We use induction on n. Evidently, $\mathbf{e}_2^T H_1(0) = 1$ and $\mathbf{e}_2^T H_1(1) = -1$. Suppose that for $n \geq 1$, $\mathbf{e}_{2^n}^T H_n(j) = (-1)^j \mathbf{1}_{\binom{n}{j}}^T$ for $j = 0, \ldots, n$. We claim that $\mathbf{e}_{2^{n+1}}^T H_{n+1}(i) = (-1)^i \mathbf{1}_{\binom{n+1}{i}}^T$ for $0 \leq i \leq n+1$. For the case $i = 0$, by Lemma 6.4.5, we have $\mathbf{e}_{2^{n+1}}^T H_{n+1}(0) = 1$. Consider $1 \leq i \leq n$. Using (ii) in Lemma 6.4.6, the row $\mathbf{e}_{2^{n+1}}^T H_{n+1}(i)$ consists of $-\mathbf{e}_{2^n}^T H_n(i-1)$ and $\mathbf{e}_{2^n}^T H_n(i)$. By the inductive hypothesis, we have $-\mathbf{e}_{2^n}^T H_n(i-1) = (-1)^i \mathbf{1}_{\binom{n}{i-1}}^T$ and $\mathbf{e}_{2^n}^T H_n(i) = (-1)^i \mathbf{1}_{\binom{n}{i}}^T$. So, by Pascal's identity, $\mathbf{e}_{2^{n+1}}^T H_{n+1}(i) = (-1)^i \mathbf{1}_{\binom{n+1}{i}}^T$. Let $i = n+1$. Applying (iv) in Lemma 6.4.6 to the last entry of $H_{n+1}(n+1)$, we have $\mathbf{e}_{2^{n+1}}^T H_{n+1}(n+1) = -\mathbf{e}_{2^n}^T H_n(n) = (-1)^{n+1}$. Therefore, the conclusion follows by induction. $\square$

Let $h_{n,j}^{l_1,l_2}(a,b)$ denote the number of columns of $H_n(j)$ whose entries are indexed by l_1 and l_2 with $l_1 \neq l_2$ are a and b, respectively. Let $h_{n,j}^{l}(a)$ denote the number of columns of $H_n(j)$ whose the l^{th} entry is a. Define $h_{n,j}^{l,l}(a,b) = 0$ if $a \neq b$, and $h_{n,j}^{l,l}(a,b) = h_{n,j}^{l}(a)$ if $a = b$. We observe that for $1 \leq l_1 \leq l_2 \leq 2^n$,

$$h_{n,j}^{l_1,l_2}(1,1) + h_{n,j}^{l_1,l_2}(-1,-1) + h_{n,j}^{l_1,l_2}(1,-1) + h_{n,j}^{l_1,l_2}(-1,1) = \binom{n}{j}. \tag{6.4.6}$$

Example 6.4.8. From Figure 6.3, we have $h_{3,0}^{5,6}(1,1) = 1$; $h_{3,1}^{5,6}(1,1) = 1$, $h_{3,1}^{5,6}(-1,-1) = 1$, and $h_{3,1}^{5,6}(1,-1) = 1$; $h_{3,2}^{5,6}(-1,-1) = 1$, $h_{3,2}^{5,6}(1,-1) = 1$, and $h_{3,2}^{5,6}(-1,1) = 1$; and $h_{3,3}^{5,6}(-1,1) = 1$.

Example 6.4.9. Let $n \geq 2$. If $0 \leq j \leq n$ for j even, then by Lemmas 6.4.5 and 6.4.7 we have $h_{n,j}^{1,2^n}(1,1) = \binom{n}{j}$; by (6.4.6) we have $h_{n,j}^{1,2^n}(1,-1) = h_{n,j}^{1,2^n}(-1,1) = h_{n,j}^{1,2^n}(-1,-1) = 0$. Similarly, for $0 \leq j \leq n$ with j odd, we have $h_{n,j}^{1,2^n}(1,-1) = \binom{n}{j}$ and $h_{n,j}^{1,2^n}(1,1) = h_{n,j}^{1,2^n}(-1,1) = h_{n,j}^{1,2^n}(-1,-1) = 0$.

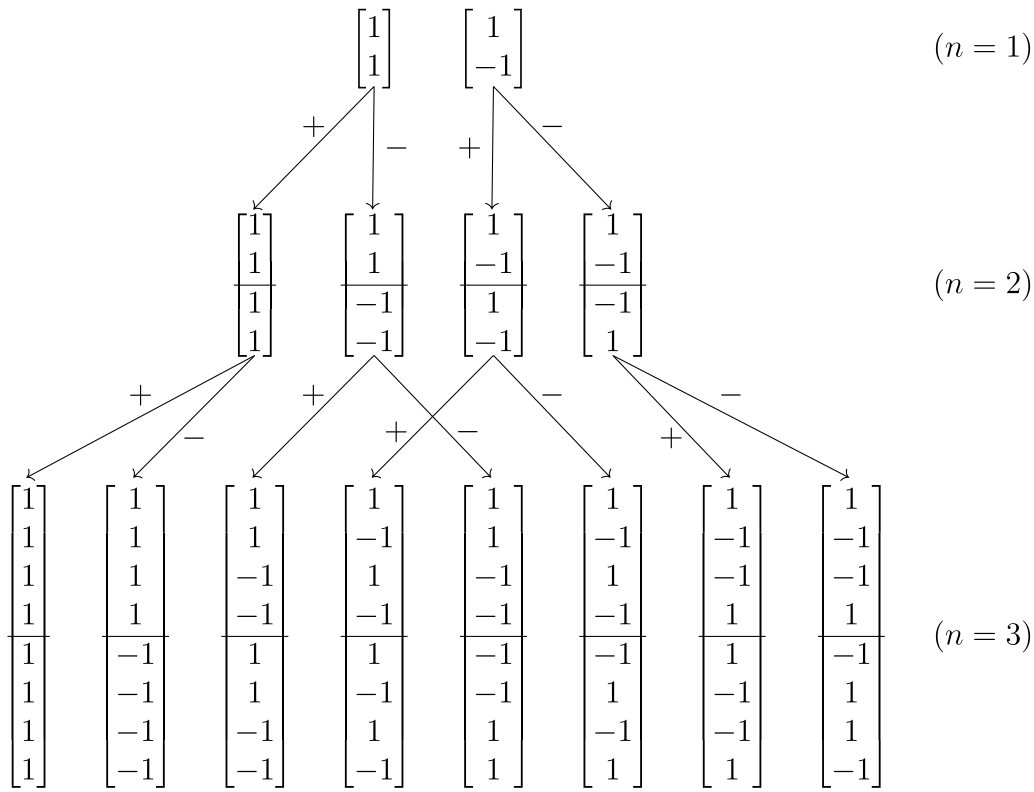


Figure 6.3: The vectors in each row corresponding to $n = 1, 2, 3$ are aligned in order of $H_n(0), \ldots, H_n(n)$, and the sign in each arrow indicates the addition or subtraction by 1 for the eigenvalue associated to the eigenvector at the starting point of the arrow.

Let $(a, b) \in \{(1, 1), (1, -1), (-1, 1), (-1, -1)\}$. We define $h_{n,j}^{l_1,l_2}(a, b) = 0$ for all $n \geq 1$ and $1 \leq l_1 \leq l_2 \leq 2^n$ whenever $j < 0$ or $j > n$.

Proposition 6.4.10. *Let $(a, b) \in \{(1, 1), (1, -1), (-1, 1), (-1, -1)\}$. Then, for $n \geq 2$ and $j = 0, \ldots, n$, we have*

$$
\begin{aligned}
&h_{n,j}^{l_1,l_2}(a, b) \\
&= \begin{cases}
h_{n-1,j-1}^{l_1,l_2}(a, b) + h_{n-1,j}^{l_1,l_2}(a, b), & \text{if } 1 \leq l_1 \leq l_2 \leq 2^{n-1}, \\
h_{n-1,j-1}^{l_1,l_2-2^{n-1}}(a, -b) + h_{n-1,j}^{l_1,l_2-2^{n-1}}(a, b), & \text{if } 1 \leq l_1 \leq 2^{n-1},\ 2^{n-1}+1 \leq l_2 \leq 2^n, \\
h_{n-1,j-1}^{l_1-2^{n-1},l_2-2^{n-1}}(-a, -b) + h_{n-1,j}^{l_1-2^{n-1},l_2-2^{n-1}}(a, b), & \text{if } 2^{n-1}+1 \leq l_1 \leq l_2 \leq 2^n,
\end{cases}
\end{aligned}
$$

with $h_{1,0}^{1,1}(1, 1) = h_{1,0}^{2,2}(1, 1) = h_{1,1}^{1,1}(1, 1) = h_{1,1}^{2,2}(-1, -1) = h_{1,0}^{1,2}(1, 1) = h_{1,1}^{1,2}(1, -1) = 1$.

Proof. Consider $h_{n,j}^{l_1,l_2}(a, b)$ for $j \in \{1, \ldots, n-1\}$. If $1 \leq l_1 \leq l_2 \leq 2^{n-1}$, then by (i) in Lemma 6.4.6, the l_1^{th} and l_2^{th} rows of $H_n(j)$ are obtained from the l_1^{th} and l_2^{th} rows of $H_{n-1}(j)$ and $H_{n-1}(j-1)$ (by an appropriate permutation). Hence, $h_{n,j}^{l_1,l_2}(a, b) =$

$h_{n-1,j-1}^{l_1,l_2}(a,b)+h_{n-1,j}^{l_1,l_2}(a,b)$. Suppose that $1 \le l_1 \le 2^{n-1}$, $2^{n-1}+1 \le l_2 \le 2^n$. Applying (i) and (ii) in Lemma 6.4.6 to the l_1^{th} and l_2^{th} rows of $H_n(j)$, respectively, we find that the l_1^{th} and l_2^{th} rows of $H_n(j)$ are obtained from the l_1^{th} and $(l_2-2^{n-1})^{\text{th}}$ rows of $H_{n-1}(j)$, and from the l_1^{th} and $(l_2-2^{n-1})^{\text{th}}$ rows of $H_{n-1}(j-1)$ with change of the sign of the $(l_2-2^{n-1})^{\text{th}}$ row. Thus, $h_{n,j}^{l_1,l_2}(a,b) = h_{n-1,j-1}^{l_1,l_2-2^{n-1}}(a,-b) + h_{n-1,j}^{l_1,l_2-2^{n-1}}(a,b)$. A similar argument applies to $2^{n-1}+1 \le l_1 \le l_2 \le 2^n$ with (ii) in Lemma 6.4.6, one can find that $h_{n,j}^{l_1,l_2}(a,b) = h_{n-1,j-1}^{l_1-2^{n-1},l_2-2^{n-1}}(-a,-b) + h_{n-1,j}^{l_1-2^{n-1},l_2-2^{n-1}}(a,b)$.

Consider $h_{n,0}^{l_1,l_2}(a,b)$. By Lemma 6.4.5, $h_{m,0}^{k_1,k_2}(1,1) = 1$ for any $m \ge 1$ and $1 \le k_1 \le k_2 \le 2^m$. Since $h_{m-1,-1}^{k_1,k_2}(a,b) = 0$ for all $m \ge 2$ and $1 \le k_1 \le k_2 \le 2^m$, our desired result for $h_{n,0}^{l_1,l_2}(a,b)$ is obtained. Using (iii) and (iv) in Lemma 6.4.6 for the case $h_{n,n}^{l_1,l_2}(a,b)$ with the fact that $h_{m-1,m}^{k_1,k_2}(a,b) = 0$ for all $m \ge 2$ and $1 \le k_1 \le k_2 \le 2^m$, the result for $h_{n,n}^{l_1,l_2}(a,b)$ can be established. □

Example 6.4.11. Let $n \ge 2$. Recursively applying Proposition 6.4.10, one can verify that $h_{n,n}^{1,2}(a,b) = h_{n-1,n-1}^{1,2}(a,b) = \cdots = h_{1,1}^{1,2}(a,b)$. Since $h_{1,1}^{1,2}(1,-1) = 1$, we have $h_{m,m}^{1,2}(1,-1) = 1$ for all $m \ge 1$. Considering the identity (6.4.6), $h_{m,m}^{1,2}(1,1) = h_{m,m}^{1,2}(-1,1) = h_{m,m}^{1,2}(-1,-1) = 0$ for all $m \ge 1$.

Example 6.4.12. By Proposition 6.4.10, we have $h_{n,j}^{1,2^{n-1}+1}(a,b) = h_{n-1,j-1}^{1,1}(a,-b) + h_{n-1,j}^{1,1}(a,b)$. Let $a=b$. Then, $h_{n,j}^{1,2^{n-1}+1}(a,b) = h_{n-1,j}^{1}(a)$. By Lemma 6.4.5, if $a=1$ then $h_{n,j}^{1,2^{n-1}+1}(a,b) = \binom{n-1}{j}$; and if $a=-1$ then $h_{n,j}^{1,2^{n-1}+1}(a,b) = 0$. Suppose $a \ne b$. A similar argument yields that if $a=1$ then $h_{n,j}^{1,2^{n-1}+1}(a,b) = \binom{n-1}{j-1}$; and if $a=-1$ then $h_{n,j}^{1,2^{n-1}+1}(a,b) = 0$.

6.4.2 $\frac{\partial \Lambda}{\partial_{k_0,l_0}}$ and particular rows of V and $\frac{\partial V}{\partial_{k_0,l_0}}$

Throughout Subsections 6.4.2–6.4.4, given Q_n, we assume that $s_0 := 1$, $k_0 := 2^{n-1}+1$, $l_0 := 2^{n-1}+2$, and $r_0 := 2^n$. By Remark 6.4.4, the antipodal vertex s_0^* of s_0 in Q_n is 2^n, and so $r_0 = s_0^*$. From the structure of A_n in form (6.4.4), we find that $d_{Q_n}(s_0,k_0) = 1$, $d_{Q_n}(s_0,l_0) = 2$, and $d_{Q_n}(k_0,l_0) = 1$.

Let $(a,b) = \{(1,1),(1,-1),(-1,1),(-1,-1)\}$. Consider $h_{n,j}^{k_0,l_0}(a,b)$ for $0 \le j \le n$. By Proposition 6.4.10, we have

$$h_{n,j}^{k_0,l_0}(a,b) = h_{n-1,j-1}^{1,2}(-a,-b) + h_{n-1,j}^{1,2}(a,b). \tag{6.4.7}$$

We now consider $h_{m,j}^{1,2}(a,b)$ for $m \ge 1$ and $0 \le j \le m$. Since the first row of H_m

is the all ones vector, we have

$$h^{1,2}_{m,j}(-1,1) = h^{1,2}_{m,j}(-1,-1) = 0 \tag{6.4.8}$$

for all $m \geq 1$ and $0 \leq j \leq m$. By Proposition 6.4.10,

$$\begin{aligned} h^{1,2}_{m,j}(1,1) &= h^{1,2}_{m-1,j-1}(1,1) + h^{1,2}_{m-1,j}(1,1), \\ h^{1,2}_{m,j}(1,-1) &= h^{1,2}_{m-1,j-1}(1,-1) + h^{1,2}_{m-1,j}(1,-1). \end{aligned}$$

From Lemma 6.4.5, we obtain $h^{1,2}_{m,0}(1,1) = 1$ for $m \geq 1$. By Example 6.4.11, we have $h^{1,2}_{m,m}(1,-1) = 1$ for $m \geq 1$. Then, labelling rows and columns as $m = 1, 2, 3, \ldots$ and $j = 0, 1, 2, \ldots$, respectively, we obtain

$$[h^{1,2}_{m,j}(1,1)] = \begin{bmatrix} 1 & 0 & \cdots & & \\ 1 & 1 & 0 & \cdots & \\ 1 & 2 & 1 & 0 & \cdots \\ 1 & 3 & 3 & 1 & 0 \\ & \vdots & & & \ddots \end{bmatrix}, \; [h^{1,2}_{m,j}(1,-1)] = \begin{bmatrix} 0 & 1 & 0 & \cdots & & \\ 0 & 1 & 1 & 0 & \cdots \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 1 & 3 & 3 & 1 \\ & \vdots & & & \ddots \end{bmatrix}.$$

Define $\binom{m}{i} = 0$ for any $m \geq 1$ whenever $i < 0$ or $i > m$. Then, one can check by induction on m and j that

$$h^{1,2}_{m,j}(1,1) = \binom{m-1}{j} \text{ and } h^{1,2}_{m,j}(1,-1) = \binom{m-1}{j-1}. \tag{6.4.9}$$

Lemma 6.4.13. *Let $n \geq 2$. Then,*

$$\begin{aligned} h^{k_0,l_0}_{n,j}(1,1) &= \binom{n-2}{j}, \; h^{k_0,l_0}_{n,j}(-1,-1) = \binom{n-2}{j-1}, \\ h^{k_0,l_0}_{n,j}(1,-1) &= \binom{n-2}{j-1}, \; h^{k_0,l_0}_{n,j}(-1,1) = \binom{n-2}{j-2}. \end{aligned}$$

Proof. By (6.4.7), we have $h^{k_0,l_0}_{n,j}(a,b) = h^{1,2}_{n-1,j-1}(-a,-b) + h^{1,2}_{n-1,j}(a,b)$ for $0 \leq j \leq n$ where $(a,b) = \{(1,1),(1,-1),(-1,1),(-1,-1)\}$. Using (6.4.8) and (6.4.9), the result can be established. □

Now, we present the algorithms for obtaining V and $\frac{\partial V}{\partial_{k_0,l_0}}$ suppressing the technical details (see Subsection 3.2 of [43] for the details).

We first introduce some notation to describe V and $\frac{\partial V}{\partial_{k_0,l_0}}$. Let $n \geq 2$, and let

$E = \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{l_0} & \mathbf{e}_{k_0} \end{bmatrix}^T$. Let $j \in \{0, \ldots, n\}$ and $m = \binom{n}{j}$. We denote by $\mathbf{x}_1^j, \ldots, \mathbf{x}_m^j$ the m unit eigenvectors of A_n associated to the eigenvalue $n - 2j$ that comprise $\frac{1}{\sqrt{2^n}} H_n(j)$. Suppose that the subspace spanned by columns of $EH_n(j)$ has dimension k. Since the rank of E is 2, we have $k \leq 2$. Furthermore, H_n is a $(1, -1)$ matrix, so $k = 1$ or $k = 2$. Without loss of generality, we assume in what follows that the first k vectors $\mathbf{x}_1^j, \ldots, \mathbf{x}_k^j$ of the vectors $\mathbf{x}_1^j, \ldots, \mathbf{x}_m^j$ satisfy that $E\mathbf{x}_1^j, \ldots, E\mathbf{x}_k^j$ form a basis of the subspace. Recall that $V = V_0$ and $\Lambda = \Lambda_0$. Let V be an orthogonal matrix obtained from the algorithm [43] described below so that $A_n = V\Lambda V^T$. Vectors $\hat{\mathbf{x}}_1^j, \ldots, \hat{\mathbf{x}}_m^j$ denote m columns in V that are eigenvectors of A_n associated to the eigenvalue $n - 2j$.

For a matrix X, we use $X^\dagger$ to denote the Moore–Penrose inverse [56] of X.

Suppose that $k = 1$. Then, $\hat{\mathbf{x}}_1^j$ is given by $\hat{\mathbf{x}}_1^j = \frac{1}{\sqrt{\sum_{i=1}^m \delta_i^2}} \sum_{i=1}^m \delta_i \mathbf{x}_i^j$ where $\delta_i = \frac{(\mathbf{x}_1^j)^T E^T E \mathbf{x}_i^j}{(\mathbf{x}_1^j)^T E^T E \mathbf{x}_1^j}$ for $i = 1, \ldots, m$. The other $(m-1)$ columns $\hat{\mathbf{x}}_2^j, \ldots, \hat{\mathbf{x}}_m^j$ in V form an orthonormal basis of $\operatorname{span}\{\delta_1 \mathbf{x}_i^j - \delta_i \mathbf{x}_1^j | i = 2, \ldots, m\}$. Furthermore, if $V\mathbf{e}_p = \hat{\mathbf{x}}_i^j$ for some $2 \leq i \leq m$, then $\frac{\partial V}{\partial_{k_0, l_0}} \mathbf{e}_p = 0$; and if $V\mathbf{e}_p = \hat{\mathbf{x}}_1^j$, then

$$\frac{\partial V}{\partial_{k_0, l_0}} \mathbf{e}_p = ((n - 2j)I - A_n)^\dagger E \hat{\mathbf{x}}_1^j. \tag{6.4.10}$$

Consider the case $k = 2$. There is a decomposition of $(n - 2j)$-eigenspace of A_n into the direct sum of $S_1 = \operatorname{span}\{\sum_{i=1}^m \alpha_i \mathbf{x}_i^j, \sum_{i=1}^m \beta_i \mathbf{x}_i^j\}$ and $S_2 = \operatorname{span}\{\mathbf{x}_i^j - \alpha_i \mathbf{x}_1^j - \beta_i \mathbf{x}_2^j | i = 3, \ldots, m\}$, where $\alpha_1 = \beta_2 = 1$, $\alpha_2 = \beta_1 = 0$ and for $3 \leq i \leq m$,

$$\begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix} = \left(\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \begin{bmatrix} \mathbf{x}_1^j & \mathbf{x}_2^j \end{bmatrix} \right)^{-1} \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^j. \tag{6.4.11}$$

Given an orthonormal basis $\{\tilde{\mathbf{x}}_1^j, \tilde{\mathbf{x}}_2^j\}$ of S_1 and an orthogonal matrix U that diagonalises $\begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix}^T E \begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix}$, we can obtain $\hat{\mathbf{x}}_1^j$ and $\hat{\mathbf{x}}_2^j$ as

$$\begin{bmatrix} \hat{\mathbf{x}}_1^j & \hat{\mathbf{x}}_2^j \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix} U.$$

We denote $\begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix}^T E \begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix}$ by B^j. The other $m - 2$ corresponding columns $\hat{\mathbf{x}}_3^j, \ldots, \hat{\mathbf{x}}_m^j$ in V form an orthonormal basis of S_2. Moreover, if $V\mathbf{e}_p = \hat{\mathbf{x}}_i^j$ for some

$3 \le i \le m$, then $\frac{\partial V}{\partial_{k_0,l_0}}\mathbf{e}_p = 0$; and if $V\begin{bmatrix}\mathbf{e}_{p_1} & \mathbf{e}_{p_2}\end{bmatrix} = \begin{bmatrix}\hat{\mathbf{x}}_1^j & \hat{\mathbf{x}}_2^j\end{bmatrix}$, then

$$\begin{aligned}
&\frac{\partial V}{\partial_{k_0,l_0}}\begin{bmatrix}\mathbf{e}_{p_1} & \mathbf{e}_{p_2}\end{bmatrix}\\
=&((n-2j)I - A_n)^{\dagger}E\begin{bmatrix}\hat{\mathbf{x}}_1^j & \hat{\mathbf{x}}_2^j\end{bmatrix} + \frac{(\hat{\mathbf{x}}_1^j)^T E((n-2j)I - A_n)^{\dagger}E\hat{\mathbf{x}}_2^j}{(\hat{\mathbf{x}}_2^j)^T E\hat{\mathbf{x}}_2^j - (\hat{\mathbf{x}}_1^j)^T E\hat{\mathbf{x}}_1^j}\begin{bmatrix}-\hat{\mathbf{x}}_2^j & \hat{\mathbf{x}}_1^j\end{bmatrix}.
\end{aligned} \tag{6.4.12}$$

We now apply the algorithms to the n-cube Q_n. We first find $\frac{\partial \Lambda}{\partial_{k_0,l_0}}$ and the rows of V indexed by s_0, k_0, l_0 and r_0, according to the dimension of the column space of $EH_n(j)$ for each $0 \le j \le n$. Since $H_n(0)$ and $H_n(n)$ both are $(1,-1)$ column vectors, the column spaces of $EH_n(0)$ and $EH_n(n)$, both, are of dimension 1. On the other hand, if $1 \le j \le n-1$, then we find from Lemma 6.4.13 with Pascal's identity that $h_{n,j}^{k_0,l_0}(1,1) + h_{n,j}^{k_0,l_0}(-1,-1) = \binom{n-1}{j} > 0$ and $h_{n,j}^{k_0,l_0}(1,-1) + h_{n,j}^{k_0,l_0}(-1,1) = \binom{n-1}{j-1} > 0$. Hence, the subspace spanned by the columns of $EH_n(j)$ has dimension 2.

Here we revisit the formula (6.4.1): for $i = 1, \dots, n$,

$$\left(\frac{\partial \Lambda}{\partial_{k_0,l_0}}\right)_{i,i} = \mathbf{e}_i^T V^T E V \mathbf{e}_i.$$

Suppose that the column space of $EH_n(j)$ is of dimension 1. Then, $j = 0$ or $j = n$. It can be checked that $\hat{\mathbf{x}}_1^0 = \mathbf{x}_1^0$ and $\hat{\mathbf{x}}_1^n = \mathbf{x}_1^n$. So, $\hat{\mathbf{x}}_1^0 = \frac{1}{\sqrt{2^n}}H_n(0)$ and $\hat{\mathbf{x}}_1^n = \frac{1}{\sqrt{2^n}}H_n(n)$. Evidently, $H_n(0) = \mathbf{1}$. By Lemma 6.4.7, $\mathbf{e}_{r_0}^T H_n(n) = (-1)^n$. From Lemma 6.4.6 and Example 6.4.11, we find that $\mathbf{e}_{k_0}^T H_n(n) = -\mathbf{e}_1^T H_{n-1}(n-1) = -1$ and $\mathbf{e}_{l_0}^T H_n(n) = -\mathbf{e}_2^T H_{n-1}(n-1) = 1$. Thus,

$$\begin{bmatrix}\mathbf{e}_{s_0}^T\\ \mathbf{e}_{k_0}^T\\ \mathbf{e}_{l_0}^T\\ \mathbf{e}_{r_0}^T\end{bmatrix}\begin{bmatrix}\hat{\mathbf{x}}_1^0 & \hat{\mathbf{x}}_1^n\end{bmatrix} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}1 & 1\\ 1 & -1\\ 1 & 1\\ 1 & (-1)^n\end{bmatrix}. \tag{6.4.13}$$

If $V\mathbf{e}_p = \hat{\mathbf{x}}_1^0$, then we have

$$\left(\frac{\partial \Lambda}{\partial_{k_0,l_0}}\right)_{p,p} = \mathbf{e}_p^T V^T E V \mathbf{e}_p = (\hat{\mathbf{x}}_1^0)^T E \hat{\mathbf{x}}_1^0 = (\hat{\mathbf{x}}_1^0)^T \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix}\begin{bmatrix}\mathbf{e}_{l_0}^T\\ \mathbf{e}_{k_0}^T\end{bmatrix}\hat{\mathbf{x}}_1^0 = \frac{1}{2^{n-1}}.$$

Similarly, if $V\mathbf{e}_p = \hat{\mathbf{x}}_1^n$ then $\left(\frac{\partial \Lambda}{\partial_{k_0,l_0}}\right)_{p,p} = -\frac{1}{2^{n-1}}$.

Suppose that the column space of $EH_n(j)$ is of dimension 2. For clarity in the following long computation, we fix $j_0 \in \{1, \ldots, n-1\}$. Let $m_0 = \binom{n}{j_0}$. Note that $h_{n,j_0}^{k_0,l_0}(-1,-1) = \binom{n-2}{j_0-1} > 0$ and $h_{n,j_0}^{k_0,l_0}(1,-1) = \binom{n-2}{j_0-1} > 0$. Without loss of generality, we may assume in the sequel that $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_1^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} -1 \\ -1 \end{bmatrix}$ and $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_2^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$.

