UNIVERSIDADE FEDERAL DO PARANÁ

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CURITIBA 2024

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ON GRAPHS WITH SIMPLY STRUCTURED EIGENSPACES

Tese apresentada ao curso de Pós-Graduação em Matemática, Setor de Ciências Exatas, Universidade Federal do Paraná, como requisito parcial à obtenção do Título de Doutora em Matemática.

Orientador: Prof. Dr. Leonardo Silva de Lima.

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ATA DE SESSÃO PÚBLICA DE DEFESA DE DOUTORADO PARA A OBTENÇÃO DO GRAU DE DOUTORA EM MATEMÁTICA

No dia vinte e cinco de novembro de dois mil e vinte e quatro às 09:00 horas, na sala de Atos, Centro Politécnico da Universidade Federal do Paraná, foram instaladas as atividades pertinentes ao rito de defesa de tese da doutoranda **HEBER CRISTINA TEIXEIRA**, intitulada: **ON GRAPHS WITH SIMPLY STRUCTURED EIGENSPACES**, sob orientação do Prof. Dr. LEONARDO SILVA DE LIMA. A Banca Examinadora, designada pelo Colegiado do Programa de Pós-Graduação MATEMÁTICA da Universidade Federal do Paraná, foi constituída pelos seguintes Membros: LEONARDO SILVA DE LIMA (UNIVERSIDADE FEDERAL DO PARANÁ), FERNANDO COLMAN TURA (UNIVERSIDADE FEDERAL DE SANTA MARIA), RENATA RAPOSO DEL VECCHIO (UNIVERSIDADE FEDERAL FLUMINENSE), JORGE FERREIRA ALENCAR LIMA (INSTITUTO FED. DE EDUC., CIÊNC. E TECN. DO TRIÂNGULO MINEIRO), ELÍAS ALFREDO GUDIÑO ROJAS (UNIVERSIDADE FEDERAL DO PARANÁ). A presidência iniciou os ritos definidos pelo Colegiado do Programa e, após exarados os pareceres dos membros do comitê examinador e da respectiva contra argumentação, ocorreu a leitura do parecer final da banca examinadora, que decidiu pela APROVAÇÃO. Este resultado deverá ser homologado pelo Colegiado do programa, mediante o atendimento de todas as indicações e correções solicitadas pela banca dentro dos prazos regimentais definidos pelo programa. A outorga de título de doutora está condicionada ao atendimento de todos os requisitos e prazos determinados no regimento do Programa de Pós-Graduação. Nada mais havendo a tratar a presidência deu por encerrada a sessão, da qual eu, LEONARDO SILVA DE LIMA, lavrei a presente ata, que vai assinada por mim e pelos demais membros da Comissão Examinadora.

CURITIBA, 25 de Novembro de 2024.

Assinatura Eletrônica 25/11/2024 18:22:14.0 LEONARDO SILVA DE LIMA Presidente da Banca Examinadora

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TERMO DE APROVAÇÃO

Os membros da Banca Examinadora designada pelo Colegiado do Programa de Pós-Graduação MATEMÁTICA da Universidade Federal do Paraná foram convocados para realizar a arguição da tese de Doutorado de **HEBER CRISTINA TEIXEIRA** intitulada: **ON GRAPHS WITH SIMPLY STRUCTURED EIGENSPACES**, sob orientação do