Let us compute α_i and β_i for $i = 1, \ldots, m_0$. As defined above, $\alpha_1 = \beta_2 = 1$ and $\alpha_2 = \beta_1 = 0$. Consider the case $3 \leq i \leq m_0$. We have

$$\left(\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \begin{bmatrix} \mathbf{x}_1^{j_0} & \mathbf{x}_2^{j_0} \end{bmatrix} \right)^{-1} = \left(\frac{1}{\sqrt{2^n}} \begin{bmatrix} -1 & 1 \\ -1 & -1 \end{bmatrix} \right)^{-1} = \sqrt{2^{n-2}} \begin{bmatrix} -1 & -1 \\ 1 & -1 \end{bmatrix}.$$

By (6.4.11), for $i = 3, \ldots, m_0$,

$$\begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix} = \begin{cases} \begin{bmatrix} -1 \\ 0 \end{bmatrix}, & \text{if } \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}; \\ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, & \text{if } \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} -1 \\ -1 \end{bmatrix}; \\ \begin{bmatrix} 0 \\ 1 \end{bmatrix}, & \text{if } \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}; \\ \begin{bmatrix} 0 \\ -1 \end{bmatrix}, & \text{if } \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} -1 \\ 1 \end{bmatrix}. \end{cases} \tag{6.4.14}$$

We shall find an orthonormal basis $\{\tilde{\mathbf{x}}_1^{j_0}, \tilde{\mathbf{x}}_2^{j_0}\}$ of $\operatorname{span}\{\sum_{i=1}^{m_0} \alpha_i \mathbf{x}_i^{j_0}, \sum_{i=1}^{m_0} \beta_i \mathbf{x}_i^{j_0}\}$. For $1 \leq i \leq m_0$, we observe that $\alpha_i = 0$ if and only if $\beta_i \neq 0$. Since the vectors $\mathbf{x}_1^{j_0}, \ldots, \mathbf{x}_{m_0}^{j_0}$ are mutually orthonormal, $\sum_{i=1}^{m_0} \alpha_i \mathbf{x}_i^{j_0}$ and $\sum_{i=1}^{m_0} \beta_i \mathbf{x}_i^{j_0}$ are orthogonal. Furthermore, using (6.4.14) and Lemma 6.4.13 with Pascal's identity,

$$\left\| \sum_{i=1}^{m_0} \alpha_i \mathbf{x}_i^{j_0} \right\|^2 = |\{i | \alpha_i \neq 0, i = 1, \ldots, m_0\}| = h_{n,j_0}^{k_0,l_0}(1,1) + h_{n,j_0}^{k_0,l_0}(-1,-1) = \binom{n-1}{j_0},$$
$$\left\| \sum_{i=1}^{m_0} \beta_i \mathbf{x}_i^{j_0} \right\|^2 = |\{i | \beta_i \neq 0, i = 1, \ldots, m_0\}| = h_{n,j_0}^{k_0,l_0}(1,-1) + h_{n,j_0}^{k_0,l_0}(-1,1) = \binom{n-1}{j_0-1}.$$

So, $\tilde{\mathbf{x}}_1^{j_0} = \frac{1}{\sqrt{\binom{n-1}{j_0}}} \sum_{i=1}^{m_0} \alpha_i \mathbf{x}_i^{j_0}$ and $\tilde{\mathbf{x}}_2^{j_0} = \frac{1}{\sqrt{\binom{n-1}{j_0-1}}} \sum_{i=1}^{m_0} \beta_i \mathbf{x}_i^{j_0}$.

Let us compute the rows of $\tilde{\mathbf{x}}_1^{j_0}$ and $\tilde{\mathbf{x}}_2^{j_0}$ that are indexed by s_0, k_0, l_0 and r_0. By Lemmas 6.4.5 and 6.4.7, we have $\mathbf{e}_{s_0}^T H_n(j_0) = \mathbf{1}_{m_0}^T$ and $\mathbf{e}_{r_0}^T H_n(j_0) = (-1)^{j_0} \mathbf{1}_{m_0}^T$. For

$i = 1, \ldots, m_0$, we see from (6.4.14) that if $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, then $\alpha_i \mathbf{e}_{s_0}^T \mathbf{x}_i^{j_0} = \frac{-1}{\sqrt{2^n}}$; if $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} -1 \\ -1 \end{bmatrix}$, then $\alpha_i \mathbf{e}_{s_0}^T \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}$; and $\alpha_i \mathbf{e}_{s_0}^T \mathbf{x}_i^{j_0} = 0$ for the other two cases in (6.4.14). By Lemma 6.4.13, we obtain

$$\begin{aligned} \mathbf{e}_{s_0}^T \tilde{\mathbf{x}}_1^{j_0} =& \frac{1}{\sqrt{\binom{n-1}{j_0}}} \sum_{i=1}^{m_0} \alpha_i \mathbf{e}_{s_0}^T \mathbf{x}_i^{j_0} \\ =& \frac{\left(-h_{n,j_0}^{k_0,l_0}(1,1) + h_{n,j_0}^{k_0,l_0}(-1,-1)\right)}{\sqrt{2^n}\sqrt{\binom{n-1}{j_0}}} = \frac{-\binom{n-2}{j_0} + \binom{n-2}{j_0-1}}{\sqrt{2^n}\sqrt{\binom{n-1}{j_0}}}. \end{aligned}$$

In a similar way, one can verify $\mathbf{e}_{r_0}^T \tilde{\mathbf{x}}_1^{j_0}$, $\mathbf{e}_{s_0}^T \tilde{\mathbf{x}}_2^{j_0}$ and $\mathbf{e}_{r_0}^T \tilde{\mathbf{x}}_2^{j_0}$ given in (6.4.15). Using (6.4.14), for $i = 1, \ldots, m_0$, we find that if $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ or $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} -1 \\ -1 \end{bmatrix}$, then $\alpha_i \mathbf{e}_{k_0}^T \mathbf{x}_i^{j_0} = \frac{-1}{\sqrt{2^n}}$; and $\alpha_i \mathbf{e}_{k_0}^T \mathbf{x}_i^{j_0} = 0$ for the other two cases in (6.4.14). Then, by Lemma 6.4.13 with Pascal's identity,

$$\begin{aligned} \mathbf{e}_{k_0}^T \tilde{\mathbf{x}}_1^{j_0} =& \frac{1}{\sqrt{\binom{n-1}{j_0}}} \sum_{i=1}^{m_0} \alpha_i \mathbf{e}_{k_0}^T \mathbf{x}_i^{j_0} \\ =& \frac{-1}{\sqrt{2^n}\sqrt{\binom{n-1}{j_0}}} \left(h_{n,j_0}^{k_0,l_0}(1,1) + h_{n,j_0}^{k_0,l_0}(-1,-1)\right) = \frac{-1}{\sqrt{2^n}} \sqrt{\binom{n-1}{j_0}}. \end{aligned}$$

By an analogous argument, one can obtain $\mathbf{e}_{l_0}^T \tilde{\mathbf{x}}_1^{j_0}$, $\mathbf{e}_{k_0}^T \tilde{\mathbf{x}}_2^{j_0}$ and $\mathbf{e}_{l_0}^T \tilde{\mathbf{x}}_2^{j_0}$; therefore,

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0} \end{bmatrix} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} \frac{1}{\sqrt{\binom{n-1}{j_0}}} \left(\binom{n-2}{j_0-1} - \binom{n-2}{j_0}\right) & \frac{1}{\sqrt{\binom{n-1}{j_0-1}}} \left(\binom{n-2}{j_0-2} - \binom{n-2}{j_0-1}\right) \\ -\sqrt{\binom{n-1}{j_0}} & -\sqrt{\binom{n-1}{j_0-1}} \\ -\sqrt{\binom{n-1}{j_0}} & \sqrt{\binom{n-1}{j_0-1}} \\ \frac{(-1)^{j_0}}{\sqrt{\binom{n-1}{j_0}}} \left(\binom{n-2}{j_0-1} - \binom{n-2}{j_0}\right) & \frac{(-1)^{j_0}}{\sqrt{\binom{n-1}{j_0-1}}} \left(\binom{n-2}{j_0-2} - \binom{n-2}{j_0-1}\right) \end{bmatrix}. \tag{6.4.15}$$

Now, we compute B^{j_0}, the particular rows of $\hat{\mathbf{x}}_1^{j_0}$ and $\hat{\mathbf{x}}_2^{j_0}$, and the entries in $\frac{\partial \Lambda}{\partial_{k_0,l_0}}$

corresponding to $\hat{\mathbf{x}}_1^{j_0}, \ldots, \hat{\mathbf{x}}_{m_0}^{j_0}$. Recall that $B^{j_0} = \begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix}^T E \begin{bmatrix} \tilde{\mathbf{x}}_1^j & \tilde{\mathbf{x}}_2^j \end{bmatrix}$. Then,

$$B^{j_0} = \begin{bmatrix} (\tilde{\mathbf{x}}_1^{j_0})^T \\ (\tilde{\mathbf{x}}_2^{j_0})^T \end{bmatrix} \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0} \end{bmatrix} = \frac{1}{2^{n-1}} \begin{bmatrix} \binom{n-1}{j_0} & 0 \\ 0 & -\binom{n-1}{j_0-1} \end{bmatrix}.$$

The matrix B^{j_0} is diagonal. This implies that $\hat{\mathbf{x}}_1^{j_0} = \tilde{\mathbf{x}}_1^{j_0}$ and $\hat{\mathbf{x}}_2^{j_0} = \tilde{\mathbf{x}}_2^{j_0}$. Thus,

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0} \end{bmatrix} = \begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0} \end{bmatrix}. \tag{6.4.16}$$

Remark 6.4.14. When we use entries of $\hat{\mathbf{x}}_1^{j_0}$ and $\hat{\mathbf{x}}_2^{j_0}$ for $1 \le j_0 \le n-1$ that are indexed by s_0, k_0, l_0 and r_0, we directly refer to (6.4.15) without the reference of (6.4.16).

Let p and q be indices such that $V \begin{bmatrix} \mathbf{e}_p & \mathbf{e}_q \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0} \end{bmatrix}$. By (6.4.1),

$$\begin{bmatrix} \mathbf{e}_p^T \\ \mathbf{e}_q^T \end{bmatrix} \frac{\partial \Lambda}{\partial_{k_0,l_0}} \begin{bmatrix} \mathbf{e}_p & \mathbf{e}_q \end{bmatrix} = \begin{bmatrix} \mathbf{e}_p^T \\ \mathbf{e}_q^T \end{bmatrix} V^T E V \begin{bmatrix} \mathbf{e}_p & \mathbf{e}_q \end{bmatrix} = B^{j_0}. \tag{6.4.17}$$

Consider the remaining entries in $\frac{\partial \Lambda}{\partial_{k_0,l_0}}$ corresponding to $\hat{\mathbf{x}}_3^{j_0}, \ldots, \hat{\mathbf{x}}_{m_0}^{j_0}$ that form an orthonormal basis of $\operatorname{span}\{\mathbf{x}_i^{j_0} - \alpha_i \mathbf{x}_1^{j_0} - \beta_i \mathbf{x}_2^{j_0} | i = 3, \ldots, m_0\}$. Note that $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_1^{j_0} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$ and $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_2^{j_0} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$. Let $i \in \{3, \ldots, m_0\}$. If $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, then we see from (6.4.14) that $\alpha_i = -1$ and $\beta_i = 0$; so,

$$\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} (\mathbf{x}_i^{j_0} - \alpha_i \mathbf{x}_1^{j_0} - \beta_i \mathbf{x}_2^{j_0}) = \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} - \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \mathbf{x}_1^{j_0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

In this manner, it can be verified that for $3 \le i \le m_0$,

$$\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} (\mathbf{x}_i^{j_0} - \alpha_i \mathbf{x}_1^{j_0} - \beta_i \mathbf{x}_2^{j_0}) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

It follows that $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} \hat{\mathbf{x}}_i^{j_0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ for $i = 3, \ldots, m_0$. Therefore, if $V\mathbf{e}_p = \hat{\mathbf{x}}_i^{j_0}$ for some

$3 \le i \le m_0$, we have

$$\mathbf{e}_p^T \frac{\partial \Lambda}{\partial_{k_0,l_0}} \mathbf{e}_p = \mathbf{e}_p^T V^T E V \mathbf{e}_p = (\hat{\mathbf{x}}_i^{j_0})^T \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{l_0} & \mathbf{e}_{k_0} \end{bmatrix}^T \hat{\mathbf{x}}_i^{j_0} = 0. \tag{6.4.18}$$

Now, we investigate the s_0^{th} and r_0^{th} rows of $\frac{\partial V}{\partial_{k_0,l_0}}$. It appears in [43] that

$$(\hat{\mathbf{x}}_1^j)^T E((n-2j)I - A_n)^\dagger E \hat{\mathbf{x}}_2^j = 0$$

for $j = 1, \ldots, n-1$. Hence, from (6.4.10) and (6.4.12), we obtain

$$\frac{\partial V}{\partial_{k_0,l_0}} \mathbf{e}_p = \begin{cases} ((n-2j)I - A_n)^\dagger E \hat{\mathbf{x}}_1^j, & \text{if } V\mathbf{e}_p = \hat{\mathbf{x}}_1^j \text{ for } j = 0 \text{ or } j = n, \\ ((n-2j)I - A_n)^\dagger E \hat{\mathbf{x}}_i^j, & \text{if } V\mathbf{e}_p = \hat{\mathbf{x}}_i^j \text{ for some } i \in \{1,2\},\ 1 \le j \le n-1, \\ 0, & \text{otherwise.} \end{cases} \tag{6.4.19}$$

Note that considering (6.4.3), we only need $\mathbf{e}_q \frac{\partial V}{\partial_{k_0,l_0}}$ for $q \in \{s_0, r_0\}$, not all of the entries in $\frac{\partial V}{\partial_{k_0,l_0}}$. Since we have explicitly shown the k_0^{th} and l_0^{th} rows of $\hat{\mathbf{x}}_1^0$, $\hat{\mathbf{x}}_1^n$, $\hat{\mathbf{x}}_1^j$ and $\hat{\mathbf{x}}_2^j$ for $1 \le j \le n-1$, we shall find the s_0^{th} and r_0^{th} rows of $((n-2j)I - A_n)^\dagger \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix}$.

Lemma 6.4.15. *[56] Let $B = UDU^T$ where U is an orthogonal matrix and D is a diagonal matrix. Then, $B^\dagger = UD^\dagger U^T$.*

Lemma 6.4.16. *[56] Let $D = \operatorname{diag}(d_1, \ldots d_n)$ for some $n \ge 1$. Then, $D^\dagger = \operatorname{diag}(\hat{d}_1, \ldots, \hat{d}_n)$ where for $1 \le i \le n$, $\hat{d}_i = \frac{1}{d_i}$ if $d_i \ne 0$, and $\hat{d}_i = 0$ otherwise.*

Reordering eigenvalues of A_n in Λ, we may assume that

$$A_n = V\Lambda V^T = \frac{1}{2^n} H_n \Lambda H_n^T.$$

Fix $j_0 = \{0, \ldots, n\}$, and let $\lambda_0 = n - 2j_0$. By Lemmas 6.4.15 and 6.4.16,

$$(\lambda_0 I - A_n)^\dagger = \frac{1}{2^n} H_n (\lambda_0 I - \Lambda)^\dagger H_n^T = \frac{1}{2^n} \sum_{\substack{0 \le j \le n, \\ j \ne j_0}} \frac{1}{2(j - j_0)} H_n(j) H_n(j)^T. \tag{6.4.20}$$

Lemma 6.4.17. *Let $n \ge 2$, $0 \le j \le n$, and $1 \le l_1 < l_2 \le 2^n$. Then,*

$$\mathbf{e}_{l_1}^T H_n(j) H_n(j)^T \mathbf{e}_{l_2} = h_{n,j}^{l_1,l_2}(1,1) + h_{n,j}^{l_1,l_2}(-1,-1) - h_{n,j}^{l_1,l_2}(1,-1) - h_{n,j}^{l_1,l_2}(-1,1).$$

Proof. Considering that $H_n(j)$ is a $(1,-1)$ matrix, the conclusion follows. □

Let $0 \leq j \leq n$. We have $\mathbf{e}_{s_0}^T H_n(j) = \mathbf{1}^T_{\binom{n}{j}}$ and $\mathbf{e}_{r_0}^T H_n(j) = (-1)^j \mathbf{1}^T_{\binom{n}{j}}$. So, $h_{n,j}^{s_0,k_0}(-1,-1) = h_{n,j}^{s_0,k_0}(-1,1) = 0$; $h_{n,j}^{k_0,r_0}(-1,-1) = h_{n,j}^{l_0,r_0}(1,-1) = 0$ for j even; and $h_{n,j}^{k_0,r_0}(-1,1) = h_{n,j}^{l_0,r_0}(1,1) = 0$ for j odd. Hence, by Lemma 6.4.17

$$\mathbf{e}_{s_0}^T H_n(j) H_n(j)^T \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} = \begin{bmatrix} h_{n,j}^{s_0,k_0}(1,1) - h_{n,j}^{s_0,k_0}(1,-1) & h_{n,j}^{s_0,l_0}(1,1) - h_{n,j}^{s_0,l_0}(1,-1) \end{bmatrix}.$$

Since the s_0^{th} row of $H_n(j)$ is all ones, $h_{n,j}^{s_0,k_0}(1,1) = h_{n,j}^{k_0,l_0}(1,1) + h_{n,j}^{k_0,l_0}(1,-1)$ and $h_{n,j}^{s_0,k_0}(1,-1) = h_{n,j}^{k_0,l_0}(-1,1) + h_{n,j}^{k_0,l_0}(-1,-1)$. Using Lemma 6.4.13, we obtain $h_{n,j}^{s_0,k_0}(1,1) = \binom{n-1}{j}$ and $h_{n,j}^{s_0,k_0}(1,-1) = \binom{n-1}{j-1}$. Similarly, one can find that $h_{n,j}^{s_0,l_0}(1,1) = \binom{n-2}{j} + \binom{n-2}{j-2}$ and $h_{n,j}^{s_0,l_0}(1,-1) = 2\binom{n-2}{j-1}$. Thus,

$$\mathbf{e}_{s_0}^T H_n(j) H_n(j)^T \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} = \begin{bmatrix} \binom{n-1}{j} - \binom{n-1}{j-1} & \binom{n-2}{j} + \binom{n-2}{j-2} - 2\binom{n-2}{j-1} \end{bmatrix}. \tag{6.4.21}$$

An analogous argument yields

$$\begin{aligned}
&\mathbf{e}_{r_0}^T H_n(j) H_n(j)^T \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \\
=&\begin{cases} \begin{bmatrix} h_{n,j}^{k_0,r_0}(1,1) - h_{n,j}^{k_0,r_0}(-1,1) & h_{n,j}^{l_0,r_0}(1,1) - h_{n,j}^{l_0,r_0}(-1,1) \end{bmatrix}, & \text{if } j \text{ is even,} \\ \begin{bmatrix} h_{n,j}^{k_0,r_0}(-1,-1) - h_{n,j}^{k_0,r_0}(1,-1) & h_{n,j}^{l_0,r_0}(-1,-1) - h_{n,j}^{l_0,r_0}(1,-1) \end{bmatrix}, & \text{if } j \text{ is odd,} \end{cases} \\
=&\begin{cases} \begin{bmatrix} \binom{n-1}{j} - \binom{n-1}{j-1} & \binom{n-2}{j} + \binom{n-2}{j-2} - 2\binom{n-2}{j-1} \end{bmatrix}, & \text{if } j \text{ is even,} \\ \begin{bmatrix} \binom{n-1}{j-1} - \binom{n-1}{j} & 2\binom{n-2}{j-1} - \binom{n-2}{j} - \binom{n-2}{j-2} \end{bmatrix}, & \text{if } j \text{ is odd,} \end{cases} \\
=&\begin{bmatrix} (-1)^j \left(\binom{n-1}{j} - \binom{n-1}{j-1} \right) & (-1)^j \left(\binom{n-2}{j} + \binom{n-2}{j-2} - 2\binom{n-2}{j-1} \right) \end{bmatrix}.
\end{aligned} \tag{6.4.22}$$

Combining (6.4.20) and (6.4.21), we have that

$$\begin{aligned}
&\mathbf{e}_{s_0}^T ((n-2j_0)I - A_n)^\dagger \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \\
=&\frac{1}{2^n} \sum_{\substack{0 \leq j \leq n \\ j \neq j_0}} \frac{1}{2(j-j_0)} \mathbf{e}_{s_0}^T H_n(j) H_n(j)^T \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \\
=&\frac{1}{2^n} \begin{bmatrix} \sum_{\substack{0 \leq j \leq n \\ j \neq j_0}} \frac{1}{2(j-j_0)} \left(\binom{n-1}{j} - \binom{n-1}{j-1} \right) & \sum_{\substack{0 \leq j \leq n \\ j \neq j_0}} \frac{1}{2(j-j_0)} \left(\binom{n-2}{j} + \binom{n-2}{j-2} - 2\binom{n-2}{j-1} \right) \end{bmatrix}.
\end{aligned} \tag{6.4.23}$$

Similarly, using (6.4.20) and (6.4.22), we find that

$$
\begin{aligned}
&\mathbf{e}_{r_0}^T((n-2j_0)I-A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix} \\
=&\frac{1}{2^n}\left[\textstyle\sum_{\substack{0\le j\le n\\ j\neq j_0}} \frac{(-1)^j}{2(j-j_0)}\left(\binom{n-1}{j}-\binom{n-1}{j-1}\right) \qquad \sum_{\substack{0\le j\le n\\ j\neq j_0}} \frac{(-1)^j}{2(j-j_0)}\left(\binom{n-2}{j}+\binom{n-2}{j-2}-2\binom{n-2}{j-1}\right)\right].
\end{aligned} \tag{6.4.24}
$$

6.4.3 The 1st and 2nd partial derivatives with respect to the weight of the edge $k_0 \sim l_0$ in Q_n

In this subsection, we shall find $\frac{\partial p(\frac{\pi}{2})}{\partial_{k_0,l_0}}$ and $\frac{\partial^2 p(\frac{\pi}{2})}{\partial_{k_0,l_0}^2}$ for Q_n.

Theorem 6.4.18. *Let G be a weighted graph. Suppose that G exhibits PST between s and r at time t_0. Then, for $k,l \in V(G)$, we have $\frac{\partial p(t_0)}{\partial_{k,l}}=0$ and $\frac{\partial^2 p(t_0)}{\partial_{k,l}^2}\le 0$.*

Proof. Suppose that A is the adjacency matrix of G and $E=\begin{bmatrix}\mathbf{e}_k & \mathbf{e}_l\end{bmatrix}\begin{bmatrix}\mathbf{e}_l & \mathbf{e}_k\end{bmatrix}^T$. Given $\epsilon>0$, let $W(h)=e^{it_0(A+hE)}$ and $q(h)=|\mathbf{e}_s^T W(h)\mathbf{e}_r|^2$ for $h\in(-\epsilon,\epsilon)$. One can verify that $W(h)$ is a unitary matrix. Since each row and column of $W(h)$ has Euclidean norm 1, we have $0\le q(h)\le 1$. Since G exhibits PST between s and r at time t_0, $q(0)=1$. Furthermore, $q(h)$ is analytic for its domain. It follows that $\frac{\partial p(t_0)}{\partial_{k,l}}=q'(0)=0$. By Taylor's theorem, for any $h\in(0,\epsilon)$, there exists $h_0\in[0,h]$ such that $q(h)=q(0)+hq'(0)+\frac{h^2}{2}q''(h_0)=1+\frac{h^2}{2}q''(h_0)\le 1$. Therefore, $\frac{\partial^2 p(t_0)}{\partial_{k,l}^2}=q''(0)\le 0$. $\square$

From Theorem 6.4.18, we immediately obtain $\frac{\partial p(\frac{\pi}{2})}{\partial_{k_0,l_0}}=0$. We also shall provide other proof (in Theorem 6.4.20) for $\frac{\partial p(\frac{\pi}{2})}{\partial_{k_0,l_0}}=0$ by using the formula in (6.4.2), in order to show how the differentiable eigenbasis V and its derivative $\frac{\partial V}{\partial_{k_0,l_0}}$ obtained in the previous section are used.

For $A_n=\frac{1}{2^n}H_n\Lambda H_n^T$ where $n\ge 2$, let $U(t)=e^{itA_n}$. Then, $U(t)=\frac{1}{2^n}H_n e^{it\Lambda}H_n^T$. There are well-known properties that $\sum_{k=0}^n\binom{n}{k}=2^n$ and $\sum_{k=0}^n(-1)^k\binom{n}{k}=0$. Note that $\mathbf{e}_{s_0}^T H_n(j) = \mathbf{1}_{\binom{n}{j}}^T$ and $\mathbf{e}_{r_0}^T H_n(j) = (-1)^j \mathbf{1}_{\binom{n}{j}}^T$ for $0 \le j \le n$. Then,

$$\begin{aligned}\left(U\left(\frac{\pi}{2}\right)\right)_{s_0,r_0} =& \frac{1}{2^n}\mathbf{e}_{s_0}^T H_n e^{\frac{\pi}{2}i\Lambda} H_n^T \mathbf{e}_{r_0} \\ =& \frac{1}{2^n}\sum_{j=0}^{n}(-1)^j e^{\frac{\pi}{2}i(n-2j)}\mathbf{1}_{\binom{n}{j}}^T \mathbf{1}_{\binom{n}{j}} \\ =& \frac{1}{2^n}\sum_{j=0}^{n}(-1)^j \left(\cos\left(\frac{(n-2j)\pi}{2}\right) + i\sin\left(\frac{(n-2j)\pi}{2}\right)\right)\binom{n}{j} \\ =& \begin{cases} 1, & \text{if } n \equiv 0 \pmod 4, \\ i, & \text{if } n \equiv 1 \pmod 4, \\ -1, & \text{if } n \equiv 2 \pmod 4, \\ -i, & \text{if } n \equiv 3 \pmod 4. \end{cases}\end{aligned}$$

Denote $\alpha + i\beta$ by $(U(\frac{\pi}{2}))_{s_0,r_0}$. Then, one can check the following according to the residues of n modulo 4: $\alpha\cos\left(\frac{(n-2j)\pi}{2}\right) + \beta\sin\left(\frac{(n-2j)\pi}{2}\right) = (-1)^j$ for $0 \le j \le n$. Hence, without loss of generality,

$$\alpha\cos\left(\frac{\pi}{2}\Lambda\right) + \beta\sin\left(\frac{\pi}{2}\Lambda\right) = \operatorname{diag}\left(\mathbf{1}_{\binom{n}{0}}^T, -\mathbf{1}_{\binom{n}{1}}^T, \ldots, (-1)^n \mathbf{1}_{\binom{n}{n}}^T\right). \tag{6.4.25}$$

Similarly, we can find that $\beta\cos\left(\frac{(n-2j)\pi}{2}\right) - \alpha\sin\left(\frac{(n-2j)\pi}{2}\right) = 0$. Thus,

$$\beta\cos\left(\frac{\pi}{2}\Lambda\right) - \alpha\sin\left(\frac{\pi}{2}\Lambda\right) = 0. \tag{6.4.26}$$

Remark 6.4.19. Let $R = \operatorname{diag}(r_1, \ldots, r_{2^n})$. Then, R can be written as $R = \sum_{p=1}^{2^n} r_p \mathbf{e}_p \mathbf{e}_p^T$. So, $\frac{\partial V}{\partial_{k_0,l_0}} R V^T = \sum_{p=1}^{2^n} r_p \frac{\partial V}{\partial_{k_0,l_0}} \mathbf{e}_p \mathbf{e}_p^T V^T$. Considering (6.4.19), we have

$$\begin{aligned}\mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{k_0,l_0}} R V^T \mathbf{e}_{r_0} =& \mathbf{e}_{s_0}^T((n-2j)I - A_n)^\dagger E(r_{a_0}\hat{\mathbf{x}}_1^0(\hat{\mathbf{x}}_1^0)^T + r_{b_n}\hat{\mathbf{x}}_1^n(\hat{\mathbf{x}}_1^n)^T)\mathbf{e}_{r_0} \\ &+ \sum_{j=1}^{n-1}\mathbf{e}_{s_0}^T((n-2j)I - A_n)^\dagger E(r_{a_j}\hat{\mathbf{x}}_1^j(\hat{\mathbf{x}}_1^j)^T + r_{b_j}\hat{\mathbf{x}}_2^j(\hat{\mathbf{x}}_2^j)^T)\mathbf{e}_{r_0},\end{aligned}$$

where $V\mathbf{e}_{a_0} = \hat{\mathbf{x}}_1^0$, $V\mathbf{e}_{b_n} = \hat{\mathbf{x}}_1^n$, and $V\begin{bmatrix}\mathbf{e}_{a_j} & \mathbf{e}_{b_j}\end{bmatrix} = \begin{bmatrix}\hat{\mathbf{x}}_1^j & \hat{\mathbf{x}}_2^j\end{bmatrix}$ for $1 \le j \le n-1$.

When we need to deal with pairs of consecutive terms as in the right side above, we shall use the following notation in this subsection in order to simplify the exposition. Set $\hat{\mathbf{y}}_1^j := \hat{\mathbf{x}}_1^j$ and $\hat{\mathbf{y}}_2^j := \hat{\mathbf{x}}_2^j$ for $1 \le j \le n-1$. Note that when we handle $\hat{\mathbf{x}}_1^0$ as an eigenvector of A_n, we may use $-\hat{\mathbf{x}}_1^0$. So, let $\hat{\mathbf{y}}_1^0 := -\hat{\mathbf{x}}_1^0$, $\hat{\mathbf{y}}_2^0 := 0$, $\hat{\mathbf{y}}_1^n := 0$, and $\hat{\mathbf{y}}_2^n = \hat{\mathbf{x}}_1^n$.

Theorem 6.4.20. *Let $n \geq 2$, and $s, r, k, l \in V(Q_n)$. Suppose that $r = s^*$, $s \sim k$ and $k \sim l$. Then, under PST between s and r at time $\frac{\pi}{2}$, we have*

$$\frac{\partial p(\frac{\pi}{2})}{\partial_{k,l}} = 0.$$

Proof. By (ii) of Proposition 2.5.1, we may assume that $s = s_0$, $k = k_0$, and $l = l_0$. Then, $r = r_0$. Let $t_0 = \frac{\pi}{2}$. Recall that $\frac{\partial p(t_0)}{\partial_{k_0,l_0}} = 2t_0X_1 + 2X_2$ where

$$\begin{aligned} X_1 =& \mathbf{e}_{s_0}^T V \frac{\partial \Lambda}{\partial_{k_0,l_0}} (\beta \mathrm{cos}(t_0\Lambda) - \alpha \mathrm{sin}(t_0\Lambda)) V^T \mathbf{e}_{r_0}, \\ X_2 =& \mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{k_0,l_0}} (\alpha \mathrm{cos}(t_0\Lambda) + \beta \mathrm{sin}(t_0\Lambda)) V^T \mathbf{e}_{r_0} + \mathbf{e}_{s_0}^T V (\alpha \mathrm{cos}(t_0\Lambda) + \beta \mathrm{sin}(t_0\Lambda)) \frac{\partial V^T}{\partial_{k_0,l_0}} \mathbf{e}_{r_0}. \end{aligned}$$

From (6.4.26), we have $X_1 = 0$. Since we deal with V and $\frac{\partial V}{\partial_{k_0,l_0}}$, we may use (6.4.25) and the notation described in Remark 6.4.19. It follows that

$$\begin{aligned} &\mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{k_0,l_0}} (\alpha \mathrm{cos}(t_0\Lambda) + \beta \mathrm{sin}(t_0\Lambda)) V^T \mathbf{e}_{r_0} \\ =& \sum_{j=0}^{n} \mathbf{e}_{s_0}^T ((n-2j)I - A_n)^\dagger \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T \end{bmatrix} ((-1)^j \hat{\mathbf{y}}_1^j (\hat{\mathbf{y}}_1^j)^T + (-1)^j \hat{\mathbf{y}}_2^j (\hat{\mathbf{y}}_2^j)^T) \mathbf{e}_{r_0}. \end{aligned} \tag{6.4.27}$$

We claim that for $0 \leq j_0 \leq n-1$,

$$\begin{aligned} &\mathbf{e}_{s_0}^T ((n-2j_0)I - A_n)^\dagger E((-1)^{j_0} \hat{\mathbf{y}}_1^{j_0} (\hat{\mathbf{y}}_1^{j_0})^T) \mathbf{e}_{r_0} \\ =& -\mathbf{e}_{s_0}^T ((n-2(j_0+1))I - A_n)^\dagger E((-1)^{j_0+1} \hat{\mathbf{y}}_2^{j_0+1} (\hat{\mathbf{y}}_2^{j_0+1})^T) \mathbf{e}_{r_0}. \end{aligned}$$

We can find from (6.4.13) and (6.4.15) that

$$\begin{aligned} \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} (-1)^{j_0} \hat{\mathbf{y}}_1^{j_0} (\hat{\mathbf{y}}_1^{j_0})^T \mathbf{e}_{r_0} =& \frac{1}{2^n} \begin{bmatrix} \binom{n-2}{j_0} - \binom{n-2}{j_0-1} \\ \binom{n-2}{j_0} - \binom{n-2}{j_0-1} \end{bmatrix}, \\ \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{l_0}^T \end{bmatrix} (-1)^{j_0+1} \hat{\mathbf{y}}_2^{j_0+1} (\hat{\mathbf{y}}_2^{j_0+1})^T \mathbf{e}_{r_0} =& \frac{1}{2^n} \begin{bmatrix} \binom{n-2}{j_0} - \binom{n-2}{j_0-1} \\ -\binom{n-2}{j_0} + \binom{n-2}{j_0-1} \end{bmatrix}. \end{aligned}$$

Let $K = \binom{n-2}{j_0} - \binom{n-2}{j_0-1}$. By (6.4.23) with Pascal's identity,

$$\begin{aligned}
&\mathbf{e}_{s_0}^T((n-2j_0)I - A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix} \begin{bmatrix}\mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T\end{bmatrix} (-1)^{j_0}\hat{\mathbf{y}}_1^{j_0}(\hat{\mathbf{y}}_1^{j_0})^T\mathbf{e}_{r_0} \\
=&\frac{K}{2^{2n}} \sum_{\substack{0\le j\le n \\ j\ne j_0}} \frac{1}{2(j-j_0)} \left(\binom{n-1}{j} - \binom{n-1}{j-1} + \binom{n-2}{j} + \binom{n-2}{j-2} - 2\binom{n-2}{j-1}\right) \\
=&\frac{K}{2^{2n}} \sum_{\substack{0\le j\le n \\ j\ne j_0}} \frac{1}{j-j_0} \left(\binom{n-2}{j} - \binom{n-2}{j-1}\right).
\end{aligned}$$

Similarly, by (6.4.23) with Pascal's identity,

$$\begin{aligned}
&\mathbf{e}_{s_0}^T((n-2(j_0+1))I - A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix} \begin{bmatrix}\mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T\end{bmatrix} (-1)^{j_0+1}\hat{\mathbf{y}}_2^{j_0+1}(\hat{\mathbf{y}}_2^{j_0+1})^T\mathbf{e}_{r_0} \\
=&-\frac{K}{2^{2n}} \sum_{\substack{0\le j\le n \\ j\ne j_0+1}} \frac{1}{j-(j_0+1)} \left(\binom{n-2}{j-1} - \binom{n-2}{j-2}\right).
\end{aligned}$$

Note that $\binom{n}{k} = 0$ whenever $k < 0$ or $k > n$. Setting $j' = j-1$, we have

$$\begin{aligned}
&\sum_{\substack{0\le j\le n \\ j\ne j_0+1}} \frac{1}{j-(j_0+1)} \left(\binom{n-2}{j-1} - \binom{n-2}{j-2}\right) \\
=&\sum_{\substack{-1\le j'\le n-1 \\ j'\ne j_0}} \frac{1}{j'-j_0} \left(\binom{n-2}{j'} - \binom{n-2}{j'-1}\right) = \sum_{\substack{0\le j'\le n \\ j'\ne j_0}} \frac{1}{j'-j_0} \left(\binom{n-2}{j'} - \binom{n-2}{j'-1}\right).
\end{aligned}$$

Therefore, our claim now follows.

Note that $\hat{\mathbf{y}}_2^0 = \hat{\mathbf{y}}_1^n = 0$. Applying our claim along with the telescoping sum to (6.4.27), we obtain $\mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{k_0,l_0}}(\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda))V^T\mathbf{e}_{r_0} = 0$.

A similar argument applies to $\mathbf{e}_{r_0}^T \frac{\partial V}{\partial_{k_0,l_0}}(\alpha\cos(\frac{\pi}{2}\Lambda)+\beta\sin(\frac{\pi}{2}\Lambda))V^T\mathbf{e}_{s_0}$ as follows. Let $j_0 \in \{0,\dots,n-1\}$. Using (6.4.13) and (6.4.15), one can find $\begin{bmatrix}\mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T\end{bmatrix} (-1)^{j_0}\hat{\mathbf{y}}_1^{j_0}(\hat{\mathbf{y}}_1^{j_0})^T\mathbf{e}_{s_0}$ and $\begin{bmatrix}\mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T\end{bmatrix} (-1)^{j_0+1}\hat{\mathbf{y}}_2^{j_0+1}(\hat{\mathbf{y}}_2^{j_0+1})^T\mathbf{e}_{s_0}$. Then, it can be verified from (6.4.24) with Pascal's identity that

$$\begin{aligned}
&\mathbf{e}_{r_0}^T((n-2j_0)I - A)^\dagger E((-1)^{j_0}\hat{\mathbf{y}}_1^{j_0}(\hat{\mathbf{y}}_1^{j_0})^T)\mathbf{e}_{s_0} \\
=&-\mathbf{e}_{r_0}^T((n-2(j_0+1))I - A)^\dagger E((-1)^{j_0+1}\hat{\mathbf{y}}_2^{j_0+1}(\hat{\mathbf{y}}_2^{j_0+1})^T)\mathbf{e}_{s_0}.
\end{aligned}$$

By the telescoping sum, one can check that $\mathbf{e}_{r_0}^T \frac{\partial V}{\partial_{k_0,l_0}}(\alpha\cos(t_0\Lambda)+\beta\sin(t_0\Lambda))V^T\mathbf{e}_{s_0} = 0$. Hence, $X_2 = 0$. Therefore, $\frac{\partial p(t_0)}{\partial_{k_0,l_0}} = 2t_0X_1 + 2X_2 = 0$. $\square$

Let $n \geq 2$, and $H(p,q,j) := \mathbf{e}_p^T((n-2j)I - A_n)^\dagger E((-1)^j\hat{\mathbf{y}}_1^j(\hat{\mathbf{y}}_1^j)^T + (-1)^j\hat{\mathbf{y}}_2^j(\hat{\mathbf{y}}_2^j)^T)\mathbf{e}_q$ for $0 \leq j \leq n$ and $(p,q) \in \{(s_0,r_0),(r_0,s_0)\}$. In the proof of Theorem 6.4.20, we see the relation between terms in $H(p,q,i)$ and $H(p,q,i+1)$ for $0 \leq i \leq n-1$. The following result describes the relation between $H(p,q,j)$ and $H(p,q,n-j)$.

Proposition 6.4.21. *Let $n \geq 2$, and let $(p,q) \in \{(s_0,r_0),(r_0,s_0)\}$. Then, for $j = 0,\ldots,n$, we have*

$$H(p,q,j) = H(p,q,n-j).$$

Proof. Let $j_0 = \{0,\ldots,n\}$. Then, $0 \leq n - j_0 \leq n$. Substituting $n - j_0$ for j_0 in (6.4.23), setting $j' = n - j$ for $0 \leq j \leq n$, and using the relation $\binom{n}{k} = \binom{n}{n-k}$ for $0 \leq k \leq n$, we obtain

$$\begin{aligned}
&\mathbf{e}_{s_0}^T((n-2(n-j_0))I - A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix} \\
=&\frac{1}{2^n}\begin{bmatrix} \sum_{\substack{0\leq j\leq n\\ j\neq n-j_0}} \frac{\left(\binom{n-1}{j}-\binom{n-1}{j-1}\right)}{2(j+j_0-n)} & \sum_{\substack{0\leq j\leq n\\ j\neq n-j_0}} \frac{\left(\binom{n-2}{j}+\binom{n-2}{j-2}-2\binom{n-2}{j-1}\right)}{2(j+j_0-n)}\end{bmatrix} \\
=&\frac{1}{2^n}\begin{bmatrix} \sum_{\substack{0\leq j'\leq n\\ j'\neq j_0}} \frac{\left(\binom{n-1}{j'}-\binom{n-1}{j'-1}\right)}{2(j'-j_0)} & \sum_{\substack{0\leq j'\leq n\\ j'\neq j_0}} \frac{-\left(\binom{n-2}{j'}+\binom{n-2}{j'-2}-2\binom{n-2}{j'-1}\right)}{2(j'-j_0)}\end{bmatrix}.
\end{aligned}$$

Note that $\mathbf{e}_{s_0}^T(-(n-2j_0)I - A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix} = \mathbf{e}_{s_0}^T((n-2(n-j_0))I - A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix}$. Comparing (6.4.23) with the last expression above yields

$$\begin{aligned}
\mathbf{e}_{s_0}^T((n-2j_0)I - A_n)^\dagger\mathbf{e}_{k_0} &= \mathbf{e}_{s_0}^T(-(n-2j_0)I - A_n)^\dagger\mathbf{e}_{k_0}, \\
\mathbf{e}_{s_0}^T((n-2j_0)I - A_n)^\dagger\mathbf{e}_{l_0} &= -\mathbf{e}_{s_0}^T(-(n-2j_0)I - A_n)^\dagger\mathbf{e}_{l_0}.
\end{aligned} \tag{6.4.28}$$

Applying an analogous argument with (6.4.24), we have

$$\begin{aligned}
&\mathbf{e}_{r_0}^T(-(n-2j_0)I - A_n)^\dagger \begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix} \\
=&\frac{1}{2^n}\begin{bmatrix} \sum_{\substack{0\leq j\leq n\\ j\neq n-j_0}} \frac{(-1)^j\left(\binom{n-1}{j}-\binom{n-1}{j-1}\right)}{2(j+j_0-n)} & \sum_{\substack{0\leq j\leq n\\ j\neq n-j_0}} \frac{(-1)^j\left(\binom{n-2}{j}+\binom{n-2}{j-2}-2\binom{n-2}{j-1}\right)}{2(j+j_0-n)}\end{bmatrix} \\
=&\frac{1}{2^n}\begin{bmatrix} \sum_{\substack{0\leq j'\leq n\\ j'\neq j_0}} \frac{(-1)^{n-j'}\left(\binom{n-1}{j'}-\binom{n-1}{j'-1}\right)}{2(j'-j_0)} & \sum_{\substack{0\leq j'\leq n\\ j'\neq j_0}} \frac{(-1)^{n-j'+1}\left(\binom{n-2}{j'-2}+\binom{n-2}{j'}-2\binom{n-2}{j'-1}\right)}{2(j'-j_0)}\end{bmatrix}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\mathbf{e}_{r_0}^T((n-2j_0)I - A_n)^\dagger\mathbf{e}_{k_0} &= (-1)^n\mathbf{e}_{r_0}^T(-(n-2j_0)I - A_n)^\dagger\mathbf{e}_{k_0}, \\
\mathbf{e}_{r_0}^T((n-2j_0)I - A_n)^\dagger\mathbf{e}_{l_0} &= (-1)^{n+1}\mathbf{e}_{r_0}^T(-(n-2j_0)I - A_n)^\dagger\mathbf{e}_{l_0}.
\end{aligned} \tag{6.4.29}$$

Recall that $\hat{\mathbf{y}}_1^{j_0} = \hat{\mathbf{x}}_1^{j_0} = \tilde{\mathbf{x}}_1^{j_0}$ and $\hat{\mathbf{y}}_2^{j_0} = \hat{\mathbf{x}}_2^{j_0} = \tilde{\mathbf{x}}_2^{j_0}$ for $1 \le j_0 \le n-1$; and $\hat{\mathbf{y}}_1^0 = -\hat{\mathbf{x}}_1^0$, $\hat{\mathbf{y}}_2^0 = 0$, $\hat{\mathbf{y}}_1^n = 0$, and $\hat{\mathbf{y}}_2^n = \hat{\mathbf{x}}_1^n$. Consider the entry $\mathbf{e}_{s_0}^T\hat{\mathbf{y}}_1^{n-j_0}$. Using (6.4.13) for $j_0 = 0$ or $j_0 = n$, and (6.4.15) for $1 \le j_0 \le n-1$, $\mathbf{e}_{s_0}^T\hat{\mathbf{y}}_1^{n-j_0}$ is given by

$$\mathbf{e}_{s_0}^T\hat{\mathbf{y}}_1^{n-j_0} = \frac{\left(\binom{n-2}{n-j_0-1} - \binom{n-2}{n-j_0}\right)}{\sqrt{2^n\binom{n-1}{n-j_0}}} = \frac{\left(\binom{n-2}{j_0-1} - \binom{n-2}{j_0-2}\right)}{\sqrt{2^n\binom{n-1}{j_0-1}}} = -\mathbf{e}_{s_0}^T\hat{\mathbf{y}}_2^{j_0}.$$

In this manner, one can check from (6.4.13) and (6.4.15) with the relation that

$$\begin{bmatrix}\mathbf{e}_{s_0}^T\\ \mathbf{e}_{k_0}^T\\ \mathbf{e}_{l_0}^T\\ \mathbf{e}_{r_0}^T\end{bmatrix}\begin{bmatrix}\hat{\mathbf{y}}_1^{n-j_0} & \hat{\mathbf{y}}_2^{n-j_0}\end{bmatrix} = \begin{bmatrix}-\mathbf{e}_{s_0}^T\hat{\mathbf{y}}_2^{j_0} & -\mathbf{e}_{s_0}^T\hat{\mathbf{y}}_1^{j_0}\\ \mathbf{e}_{k_0}^T\hat{\mathbf{y}}_2^{j_0} & \mathbf{e}_{k_0}^T\hat{\mathbf{y}}_1^{j_0}\\ -\mathbf{e}_{l_0}^T\hat{\mathbf{y}}_2^{j_0} & -\mathbf{e}_{l_0}^T\hat{\mathbf{y}}_1^{j_0}\\ (-1)^{n+1}\mathbf{e}_{r_0}^T\hat{\mathbf{y}}_2^{j_0} & (-1)^{n+1}\mathbf{e}_{r_0}^T\hat{\mathbf{y}}_1^{j_0}\end{bmatrix}. \tag{6.4.30}$$

For simplicity, let $\lambda_0 = n - 2j_0$. Using (6.4.28) and (6.4.30), we have

$$\begin{aligned}
&H(s_0, r_0, n-j_0)\\
=&\mathbf{e}_{s_0}^T(-\lambda_0 I - A_n)^\dagger\begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix}\begin{bmatrix}\mathbf{e}_{l_0}^T\\ \mathbf{e}_{k_0}^T\end{bmatrix}(-1)^{n-j_0}(\hat{\mathbf{y}}_1^{n-j_0}(\hat{\mathbf{y}}_1^{n-j_0})^T + \hat{\mathbf{y}}_2^{n-j_0}(\hat{\mathbf{y}}_2^{n-j_0})^T)\mathbf{e}_{r_0}\\
=&\mathbf{e}_{s_0}^T(\lambda_0 I - A_n)^\dagger\begin{bmatrix}\mathbf{e}_{k_0} & -\mathbf{e}_{l_0}\end{bmatrix}\begin{bmatrix}\mathbf{e}_{l_0}^T\\ -\mathbf{e}_{k_0}^T\end{bmatrix}(-1)^{2n-j_0}(\hat{\mathbf{y}}_2^{j_0}(\hat{\mathbf{y}}_2^{j_0})^T + \hat{\mathbf{y}}_1^{j_0}(\hat{\mathbf{y}}_1^{j_0})^T)\mathbf{e}_{r_0}\\
=&\mathbf{e}_{s_0}^T(\lambda_0 I - A_n)^\dagger\begin{bmatrix}\mathbf{e}_{k_0} & \mathbf{e}_{l_0}\end{bmatrix}\begin{bmatrix}\mathbf{e}_{l_0}^T\\ \mathbf{e}_{k_0}^T\end{bmatrix}(-1)^{j_0}(\hat{\mathbf{y}}_1^{j_0}(\hat{\mathbf{y}}_1^{j_0})^T + \hat{\mathbf{y}}_2^{j_0}(\hat{\mathbf{y}}_2^{j_0})^T)\mathbf{e}_{r_0}\\
=&H(s_0, r_0, j_0).
\end{aligned}$$

Similarly, applying (6.4.29) and (6.4.30), one can establish $H(r_0, s_0, j_0) = H(r_0, s_0, n-j_0)$ for $0 \le j_0 \le n$. □

Now, we provide the second derivative $\frac{\partial^2 p(t_0)}{\partial^2_{k_0,l_0}}$ under PST between s_0 and r_0 in Q_n where $t_0 = \frac{\pi}{2}$. Recall that $\frac{\partial^2 p(t_0)}{\partial^2_{k,l}} = -2t_0^2 Y_1 - 2Y_2$ where

$$\begin{aligned}
Y_1 =&\mathbf{e}_s^T V\left(\frac{\partial\Lambda}{\partial_{k,l}}\right)^2 V^T\mathbf{e}_s - \left(\mathbf{e}_s^T V\frac{\partial\Lambda}{\partial_{k,l}}V^T\mathbf{e}_s\right)^2,\\
Y_2 =&\mathbf{e}_s^T\frac{\partial V}{\partial_{k,l}}\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_s + \mathbf{e}_r^T\frac{\partial V}{\partial_{k,l}}\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_r - 2\mathbf{e}_s^T\frac{\partial V}{\partial_{k,l}}(\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda))\frac{\partial V^T}{\partial_{k,l}}\mathbf{e}_r.
\end{aligned}$$

Note that we may use the notation introduced in Remark 6.4.19 for computations of Y_1 and Y_2. Here we revisit (6.4.17) and (6.4.18): for $j = 1, \ldots, n-1$, if $V\mathbf{e}_p = \hat{\mathbf{y}}_i^j$ for some $3 \le i \le m$ where $m = \binom{n}{j}$, we have $\mathbf{e}_p^T \frac{\partial \Lambda}{\partial_{k_0,l_0}} \mathbf{e}_p = 0$; and if $V \begin{bmatrix} \mathbf{e}_{p_1} & \mathbf{e}_{p_2} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{y}}_1^j & \hat{\mathbf{y}}_2^j \end{bmatrix}$, then

$$\begin{bmatrix} \mathbf{e}_{p_1}^T \\ \mathbf{e}_{p_2}^T \end{bmatrix} \frac{\partial \Lambda}{\partial_{k_0,l_0}} \begin{bmatrix} \mathbf{e}_{p_1} & \mathbf{e}_{p_2} \end{bmatrix} = B^j = \frac{1}{2^{n-1}} \begin{bmatrix} \binom{n-1}{j} & 0 \\ 0 & -\binom{n-1}{j-1} \end{bmatrix}.$$

From the fact that if $V\mathbf{e}_p = \hat{\mathbf{y}}_1^0$ then $\mathbf{e}_p^T \frac{\partial \Lambda}{\partial_{k_0,l_0}} \mathbf{e}_p = \frac{1}{2^{n-1}}$; and if $V\mathbf{e}_p = \hat{\mathbf{y}}_2^n$ then $\mathbf{e}_p^T \frac{\partial \Lambda}{\partial_{k_0,l_0}} \mathbf{e}_p = \frac{-1}{2^{n-1}}$, we define $B^0 = \frac{1}{2^{n-1}} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and $B^n = \frac{1}{2^{n-1}} \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$.

Using (6.4.13) and (6.4.15) along with the telescoping sum yields

$$\begin{aligned}
&\left(\mathbf{e}_{s_0}^T V \frac{\partial \Lambda}{\partial_{k_0,l_0}} V^T \mathbf{e}_{s_0} \right)^2 \\
=&\left(\sum_{j=0}^{n} \mathbf{e}_{s_0}^T \begin{bmatrix} \hat{\mathbf{y}}_1^j & \hat{\mathbf{y}}_2^j \end{bmatrix} B^j \begin{bmatrix} (\hat{\mathbf{y}}_1^j)^T \\ (\hat{\mathbf{y}}_2^j)^T \end{bmatrix} \mathbf{e}_{s_0} \right)^2 \\
=&\left(\frac{1}{2^{2n-1}} \sum_{j=0}^{n} \left[\left(\binom{n-2}{j-1} - \binom{n-2}{j} \right)^2 - \left(\binom{n-2}{j-2} - \binom{n-2}{j-1} \right)^2 \right] \right)^2 \\
=&0
\end{aligned}$$

By (6.4.13) and (6.4.15) with the telescoping sum and the identity $\binom{n-2}{j} - \binom{n-2}{j-1} = \frac{n-1-2j}{n-1}\binom{n-1}{j}$ for $0 \le j \le n-1$, we obtain

$$\begin{aligned}
&\mathbf{e}_{s_0}^T V \left(\frac{\partial \Lambda}{\partial_{k_0,l_0}} \right)^2 V^T \mathbf{e}_{s_0} \\
=&\sum_{j=0}^{n} \mathbf{e}_{s_0}^T \begin{bmatrix} \hat{\mathbf{y}}_1^j & \hat{\mathbf{y}}_2^j \end{bmatrix} (B^j)^2 \begin{bmatrix} (\hat{\mathbf{y}}_1^j)^T \\ (\hat{\mathbf{y}}_2^j)^T \end{bmatrix} \mathbf{e}_{s_0} \\
=&\frac{1}{2^{3n-2}} \sum_{j=0}^{n} \left[\binom{n-1}{j} \left(\binom{n-2}{j} - \binom{n-2}{j-1} \right)^2 + \binom{n-1}{j-1} \left(\binom{n-2}{j-1} - \binom{n-2}{j-2} \right)^2 \right] \\
=&\frac{1}{2^{3n-3}} \sum_{j=0}^{n-1} \binom{n-1}{j} \left(\binom{n-2}{j} - \binom{n-2}{j-1} \right)^2 = \frac{1}{2^{3n-3}} \sum_{j=0}^{n-1} \frac{(n-2j-1)^2}{(n-1)^2} \binom{n-1}{j}^3.
\end{aligned}$$

Hence, Y_1 is completely determined with respect to n.

We now consider Y_2. Regarding computation of Y_2, we may use (6.4.25). Then,

Y_2 can be recast as follows:

$$\begin{aligned}
Y_2 =& \mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{k_0,l_0}} \frac{\partial V^T}{\partial_{k_0,l_0}} \mathbf{e}_{s_0} + \mathbf{e}_{r_0}^T \frac{\partial V}{\partial_{k_0,l_0}} \frac{\partial V^T}{\partial_{k_0,l_0}} \mathbf{e}_{r_0} \\
& - 2\mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{k_0,l_0}} \mathrm{diag}\left(\mathbf{1}_{\binom{n}{0}}^T, -\mathbf{1}_{\binom{n}{1}}^T, \ldots, (-1)^n \mathbf{1}_{\binom{n}{n}}^T\right) \frac{\partial V^T}{\partial_{k_0,l_0}} \mathbf{e}_{r_0} \\
=& (\mathbf{e}_{s_0} + \mathbf{e}_{r_0})^T \frac{\partial V}{\partial_{k_0,l_0}} \mathrm{diag}\left(\delta_0 \mathbf{0}_{\binom{n}{0}}^T, \delta_1 \mathbf{1}_{\binom{n}{1}}^T, \ldots, (-1)^n \delta_n \mathbf{1}_{\binom{n}{n}}^T\right) \frac{\partial V^T}{\partial_{k_0,l_0}} (\mathbf{e}_{s_0} + \mathbf{e}_{r_0}) \\
& + (\mathbf{e}_{s_0} - \mathbf{e}_{r_0})^T \frac{\partial V}{\partial_{k_0,l_0}} \mathrm{diag}\left(\delta_1 \mathbf{1}_{\binom{n}{0}}^T, \delta_2 \mathbf{0}_{\binom{n}{1}}^T, \ldots, (-1)^n \delta_{n+1} \mathbf{1}_{\binom{n}{n}}^T\right) \frac{\partial V^T}{\partial_{k_0,l_0}} (\mathbf{e}_{s_0} - \mathbf{e}_{r_0}),
\end{aligned}$$

where $\delta_i = \mathrm{mod}(i,2)$ for $0 \le i \le n$. We find from (6.4.23) and (6.4.24) that for $j = 0, \ldots, n$

$$\begin{aligned}
& (\mathbf{e}_{s_0} + \mathbf{e}_{r_0})^T ((n-2j)I - A_n)^\dagger \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \\
&= \frac{1}{2^n} \begin{bmatrix} \sum_{\substack{i:\text{even} \\ i \neq j}} \frac{1}{i-j} \left(\binom{n-1}{i} - \binom{n-1}{i-1}\right) & \sum_{\substack{i:\text{even} \\ i \neq j}} \frac{1}{i-j} \left(\binom{n-2}{i} + \binom{n-2}{i-2} - 2\binom{n-2}{i-1}\right) \end{bmatrix} \\
&=: \begin{bmatrix} m_1(j) & m_2(j) \end{bmatrix},
\end{aligned}$$

and

$$\begin{aligned}
& (\mathbf{e}_{s_0} - \mathbf{e}_{r_0})^T ((n-2j)I - A_n)^\dagger \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{l_0} \end{bmatrix} \\
&= \frac{1}{2^n} \begin{bmatrix} \sum_{\substack{i:\text{odd} \\ i \neq j}} \frac{1}{i-j} \left(\binom{n-1}{i} - \binom{n-1}{i-1}\right) & \sum_{\substack{i:\text{odd} \\ i \neq j}} \frac{1}{i-j} \left(\binom{n-2}{i} + \binom{n-2}{i-2} - 2\binom{n-2}{i-1}\right) \end{bmatrix} \\
&=: \begin{bmatrix} m_3(j) & m_4(j) \end{bmatrix}.
\end{aligned}$$

Applying Pascal's identity to $\binom{n-1}{i}$ and $\binom{n-1}{i-1}$, using the identity $\binom{n-2}{i} - \binom{n-2}{i-1} = \frac{n-1-2i}{n-1}\binom{n-1}{i}$ for $0 \le i \le n-1$, we obtain

$$\begin{aligned}
m_1(j) + m_2(j) &= \frac{1}{2^{n-1}} \sum_{\substack{i:\text{even} \\ i \neq j}} \frac{n-2i-1}{(n-1)(i-j)} \binom{n-1}{i}, \\
m_3(j) + m_4(j) &= \frac{1}{2^{n-1}} \sum_{\substack{i:\text{odd} \\ i \neq j}} \frac{n-2i-1}{(n-1)(i-j)} \binom{n-1}{i}.
\end{aligned}$$

We find from (6.4.13) and (6.4.15) with Pascal's identity that for $j = 0, \ldots, n$,

$$\begin{bmatrix} \mathbf{e}_{l_0}^T \\ \mathbf{e}_{k_0}^T \end{bmatrix} (\hat{\mathbf{y}}_1^j (\hat{\mathbf{y}}_1^j)^T + \hat{\mathbf{y}}_2^j (\hat{\mathbf{y}}_2^j)^T) \begin{bmatrix} \mathbf{e}_{l_0} & \mathbf{e}_{k_0} \end{bmatrix} = \frac{1}{2^n} \begin{bmatrix} \binom{n}{j} & \binom{n-1}{j} - \binom{n-1}{j-1} \\ \binom{n-1}{j} - \binom{n-1}{j-1} & \binom{n}{j} \end{bmatrix}.$$

Thus, it follows from (6.4.19) that

$$
\begin{aligned}
&(\mathbf{e}_{s_0}+\mathbf{e}_{r_0})^T\frac{\partial V}{\partial_{k_0,l_0}}\mathrm{diag}\left(\delta_0\mathbf{0}^T_{\binom{n}{0}},\delta_1\mathbf{1}^T_{\binom{n}{1}},\dots,(-1)^n\delta_n\mathbf{1}^T_{\binom{n}{n}}\right)\frac{\partial V^T}{\partial_{k_0,l_0}}(\mathbf{e}_{s_0}+\mathbf{e}_{r_0})\\
=&\sum_{\substack{0\le j\le n\\ j:\text{odd}}}\begin{bmatrix}m_1(j) & m_2(j)\end{bmatrix}\begin{bmatrix}\mathbf{e}^T_{l_0}\\ \mathbf{e}^T_{k_0}\end{bmatrix}(\hat{\mathbf{y}}^j_1(\hat{\mathbf{y}}^j_1)^T+\hat{\mathbf{y}}^j_2(\hat{\mathbf{y}}^j_2)^T)\begin{bmatrix}\mathbf{e}_{l_0} & \mathbf{e}_{k_0}\end{bmatrix}\begin{bmatrix}m_1(j)\\ m_2(j)\end{bmatrix}\\
=&\frac{1}{2^n}\sum_{\substack{0\le j\le n\\ j:\text{odd}}}\left((m_1(j)^2+m_2(j)^2)\binom{n}{j}+2m_1(j)m_2(j)\left(\binom{n-1}{j}-\binom{n-1}{j-1}\right)\right)\\
=&\frac{1}{2^n}\sum_{\substack{0\le j\le n\\ j:\text{odd}}}\left((m_1(j)+m_2(j))^2\binom{n}{j}-4m_1(j)m_2(j)\binom{n-1}{j-1}\right). \qquad (6.4.31)
\end{aligned}
$$

Similarly, one can find that

$$
\begin{aligned}
&(\mathbf{e}_{s_0}-\mathbf{e}_{r_0})^T\frac{\partial V}{\partial_{k_0,l_0}}\mathrm{diag}\left(\delta_1\mathbf{1}^T_{\binom{n}{0}},\delta_2\mathbf{0}^T_{\binom{n}{1}},\dots,(-1)^n\delta_{n+1}\mathbf{1}^T_{\binom{n}{n}}\right)\frac{\partial V^T}{\partial_{k_0,l_0}}(\mathbf{e}_{s_0}-\mathbf{e}_{r_0})\\
=&\frac{1}{2^n}\sum_{\substack{0\le j\le n\\ j:\text{even}}}\left((m_3(j)+m_4(j))^2\binom{n}{j}-4m_3(j)m_4(j)\binom{n-1}{j-1}\right). \qquad (6.4.32)
\end{aligned}
$$

Hence, Y_2 is the sum of the expressions (6.4.31) and (6.4.32). Therefore, considering (ii) of Proposition 2.5.1, we have the following theorem.

Theorem 6.4.22. *Let $n\ge 2$, and $s,r,k,l\in V(Q_n)$. Suppose that $r=s^*$, $s\sim k$ and $k\sim l$. Then, under perfect state transfer between s and r at time $\frac{\pi}{2}$, we have*

$$
\begin{aligned}
\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{k,l}}=&-\frac{\pi^2}{2^{3n-2}}\sum_{j=0}^{n-1}\frac{(n-2j-1)^2}{(n-1)^2}\binom{n-1}{j}^3\\
&-\frac{1}{2^{n-1}}\sum_{\substack{0\le j\le n\\ j:odd}}\left((m_1(j)+m_2(j))^2\binom{n}{j}-4m_1(j)m_2(j)\binom{n-1}{j-1}\right)\\
&-\frac{1}{2^{n-1}}\sum_{\substack{0\le j\le n\\ j:even}}\left((m_3(j)+m_4(j))^2\binom{n}{j}-4m_3(j)m_4(j)\binom{n-1}{j-1}\right).
\end{aligned}
$$

6.4.4 The 1st and 2nd derivatives with respect to the weight of edge $s_0 \sim k_0$ in Q_n

Given Q_n, under PST between s_0 and r_0 at time $\frac{\pi}{2}$, we shall find $\frac{\partial p(\frac{\pi}{2})}{\partial_{s_0,k_0}}$ and $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{s_0,k_0}}$. In this subsection, we use the same notation introduced in Subsection 6.4.2 except

$$E = \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{s_0} \end{bmatrix}^T.$$

As noted, V depends on the choice of an edge for changes of the weight, *i.e.* here $\hat{\mathbf{x}}_1^j, \dots, \hat{\mathbf{x}}^j_{\binom{n}{j}}$ are not necessarily the same as those in Subsection 6.4.2. Procedures for finding $\frac{\partial \Lambda}{\partial_{s_0,k_0}}$, particular rows of V and $\frac{\partial V}{\partial_{s_0,k_0}}$, $\frac{\partial p(\frac{\pi}{2})}{\partial_{s_0,k_0}}$, and $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{s_0,k_0}}$ are the same as those as done in Subsections 6.4.2 and 6.4.3. Hence, we shall present the results with brief explanations.

From Example 6.4.12, we have

$$h_{n,j}^{s_0,k_0}(1,1) = \binom{n-1}{j}, \; h_{n,j}^{s_0,k_0}(1,-1) = \binom{n-1}{j-1}.$$

Let $\hat{\mathbf{x}}_1^{j_0} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\hat{\mathbf{x}}_2^{j_0} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ for $1 \le j_0 \le n-1$. Then, as done in order to obtain (6.4.13)–(6.4.16), one can find the following:

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}}_1^0 & \hat{\mathbf{x}}_1^n \end{bmatrix} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & (-1)^n \end{bmatrix},$$

and for $j_0 = 1, \dots, n-1$,

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0} \end{bmatrix} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} \sqrt{\binom{n-1}{j_0}} & \sqrt{\binom{n-1}{j_0-1}} \\ \sqrt{\binom{n-1}{j_0}} & -\sqrt{\binom{n-1}{j_0-1}} \\ (-1)^{j_0}\sqrt{\binom{n-1}{j_0}} & (-1)^{j_0}\sqrt{\binom{n-1}{j_0-1}} \end{bmatrix}.$$

Furthermore, $B^{j_0} = \frac{1}{2^{n-1}} \begin{bmatrix} \binom{n-1}{j_0} & 0 \\ 0 & -\binom{n-1}{j_0-1} \end{bmatrix}$. Using the arguments to obtain (6.4.21)–

(6.4.24), one can establish that for $0 \le j \le n$,

$$\begin{aligned}\mathbf{e}_{s_0}^T((n-2j_0)I-A_n)^\dagger \begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix} &= \frac{1}{2^n}\begin{bmatrix}\sum_{\substack{0\le j\le n\\ j\neq j_0}} \frac{\binom{n}{j}}{2(j-j_0)} & \sum_{\substack{0\le j\le n\\ j\neq j_0}} \frac{\binom{n-1}{j}-\binom{n-1}{j-1}}{2(j-j_0)}\end{bmatrix},\\ \mathbf{e}_{r_0}^T((n-2j_0)I-A_n)^\dagger \begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix} &= \frac{1}{2^n}\begin{bmatrix}\sum_{\substack{0\le j\le n\\ j\neq j_0}} \frac{(-1)^j\binom{n}{j}}{2(j-j_0)} & \sum_{\substack{0\le j\le n\\ j\neq j_0}} \frac{(-1)^j\left(\binom{n-1}{j}-\binom{n-1}{j-1}\right)}{2(j-j_0)}\end{bmatrix}.\end{aligned} \tag{6.4.33}$$

Set $\hat{\mathbf{y}}_1^j = \hat{\mathbf{x}}_1^j$ and $\hat{\mathbf{y}}_2^j = \hat{\mathbf{x}}_2^j$ for $j = 1, \ldots, n-1$. Define $\hat{\mathbf{y}}_1^0 = \hat{\mathbf{x}}_1^0$, $\hat{\mathbf{y}}_2^0 = 0$, $\hat{\mathbf{y}}_1^n = 0$, and $\hat{\mathbf{y}}_2^n = \hat{\mathbf{x}}_1^n$.

Theorem 6.4.23. *Let $n \ge 2$, and $s, k \in V(Q_n)$. Suppose $s \sim k$. Then, under PST between s and s^* at time $\frac{\pi}{2}$, we have*

$$\frac{\partial p(\frac{\pi}{2})}{\partial_{s,k}} = 0.$$

Proof. It is straightforward from Theorem 6.4.18. □

Define $B^0 = \frac{1}{2^{n-1}}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}$ and $B^n = \frac{1}{2^{n-1}}\begin{bmatrix}0 & 0\\ 0 & -1\end{bmatrix}$. It can be found that

$$\left(\mathbf{e}_{s_0}^T V \frac{\partial \Lambda}{\partial_{s_0,k_0}} V^T \mathbf{e}_{s_0}\right)^2 = 0 \text{ and } \mathbf{e}_{s_0}^T V \left(\frac{\partial \Lambda}{\partial_{s_0,k_0}}\right)^2 V^T \mathbf{e}_{s_0} = \frac{1}{2^{3n-3}} \sum_{j=0}^{n-1} \binom{n-1}{j}^3.$$

Furthermore, one can verify that for $j = 0, \ldots, n$,

$$\begin{aligned}(\mathbf{e}_{s_0}+\mathbf{e}_{r_0})^T((n-2j)I-A_n)^\dagger \begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix} &= \frac{1}{2^n}\begin{bmatrix}\sum_{\substack{i:\text{even}\\ i\neq j}} \frac{\binom{n}{i}}{i-j} & \sum_{\substack{i:\text{even}\\ i\neq j}} \frac{\binom{n-1}{i}-\binom{n-1}{i-1}}{i-j}\end{bmatrix}\\ &=: \begin{bmatrix}n_1(j) & n_2(j)\end{bmatrix},\end{aligned}$$

and

$$\begin{aligned}(\mathbf{e}_{s_0}-\mathbf{e}_{r_0})^T((n-2j)I-A_n)^\dagger \begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix} &= \frac{1}{2^n}\begin{bmatrix}\sum_{\substack{i:\text{odd}\\ i\neq j}} \frac{\binom{n}{i}}{i-j} & \sum_{\substack{i:\text{odd}\\ i\neq j}} \frac{\binom{n-1}{i}-\binom{n-1}{i-1}}{i-j}\end{bmatrix}\\ &=: \begin{bmatrix}n_3(j) & n_4(j)\end{bmatrix}.\end{aligned}$$

Theorem 6.4.24. *Let $n \ge 2$, and $s, k \in V(Q_n)$. Suppose that $s \sim k$. Then, under* *perfect state transfer between s and s^* at time $\frac{\pi}{2}$, we have*

$$\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{s,k}} = \frac{-\pi^2}{2^{3n-2}} \sum_{j=0}^{n-1} \binom{n-1}{j}^3 - \frac{1}{2^{n-1}} \sum_{\substack{0\le j\le n\\ j:odd}} \left((n_1(j)+n_2(j))^2 \binom{n}{j} - 4n_1(j)n_2(j)\binom{n-1}{j-1} \right)$$
$$- \frac{1}{2^{n-1}} \sum_{\substack{0\le j\le n\\ j:even}} \left((n_3(j)+n_4(j))^2 \binom{n}{j} - 4n_3(j)n_4(j)\binom{n-1}{j-1} \right).$$

6.5 Sensitivity of the fidelity under PST to edge weight errors in the $(2,2,2,\{3,3\})$-switched hypercube

Our ultimate goal of this subsection is to compare the sensitivity of the fidelity of state transfer under PST to changes in the weight of an edge in Q_n and in 'the' equidistant switched n-cube $\widetilde{Q}_n^{(M)}$ where M is a $(2,2,2,\{3,3\})$-matching in Q_n (note Remark 6.3.26). The comparison of the sensitivity depends on the choice of an edge (as seen in Theorems 6.4.22 and 6.4.24). Since the edges in M are not in $\widetilde{Q}_n^{(M)}$, selecting an edge in M results in 'comparing apples and oranges'. Therefore, we conduct a sensitivity analysis particularly by choosing an edge incident to one of the edges in M.

Then, we need to obtain the first and second partial derivatives of the fidelity under PST with respect to the selected edge-weight for $\widetilde{Q}_n^{(M)}$. In Subsection 6.5.1, we shall investigate spectral properties of $A(\widetilde{Q}_n^{(M)})$ by using equitable partitions and rank one updated matrices. Furthermore, we shall find particular entries of eigenvectors of $A(\widetilde{Q}_n^{(M)})$ that correspond to vertices s, k and r in $V(\widetilde{Q}_n^{(M)})$ where $r = s^*$ and $s \sim k$ is incident to an edge in M; here we note that there are three types of vertices l in $V(\widetilde{Q}_n^{(M)})$ such that $l \sim k$ is incident to an edge in M (Remark 6.5.21), and we leave related tasks for future works. In Subsection 6.5.2, we produce all necessary results in explicit form in order to obtain our desired derivatives. We remark about formulating the derivatives, provide numerical results regarding our goal, and finally pose a related conjecture.

6.5.1 Spectral properties of the adjacency matrix of $\widetilde{Q}_n$

Let $n \geq 3$, and M be a $(2,2,2,\{3,3\})$-matching in Q_n. For ease of notation, we denote, in what follows, the $(2,2,2,\{3,3\})$-switched n-cube $\widetilde{Q}_n^{(M)}$ by $\widetilde{Q}_n$. We shall find an equitable partition π of $V(\widetilde{Q}_n)$ that produces 2^{n-1} eigen-pairs of $A(\widetilde{Q}_n)$. In order to obtain such a partition, we first construct the adjacency matrix of Q_n in a particular form.

For an ordered set X of binary strings and $a \in \{0,1\}$, we use $X+a$ to denote the ordered set obtained from X by attaching an a at the end of each binary string (on the right).

Consider the following ordered sets: $\alpha_1^{(3)} = \{000, 011\}$, $\alpha_2^{(3)} = \{101, 110\}$, $\beta_1^{(3)} = \{100, 111\}$ and $\beta_2^{(3)} = \{001, 010\}$. Then, labelling $V(Q_3)$ in order of $\alpha_1^{(3)}, \alpha_2^{(3)}, \beta_1^{(3)}$ and $\beta_2^{(3)}$, we have

$$A(Q_3) = \left[\begin{array}{cc|cc} 0 & 0 & I_2 & J_2 \\ 0 & 0 & J_2 & I_2 \\ \hline I_2 & J_2 & 0 & 0 \\ J_2 & I_2 & 0 & 0 \end{array}\right].$$

Suppose that for $n \geq 4$, $\alpha_i^{(n)} = \left(\alpha_i^{(n-1)} + 0\right) \cup_L \left(\beta_i^{(n-1)} + 1\right)$ and $\beta_i^{(n)} = \left(\beta_i^{(n-1)} + 0\right) \cup_L \left(\alpha_i^{(n-1)} + 1\right)$ for $i = 1, 2$ (recall that $\cup_L$ is the linear sum). We claim that labelling $V(Q_n)$ in order of $\alpha_1^{(n)}, \alpha_2^{(n)}, \beta_1^{(n)}$ and $\beta_2^{(n)}$, we obtain the adjacency matrix $A(Q_n)$ in the form of (6.5.1) below. We shall check the first row partition of $A(Q_n)$ by induction, and leave the remaining task to the reader.

No vertex in $\alpha_1^{(n-1)}$ $\left(\text{resp. } \beta_1^{(n-1)}\right)$ is adjacent to all vertices in $\alpha_j^{(n-1)}$ $\left(\text{resp. } \beta_j^{(n-1)}\right)$ for $j = 1, 2$. This implies that any vertex in $\alpha_1^{(n-1)} + 0$ $\left(\text{resp. } \beta_1^{(n-1)} + 1\right)$ is not adjacent to all vertices in $\alpha_j^{(n-1)} + 0$ $\left(\text{resp. } \beta_j^{(n-1)} + 1\right)$ for $j \in \{1, 2\}$. For two distinct binary strings, attaching a 0 at the end of one of them and a 1 at the end of the other results in two binary strings whose distance is more than 1. So, any vertex in $\alpha_1^{(n-1)} + 0$ $\left(\text{resp. } \beta_1^{(n-1)} + 1\right)$ is not adjacent to all vertices in $\left(\cup_{j=1}^2 \left(\beta_j^{(n-1)} + 1\right)\right) \cup \left(\alpha_2^{(n-1)} + 1\right)$ $\left(\text{resp. } \left(\cup_{j=1}^2 \left(\alpha_j^{(n-1)} + 0\right)\right) \cup \left(\beta_2^{(n-1)} + 0\right)\right)$. Given a binary string, the string obtained by attaching a 0 to the end is adjacent to the string obtained by attaching a 1 to the end. Thus, k^{th} vertex in $\alpha_1^{(n-1)} + 0$ (resp. $\beta_1^{(n-1)} + 1$) is only adjacent to k^{th} vertex in $\alpha_1^{(n-1)} + 1$ (resp. $\beta_1^{(n-1)} + 0$). Finally, the remaining parts in the first row partition of $A(Q_n)$ are filled by induction. Therefore, we have the following:

$$A(Q_n) = \left[\begin{array}{cc|cc} 0 & 0 & B_n & I_{2^{n-3}} \otimes J_2 \\ 0 & 0 & I_{2^{n-3}} \otimes J_2 & B_n \\ \hline B_n & I_{2^{n-3}} \otimes J_2 & 0 & 0 \\ I_{2^{n-3}} \otimes J_2 & B_n & 0 & 0 \end{array}\right] \tag{6.5.1}$$

where $B_3 = I_2$, and while for $n \geq 4$, $B_n = \begin{bmatrix} B_{n-1} & I_{2^{n-3}} \\ I_{2^{n-3}} & B_{n-1} \end{bmatrix}$.

From $A(Q_n)$ in (6.5.1) with $\alpha_1^{(n)}$, we observe that the first and second vertices v_1 and v_2 in $V(Q_n)$ correspond the binary strings $0\dots0$ and $0110\dots0$, respectively. Considering $\beta_1^{(n)}$, the $(2^{n-1}+1)^{\text{th}}$ and $(2^{n-1}+2)^{\text{th}}$ vertices w_1 and w_2 correspond $10\dots0$ and $1110\dots0$, respectively. Then, $\{v_1 \sim w_1, v_2 \sim w_2\}$ is a $(2,2,2;\{3,3\})$-matching in Q_n. By Proposition 6.3.25, we may assume in this section that $M = \{v_1 \sim w_1, v_2 \sim w_2\}$. Hence,

$$A(\widetilde{Q}_n) = \left[\begin{array}{cc|cc} 0 & 0 & \widetilde{B}_n & I_{2^{n-3}} \otimes J_2 \\ 0 & 0 & I_{2^{n-3}} \otimes J_2 & B_n \\ \hline \widetilde{B}_n & I_{2^{n-3}} \otimes J_2 & 0 & 0 \\ I_{2^{n-3}} \otimes J_2 & B_n & 0 & 0 \end{array}\right] \tag{6.5.2}$$

where $\widetilde{B}_3 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, and while $n \geq 4$, $\widetilde{B}_n = \begin{bmatrix} \widetilde{B}_{n-1} & I_{2^{n-3}} \\ I_{2^{n-3}} & B_{n-1} \end{bmatrix}$.

In the sequel, we assume that $V(\widetilde{Q}_n)$ is defined as $\{1,\dots,2^n\}$, and adjacency of vertices in $\widetilde{Q}_n$ is given by entries of the matrix $A(\widetilde{Q}_n)$ in (6.5.2): vertices k and l are adjacent if and only if $(A(\widetilde{Q}_n))_{k,l} = 1$. Furthermore, let $k_0 := 1$ and $s_0 := 2^{n-1} + 2^{n-2} + 1$. As seen in (6.5.2), k_0 is adjacent to s_0. Since s_0 corresponds to the first element in $\beta_2^{(n)}$, s_0 can be regarded as the string $0010\dots0$. Let $r_0 := s_0^*$. Then r_0 corresponds to $1101\dots1$. It can be checked that $1101\dots1$ is the last element in $\alpha_2^{(n)}$ if n is odd, and the last element in $\beta_2^{(n)}$ if n is even. Therefore, $r_0 = 2^{n-1}$ if n odd, and $r_0 = 2^n$ if n is even.

Given a $(0,1)$ symmetric matrix B, let G be the undirected graph with or without loops associated to B. If there exists an equitable partition π of G, then we use $B^{(\pi)}$ to denote the adjacency matrix of the quotient graph G/π.

Consider a partition $\pi = \bigcup_{i=1}^{2^{n-1}} \{2i-1, 2i\}$ of $V(\widetilde{Q}_n)$. We can find from (6.5.1) and (6.5.2) that by induction each block in the partitioned matrix for $A(\widetilde{Q}_n)$ according to

π is one of the following: $\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, and $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$. Hence, π is equitable, and so we have

$$A(\widetilde{Q}_n/\pi) = \left[\begin{array}{cc|cc} 0 & 0 & B_n^{(\tau_n)} & 2I_{2^{n-3}} \\ 0 & 0 & 2I_{2^{n-3}} & B_n^{(\tau_n)} \\ \hline B_n^{(\tau_n)} & 2I_{2^{n-3}} & 0 & 0 \\ 2I_{2^{n-3}} & B_n^{(\tau_n)} & 0 & 0 \end{array}\right]$$

where $\tau_n = \bigcup_{i=1}^{2^{n-3}} \{2i-1, 2i\}$, $B_3^{(\tau_3)} = [1]$ and for $n \geq 4$,

$$B_n^{(\tau_n)} = \begin{bmatrix} B_{n-1}^{(\tau_{n-1})} & I_{2^{n-4}} \\ I_{2^{n-4}} & B_{n-1}^{(\tau_{n-1})} \end{bmatrix}.$$

Then, 2^{n-1} eigen-pairs of $A(\widetilde{Q}_n)$ can be obtained from $A(\widetilde{Q}_n/\pi)$ by Proposition 2.5.3. (Since the subindex n of τ_n is clear from $B_n^{(\tau_n)}$, we simply write $B_n^{(\tau_n)}$ as $B_n^{(\tau)}$.)

We consider the remaining 2^{n-1} eigen-pairs of $A(\widetilde{Q}_n)$. Consider the following equations:

$$A(\widetilde{Q}_n)\begin{bmatrix} \mathbf{u}\otimes\mathbf{c} \\ 0 \\ \mathbf{u}\otimes\mathbf{c} \\ 0 \end{bmatrix} = \lambda_1 \begin{bmatrix} \mathbf{u}\otimes\mathbf{c} \\ 0 \\ \mathbf{u}\otimes\mathbf{c} \\ 0 \end{bmatrix}, \quad A(\widetilde{Q}_n)\begin{bmatrix} 0 \\ \mathbf{v}\otimes\mathbf{c} \\ 0 \\ \mathbf{v}\otimes\mathbf{c} \end{bmatrix} = \lambda_2 \begin{bmatrix} 0 \\ \mathbf{v}\otimes\mathbf{c} \\ 0 \\ \mathbf{v}\otimes\mathbf{c} \end{bmatrix} \tag{6.5.3}$$

where $\lambda_1, \lambda_2 \in \mathbb{R}$, $\mathbf{u}, \mathbf{v} \in \mathbb{R}^{2^{n-3}}$, and $\mathbf{c} := \begin{bmatrix} 1 \\ -1 \end{bmatrix}$. Then, we are led to equations

$$\widetilde{B}_n(\mathbf{u}\otimes\mathbf{c}) = \lambda_1(\mathbf{u}\otimes\mathbf{c}) \text{ and } B_n(\mathbf{v}\otimes\mathbf{c}) = \lambda_2(\mathbf{v}\otimes\mathbf{c}). \tag{6.5.4}$$

In order to consider the following lemma, for $n \geq 3$, we define a matrix C_n to be

$$C_n = B_n^{(\tau)} - 2\mathbf{e}_1\mathbf{e}_1^T.$$

Then, for $n \geq 4$, C_n can be expressed as $C_n = \begin{bmatrix} C_{n-1} & I_{2^{n-4}} \\ I_{2^{n-4}} & B_{n-1}^{(\tau)} \end{bmatrix}$.

Lemma 6.5.1. *Let $n \geq 3$, $\lambda \in \mathbb{R}$, and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2^{n-3}}$. Then, $B_n(\mathbf{x}\otimes\mathbf{c}) = \lambda(\mathbf{y}\otimes\mathbf{c})$ if and only if $B_n^{(\tau)}\mathbf{x} = \lambda\mathbf{y}$; and $\widetilde{B}_n(\mathbf{x}\otimes\mathbf{c}) = \lambda(\mathbf{y}\otimes\mathbf{c})$ if and only if $C_n\mathbf{x} = \lambda\mathbf{y}$.*

Proof. We shall use induction on n. Let $n = 3$. We have $B_3 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and $B_3^{(\tau)} = [1]$, so the statement holds. Suppose that for $n \geq 3$ and $\mathbf{u}, \mathbf{v} \in \mathbb{R}^{2^{n-3}}$, $B_n(\mathbf{u} \otimes \mathbf{c}) = \lambda(\mathbf{v} \otimes \mathbf{c})$ if and only if $B_n^{(\tau)}\mathbf{u} = \lambda\mathbf{v}$. Let $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \otimes \mathbf{c}$ and $\mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} \otimes \mathbf{c}$ where $\mathbf{x}_1, \mathbf{x}_2, \mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^{2^{n-3}}$. We first assume for the sufficiency that $B_{n+1}(\mathbf{x} \otimes \mathbf{c}) = \lambda(\mathbf{y} \otimes \mathbf{c})$. Then, we have

$$\begin{aligned}
\lambda \begin{bmatrix} \mathbf{y}_1 \otimes \mathbf{c} \\ \mathbf{y}_2 \otimes \mathbf{c} \end{bmatrix} = \lambda \left(\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} \otimes \mathbf{c} \right) &= B_{n+1} \left(\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \otimes \mathbf{c} \right) \\
&= \begin{bmatrix} B_n & I_{2^{n-2}} \\ I_{2^{n-2}} & B_n \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \otimes \mathbf{c} \\ \mathbf{x}_2 \otimes \mathbf{c} \end{bmatrix} = \begin{bmatrix} B_n(\mathbf{x}_1 \otimes \mathbf{c}) + \mathbf{x}_2 \otimes \mathbf{c} \\ \mathbf{x}_1 \otimes \mathbf{c} + B_n(\mathbf{x}_2 \otimes \mathbf{c}) \end{bmatrix}.
\end{aligned}$$

This implies that $B_n(\mathbf{x}_1 \otimes \mathbf{c}) = (\lambda\mathbf{y}_1 - \mathbf{x}_2) \otimes \mathbf{c}$ and $B_n(\mathbf{x}_2 \otimes \mathbf{c}) = (\lambda\mathbf{y}_2 - \mathbf{x}_1) \otimes \mathbf{c}$. By the inductive hypothesis, $B_n^{(\tau)}\mathbf{x}_1 = \lambda\mathbf{y}_1 - \mathbf{x}_2$ and $B_n^{(\tau)}\mathbf{x}_2 = \lambda\mathbf{y}_2 - \mathbf{x}_1$. Hence,

$$B_{n+1}^{(\tau)} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} B_n^{(\tau)} & I_{2^{n-3}} \\ I_{2^{n-3}} & B_n^{(\tau)} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}.$$

By induction, $B_n(\mathbf{x} \otimes \mathbf{c}) = \lambda(\mathbf{y} \otimes \mathbf{c})$ implies $B_n^{(\tau)}\mathbf{x} = \lambda\mathbf{y}$ for $n \geq 3$. The converse follows readily.

An analogous argument applies to the remaining case. One can check that $\lambda \left(\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} \otimes \mathbf{c} \right) = \widetilde{B}_{n+1} \left(\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \otimes \mathbf{c} \right)$ if and only if $\widetilde{B}_n(\mathbf{x}_1 \otimes \mathbf{c}) = (\lambda\mathbf{y}_1 - \mathbf{x}_2) \otimes \mathbf{c}$ and $B_n(\mathbf{x}_2 \otimes \mathbf{c}) = (\lambda\mathbf{y}_2 - \mathbf{x}_1) \otimes \mathbf{c}$. Therefore, applying induction for $\widetilde{B}_n(\mathbf{x}_1 \otimes \mathbf{c}) = (\lambda\mathbf{y}_1 - \mathbf{x}_2) \otimes \mathbf{c}$, and using the result above for $B_n(\mathbf{x}_2 \otimes \mathbf{c}) = (\lambda\mathbf{y}_2 - \mathbf{x}_1) \otimes \mathbf{c}$, the desired conclusion can be established. $\square$

By (6.5.3) and (6.5.4) with Lemma 6.5.1, we can obtain 2^{n-3} eigen-pairs of $A(\widetilde{Q}_n)$ from $B_n^{(\tau)}$ (resp. C_n). Since $\widetilde{Q}_n$ is a bipartite graph, we see that if $\begin{bmatrix} \mathbf{x}^T & \mathbf{y}^T \end{bmatrix}$ for some $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2^{n-1}}$ is an eigenvector of $A(\widetilde{Q}_n)$ associated to an eigenvalue λ, then so is $\begin{bmatrix} \mathbf{x}^T & -\mathbf{y}^T \end{bmatrix}$ associated to $-\lambda$. Hence, each eigen-pair $(\lambda_1, \mathbf{u})$ of C_n generates two eigen-pairs of $A(\widetilde{Q}_n)$:

$$\left(\lambda_1, \begin{bmatrix} (\mathbf{u} \otimes \mathbf{c})^T & 0^T & (\mathbf{u} \otimes \mathbf{c})^T & 0^T \end{bmatrix}\right) \text{ and } \left(-\lambda_1, \begin{bmatrix} (\mathbf{u} \otimes \mathbf{c})^T & 0^T & -(\mathbf{u} \otimes \mathbf{c})^T & 0^T \end{bmatrix}\right). \tag{6.5.5}$$

Similarly, each eigen-pair $(\lambda_2, \mathbf{v})$ of $B_n^{(\tau)}$ generates two eigen-pairs of $A(\widetilde{Q}_n)$:

$$\left(\lambda_2, \left[0^T \quad (\mathbf{v}\otimes\mathbf{c})^T \quad 0^T \quad (\mathbf{v}\otimes\mathbf{c})^T\right]\right) \text{ and } \left(-\lambda_2, \left[0^T \quad (\mathbf{v}\otimes\mathbf{c})^T \quad 0^T \quad -(\mathbf{v}\otimes\mathbf{c})^T\right]\right). \tag{6.5.6}$$

Furthermore, since any eigenvector $\mathbf{z}$ of $A(\widetilde{Q}_n)$ obtained from an eigenvector of $A(\widetilde{Q}_n/\pi)$ by Proposition 2.5.3 is in form $\mathbf{z}_1 \otimes \mathbf{1}_2$ for some $\mathbf{z}_1 \in \mathbb{R}^{2^{n-1}}$, we see that no eigenvector of $A(\widetilde{Q}_n)$ in form $\left[0^T \quad (\mathbf{v}\otimes\mathbf{c})^T \quad 0^T \quad (\mathbf{v}\otimes\mathbf{c})^T\right]$ can be expressed as a linear combination of vectors in form $\mathbf{z}_1 \otimes \mathbf{1}_2$ or $\left[(\mathbf{u}\otimes\mathbf{c})^T \quad 0^T \quad (\mathbf{u}\otimes\mathbf{c})^T \quad 0^T\right]$. We also can see that any non-zero vector in form $\mathbf{z}_1 \otimes \mathbf{1}_2$ is linearly independent of any vector in form $\left[(\mathbf{u}\otimes\mathbf{c})^T \quad 0^T \quad (\mathbf{u}\otimes\mathbf{c})^T \quad 0^T\right]$. Therefore, the remaining 2^{n-1} eigen-pairs of $A(\widetilde{Q}_n)$ can be completely determined by eigen-pairs of $B_n^{(\tau)}$ and C_n as in forms (6.5.5) and (6.5.6).

Here is an outline for establishing our main result of this subsection (Theorem 6.5.14) about the spectral properties of $A(\widetilde{Q}_n)$:

- In Step 1, 2^{n-1} eigen-pairs of $A(\widetilde{Q}_n)$ are obtained from those of $A(\widetilde{Q}_n/\pi)$ by Proposition 2.5.3.
- In Step 2, another 2^{n-2} eigen-pairs of $A(\widetilde{Q}_n)$ are constructed from 2^{n-3} eigen-pairs of $B_n^{(\tau)}$ as in form (6.5.6).
- In Step 3, another $2^{n-2} - 2(n-2)$ eigen-pairs of $A(\widetilde{Q}_n)$ are constructed from $2^{n-3} - (n-2)$ eigen-pairs of C_n as in form (6.5.5).
- In Step 4, the other $2(n-2)$ eigen-pairs of $A(\widetilde{Q}_n)$ are constructed from $(n-2)$ eigen-pairs of C_n as in form (6.5.5).
- In all the steps, we find the k_0^{th}, s_0^{th}, and r_0^{th} entries of each eigenvector, and the multiplicity of the corresponding eigenvalue.

6.5.1.1 Step 1

We claim that for $n \geq 3$, the columns in H_{n-1} consist of eigenvectors of $A(\widetilde{Q}_n/\pi)$. In order to establish the claim, using induction, we first show that for $n \geq 3$ the columns of H_{n-3} consist of eigenvectors of $B_n^{(\tau)}$ where $H_0 := [1]$. (We may extend the inductive construction of H_n in (6.4.5) for $n \geq 0$.) For $n = 3$, it is trivial that the eigenvalue of $B_3^{(\tau)}$ is 1. Suppose that for $n \geq 3$, $B_n^{(\tau)} H_{n-3} = H_{n-3} D_n$ where D_n

is a diagonal matrix. Then,

$$B_{n+1}^{(\tau)}H_{n-2} = \begin{bmatrix} B_n^{(\tau)} & I \\ I & B_n^{(\tau)} \end{bmatrix} \begin{bmatrix} H_{n-3} & H_{n-3} \\ H_{n-3} & -H_{n-3} \end{bmatrix} = \begin{bmatrix} H_{n-3} & H_{n-3} \\ H_{n-3} & -H_{n-3} \end{bmatrix} \begin{bmatrix} D_n + I & 0 \\ 0 & D_n - I \end{bmatrix}.$$

Thus, by induction, H_{n-3} diagonalises $B_n^{(\tau)}$ for $n \geq 3$. Let

$$D_n := \frac{1}{2^{n-3}} H_{n-3}^T B_n^{(\tau)} H_{n-3}.$$

Considering $D_3 = [1]$ and the inductive relation between D_n and $D_{n+1} = \mathrm{diag}(D_n + I, D_n - I)$, eigenvalues of $B_n^{(\tau)}$ (the main diagonal entries of D_n) are given by $(n-2) - 2i$ for $i = 0, \ldots, n-3$ with respective multiplicity $\binom{n-3}{i}$. Furthermore, it can be checked that

$$\begin{aligned} A(\widetilde{Q}_n/\pi)H_{n-1} =& A(\widetilde{Q}_n/\pi) \begin{bmatrix} H_{n-3} & H_{n-3} & H_{n-3} & H_{n-3} \\ H_{n-3} & -H_{n-3} & H_{n-3} & -H_{n-3} \\ H_{n-3} & H_{n-3} & -H_{n-3} & -H_{n-3} \\ H_{n-3} & -H_{n-3} & -H_{n-3} & H_{n-3} \end{bmatrix} \\ =& H_{n-1}\mathrm{diag}(D_n + 2I, D_n - 2I, -D_n - 2I, -D_n + 2I). \end{aligned} \tag{6.5.7}$$

Hence, H_{n-1} diagonalises $A(\widetilde{Q}_n/\pi)$. Then, the distinct eigenvalues of $A(\widetilde{Q}_n/\pi)$ are given by $n-2j$ for $j = 0, \ldots, n$. We denote $\frac{1}{\sqrt{2^n}} H_{n-1} \otimes \mathbf{1}_2$ by X_1. By Proposition 2.5.3, X_1 consists of 2^{n-1} eigenvectors of $A(\widetilde{Q}_n)$ such that $X_1^T X_1 = I$. Let Λ_1 denote the diagonal matrix such that $A(\widetilde{Q}_n)X_1 = X_1\Lambda_1$. For $j = 0, \ldots, n$, we use $X_1(j)$ to denote the submatrix of X_1 that consists of all columns in X_1 that are eigenvectors of $A(\widetilde{Q}_n)$ corresponding to the eigenvalue $n-2j$.

We consider the multiplicity of eigenvalue $n-2j$ of $A(\widetilde{Q}_n/\pi)$ for $j = 0, \ldots, n$, and examine sign patterns of the rows of $X_1(j)$ indexed by $k_0 = 1$, $s_0 = 2^{n-1} + 2^{n-2} + 1$, $r_0 = 2^n$ (if n is even), and $r_0 = 2^{n-1}$ (if n is odd). From the structure of $X_1 = \frac{1}{\sqrt{2^n}} H_{n-1} \otimes \mathbf{1}_2$, for the sign patterns we may consider the rows of H_{n-1} indexed by 1, $2^{n-2} + 2^{n-3} + 1$, 2^{n-1} (if n is even), and 2^{n-2} (if n is odd). We observe from (6.5.7) that the multiplicity of $n-2j$ is derived from the $\binom{n-3}{j}$ entries $(n-2)-2j$ in D_n by adding 2; from the $\binom{n-3}{j-2}$ entries $(n-2)-2(j-2)$ in D_n by adding -2; from the $\binom{n-3}{n-j}$ entries $-(n-2)+2(n-j)$ in $-D_n$ by adding -2; and from the $\binom{n-3}{n-j-2}$ entries $-(n-2)+2(n-j-2)$ in $-D_n$ by adding 2. This implies from Pascal's identity that the multiplicity of $n-2j$ is $\binom{n-2}{j} + \binom{n-2}{j-2}$. In other words, there are $\binom{n-2}{j} + \binom{n-2}{j-2}$ columns in $X_1(j)$.

Remark 6.5.2. Recall that for $0 \le j \le n-3$, $H_{n-3}(j)$ consists of all columns in H_{n-3} that are eigenvectors of A_{n-3} associated to the eigenvalue $(n-3)-2j$; and the first and last rows of $H_{n-3}(j)$ are $\mathbf{1}^T_{\binom{n-3}{j}}$ and $(-1)^j\mathbf{1}^T_{\binom{n-3}{j}}$, respectively. Comparing the arguments for recursively finding the eigenvalues of A_{n-3} and $B_n^{(\tau)}$ by using the standard Hadamard matrix H_{n-3}, we can see that each column of $H_{n-3}(j)$ is an eigenvector $\mathbf{x}$ of $B_n^{(\tau)}$ corresponding to the eigenvalue $(n-2)-2j$. Therefore, the first and last entries of $\mathbf{x}$ are 1 and $(-1)^j$, respectively.

Considering the four column partitions of H_{n-1} in (6.5.7) and the corresponding four diagonal matrices with the argument above about the multiplicity of $n-2j$, we can find from Remark 6.5.2 that

$$\begin{bmatrix} \mathbf{e}^T_{k_0} \\ \mathbf{e}^T_{s_0} \end{bmatrix} \left(\sqrt{2^n}X_1(j)\right) = \begin{bmatrix} \mathbf{1}^T_{\binom{n-3}{j}} & \mathbf{1}^T_{\binom{n-3}{j-2}} & \mathbf{1}^T_{\binom{n-3}{j-3}} & \mathbf{1}^T_{\binom{n-3}{j-1}} \\ \mathbf{1}^T_{\binom{n-3}{j}} & -\mathbf{1}^T_{\binom{n-3}{j-2}} & -\mathbf{1}^T_{\binom{n-3}{j-3}} & \mathbf{1}^T_{\binom{n-3}{j-1}} \end{bmatrix}, \tag{6.5.8}$$

and by checking two cases that n is even or odd,

$$\begin{aligned}
&\mathbf{e}^T_{r_0}\left(\sqrt{2^n}X_1(j)\right) \\
=&\begin{cases} \left[(-1)^j\mathbf{1}^T_{\binom{n-3}{j}} \quad -(-1)^{j-2}\mathbf{1}^T_{\binom{n-3}{j-2}} \quad -(-1)^{n-j}\mathbf{1}^T_{\binom{n-3}{j-3}} \quad (-1)^{n-j-2}\mathbf{1}^T_{\binom{n-3}{j-1}}\right], & \text{if } n \text{ is even,} \\ \left[(-1)^j\mathbf{1}^T_{\binom{n-3}{j}} \quad -(-1)^{j-2}\mathbf{1}^T_{\binom{n-3}{j-2}} \quad (-1)^{n-j}\mathbf{1}^T_{\binom{n-3}{j-3}} \quad -(-1)^{n-j-2}\mathbf{1}^T_{\binom{n-3}{j-1}}\right], & \text{if } n \text{ is odd,} \end{cases} \\
=&(-1)^j\left[\mathbf{1}^T_{\binom{n-3}{j}} \quad -\mathbf{1}^T_{\binom{n-3}{j-2}} \quad -\mathbf{1}^T_{\binom{n-3}{j-3}} \quad \mathbf{1}^T_{\binom{n-3}{j-1}}\right].
\end{aligned} \tag{6.5.9}$$

6.5.1.2 Step 2

Let us consider $B_n^{(\tau)}$. As explained in Step 1, we have that $B_n^{(\tau)}H_{n-3} = H_{n-3}D_n$ for $n \ge 3$, and the eigenvalues of $B_n^{(\tau)}$ are given by $(n-2)-2i$ for $i = 0, \dots, n-3$ with respective multiplicity $\binom{n-3}{i}$. By Lemma 6.5.1, $B_n(H_{n-3} \otimes \mathbf{c}) = (H_{n-3} \otimes \mathbf{c})D_n$. So, we let

$$X_2 := \frac{1}{\sqrt{2^{n-1}}}\begin{bmatrix} 0 & 0 \\ H_{n-3} \otimes \mathbf{c} & H_{n-3} \otimes \mathbf{c} \\ 0 & 0 \\ H_{n-3} \otimes \mathbf{c} & -H_{n-3} \otimes \mathbf{c} \end{bmatrix}.$$

Then, X_2 consists of 2^{n-2} eigenvectors of $A(\widetilde{Q}_n)$ such that $X_2^TX_2 = I$. Denote by Λ_2 the diagonal matrix such that $A(\widetilde{Q}_n)X_2 = X_2\Lambda_2$. Then, $\Lambda_2 = \operatorname{diag}(D_n, -D_n)$. For $j = 1, \dots, n-1$, we use $X_2(j)$ to denote the submatrix of X_2 that consists of all columns in X_2 that are eigenvectors of $A(\widetilde{Q}_n)$ corresponding to the eigenvalue

$n-2j$. We observe that for $j=1,\dots,n-1$, the entries $n-2j$ on the main diagonal of Λ_2 are derived from the $\binom{n-3}{j-1}$ eigenvalues $(n-2)-2(j-1)$ of $B_n^{(\tau)}$, and from the $\binom{n-3}{n-j-1}$ eigenvalues $(n-2)-2(n-j-1)$ of $B_n^{(\tau)}$ by changing their signs. Hence, there are $\binom{n-2}{j-1}$ columns in $X_2(j)$. Furthermore, considering the fact $\mathbf{c} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ concerning computation for $\mathbf{e}_{r_0}^T\left(\sqrt{2^n}X_2(j)\right)$, it follows from Remark 6.5.2 that

$$\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \left(\sqrt{2^n}X_2(j)\right) = \sqrt{2}\begin{bmatrix} \mathbf{0}^T_{\binom{n-3}{j-1}} & \mathbf{0}^T_{\binom{n-3}{j-2}} \\ \mathbf{1}^T_{\binom{n-3}{j-1}} & -\mathbf{1}^T_{\binom{n-3}{j-2}} \\ (-1)^j\mathbf{1}^T_{\binom{n-3}{j-1}} & (-1)^{j+1}\mathbf{1}^T_{\binom{n-3}{j-2}} \end{bmatrix}. \tag{6.5.10}$$

6.5.1.3 Step 3

We now consider spectral properties of $C_n = B_n^{(\tau)} - 2\mathbf{e}_1\mathbf{e}_1^T$ where $n \geq 3$. Since $D_n = \frac{1}{2^{n-3}}H_{n-3}^T B_n^{(\tau)} H_{n-3}$ and $\mathbf{e}_1^T H_{n-3} = \mathbf{1}^T$, we have

$$\frac{1}{2^{n-3}}H_{n-3}^T C_n H_{n-3} = D_n - \frac{1}{2^{n-4}}\mathbf{1}\mathbf{1}^T.$$

By a similarity transformation on C_n, the spectrum of C_n is the same as that of $D_n - \frac{1}{2^{n-4}}\mathbf{1}\mathbf{1}^T$, and any eigenvector of C_n can be expressed as $H_{n-3}\mathbf{x}$ for some eigenvector $\mathbf{x}$ of $D_n - \frac{1}{2^{n-4}}\mathbf{1}\mathbf{1}^T$.

Lemma 6.5.3. *[36] Let $C = D + \sigma\mathbf{u}\mathbf{u}^T$ where $\sigma \leq 0$, $\mathbf{u} \in \mathbb{R}^n$ and $D = \operatorname{diag}(d_1,\dots,d_n)$ with $d_1 \geq \cdots \geq d_n$. Suppose that $c_1,\dots,c_n$ are the eigenvalues of C where $c_1 \geq \cdots \geq c_n$. Then,*

$$\begin{cases} d_{i+1} \leq c_i \leq d_i, & i = 1,\dots,n-1, \\ d_n + \sigma\mathbf{u}^T\mathbf{u} \leq c_n \leq d_n. \end{cases}$$

Lemma 6.5.4. *[1] Let $C = D + \sigma\mathbf{u}\mathbf{v}^T$ where $\sigma \in \mathbb{R}$, $\mathbf{u},\mathbf{v} \in \mathbb{R}^n$ and $D = \operatorname{diag}(d_1,\dots,d_n)$. Then, the characteristic polynomial $p(x)$ of C is*

$$p(x) = \prod_{i=1}^{n}(d_i - x) + \sigma\sum_{i=1}^{n} u_i v_i \prod_{\substack{j=1 \\ j\neq i}}^{n}(d_j - x).$$

Furthermore, if λ is not in the spectrum of D, then λ is an eigenvalue of C if and only if

$$q(\lambda) = 1 + \sigma \sum_{i=1}^{n} \frac{u_i v_i}{(d_i - \lambda)} = 0.$$

Lemma 6.5.5. *[27] Let $\sigma \in \mathbb{R}$, $\mathbf{u} \in \mathbb{R}^n$ and $D = \operatorname{diag}(d_1, \ldots, d_n)$. Suppose that λ is not in the spectrum of D. If λ is an eigenvalue of $D + \sigma \mathbf{u}\mathbf{u}^T$, then $(D - \lambda I)^{-1}\mathbf{u}$ is an eigenvector of $D + \sigma \mathbf{u}\mathbf{u}^T$ associated to λ.*

The spectral property of $C_3 = [-1]$ is obvious. We assume $n \geq 4$. By Lemma 6.5.4, the characteristic polynomial $\phi(x)$ of $D_n - \frac{1}{2^{n-4}}\mathbf{1}\mathbf{1}^T$ is given by

$$\phi(x) = \prod_{j=0}^{n-3} (\lambda_j - x)^{\binom{n-3}{j}} - \frac{1}{2^{n-4}} \sum_{i=0}^{n-3} \binom{n-3}{i} (\lambda_i - x)^{\binom{n-3}{i}-1} \prod_{\substack{j=0 \\ j \neq i}}^{n-3} (\lambda_j - x)^{\binom{n-3}{j}}$$

where $\lambda_j = (n-2) - 2j$ for $j = 0, \ldots, n-3$. It can be checked that $\phi(\lambda_0) \neq 0$ and $\phi(\lambda_{n-3}) \neq 0$. Clearly, $\phi(\lambda_j) = 0$ for $j = 1, \ldots, n-4$. Fix $j_0 \in \{1, \ldots, n-4\}$. Note that $(\lambda_{j_0} - x)^{\binom{n-3}{j_0}}$ is a factor of $\prod_{j=0}^{n-3} (\lambda_j - x)^{\binom{n-3}{j}}$, and is also a factor of $\frac{1}{2^{n-4}} \binom{n-3}{i} (\lambda_i - x)^{\binom{n-3}{i}-1} \prod_{\substack{j=0 \\ j \neq i}}^{n-3} (\lambda_j - x)^{\binom{n-3}{j}}$ for $i \in \{0, \ldots, n-3\}$ with $i \neq j_0$. Considering the term $\frac{1}{2^{n-4}} \binom{n-3}{j_0} (\lambda_{j_0} - x)^{\binom{n-3}{j_0}-1} \prod_{\substack{j=0 \\ j \neq j_0}}^{n-3} (\lambda_j - x)^{\binom{n-3}{j}}$ in $\phi(x)$, we find that $\phi^{(k)}(\lambda_{j_0}) = 0$ for $1 \leq k \leq \binom{n-3}{j_0} - 2$, and $\phi^{\left(\binom{n-3}{j_0}-1\right)}(\lambda_{j_0}) \neq 0$. Thus, the multiplicity of eigenvalue λ_{j_0} of C_n for $j_0 = 1, \ldots, n-4$ is $\binom{n-3}{j_0} - 1$. Therefore, the $2^{n-3} - (n-2)$ eigenvalues of C_n are given by $(n-2) - 2j$ for $1 \leq j \leq n-4$ with respective multiplicity $\binom{n-3}{j} - 1$, and the remaining $n-2$ eigenvalues of C_n are not in the spectrum of $B_n^{(\tau)}$ (and D_n).

Now, we consider eigenvectors corresponding to the $2^{n-3} - (n-2)$ eigenvalues of C_n that are in the spectrum of D_n, where $n \geq 5$. Let $j \in \{1, \ldots, n-4\}$, and $m = \binom{n-3}{j}$. Suppose that $p_1, \ldots, p_m$ are indices such that $\mathbf{e}_{p_s}^T D_n \mathbf{e}_{p_s} = \lambda_j$ for $s = 1, \ldots, m$. Then, for $1 \leq i \leq m-1$, we have

$$\left(D_n - \frac{1}{2^{n-4}} J\right) \left(\sum_{k=1}^{i} \mathbf{e}_{p_k} - i\mathbf{e}_{p_{i+1}}\right) = \lambda_j \left(\sum_{k=1}^{i} \mathbf{e}_{p_k} - i\mathbf{e}_{p_{i+1}}\right).$$

So, $\left(\sum_{k=1}^{i} \mathbf{e}_{p_k} - i\mathbf{e}_{p_{i+1}}\right)$ is an eigenvector of $D_n - \frac{1}{2^{n-4}} J$. It follows from Remark 6.5.2 that the first and last entries of $H_{n-3} \left(\sum_{k=1}^{i} \mathbf{e}_{p_k} - i\mathbf{e}_{p_{i+1}}\right)$ are zero. Hence, there exist $\binom{n-3}{j} - 1$ mutually orthonormal eigenvectors $\mathbf{y}$ of $D_n - \frac{1}{2^{n-4}}J$ corresponding to eigenvalue $(n-2) - 2j$ for $1 \leq j \leq n-4$ such that the first and last entries of $H_{n-3}\mathbf{y}$ are zero. We denote by Y_1 the matrix that consists of those $2^{n-3} - (n-2)$ eigenvectors. We note that eigenvectors corresponding to distinct eigenvalues of a symmetric matrix are orthogonal. Thus, $Y_1^T Y_1 = I$. Let

$$X_3 := \frac{1}{\sqrt{2^{n-1}}} \begin{bmatrix} H_{n-3}Y_1 \otimes \mathbf{c} & H_{n-3}Y_1 \otimes \mathbf{c} \\ 0 & 0 \\ H_{n-3}Y_1 \otimes \mathbf{c} & -H_{n-3}Y_1 \otimes \mathbf{c} \\ 0 & 0 \end{bmatrix}.$$

Then, for each column $\mathbf{y}$ of Y_1, $(\mathbf{y}^T H_{n-3}^T \otimes \mathbf{c}^T)(H_{n-3}\mathbf{y} \otimes \mathbf{c}) = 2^{n-2}$. This implies that X_3 consists of $2^{n-2} - 2(n-2)$ eigenvectors of $A(\widetilde{Q}_n)$ such that $X_3^T X_3 = I$. We denote by Λ_3 the diagonal matrix such that $A(\widetilde{Q}_n)X_3 = X_3\Lambda_3$.

For $2 \leq j \leq n-2$, we use $X_3(j)$ to denote the submatrix of X_3 that consists of all columns in X_3 that are eigenvectors of $A(\widetilde{Q}_n)$ associated to the eigenvalue $n-2j$. Note (6.5.3) and (6.5.4) with Lemma 6.5.1. The entries $n-2j$ on the main diagonal of Λ_3 are derived from the $\binom{n-3}{j-1} - 1$ eigenvalues $(n-2) - 2(j-1)$ of C_n, and from the $\binom{n-3}{n-j-1} - 1$ eigenvalues $(n-2) - 2(n-j-1)$ of C_n by changing their signs. Thus, there are $\binom{n-2}{j-1} - 2$ columns in $X_3(j)$.

From the first and last rows of $H_{n-3}Y_1$, we have $\mathbf{e}_i^T X_3 = 0$ for

$$i \in \{1, 2, 2^{n-2} - 1, 2^{n-2}, 2^{n-1} + 1, 2^{n-1} + 2, 2^{n-1} + 2^{n-2} - 1, 2^{n-1} + 2^{n-2}\}.$$

Moreover,

$$\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} X_3 = 0. \tag{6.5.11}$$

6.5.1.4 Step 4

Let $n \geq 4$. We shall consider the $(n-2)$ eigenvalues of C_n not in the spectrum of D_n (explained in Step 3) and corresponding eigenvectors, where $\frac{1}{2^{n-3}} H_{n-3}^T C_n H_{n-3} = D_n - \frac{1}{2^{n-4}}J$. We denote by $\mu_1, \ldots, \mu_{n-2}$ those $(n-2)$ eigenvalues. We assume $\mu_1 \geq \cdots \geq \mu_{n-2}$. Let $\lambda_j = (n-2) - 2j$ for $j = 0, \ldots, n-3$. Since $\mu_1, \ldots, \mu_{n-2}$ are not in the spectrum of D_n, it follows from Lemma 6.5.3 that

$$\begin{cases} \lambda_j < \mu_j < \lambda_{j-1}, & \text{for } j = 1, \dots, n-3, \\ -n+2 \leq \mu_{n-2} < \lambda_{n-3}. \end{cases} \tag{6.5.12}$$

Let $i = 1, \dots, n-2$. By Lemma 6.5.5, $(D_n - \mu_i I)^{-1}\mathbf{1}$ is an eigenvector of $D_n - \frac{1}{2^{n-4}}J$ associated to μ_i. Without loss of generality, the eigenvector $(D_n - \mu_i I)^{-1}\mathbf{1}$ is of the form

$$\mathbf{v}_i^T = \begin{bmatrix} v_0 \mathbf{1}^T_{\binom{n-3}{0}} & v_1 \mathbf{1}^T_{\binom{n-3}{1}} & \cdots & v_{n-3}\mathbf{1}^T_{\binom{n-3}{n-3}} \end{bmatrix} \tag{6.5.13}$$

where $v_j = \frac{1}{\lambda_j - \mu_i}$ for $0 \leq j \leq n-3$. Let $\hat{\mathbf{v}}_i = (v_0, \dots, v_{n-3})^T$. Then, $(D_n - \frac{1}{2^{n-4}}J)\mathbf{v}_i = \mu_i \mathbf{v}_i$ implies that $(\mu_i, \hat{\mathbf{v}}_i)$ is an eigen-pair of the matrix given by

$$\widehat{D}_n := \operatorname{diag}(\lambda_0, \dots, \lambda_{n-3}) - \frac{1}{2^{n-4}}\mathbf{1}_{n-2}\left[\binom{n-3}{0} \quad \cdots \quad \binom{n-3}{n-3}\right]. \tag{6.5.14}$$

Therefore, the $(n-2)$ eigenvalues of C_n not in the spectrum of D_n are the same as those of $\widehat{D}_n$.

Remark 6.5.6. One can find an equitable partition on $D_n - \frac{1}{2^{n-4}}J$ to deduce $\widehat{D}_n$.

Now, we consider the k_0^{th}, s_0^{th}, and r_0^{th} entries of the eigenvectors of $A(\widetilde{Q}_n)$ corresponding to the eigenvalues $\pm\mu_1, \dots, \pm\mu_{n-2}$ where $n \geq 4$. Since $\mu_1, \dots, \mu_{n-2}$ are not in the spectrum of $\operatorname{diag}(\lambda_0, \dots, \lambda_{n-3})$, we find from Lemma 6.5.4 that the eigenvalues of $\widehat{D}_n$ are given by the roots of a polynomial

$$q_1(x) = 2^{n-4} - \sum_{j=0}^{n-3} \frac{\binom{n-3}{j}}{\lambda_j - x}. \tag{6.5.15}$$

Define Y_2 to be the $2^{n-3} \times (n-2)$ matrix whose i^{th} column is $\frac{1}{\nu_i}(D_n - \mu_i I)^{-1}\mathbf{1}$ for $i = 1, \dots, n-2$ where

$$\nu_i := \left\| (D_n - \mu_i I)^{-1}\mathbf{1} \right\| = \sqrt{\sum_{j=0}^{n-3} \frac{\binom{n-3}{j}}{(\lambda_j - \mu_i)^2}}.$$

Then, Y_2 consists of $(n-2)$ unit eigenvectors of $D_n - \frac{1}{2^{n-4}}J$. Let

$$X_4 := \frac{1}{\sqrt{2^{n-1}}}\begin{bmatrix} H_{n-3}Y_2 \otimes \mathbf{c} & H_{n-3}Y_2 \otimes \mathbf{c} \\ 0 & 0 \\ H_{n-3}Y_2 \otimes \mathbf{c} & -H_{n-3}Y_2 \otimes \mathbf{c} \\ 0 & 0 \end{bmatrix}.$$

Then, X_4 consists of $2(n-2)$ unit eigenvectors of $A(\widetilde{Q}_n)$ corresponding to the eigenvalues $\pm\mu_1, \dots, \pm\mu_{n-2}$. Furthermore, we use Λ_4 to denote the diagonal matrix such that $A(\widetilde{Q}_n)X_4 = X_4\Lambda_4$. Since $q_1(\mu_i) = 0$ for $i = 1, \dots, n-2$, we see from (6.5.13) and (6.5.15) that

$$\mathbf{1}^T(D_n - \mu_i I)^{-1}\mathbf{1} = \sum_{j=0}^{n-3} \frac{\binom{n-3}{j}}{\lambda_j - \mu_i} = 2^{n-4}.$$

Hence, for $n \geq 4$, we have

$$\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} X_4 = \frac{2^{n-4}}{\sqrt{2^{n-1}}}\begin{bmatrix} \frac{1}{\nu_1} & \cdots & \frac{1}{\nu_{n-2}} & \frac{1}{\nu_1} & \cdots & \frac{1}{\nu_{n-2}} \\ 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix}. \tag{6.5.16}$$

Now, we claim that columns in X_4 are mutually orthogonal. In order to establish this claim, we first consider the case X_4 when $n = 4$ in Remark 6.5.7, and then we show that for $n \geq 5$, the spectrum of $\mathrm{diag}(\widehat{D}_n, -\widehat{D}_n)$ consists of simple eigenvalues—that is, $\pm\mu_1, \dots, \pm\mu_{n-2}$ are distinct.

Remark 6.5.7. It can be checked that two eigenvectors $(D_4 - \sqrt{2}I)^{-1}\mathbf{1}$ and $(D_4 + \sqrt{2}I)^{-1}\mathbf{1}$ of $D_4 - J$ are orthogonal where $D_4 = \mathrm{diag}(2, 0)$. It follows that $X_4^T X_4 = I$ for $n = 4$. Furthermore, one can find that $\widehat{D}_4 = \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix}$ and $-\widehat{D}_4$ have the same eigenvalues as $\pm\sqrt{2}$; so, the eigenvalues of $\mathrm{diag}(\widehat{D}_4, -\widehat{D}_4)$ are not simple.

Consider $n \geq 5$. Note that $\lambda_j = -\lambda_{n-2-j}$ for $j = 1, \dots, n-3$. Let $\lambda_{n-2} = (n-2) - 2(n-2)$. Then, $\lambda_0 = -\lambda_{n-2}$. So, $-\widehat{D}_n$ can be recast as

$$-\widehat{D}_n = \mathrm{diag}(\lambda_{n-2}, \lambda_{n-3}, \lambda_{n-4}, \dots, \lambda_1) + \frac{1}{2^{n-4}}\mathbf{1}_{n-2}\left[\binom{n-3}{0} \quad \cdots \quad \binom{n-3}{n-3}\right].$$

From Lemma 6.5.4, the eigenvalues of $-\widehat{D}_n$ are given by the roots of a polynomial

$$q_2(x) = 2^{n-4} + \sum_{j=1}^{n-2} \frac{\binom{n-3}{j-1}}{\lambda_j - x}.$$

We note that $-\mu_1,\ldots,-\mu_{n-2}$ are the roots of $q_2(x)$; and by (6.5.12), $-\lambda_{i-1} < -\mu_i < -\lambda_i$ for $i = 1,\ldots,n-3$, and $-\lambda_{n-3} < -\mu_{n-2} \le n-2$. That is, $\lambda_{j+1} < -\mu_{n-2-j} < \lambda_j$ for $1 \le j \le n-3$ and $\lambda_1 < -\mu_{n-2} \le \lambda_0$. Hence, $q_1(x)$ and $q_2(x)$ have exactly one root in each interval $(\lambda_{i+1},\lambda_i)$ for $i = 1,\ldots,n-4$; in $(\lambda_1,\lambda_0]$; and in $[\lambda_{n-2},\lambda_{n-3})$. Therefore, we only need to show that in each of those intervals, $q_1(x)$ and $q_2(x)$ do not have a common root in order to prove that $\pm\mu_1,\ldots,\pm\mu_{n-2}$ are distinct.

Lemma 6.5.8. *Let $n \ge 5$. Then, $2^{n-4} \ge \binom{n-3}{\frac{n-3}{2}}$ for $n-3$ even; $2^{n-4} \ge \frac{4}{3}\binom{n-3}{\lceil\frac{n-3}{2}\rceil}$ for $n-3$ odd; and $2^{n-4} > \frac{1}{3}\binom{n-3}{\frac{n-3}{2}} + \frac{6}{5}\binom{n-3}{\frac{n-3}{2}+1}$ for $n-3$ even.*

Proof. We shall use induction on n to prove $2^{n-4} \ge \binom{n-3}{\frac{n-3}{2}}$ for $n-3$ even. Clearly, it holds for $n = 5$. Suppose that for $k \ge 5$ with $k-3$ even, $2^{k-4} \ge \binom{k-3}{\frac{k-3}{2}}$. Since $\binom{k-1}{\frac{k-1}{2}} = \frac{4(k-1)(k-2)}{(k-1)^2}\binom{k-3}{\frac{k-3}{2}} < 4\binom{k-3}{\frac{k-3}{2}}$, we have

$$2^{k-2} = 4\cdot 2^{k-4} \ge 4\binom{k-3}{\frac{k-3}{2}} > \binom{k-1}{\frac{k-1}{2}}.$$

By induction, we obtain the result, as desired. Similarly, one can establish the remaining results from induction. $\square$

Lemma 6.5.9. *Let $n \ge 5$. Then, for $j = 0,\ldots,n-3$,*

$$q_1(n-3-2j) > 0 \text{ and } q_2(n-3-2j) > 0.$$

Proof. Let $\lambda_j = (n-2)-2j$ for $0 \le j \le n-3$. Given $x_0 = n-3-2j_0$ for $0 \le j_0 \le n-3$, we have $\lambda_j - x_0 = 1 + 2(j_0 - j)$. So, from $2^{n-4} = \frac{1}{2}\sum_{j=0}^{n-3}\binom{n-3}{j}$, $q_1(x_0)$ can be written as

$$\begin{aligned} q_1(x_0) = {} & \left(\frac{1}{2} - \frac{1}{1+2j_0}\right)\binom{n-3}{0} + \cdots + \left(\frac{1}{2} - \frac{1}{1+2}\right)\binom{n-3}{j_0-1} + \left(\frac{1}{2} - \frac{1}{1}\right)\binom{n-3}{j_0} \\ & + \left(\frac{1}{2} - \frac{1}{1-2}\right)\binom{n-3}{j_0+1} + \cdots + \left(\frac{1}{2} - \frac{1}{1+2(j_0-(n-3))}\right)\binom{n-3}{n-3}. \end{aligned}$$

Evidently, $\frac{1}{2} - \frac{1}{1+2(j_0-j)} < 0$ if and only if $j = j_0$. If $\binom{n-3}{j_0} \le \binom{n-3}{j_0+1}$ then $q_1(x_0) > 0$. By the unimodality of the binomial coefficients, we only consider the case $j_0 \ge \lceil\frac{n-3}{2}\rceil$. For $k = 0,\ldots,n-3$, let $p(k) = \left(\frac{1}{2} - \frac{1}{1+2(j_0-k)}\right)\binom{n-3}{k} + \left(\frac{1}{2} - \frac{1}{1+2(j_0-(n-3-k))}\right)\binom{n-3}{n-3-k}$. Note that $\binom{n-3}{k} = \binom{n-3}{n-3-k}$ and $p(k) = p(n-3-k)$. Since $\frac{1}{1+2(j_0-k)} + \frac{1}{1+2(j_0-(n-3-k))} = \frac{2+4j_0-2(n-3)}{(1+2(j_0-k))(1+2(j_0-(n-3-k)))}$, we find from $j_0 \ge \lceil\frac{n-3}{2}\rceil$ that if $1+2(j_0-k) > 0$ and $1+2(j_0-(n-3-k)) < 0$, then $p(k) > \frac{1}{2}\binom{n-3}{k} + \frac{1}{2}\binom{n-3}{n-3-k}$.

Suppose that $n-3$ is even and $j_0 = \frac{n-3}{2}$. Then, for $0 \le i \le \frac{n-3}{2} - 1$, we have $1 + 2(j_0 - i) > 0$ and $1 + 2(j_0 - (n-3-i) < 0$. So, $p(i) > \frac{1}{2}\binom{n-3}{i} + \frac{1}{2}\binom{n-3}{n-3-i}$. By Lemma 6.5.8, we obtain

$$q_1(x_0) = -\frac{1}{2}\binom{n-3}{\frac{n-3}{2}} + \sum_{i=0}^{\frac{n-3}{2}-1} p(i) > -\binom{n-3}{\frac{n-3}{2}} + \frac{1}{2}\sum_{j=0}^{n-3}\binom{n-3}{j} = 2^{n-4} - \binom{n-3}{\frac{n-3}{2}} \ge 0.$$

Assume that $n-3$ is odd and $j_0 = \lceil \frac{n-3}{2} \rceil$, *i.e.*, $j_0 = \frac{n-3}{2} + \frac{1}{2}$. By a similar argument as in the previous case, we obtain $p(i) > \frac{1}{2}\binom{n-3}{i} + \frac{1}{2}\binom{n-3}{n-3-i}$ for $i = 0, \ldots, \frac{n-3}{2} - \frac{3}{2}$. Note that $p(j_0) = (\frac{1}{2} - \frac{1}{3})\binom{n-3}{j_0-1} + (\frac{1}{2} - 1)\binom{n-3}{j_0}$. By Lemma 6.5.8, $q_1(x) = p(j_0) + \sum_{i=0}^{\frac{n-3}{2}-\frac{3}{2}} p(i) > -\frac{4}{3}\binom{n-3}{\lceil\frac{n-3}{2}\rceil} + \frac{1}{2}\sum_{j=0}^{n-3}\binom{n-3}{j} = 2^{n-4} - \frac{4}{3}\binom{n-3}{\lceil\frac{n-3}{2}\rceil} \ge 0$.

Consider the case $j_0 = \lceil \frac{n-3}{2} \rceil + 1$. If $n-3$ is odd, then $p(j_0) = -\frac{1}{7}\binom{n-3}{j_0}$ and $p(j_0 - 1) = \frac{7}{15}\binom{n-3}{j_0-1}$. Since $\binom{n-3}{j_0-1} > \binom{n-3}{j_0}$, we have $p(j_0-1) + p(j_0) > 0$. It follows that $q_1(x_0) > 0$. Let $n-3$ be even. One can check that $p(i) > \frac{1}{2}\binom{n-3}{i} + \frac{1}{2}\binom{n-3}{n-3-i}$ for $i = 0, \ldots, \frac{n-3}{2} - 2$. Then, $q_1(x_0) = \frac{1}{6}\binom{n-3}{\frac{n-3}{2}} - \frac{1}{5}\binom{n-3}{\frac{n-3}{2}-1} + \sum_{i=0}^{\frac{n-3}{2}-2} p(i)$. From Lemma 6.5.8, $q_1(x_0) > -\frac{1}{3}\binom{n-3}{\frac{n-3}{2}} - \frac{6}{5}\binom{n-3}{\frac{n-3}{2}+1} + \frac{1}{2}\sum_{j=0}^{n-3}\binom{n-3}{j} = 2^{n-4} - \frac{1}{3}\binom{n-3}{\frac{n-3}{2}} - \frac{6}{5}\binom{n-3}{\frac{n-3}{2}+1} > 0$.

Finally, suppose $j_0 \ge \lceil \frac{n-3}{2} \rceil + 2$. Then, $p(j_0) \ge -\frac{1}{9}\binom{n-3}{j_0}$ and $p(j_0 - 1) \ge \frac{11}{21}\binom{n-3}{j_0-1}$ where both equalities hold for $j_0 = \lceil \frac{n-3}{2} \rceil + 2$ with $n-3$ even. So, $p(j_0-1) + p(j_0) > 0$. Hence, $q_1(x_0) > 0$. Therefore, $q_1(n-3-2j) > 0$ for $0 \le j \le n-3$, as desired.

An analogous argument applies for $q_2(n-3-2j) > 0$ for $0 \le j \le n-3$. Then, one can see in a similar setting as above that the argument goes in a reverse way; if $\binom{n-3}{j_0-1} \ge \binom{n-3}{j_0}$ then $q_2(n-3-2j_0) > 0$, and so we consider $j_0 \le \lfloor \frac{n-3}{2} \rfloor$. As done above with Lemma 6.5.8, our desired result can be established. $\square$

Remark 6.5.10. Let $n = 4$. Then, $q_1(-1) < 0$, $q_2(-1) > 0$, $q_1(1) > 0$ and $q_2(1) < 0$.

Proposition 6.5.11. *For $n \ge 5$, all eigenvalues of* $\operatorname{diag}\left(\widehat{D}_n, -\widehat{D}_n\right)$ *are simple.*

Proof. Let $\lambda_j = (n-2) - 2j$ for $0 \le j \le n-2$. Consider the graph of $q_1(x)$. For $0 \le j \le n-3$, each line $x = \lambda_j$ is a vertical asymptote of $q_1(x)$. Moreover, $q_1'(x) < 0$ except at $x = \lambda_j$ for $0 \le j \le n-3$. Similarly, $q_2(x)$ has vertical asymptotes $x = \lambda_i$ for $i = 1 \le i \le n-2$, and $q_2(x)$ is strictly increasing except at $x = \lambda_i$ for $1 \le i \le n-2$. By Lemma 6.5.9, there is a number c in $(\lambda_{i+1}, \lambda_i)$ for $i = 0, \ldots, n-3$ such that $q_1(c) > 0$ and $q_2(c) > 0$. It follows from the intermediate value theorem that $q_1(x)$ and $q_2(x)$ have a root in $(c, \lambda_i]$ and $[\lambda_{i+1}, c)$, respectively. Hence, $q_1(x)$ and $q_2(x)$ do not have a common root in each interval $[\lambda_{i+1}, \lambda_i]$ for $i = 0, \ldots, n-3$. As explained in the earlier part of Lemma 6.5.8, this is enough to establish the conclusion. $\square$

Corollary 6.5.12. *Let $n \geq 5$. The eigenvalues $\pm\mu_1, \ldots, \pm\mu_{n-2}$ of $A(\widetilde{Q}_n)$ are distinct, and so X_4 consists of $2(n-2)$ mutually orthonormal columns.*

Remark 6.5.13. Let $n \geq 5$. Define μ_{n-2+i} to be $-\mu_i$ for $1 \leq i \leq n-2$. Then, for $1 \leq j \leq 2(n-2)$, j^{th} column of X_4 is an eigenvector of $A(\widetilde{Q}_n)$ associated to μ_j.

Let $n \geq 4$, and let

$$X := \begin{bmatrix} X_1 & X_2 & X_3 & X_4 \end{bmatrix} \text{ and } \Lambda := \operatorname{diag}(\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4). \tag{6.5.17}$$

Note that for any vectors $\mathbf{x}$ and $\mathbf{y}$ of the same size, $\mathbf{x} \otimes \mathbf{c}$ and $\mathbf{y} \otimes \mathbf{1}_2$ are orthogonal; that each column of X_2, X_3, and X_4 is in the form (6.5.3) or (6.5.4); that any entry on the main diagonal of Λ_4 does not appear on main diagonals of Λ_i for $i = 1, 2, 3$. It follows that X is orthogonal. Moreover, X diagonalises $A(\widetilde{Q}_n)$ so that $X^T A(\widetilde{Q}_n) X = \Lambda$. For $j = 0, \ldots, n$, $X(j)$ denotes the submatrix of X that consists of all columns in X that are eigenvectors of $A(\widetilde{Q}_n)$ corresponding to the eigenvalue $n - 2j$. We denote by $\tilde{h}_{n,j}^{l_1,l_2}(a, b)$ the number of columns in $\sqrt{2^n} X(j)$ whose entries indexed by l_1 and l_2 with $l_1 \neq l_2$ are a and b, respectively.

Summarizing this subsection about the spectral properties of $A(\widetilde{Q}_n)$, we have the following theorem.

Theorem 6.5.14. *Let $n \geq 4$, and let M be a $(2, 2, 2, \{3, 3\})$-matching with a distance-partite set $\{v_1, v_2\}$. Let $\widetilde{Q}_n = \widetilde{Q}_n^{(M)}$. Suppose that $s \in S_1(\{v_1, v_2\})$ and $k = v_1$. Then, the following hold:*

(i) The eigenvalues of $A(\widetilde{Q}_n)$ are given by $n - 2j$ for $0 \leq j \leq n$, and $\pm\mu_i$ for $1 \leq i \leq n-2$ where $\mu_1, \ldots, \mu_{n-2}$ are the eigenvalues of the matrix $\widehat{D}_n$ in (6.5.14)*.*

(ii) We have that $am(n) = am(-n) = 1$, $am(n-2) = am(-n+2) = n-1$, and $am(n-2j) = \binom{n}{j} - 2$ for $j = 2, \ldots, n-2$.

(iii) If $n = 4$, then $\mu_1 = -\mu_2$ and $\mu_2 = -\mu_1$. If $n \geq 5$, then $am(\mu_i) = am(-\mu_i) = 1$ for $i = 1, \ldots, n-2$.

(iv) The orthogonal matrix X in (6.5.17) *diagonalises $A(\widetilde{Q}_n)$ so that $X^T A(\widetilde{Q}_n) X = \Lambda$.*

(v) For $j = 0, \ldots, n$, $\tilde{h}_{n,j}^{k,s}(1, 1) = \binom{n-2}{j}$, $\tilde{h}_{n,j}^{k,s}(1, -1) = \binom{n-2}{j-2}$, $\tilde{h}_{n,j}^{k,s}(0, \sqrt{2}) = \binom{n-3}{j-1}$, $\tilde{h}_{n,j}^{k,s}(0, -\sqrt{2}) = \binom{n-3}{j-2}$, and $\tilde{h}_{n,j}^{k,s}(0, 0) = \binom{n-2}{j-1}$.

Proof. Inspecting Steps 1–4, the results can be established. In particular, from (6.5.8), (6.5.10) and (6.5.11), we obtain (v). $\square$

6.5.2 $\frac{\partial \Lambda}{\partial_{s_0,k_0}}$ and particular rows of V and $\frac{\partial V}{\partial_{s_0,k_0}}$ for $\widetilde{Q}_n$

We begin with modifying some conditions—unless stated otherwise in this subsection, we assume the same condition—for the notation introduced in Subsection 6.4.2. Assume that $n \geq 4$ and $\widetilde{A}_n = A(\widetilde{Q}_n)$ where $A(\widetilde{Q}_n)$ is of form (6.5.2). Recall that $s_0 = 2^{n-1} + 2^{n-2} + 1$, $k_0 = 1$, $r_0 = 2^n$ (if n is even), and $r_0 = 2^{n-1}$ (if n is odd). We consider the weight of the edge $s_0 \sim k_0$. Let $E = \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{s_0} \end{bmatrix}^T$. Assume that $\widetilde{A}_n = V \Lambda V^T$, where Λ is the diagonal matrix in (6.5.17), and columns of V consist of vectors in a differentiable eigenbasis evaluated at $h = 0$ in the context of $\widetilde{A}_n + hE$ as explained in Subsection 6.4.2. Let $j = 0, \ldots, n$, and $m = am(n - 2j)$. We use $\mathbf{x}_1^j, \ldots, \mathbf{x}_m^j$ to denote the columns of $X(j)$. Suppose that V is obtained from the algorithms described in Subsection 6.4.2, Vectors $\hat{\mathbf{x}}_1^j, \ldots, \hat{\mathbf{x}}_m^j$ denote m columns in V that are eigenvectors of $\widetilde{A}_n$ associated to eigenvalue $n - 2j$. Here we revisit the formula (6.4.1): for $i = 1, \ldots, 2^n$, $\left(\frac{\partial \Lambda}{\partial_{s_0,k_0}}\right)_{i,i} = \mathbf{e}_i^T V^T E V \mathbf{e}_i$.

We first consider the case that for an eigenspace Z corresponding to an eigenvalue of $\widetilde{A}_n$, the subspace spanned by columns of EZ is of dimension 1. If an eigenvalue of $\widetilde{A}_n$ is simple, then its corresponding column in V can be taken as that in X. Evidently, $am(n) = am(-n) = 1$. From (6.5.8) and (6.5.9), we have

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}}_1^0 & \hat{\mathbf{x}}_1^n \end{bmatrix} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \\ 1 & (-1)^{n+1} \end{bmatrix}. \tag{6.5.18}$$

For $V\mathbf{e}_{m_1} = \hat{\mathbf{x}}_1^0$ and $V\mathbf{e}_{m_2} = \hat{\mathbf{x}}_1^n$, we can see that

$$\left(\frac{\partial \Lambda}{\partial_{s_0,k_0}}\right)_{m_1,m_1} = \frac{1}{2^{n-1}} \text{ and } \left(\frac{\partial \Lambda}{\partial_{s_0,k_0}}\right)_{m_2,m_2} = -\frac{1}{2^{n-1}}. \tag{6.5.19}$$

Let $n \geq 5$. By (iii) of Theorem 6.5.14 and Remark 6.5.13, $am(\mu_i) = 1$ for $i = 1, \ldots, 2(n-2)$. Let $\mathbf{z}_1^i$ (resp. $\hat{\mathbf{z}}_1^i$) denote the column in X_4 (resp. V) corresponding to eigenvalue μ_i of $\widetilde{A}_n$ for $i = 1, \ldots, 2(n-2)$. Thus, from (6.5.16), for $i = 1, \ldots, 2(n-2)$,

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \hat{\mathbf{z}}_1^i = \frac{2^{n-4}}{\sqrt{2^{n-1}}} \begin{bmatrix} 0 \\ \frac{1}{\nu_i} \\ 0 \end{bmatrix} \tag{6.5.20}$$

where $\nu_{n-2+j} = \nu_j$ for $j = 1, \ldots, n-2$. It is straightforward that for $1 \leq i \leq 2(n-2)$ if $V\mathbf{e}_m = \hat{\mathbf{z}}_1^i$, then $\left(\frac{\partial \Lambda}{\partial_{s_0,k_0}}\right)_{m,m} = 0$.

Consider $n = 4$. Then, $am(\mu_1) = am(\mu_2) = 2$ where $\mu_1 = -\mu_2$. Let $\mathbf{z}_1^i$ and $\mathbf{z}_2^i$ (resp. $\hat{\mathbf{z}}_1^i$ and $\hat{\mathbf{z}}_2^i$) denote the columns in X_4 (resp. V) corresponding to eigenvalue μ_i for $i = 1, 2$. It follows from (6.5.16) that for $i = 1, 2$, the subspace spanned by $E\mathbf{z}_1^i$ and $E\mathbf{z}_2^i$ is of dimension 1. According to the algorithm with the notation described in Subsection 6.4.2, one can verify that $\delta_1 = 1$ and $\delta_2 = \frac{\nu_1}{\nu_2}$. Thus, $\hat{\mathbf{z}}_1^i = \frac{1}{\sqrt{\nu_1^2+\nu_2^2}}(\nu_2\mathbf{z}_1^i + \nu_1\mathbf{z}_2^i)$. Since $\mathbf{z}_1^i$ and $\mathbf{z}_2^i$ are orthogonal, it can be checked that $\hat{\mathbf{z}}_2^i = \frac{1}{\sqrt{\nu_1^2+\nu_2^2}}(-\nu_1\mathbf{z}_1^i + \nu_2\mathbf{z}_2^i)$. Then, $\mathbf{e}_{k_0}^T\hat{\mathbf{z}}_1^i = \frac{\sqrt{\nu_1^2+\nu_2^2}}{\sqrt{2^3}\nu_1\nu_2}$ and $\mathbf{e}_{k_0}^T\hat{\mathbf{z}}_2^i = 0$. By computations of ν_1 and ν_2, we can find that for $i \in \{1, 2\}$,

$$\begin{bmatrix} \mathbf{e}_{s_0}^T \\ \mathbf{e}_{k_0}^T \\ \mathbf{e}_{r_0}^T \end{bmatrix} \begin{bmatrix} \hat{\mathbf{z}}_1^i & \hat{\mathbf{z}}_2^i \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & 0 \\ 0 & 0 \end{bmatrix}. \tag{6.5.21}$$

For $V\mathbf{e}_{m_1} = \hat{\mathbf{z}}_1^i$ and $V\mathbf{e}_{m_2} = \hat{\mathbf{z}}_2^i$, we obtain $\left(\frac{\partial\Lambda}{\partial_{s_0,k_0}}\right)_{m_1,m_1} = \left(\frac{\partial\Lambda}{\partial_{s_0,k_0}}\right)_{m_2,m_2} = 0$.

Now, we investigate the case that for an eigenspace Z corresponding to an eigenvalue of $\widetilde{A}_n$, the subspace spanned by columns of EZ is of dimension 2. Let $j_0 = 1, \ldots, n-1$ and $m_0 = am(n-2j_0)$. By (v) of Theorem 6.5.14, we have $\tilde{h}_{n,j_0}^{k_0,s_0}(1,1) = \binom{n-2}{j_0}$, $\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1) = \binom{n-2}{j_0-2}$, $\tilde{h}_{n,j_0}^{k_0,s_0}(0,\sqrt{2}) = \binom{n-3}{j_0-1}$, and $\tilde{h}_{n,j_0}^{k_0,s_0}(0,-\sqrt{2}) = \binom{n-3}{j_0-2}$. For $1 \le j_0 \le n-2$, $\tilde{h}_{n,j_0}^{k_0,s_0}(1,1), \tilde{h}_{n,j_0}^{k_0,s_0}(0,\sqrt{2}) > 0$, and for $2 \le j_0 \le n-1$, $\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1), \tilde{h}_{n,j_0}^{k_0,s_0}(0,-\sqrt{2}) > 0$. So, the subspace spanned by $E\mathbf{x}_i^{j_0}$ for $1 \le i \le m_0$ is of dimension 2. We may assume that $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \mathbf{x}_1^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \mathbf{x}_2^{j_0} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 0 \\ \sqrt{2} \end{bmatrix}$ for $1 \le j_0 \le n-2$; and $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \mathbf{x}_1^{n-1} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ and $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \mathbf{x}_2^{n-1} = \frac{1}{\sqrt{2^n}} \begin{bmatrix} 0 \\ -\sqrt{2} \end{bmatrix}$.

We shall compute the entries of $\tilde{\mathbf{x}}_1^{j_0}$ and $\tilde{\mathbf{x}}_2^{j_0}$ that are indexed by s_0, k_0, and r_0 for $1 \le j_0 \le n-1$. Then, we need to consider two cases $1 \le j_0 \le n-2$ and $j_0 = n-1$ for the computations since $\begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \mathbf{x}_i^{j_0} \neq \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \mathbf{x}_i^{n-1}$ for $1 \le j_0 \le n-2$ and $i = 1, 2$. In order to obtain the related result (6.5.23), we consider the case $1 \le j_0 \le n-2$, and leave the remaining task for $j_0 = n-1$ to the reader—we note that $-\tilde{\mathbf{x}}_2^{n-1}$ is used in (6.5.23) for ease of exposition.

Let $j_0 = 1, \ldots, n-2$, and let us compute α_i and β_i for $i = 1, \ldots, m_0$. As explained in Subsection 6.4.2, $\alpha_1 = \beta_2 = 1$ and $\alpha_2 = \beta_1 = 0$. Consider the case $3 \le i \le m_0$.

We have

$$\left(\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\begin{bmatrix}\mathbf{x}_1^{j_0} & \mathbf{x}_2^{j_0}\end{bmatrix}\right)^{-1} = \left(\frac{1}{\sqrt{2^n}}\begin{bmatrix}1 & 0\\ 1 & \sqrt{2}\end{bmatrix}\right)^{-1} = \sqrt{2^n}\begin{bmatrix}1 & 0\\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}.$$

Note that for $3 \le i \le m_0$, either $\mathbf{e}_{k_0}^T\mathbf{x}_i^{j_0} = 1$ or $\mathbf{e}_{k_0}^T\mathbf{x}_i^{j_0} = 0$. So,

$$\begin{bmatrix}\alpha_i\\ \beta_i\end{bmatrix} = \begin{cases}\begin{bmatrix}1\\ 0\end{bmatrix}, & \text{if } \begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}1\\ 1\end{bmatrix};\\ \begin{bmatrix}1\\ -\sqrt{2}\end{bmatrix}, & \text{if } \begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}1\\ -1\end{bmatrix};\\ \begin{bmatrix}0\\ 1\end{bmatrix}, & \text{if } \begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}0\\ \sqrt{2}\end{bmatrix};\\ \begin{bmatrix}0\\ -1\end{bmatrix}, & \text{if } \begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}0\\ -\sqrt{2}\end{bmatrix}.\end{cases} \tag{6.5.22}$$

Remark 6.5.15. Let $3 \le i \le n-1$. By (v) of Theorem 6.5.14, we find that $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{n-1}$ is either $\begin{bmatrix}1\\ -1\end{bmatrix}$ or $\begin{bmatrix}0\\ -\sqrt{2}\end{bmatrix}$. One can verify that $\begin{bmatrix}\alpha_i\\ \beta_i\end{bmatrix} = \begin{bmatrix}1\\ 0\end{bmatrix}$ if $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{n-1} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}1\\ -1\end{bmatrix}$; and $\begin{bmatrix}\alpha_i\\ \beta_i\end{bmatrix} = \begin{bmatrix}0\\ 1\end{bmatrix}$ if $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{n-1} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}0\\ -\sqrt{2}\end{bmatrix}$.

We shall find an orthonormal basis $\{\tilde{\mathbf{x}}_1^{j_0}, \tilde{\mathbf{x}}_2^{j_0}\}$ of $\operatorname{span}\{\sum_{i=1}^{m_0}\alpha_i\mathbf{x}_i^{j_0}, \sum_{i=1}^{m_0}\beta_i\mathbf{x}_i^{j_0}\}$. Since the vectors $\mathbf{x}_1^{j_0}, \ldots, \mathbf{x}_{m_0}^{j_0}$ are mutually orthonormal,

$$\begin{aligned}\left\|\sum_{i=1}^{m_0}\alpha_i\mathbf{x}_i^{j_0}\right\|^2 =& |\{i|\alpha_i \neq 0, i = 1, \ldots, m_0\}|\\ =& \tilde{h}_{n,j_0}^{k_0,s_0}(1,1) + \tilde{h}_{n,j_0}^{k_0,s_0}(1,-1) = \binom{n-2}{j_0} + \binom{n-2}{j_0-2}.\end{aligned}$$

Let $\tilde{\mathbf{x}}_1^{j_0} = \frac{1}{\sqrt{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}}\sum_{i=1}^{m_0}\alpha_i\mathbf{x}_i^{j_0}$. Considering the orthogonality of $\mathbf{x}_1^{j_0}, \ldots, \mathbf{x}_{m_0}^{j_0}$ and the relation between the α_i's and β_i's in (6.5.22), the dot product of $\sum_{i=1}^{m_0}\alpha_i\mathbf{x}_i^{j_0}$ and $\sum_{i=1}^{m_0}\beta_i\mathbf{x}_i^{j_0}$ is $(-\sqrt{2})\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1) = -\sqrt{2}\binom{n-2}{j_0-2}$. Applying the Gram–Schmidt process to $\sum_{i=1}^{m_0}\alpha_i\mathbf{x}_i^{j_0}$ and $\sum_{i=1}^{m_0}\beta_i\mathbf{x}_i^{j_0}$, we obtain

$$\mathbf{u}_2^{j_0} = \sum_{i=1}^{m_0}\beta_i\mathbf{x}_i^{j_0} + \frac{\sqrt{2}\binom{n-2}{j_0-2}}{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}\sum_{i=1}^{m_0}\alpha_i\mathbf{x}_i^{j_0}.$$

For simplicity, let $\delta = \frac{\sqrt{2}\binom{n-2}{j_0-2}}{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}$. From the α_i's and β_i's in (6.5.22), we have

$$\begin{aligned}
\left\|\mathbf{u}_2^{j_0}\right\|^2 =& \left\|\sum_{i=1}^{m_0}(\delta\alpha_i+\beta_i)\mathbf{x}_i^{j_0}\right\|^2 \\
=&\sum_{i=1}^{m_0}(\delta^2\alpha_i^2+2\delta\alpha_i\beta_i+\beta_i^2) \\
=&\delta^2\tilde{h}_{n,j_0}^{k_0,s_0}(1,1)+(\delta-\sqrt{2})^2\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1)+\tilde{h}_{n,j_0}^{k_0,s_0}(0,\sqrt{2})+\tilde{h}_{n,j_0}^{k_0,s_0}(0,-\sqrt{2}) \\
=&\frac{2\binom{n-2}{j_0}\binom{n-2}{j_0-2}+\binom{n-2}{j_0-1}\left(\binom{n-2}{j_0}+\binom{n-2}{j_0-2}\right)}{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}.
\end{aligned}$$

So, we obtain $\tilde{\mathbf{x}}_2^{j_0} = \frac{1}{\|\mathbf{u}_2^{j_0}\|}\mathbf{u}_2^{j_0}$.

We compute the s_0^{th}, k_0^{th} and r_0^{th} rows of $\tilde{\mathbf{x}}_1^{j_0}$ and $\tilde{\mathbf{x}}_2^{j_0}$. By the α_i's in (6.5.22), we obtain

$$\begin{aligned}
\mathbf{e}_{s_0}^T\tilde{\mathbf{x}}_1^{j_0} =& \frac{1}{\sqrt{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}}\sum_{i=1}^{m_0}\alpha_i\mathbf{e}_{s_0}^T\mathbf{x}_i^{j_0} \\
=&\frac{\left(\tilde{h}_{n,j_0}^{k_0,s_0}(1,1)-\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1)\right)}{\sqrt{2^n}\sqrt{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}} = \frac{\binom{n-2}{j_0}-\binom{n-2}{j_0-2}}{\sqrt{2^n}\sqrt{\binom{n-2}{j_0}+\binom{n-2}{j_0-2}}}.
\end{aligned}$$

Similarly, one can find $\mathbf{e}_{k_0}^T\tilde{\mathbf{x}}_1^{j_0}$ as in (6.5.23). By the α_i's and β_i's in (6.5.22), we can find that

$$\begin{aligned}
\mathbf{e}_{s_0}^T\tilde{\mathbf{x}}_2^{j_0} =& \frac{1}{\|\mathbf{u}_2^{j_0}\|}\left(\sum_{i=1}^{m_0}\beta_i\mathbf{e}_{s_0}^T\mathbf{x}_i^{j_0}+\delta\sum_{i=1}^{m_0}\alpha_i\mathbf{e}_{s_0}^T\mathbf{x}_i^{j_0}\right) \\
=&\frac{1}{\|\mathbf{u}_2^{j_0}\|}\left(\frac{\sqrt{2}}{\sqrt{2^n}}\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1)+\frac{\sqrt{2}}{\sqrt{2^n}}\left(\tilde{h}_{n,j_0}^{k_0,s_0}(0,\sqrt{2})+\tilde{h}_{n,j_0}^{k_0,s_0}(0,-\sqrt{2})\right)\right) \\
&+\frac{1}{\|\mathbf{u}_2^{j_0}\|}\left(\delta\frac{1}{\sqrt{2^n}}\left(\tilde{h}_{n,j_0}^{k_0,s_0}(1,1)-\tilde{h}_{n,j_0}^{k_0,s_0}(1,-1)\right)\right) = \frac{\sqrt{2}\|\mathbf{u}_2^{j_0}\|}{\sqrt{2^n}}.
\end{aligned}$$

By a similar argument, $\mathbf{e}_{k_0}^T\tilde{\mathbf{x}}_2^{j_0}$ can be found as in (6.5.23). Moreover, (6.5.8), (6.5.9) and (6.5.10) yield that for $i=1,\dots,m_0$, $\mathbf{e}_{r_0}^T\mathbf{x}_i^{j_0} = \frac{(-1)^{j_0}}{\sqrt{2^n}}$ if $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}1\\1\end{bmatrix}$; $\mathbf{e}_{r_0}^T\mathbf{x}_i^{j_0} = \frac{(-1)^{j_0+1}}{\sqrt{2^n}}$ if $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}1\\-1\end{bmatrix}$; $\mathbf{e}_{r_0}^T\mathbf{x}_i^{j_0} = \frac{(-1)^{j_0}\sqrt{2}}{\sqrt{2^n}}$ if $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}0\\\sqrt{2}\end{bmatrix}$; and $\mathbf{e}_{r_0}^T\mathbf{x}_i^{j_0} = \frac{(-1)^{j_0+1}\sqrt{2}}{\sqrt{2^n}}$ if $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0} = \frac{1}{\sqrt{2^n}}\begin{bmatrix}0\\-\sqrt{2}\end{bmatrix}$. Then, as done for finding $\mathbf{e}_{s_0}^T\tilde{\mathbf{x}}_1^{j_0}$

and $\mathbf{e}_{s_0}^T\tilde{\mathbf{x}}_2^{j_0}$, one can check $\mathbf{e}_{r_0}^T\tilde{\mathbf{x}}_1^{j_0}$ and $\mathbf{e}_{r_0}^T\tilde{\mathbf{x}}_2^{j_0}$. Furthermore, computing $\tilde{\mathbf{x}}_1^{n-1}$ and $-\tilde{\mathbf{x}}_2^{n-1}$ wit Remark 6.5.15 as done above, we establish

$$\begin{aligned}&\begin{bmatrix}\mathbf{e}_{s_0}^T\\ \mathbf{e}_{k_0}^T\\ \mathbf{e}_{r_0}^T\end{bmatrix}\begin{bmatrix}\tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0}\end{bmatrix}\\ =&\frac{1}{\sqrt{2^n\omega_0}}\begin{bmatrix}\binom{n-2}{j_0}-\binom{n-2}{j_0-2} & \sqrt{4\binom{n-2}{j_0}\binom{n-2}{j_0-2}+2\omega_0\binom{n-2}{j_0-1}}\\ \binom{n-2}{j_0}+\binom{n-2}{j_0-2} & 0\\ (-1)^{j_0}\left(\binom{n-2}{j_0}-\binom{n-2}{j_0-2}\right) & (-1)^{j_0}\sqrt{4\binom{n-2}{j_0}\binom{n-2}{j_0-2}+2\omega_0\binom{n-2}{j_0-1}}\end{bmatrix}\end{aligned} \tag{6.5.23}$$

where $\omega_0=\binom{n-2}{j_0}+\binom{n-2}{j_0-2}$.

Now, we compute the rows of $\hat{\mathbf{x}}_1^{j_0}$ and $\hat{\mathbf{x}}_2^{j_0}$ that are indexed by s_0, k_0 and r_0, and the remaining diagonal entries in $\frac{\partial\Lambda}{\partial_{s_0,k_0}}$. Recall that $B^{j_0}=\begin{bmatrix}\tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0}\end{bmatrix}^T E\begin{bmatrix}\tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0}\end{bmatrix}$. For simplicity, let $a_0=\binom{n-2}{j_0}-\binom{n-2}{j_0-2}$ and $b_0=\sqrt{4\binom{n-2}{j_0}\binom{n-2}{j_0-2}+2\omega_0\binom{n-2}{j_0-1}}$. Then,

$$B^{j_0}=\frac{1}{2^n}\begin{bmatrix}2a_0 & b_0\\ b_0 & 0\end{bmatrix}.$$

Let $c_0=\sqrt{\omega_0\binom{n}{j_0}}$. Then, $a_0^2+b_0^2=c_0^2$. One can verify that B^{j_0} can be diagonalised by an orthogonal matrix

$$U=\frac{1}{\sqrt{2c_0(c_0-a_0)}}\begin{bmatrix}b_0 & a_0-c_0\\ -a_0+c_0 & b_0\end{bmatrix}.$$

Then, we obtain

$$\begin{bmatrix}\mathbf{e}_{s_0}^T\\ \mathbf{e}_{k_0}^T\\ \mathbf{e}_{r_0}^T\end{bmatrix}\begin{bmatrix}\hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0}\end{bmatrix}=\begin{bmatrix}\mathbf{e}_{s_0}^T\\ \mathbf{e}_{k_0}^T\\ \mathbf{e}_{r_0}^T\end{bmatrix}\begin{bmatrix}\tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0}\end{bmatrix}U=\frac{1}{\sqrt{2^n}}\begin{bmatrix}\frac{b_0\sqrt{c_0}}{\sqrt{2\omega_0(c_0-a_0)}} & \frac{\sqrt{c_0(c_0-a_0)}}{\sqrt{2\omega_0}}\\ \frac{b_0\sqrt{\omega_0}}{\sqrt{2c_0(c_0-a_0)}} & -\frac{\sqrt{\omega_0(c_0-a_0)}}{\sqrt{2c_0}}\\ \frac{(-1)^{j_0}b_0\sqrt{c_0}}{\sqrt{2\omega_0(c_0-a_0)}} & \frac{(-1)^{j_0}\sqrt{c_0(c_0-a_0)}}{\sqrt{2\omega_0}}\end{bmatrix}. \tag{6.5.24}$$

Furthermore, let p and q be indices such that $V\begin{bmatrix}\mathbf{e}_p & \mathbf{e}_q\end{bmatrix}=\begin{bmatrix}\hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0}\end{bmatrix}$. Since the eigenvalues of B^{j_0} comprise the main diagonal of $\begin{bmatrix}\mathbf{e}_p^T\\ \mathbf{e}_q^T\end{bmatrix}\frac{\partial\Lambda}{\partial_{s_0,k_0}}\begin{bmatrix}\mathbf{e}_p & \mathbf{e}_q\end{bmatrix}$, it can be checked that

$$\begin{bmatrix}\mathbf{e}_p^T\\ \mathbf{e}_q^T\end{bmatrix}\frac{\partial\Lambda}{\partial_{s_0,k_0}}\begin{bmatrix}\mathbf{e}_p & \mathbf{e}_q\end{bmatrix}=\frac{1}{2^n}\begin{bmatrix}a_0+c_0 & 0\\ 0 & a_0-c_0\end{bmatrix}. \tag{6.5.25}$$

Remark 6.5.16. Regarding $\frac{\partial V}{\partial_{s_0,k_0}}$, we use the following later:

$$(\hat{\mathbf{x}}_1^{j_0})^T E\hat{\mathbf{x}}_1^{j_0}=(U\mathbf{e}_1)^T\begin{bmatrix}(\tilde{\mathbf{x}}_1^{j_0})^T\\ (\tilde{\mathbf{x}}_2^{j_0})^T\end{bmatrix}E\begin{bmatrix}\tilde{\mathbf{x}}_1^{j_0} & \tilde{\mathbf{x}}_2^{j_0}\end{bmatrix}(U\mathbf{e}_1)=(U\mathbf{e}_1)^TB^{j_0}(U\mathbf{e}_1)=\frac{1}{2^n}(a_0+c_0),$$

and similarly, $(\hat{\mathbf{x}}_2^{j_0})^T E\hat{\mathbf{x}}_2^{j_0}=\frac{1}{2^n}(a_0-c_0)$.

We note that $\hat{\mathbf{x}}_3^{j_0},\ldots,\hat{\mathbf{x}}_{m_0}^{j_0}$ can be obtained from an orthonormal basis of $\mathrm{span}\{\mathbf{x}_i^{j_0}-\alpha_i\mathbf{x}_1^{j_0}-\beta_i\mathbf{x}_2^{j_0}|i=3,\ldots,m_0\}$. Considering all cases that $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}\mathbf{x}_i^{j_0}$ is $\begin{bmatrix}1\\1\end{bmatrix}$, $\begin{bmatrix}1\\-1\end{bmatrix}$, $\begin{bmatrix}0\\ \sqrt{2}\end{bmatrix}$ or $\begin{bmatrix}0\\ -\sqrt{2}\end{bmatrix}$, and using the α_i's and β_i's in (6.5.22) for $1\le j_0\le n-2$ and in Remark 6.5.15 for $j_0=n-1$, it can be verified that $\begin{bmatrix}\mathbf{e}_{k_0}^T\\ \mathbf{e}_{s_0}^T\end{bmatrix}(\mathbf{x}_i^{j_0}-\alpha_i\mathbf{x}_1^{j_0}-\beta_i\mathbf{x}_2^{j_0})=0$ for $i=3,\ldots,m_0$. This implies that if $V\mathbf{e}_m=\hat{\mathbf{x}}_i^{j_0}$ for some $3\le i\le m_0$, we have

$$\mathbf{e}_m^T\frac{\partial\Lambda}{\partial_{s_0,k_0}}\mathbf{e}_m=0.$$

Remark 6.5.17. For ease of exposition, we define $X_2(k_1)$ and $X_3(k_2)$ for $k_1\in\{0,n\}$ and $k_2\in\{0,1,n-1,n\}$ as the zero column.

Now, we consider $\mathbf{e}_p^T(\lambda I-\widetilde{A}_n)^\dagger\begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix}$ where $p\in\{s_0,r_0\}$, in order to find $\frac{\partial V}{\partial_{s_0,k_0}}$. We note that $(\lambda I-\widetilde{A}_n)^\dagger=X(\lambda I-\Lambda)^{-1}X^T$. From (6.5.8), (6.5.10) and (6.5.11), for $j=0,\ldots,n$,

$$\begin{aligned}&\mathbf{e}_{s_0}^TX(j)X(j)^T\begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix}\\ =&\begin{bmatrix}\mathbf{e}_{s_0}^TX_1(j) & \mathbf{e}_{s_0}^TX_2(j) & \mathbf{e}_{s_0}^TX_3(j)\end{bmatrix}\begin{bmatrix}\mathbf{e}_{s_0}^TX_1(j) & \mathbf{e}_{s_0}^TX_2(j) & \mathbf{e}_{s_0}^TX_3(j)\\ \mathbf{e}_{k_0}^TX_1(j) & \mathbf{e}_{k_0}^TX_2(j) & \mathbf{e}_{k_0}^TX_3(j)\end{bmatrix}^T\\ =&\frac{1}{2^n}\begin{bmatrix}\binom{n}{j} & \binom{n-2}{j}-\binom{n-2}{j-2}\end{bmatrix}.\end{aligned}$$

In a similar way, it can be found from (6.5.8), (6.5.9), (6.5.10) and (6.5.11) that

$$\mathbf{e}_{r_0}^TX(j)X(j)^T\begin{bmatrix}\mathbf{e}_{s_0} & \mathbf{e}_{k_0}\end{bmatrix}=\frac{(-1)^j}{2^n}\begin{bmatrix}\binom{n}{j} & \binom{n-2}{j}-\binom{n-2}{j-2}\end{bmatrix}.$$

From (6.5.16), $\mathbf{e}_{s_0}^T X_4 = \mathbf{e}_{r_0}^T X_4 = 0$. So, for $n \geq 5$, $1 \leq i \leq 2(n-2)$, and $p \in \{s_0, r_0\}$, we have

$$\mathbf{e}_p^T \mathbf{z}_1^i (\mathbf{z}_1^i)^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = 0.$$

Similarly, for $n = 4$, $i = 1, 2$, and $p \in \{s_0, r_0\}$, we have

$$\mathbf{e}_p^T \begin{bmatrix} \mathbf{z}_1^i & \mathbf{z}_2^i \end{bmatrix} \begin{bmatrix} \mathbf{z}_1^i & \mathbf{z}_2^i \end{bmatrix}^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = 0. \tag{6.5.26}$$

Let λ be an eigenvalue of $\widetilde{A}_n$. Let $\lambda_j = n - 2j$ for $j = 0, \ldots, n$. Then, for $n \geq 5$,

$$\begin{aligned}
&\mathbf{e}_{s_0}^T (\lambda I - \widetilde{A}_n)^\dagger \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \\
=&\mathbf{e}_{s_0}^T X (\lambda I - \Lambda)^{-1} X^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \\
=&\sum_{\substack{0 \leq j \leq n, \\ \lambda_j \neq \lambda}} \frac{1}{\lambda - \lambda_j} \mathbf{e}_{s_0}^T X(j) X(j) \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} + \sum_{\substack{1 \leq i \leq 2(n-2), \\ \mu_i \neq \lambda}} \frac{1}{\lambda - \mu_i} \mathbf{e}_{s_0}^T \mathbf{z}_1^i (\mathbf{z}_1^i)^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \\
=&\frac{1}{2^n} \begin{bmatrix} \sum_{\substack{0 \leq j \leq n, \\ \lambda_j \neq \lambda}} \frac{1}{\lambda - \lambda_j} \binom{n}{j} & \sum_{\substack{0 \leq j \leq n, \\ \lambda_j \neq \lambda}} \frac{1}{\lambda - \lambda_j} \left(\binom{n-2}{j} - \binom{n-2}{j-2} \right) \end{bmatrix}.
\end{aligned} \tag{6.5.27}$$

We can find from (6.5.26) that $\mathbf{e}_{s_0}^T (\lambda I - \widetilde{A}_4)^\dagger \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix}$ can be obtained by setting $n = 4$ in (6.5.27). An analogous argument yields that for $n \geq 4$,

$$\mathbf{e}_{r_0}^T (\lambda I - \widetilde{A}_n)^\dagger \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = \frac{1}{2^n} \begin{bmatrix} \sum_{\substack{0 \leq j \leq n, \\ \lambda_j \neq \lambda}} \frac{(-1)^j}{\lambda - \lambda_j} \binom{n}{j} & \sum_{\substack{0 \leq j \leq n, \\ \lambda_j \neq \lambda}} \frac{(-1)^j}{\lambda - \lambda_j} \left(\binom{n-2}{j} - \binom{n-2}{j-2} \right) \end{bmatrix}. \tag{6.5.28}$$

Remark 6.5.18. Pascal's identity yields $\binom{n-1}{k} - \binom{n-1}{k-1} = \binom{n-2}{k} - \binom{n-2}{k-2}$ for $0 \leq k \leq n$. Comparing (6.5.27) and (6.5.28) with (6.4.33), we obtain that for $0 \leq j \leq n$ and $p \in \{s_0, r_0\}$,

$$\mathbf{e}_p^T ((n-2j)I - \widetilde{A}_n)^\dagger \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = \mathbf{e}_p^T ((n-2j)I - A_n)^\dagger \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix}.$$

Now, we shall find the s_0^{th} and r_0^{th} rows in $\frac{\partial V}{\partial_{s_0,k_0}}$. We first consider the dimension one cases—that is, the subspace spanned by the vectors $E\mathbf{y}$ for eigenvectors $\mathbf{y}$ corresponding to some eigenvalue of $\widetilde{A}_n$ is of dimension 1. Then, there are 4 cases: an eigenvalue of $\widetilde{A}_n$ is n, $-n$, one of the μ_i's ($i = 1, 2$) when $n = 4$, or one of the μ_i's ($1 \leq i \leq 2(n-2)$) when $n \geq 5$. Given $n \geq 5$ and $V\mathbf{e}_m = \hat{\mathbf{z}}_1^i$ for $1 \leq i \leq 2(n-2)$, we find from (6.5.20) and (6.5.27) that

$$\begin{aligned}\mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{s_0,k_0}} \mathbf{e}_m =& \mathbf{e}_{s_0}^T (\lambda I - \widetilde{A}_n)^\dagger \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \hat{\mathbf{z}}_1^i \\ =& \frac{2^{n-4}}{2^n\sqrt{2^{n-1}}} \sum_{j=0}^{n} \frac{1}{\nu_i(\mu_i - \lambda_j)} \binom{n}{j}.\end{aligned} \tag{6.5.29}$$

We leave to the reader the other three cases.

Next, consider the dimension two case. Let $j_0 \in \{1, \dots, n-1\}$. Here we revisit the formula (6.4.12): for $V \begin{bmatrix} \mathbf{e}_p & \mathbf{e}_q \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0} \end{bmatrix}$, we have

$$\begin{aligned}&\frac{\partial V}{\partial_{s_0,k_0}} \begin{bmatrix} \mathbf{e}_p & \mathbf{e}_q \end{bmatrix} \\ =& ((n-2j_0)I - \widetilde{A}_n)^\dagger E \begin{bmatrix} \hat{\mathbf{x}}_1^{j_0} & \hat{\mathbf{x}}_2^{j_0} \end{bmatrix} + \frac{(\hat{\mathbf{x}}_1^{j_0})^T E((n-2j_0)I - \widetilde{A}_n)^\dagger E \hat{\mathbf{x}}_2^{j_0}}{(\hat{\mathbf{x}}_2^{j_0})^T E \hat{\mathbf{x}}_2^{j_0} - (\hat{\mathbf{x}}_1^{j_0})^T E \hat{\mathbf{x}}_1^{j_0}} \begin{bmatrix} -\hat{\mathbf{x}}_2^{j_0} & \hat{\mathbf{x}}_1^{j_0} \end{bmatrix}.\end{aligned}$$

Let us compute $(\hat{\mathbf{x}}_1^{j_0})^T E((n-2j_0)I - \widetilde{A}_n)^\dagger E \hat{\mathbf{x}}_2^{j_0}$. From (6.5.8), (6.5.10) and (6.5.11), for $j = 0, \dots, n$, it can be found that

$$\begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{s_0} \end{bmatrix}^T X(j) X(j)^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = \frac{1}{2^n} \begin{bmatrix} \binom{n-2}{j} - \binom{n-2}{j-2} & \binom{n-2}{j} + \binom{n-2}{j-2} \\ \binom{n}{j} & \binom{n-2}{j} - \binom{n-2}{j-2} \end{bmatrix}.$$

Since $\mathbf{e}_{s_0}^T X_4 = \mathbf{e}_{r_0}^T X_4 = 0$, we have $\begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{s_0} \end{bmatrix}^T \mathbf{z}_1^i (\mathbf{z}_1^i)^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = 0$ for $n \geq 5$ and $1 \leq i \leq 2(n-2)$; and we have $\begin{bmatrix} \mathbf{e}_{k_0} & \mathbf{e}_{s_0} \end{bmatrix}^T \begin{bmatrix} \mathbf{z}_1^i & \mathbf{z}_2^i \end{bmatrix} \begin{bmatrix} \mathbf{z}_1^i & \mathbf{z}_2^i \end{bmatrix}^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} = 0$ for $n = 4$ and $i \in \{1, 2\}$. By Remark 6.5.16 and (6.5.24), for $1 \leq j_0 \leq n-1$, we have

$$\begin{aligned}&\frac{(\hat{\mathbf{x}}_1^{j_0})^T E((n-2j_0)I - \widetilde{A}_n)^\dagger E \hat{\mathbf{x}}_2^{j_0}}{(\hat{\mathbf{x}}_2^{j_0})^T E \hat{\mathbf{x}}_2^{j_0} - (\hat{\mathbf{x}}_1^{j_0})^T E \hat{\mathbf{x}}_1^{j_0}} \\ =& \frac{2^n}{-2^2 c_0} \sum_{\substack{0 \leq j \leq n, \\ j \neq j_0}} \frac{1}{j - j_0} (\hat{\mathbf{x}}_1^{j_0})^T \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} X(j) X(j) \begin{bmatrix} \mathbf{e}_{s_0} & \mathbf{e}_{k_0} \end{bmatrix} \begin{bmatrix} \mathbf{e}_{k_0}^T \\ \mathbf{e}_{s_0}^T \end{bmatrix} \hat{\mathbf{x}}_2^{j_0} \\ =& \sum_{\substack{0 \leq j \leq n, \\ j \neq j_0}} \frac{b_0}{2^{n+3}(j - j_0)} \left(\frac{\binom{n}{j}}{\binom{n}{j_0}} - \frac{\binom{n-2}{j} + \binom{n-2}{j-2}}{\binom{n-2}{j_0} + \binom{n-2}{j_0-2}} \right).\end{aligned}$$

Hence, if $V\mathbf{e}_m = \hat{\mathbf{x}}_1^{j_0}$, then

$$
\begin{aligned}
&\mathbf{e}_{s_0}^T \frac{\partial V}{\partial_{s_0,k_0}} \mathbf{e}_m \\
=&\mathbf{e}_{s_0}^T ((n-2j_0)I - \widetilde{A}_n)^\dagger E \hat{\mathbf{x}}_1^{j_0} - \frac{(\hat{\mathbf{x}}_1^{j_0})^T E((n-2j_0)I - \widetilde{A}_n)^\dagger E \hat{\mathbf{x}}_2^{j_0}}{(\hat{\mathbf{x}}_2^{j_0})^T E \hat{\mathbf{x}}_2^{j_0} - (\hat{\mathbf{x}}_1^{j_0})^T E \hat{\mathbf{x}}_1^{j_0}} \mathbf{e}_{s_0}^T \hat{\mathbf{x}}_2^{j_0} \\
=&\frac{b_0}{2^{n+1}\sqrt{2^{n+1}\omega_0}} \sum_{\substack{0 \le j \le n, \\ j \ne j_0}} \frac{1}{j-j_0} \left(\frac{\omega_0 \binom{n}{j} + c_0 \left(\binom{n-2}{j} - \binom{n-2}{j-2} \right)}{\sqrt{c_0(c_0-a_0)}} \right) \\
&- \frac{b_0}{2^{n+1}\sqrt{2^{n+1}\omega_0}} \sum_{\substack{0 \le j \le n, \\ j \ne j_0}} \frac{\sqrt{c_0(c_0-a_0)}}{4(j-j_0)} \left(\frac{\binom{n}{j}}{\binom{n}{j_0}} - \frac{\binom{n-2}{j} + \binom{n-2}{j-2}}{\binom{n-2}{j_0} + \binom{n-2}{j_0-2}} \right).
\end{aligned}
\tag{6.5.30}
$$

We leave to the reader the computations for $\mathbf{e}_{r_0}^T \frac{\partial V}{\partial_{s_0,k_0}} \mathbf{e}_m$ and $\mathbf{e}_{p_1}^T \frac{\partial V}{\partial_{s_0,k_0}} \mathbf{e}_{p_2}$ where $p_1 \in \{s_0, r_0\}$ and $V\mathbf{e}_{p_2} = \hat{\mathbf{x}}_2^{j_0}$.

Remark 6.5.19. Summing this subsection up, we have found the s_0^{th}, k_0^{th}, and r_0^{th} rows of V in (6.5.18), (6.5.20), (6.5.21), and (6.5.24). Furthermore, non-zero entries of $\frac{\partial \Lambda}{\partial_{s_0,k_0}}$ can be found in (6.5.19) and (6.5.25), and the remaining entries in $\frac{\partial \Lambda}{\partial_{s_0,k_0}}$ are zeros. Finally, the s_0^{th} and r_0^{th} entries of a non-zero column in $\frac{\partial V}{\partial_{s_0,k_0}}$ can be obtained as done in (6.5.29) and (6.5.30).

Recall that $\widetilde{Q}_n$ is the $(2,2,2,\{3,3\})$-switched n-cube and $A(\widetilde{Q}_n) = \widetilde{A}_n$.

Remark 6.5.20. As seen in (6.5.30), quantity $(\hat{\mathbf{x}}_1^j)^T E((n-2j)I - A(\widetilde{Q}_n))^\dagger E \hat{\mathbf{x}}_2^j$ for $j = 1, \dots, n-1$ is not necessarily zero while those quantities are zeros for Q_n so that we compute the s_0^{th} and r_0^{th} rows of each column of $\frac{\partial V}{\partial_{s_0,k_0}}$ for Q_n with less complexity, and without distinction between the dimension one and dimension two cases. This difference complicates obtaining the desired derivatives for $\widetilde{Q}_n$ in explicit form (which can be obtained), and comparing them between Q_n and $\widetilde{Q}_n$. Thus, we close this chapter after reporting some numerical results for the comparison and making a related conjecture.

Remark 6.5.21. Let $n \ge 4$. Consider $A(Q_n)$ and $A(\widetilde{Q}_n)$ of the forms (6.5.1) and (6.5.2). Let $M = \{k \sim w_1, v_2 \sim w_2\}$ where $k = 1$, $v_2 = 2$, $w_1 = 2^{n-1} + 1$, and $w_2 = 2^{n-1} + 2$. Then, M is the $(2,2,2;\{3,3\})$-matching used for obtaining $\widetilde{Q}_n$. Furthermore, $S_1(\{k, v_2\}) = \{s, l_1\}$ where $s = 2^{n-1} + 2^{n-2} + 1$ and $l_1 = 2^{n-1} + 2^{n-2} + 2$. We note that s and s^* pair up to have PST in $\widetilde{Q}_n$.

Suppose that l is adjacent to k and $l \ne w_1$. Consider $\frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial_{k,l}^2}$ for $n \ge 5$, where $p_{\widetilde{Q}_n}(t) = |(U(t))_{s,s^*}|^2$ for $U(t) = e^{itA(\widetilde{Q}_n)}$ $(t \ge 0)$. Even though s and l_1 are the common neighbours of k and v_2, since we consider PST between s and s^* in $\widetilde{Q}_n$, we need to distinguish s from l_1. Furthermore, if l is neither s nor l_1, then by (ii) of Proposition 2.5.1 regarding P_3-transitivity, we may assume $l = l_2$ where $l_2 = 2^{n-1}+3$.

Remark 6.5.22. Let $n \geq 4$, and $s, r, k, l \in V(\widetilde{Q}_n)$. Suppose that $r = s^*$, $s \sim k$, and $k \sim l$. By Theorem 6.4.18, under PST between s and r at time $\frac{\pi}{2}$ in $\widetilde{Q}_n$, we have

$$\frac{\partial p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial_{s,k}} = \frac{\partial p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial_{k,l}} = 0.$$

Example 6.5.23. Maintaining the notation and result of Remark 6.5.21, let $r = 2^n$. We note that $\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}} = \frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_2}}$. Using MATLAB®, we have the following table:

	$\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{s,k}}$	$\frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{s,k}}$	$\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}}$	$\frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}}$	$\frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l_2}}$
$n = 4$	-0.720300	-0.717532	-0.174329	-0.173932	-0.175813
$n = 5$	-0.555745	-0.552891	-0.096518	-0.096284	-0.096788
$n = 6$	-0.452203	-0.449722	-0.061181	-0.061050	-0.061226
$n = 7$	-0.381113	-0.379031	-0.042215	-0.042139	-0.042213
$n = 8$	-0.329308	-0.327567	-0.030874	-0.030827	-0.030862

Conjecture 6.5.24. *Let $n \geq 4$, and let us maintain the notation in Remark 6.5.21. Prove that under PST between s and $r = s^*$ at time $\frac{\pi}{2}$ in Q_n and $\widetilde{Q}_n$,*

$$\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{s,k}} < \frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{s,k}} < 0 \text{ and } \frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}} < \frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}} < 0$$

and for $n \geq 7$,

$$\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_2}} < \frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l_2}} < 0.$$

7

Future work

In this chapter, we restate the problems and conjectures described in Chapters 3–6 with extra commentaries.

7.1 Gram mates

In Chapter 3, we mainly discussed Gram mates via realizable matrices—that is, given a realizable matrix E, we studied Gram mates A and $A+E$. Instead of starting with a realizable matrix, it would be interesting to begin with two non-negative integral vectors, and to consider Gram mates with them as row and column sum vectors.

Research direction 1. (Problem 3.5.7) Given non-negative integral vectors R and S, does there exist a pair of Gram mates in $\mathcal{U}(R, S)$? We shall pose a concrete question under the following assumption. Suppose that each distinct integer in R (resp. S) appears an even number of times and $R^* \succ S$. Prove or disprove that there exists a pair of Gram mates A and B in $\mathcal{U}(R, S)$. One could check if such Gram mates A and B can be constructed as $A = \begin{bmatrix} A_1 & A_2 \\ A_2 & A_1 \end{bmatrix}$ and $B = \begin{bmatrix} A_2 & A_1 \\ A_1 & A_2 \end{bmatrix}$ for some A_1 and A_2 with $A_1 \neq A_2$.

Motivated by Gram mates via realizable matrices, we dealt with Gram mates via unitary (orthogonal) matrices in Section 3.7.

Research direction 2. (Problems 3.7.8, 3.7.9) Given a unitary (or an orthogonal) matrix U, develop a systematic way to find Gram mates via U. If U is the $n \times n$ DFT matrix and $|\{j | 1 \leq j \leq n,\ \gcd(j, n) > \sqrt{n}\}| \geq \sqrt{n}$, then characterize Gram mates via U.

It is important to find non-isomorphic Gram mates A and B in order to discern that the two-mode network corresponding to A retains the information in the conversion approach. Such A and B can be analysed through the automorphism groups $\Gamma(AA^T)$ and $\Gamma(A^TA)$ in that if $\Gamma(AA^T) = \Gamma(A^TA) = \emptyset$, then any Gram mate to A is non-isomorphic to A. As explained in Problem 3.4.8, we may study $(0,1)$ matrices X such that $\Gamma(X) = \emptyset$ in order to understand A with $\Gamma(AA^T) = \Gamma(A^TA) = \emptyset$.

Research direction 3. (Problem 3.4.8) Characterize $(0,1)$ matrices X such that $\Gamma(X) = \emptyset$.

Moreover, regarding non-isomorphic Gram mates, we have the following.

Conjecture 4. (Conjecture 3.4.12) Let A and B be Gram mates where $\text{rank}(A - B) = 1$. Prove that A and B are isomorphic if and only if the remaining matrix of A and B is fixable.

In Section 3.6, we investigated Gram mates in several classes of $(0,1)$ matrices. We particularly posed problems concerning circulant Gram mates from combinatorial and algebraic viewpoints. Recall that D_{2n} is the dihedral group of order $2n$.

Research direction 5. (Problem 3.6.14) Let $\mathbf{a}^T$ be a $(0,1)$ row vector of size n, and $\omega_{\mathbf{a}^T} = (\omega_0, \dots, \omega_{n-1})$ where $\omega_i = \mathbf{a}^T P^i \mathbf{a}$ for $i = 0, \dots, n-1$ and $P = \text{circ}(0, 1, 0, \dots, 0)$. (a) Provide combinatorial interpretations for $\omega_2, \dots, \omega_{\lfloor \frac{n}{2} \rfloor}$, and bounds on each ω_i for $2 \le i \le \lfloor \frac{n}{2} \rfloor$; (b) Find a $(0,1)$ row vector $\mathbf{b}^T$ such that $\omega_{\mathbf{a}^T} = \omega_{\mathbf{b}^T}$ and $\mathbf{b}^T \notin \mathcal{O}_{\mathbf{a}^T}$.

Research direction 6. (Problem 3.6.15) Let $\mathbf{a}^T$ be a $(0,1)$ row vector of size n with m ones. Prove or disprove that $|\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n}| \le n$. Investigate the relationship between m and $|\mathcal{E}_{n,m}^{\mathbf{a}^T}/D_{2n}|$.

7.2 Fiedler vectors with unbalanced sign patterns

In Chapter 4, we investigated graphs G with $i(G) = 1$ or $i(G) = 2$ in order to study the robustness of spectral bisection. Since we completely characterized graphs G with $i(G) = 1$, it would be interesting to find more classes with the characterization in addition to the classes described in Section 4.4; then, one could consider cographs, split graphs, and Laplacian integral graphs. Furthermore, we need to fully characterize graphs G with $i(G) = 2$.

Research direction 7. (Problem 4.4.9) Find classes of graphs G with $i(G) = 1$, and investigate $am(\alpha(G))$ for graphs in those classes.

Research direction 8. (Problem 4.5.16) Completely characterize non-regular graphs with $i(G) = 2$.

If we develop a systematic tool to find $i(G)$ where G is a connected graph, then it would be helpful to characterize graphs G with $i(G) \geq 2$. As discussed in Problem 4.5.9, one could use oriented matroids to develop such a tool.

Research direction 9. (Problem 4.5.9) Given a connected graph G, how can we find $i(G)$?

Considering the equivalent conditions in Theorem 4.2.8 for a connected graph G to have $i(G) = 1$, G could be regarded as a highly structured graph. In order to see if such G is rarely seen in empirical settings, we need to understand the probability of G to have $i(G) = 1$.

Research direction 10. (Problem 4.2.9) Find bounds on the probability of a connected graph G to have $i(G) = 1$.

Given a connected graph G of order n such that $\frac{i(G)}{n} < 0.1$, say, one might consider G as a pathological graph with respect to spectral bisection. So, it would be helpful to provide a probability of a randomly chosen graph H of order n to have $\frac{i(H)}{n} < 0.1$.

Research direction 11. (Problem 4.2.9) Given $\varepsilon > 0$, find the probability of a random graph G of order n in the Erdös–Rényi model to have $\frac{i(G)}{n} < \varepsilon$.

7.3 Families of graphs with the Braess edge on twin pendent paths

In Chapter 5, we considered graphs with twin pendent paths, and investigated if the non-edge between the two pendent vertices on the twin pendent paths is a Braess edge or not. One could generalise the works in Chapter 5 by considering any non-edge on the twin pendent paths.

Research direction 12. (Problems 5.2.9, 5.2.23, and 5.4.10) Let G be a connected graph with a vertex v, and $P_{k_1} = (v_0, \ldots, v_{k_1})$ and $P_{k_2} = (w_0, \ldots, w_{k_2})$ where $k_1, k_2 \geq 0$ with $k_1 + k_2 \geq 2$. Let $\widetilde{G}(v, k_1, k_2)$ be the graph obtained from G, P_{k_1} and P_{k_2} by identifying the vertices v, v_0 and w_0. Suppose that H is the graph obtained from $\widetilde{G}(v, k_1, k_2)$ by adding an edge $v_i \sim w_j$ for some $0 \leq i \leq k_1$ and $1 \leq j \leq k_2$ with $i+j \geq 2$. Establish an equivalent condition for $\kappa(H) > \kappa(\widetilde{G}(v, k_1, k_2))$ as in Theorem 5.2.8. Next, apply the equivalent condition to the graphs K_n, C_n, P_n, and S_n as done in Section 5.2. Finally, establish analogous results as done in Sections 5.3 and 5.4.

7.4 Equidistant switched hypercubes: their properties and sensitivity analysis under PST

The ultimate goal of Chapter 6 is to prove that the switched n-cube $\widetilde{Q}_n^{(M)}$ where M is a $(2, 2, 2, \{3, 3\})$-matching in Q_n is less sensitive to changes in the weight of some particular edge than Q_n. To achieve that goal, we only need to resolve the following problem.

Conjecture 13. (Conjecture 6.5.24) Let $n \geq 4$, and $\widetilde{Q}_n^{(M)}$ be the switched n-cube where $M = \{k \sim w_1, v_2 \sim w_2\}$ is a $(2, 2, 2, \{3, 3\})$-matching in Q_n with distant partite sets $\{k, v_2\}$ and $\{w_1, w_2\}$. For simplicity, let $\widetilde{Q}_n = \widetilde{Q}_n^{(M)}$. Choose a vertex $s \in V(Q_n)$ such that $s \neq w_1$ and s is adjacent to k in Q_n. Suppose that l is adjacent to k in Q_n and $\widetilde{Q}_n$. Then, $l \neq w_1$ and $l \neq w_2$. When it comes to evaluating $\frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l}}$ under PST between s and s^* at time $\frac{\pi}{2}$, by Remark 6.5.21, l can be considered as one of the following cases: (i) $l = s$, (ii) $l \neq s$ and l is a common neighbour of k and v_2, say $l = l_1$, (iii) otherwise, say $l = l_2$. Prove that under PST between s and s^* at time $\frac{\pi}{2}$ in Q_n and $\widetilde{Q}_n$,

$$\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{s,k}} < \frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{s,k}} < 0 \text{ and } \frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}} < \frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l_1}} < 0$$

and for $n \geq 7$,

$$\frac{\partial^2 p_{Q_n}(\frac{\pi}{2})}{\partial^2_{k,l_2}} < \frac{\partial^2 p_{\widetilde{Q}_n}(\frac{\pi}{2})}{\partial^2_{k,l_2}} < 0.$$

In quantum spin networks, it is crucial to understand under what circumstances a graph exhibits PST. So, we need to characterize pairs of vertices exhibiting PST in an equidistant switched hypercube.

Conjecture 14. (Conjecture 6.3.15) Let $k \geq 2$, and let $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ be an equidistant matching in Q_n with distance-partite sets $M_1 = \{v_1, \ldots, v_k\}$ and

$M_2 = \{w_1, \ldots, w_k\}$. Suppose that x and x^* pair up to exhibit PST at time $\frac{\pi}{2}$ in $\widetilde{Q}_n^{(M_\tau)}$ for any $\tau \in \mathcal{S}_k$. Prove that $d_{Q_n}(x, v_1) = \cdots = d_{Q_n}(x, v_k)$ and $d_{Q_n}(x, w_1) = \cdots = d_{Q_n}(x, w_k)$.

If Problem 14 is resolved, then we immediately obtain the following: (i) for a $(2, a, b; \Gamma)$-matching M with a and b odd, $\widetilde{Q}_n^{(M)}$ does not exhibit PST between any pair of vertices at time $\frac{\pi}{2}$; (ii) the number of pairs exhibiting PST in Proposition 6.3.19 is exactly given.

Recall that given Q_n with a subset X of $V(Q_n)$, $S_r(X)$ is the set of vertices v in Q_n such that $d(v, x) = r$ for all $x \in X$. Considering Theorem 6.3.12, counting pairs of vertices exhibiting PST in an equidistant switched hypercube is related to understanding the cardinality of $|S_r(X)|$. In general, it is not easy to compute $|S_r(X)|$ without constraints. We pose a related problem under some circumstance.

Research direction 15. (Problem 6.3.24) Given a $(k, 2\alpha, 2\alpha; \{(2\alpha+1)^k\})$-matching M in Q_n where $k \geq 3$, find $|\bigcup_{i=\alpha}^{n-\alpha} S_i(M^{2\alpha})|$. This provides a lower bound on the number of pairs of vertices exhibiting PST at time $\frac{\pi}{2}$ in $\widetilde{Q}_n^{(M_\tau)}$ for any $\tau \in \mathcal{S}_k$. Further, if Problem 14 is proved, then we obtain the exact number as $|\bigcup_{i=\alpha}^{n-\alpha} S_i(M^{2\alpha})|$.

Given an equidistant matching M in a graph G, when we apply an equidistant switch with M on a graph, we need to consider orderings of the edges in M and transitivity of M in Q_n. We refer the interested reader to Example 6.3.3, Remarks 6.3.2 and 6.3.26 for understanding. Hence, we discussed classification of $(k, a, b; \Gamma)$-switched n-cubes (or graphs) up to isomorphism in Section 6.3. We shall introduce the following related problems.

Research direction 16. (Problems 6.3.4, 6.3.6) Given an equidistant matching M of size $k \geq 3$ in a graph G, find conditions in order that an equidistant switched graph is uniquely determined up to permutations of the edges in M. Further, we pose a concrete question about Q_n. Let $n \geq 4$ and $k \geq 3$. Let $M = \{v_i \sim w_i | i = 1, \ldots, k\}$ be an equidistant matching in Q_n with distance-partite sets $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$. Prove or disprove that if there exists a vertex x in Q_n such that $d(x, v_1) = \cdots = d(x, v_k)$ and $d(x, w_1) = \cdots = d(x, w_k)$, then an equidistant switched n-cube is uniquely determined up to permutations of the edges in M.

Before we consider quadruples $(k, \alpha, \beta, \Gamma)$ that allow attaining transitivity of a $(k, \alpha, \beta; \Gamma)$-matching in a graph G, we need to understand what quadruples (k, a, b, Γ) guarantee the existence of a $(k, \alpha, \beta, \Gamma)$-matching in G.

Research direction 17. (Problems 6.2.6, 6.3.27) Given a graph G, investigate quadruples (k, a, b, Γ) that guarantee the existence of a $(k, a, b; \Gamma)$-matching in G. One might explore, using Menger's theorem, the range of k by considering graph parameters such as vertex-connectivity. After that, determine quadruples $(k, \alpha, \beta, \Gamma)$ that allow transitivity of a $(k, \alpha, \beta; \Gamma)$-matching. One could consider G as a hypercube, or more generally as any bipartite graph.

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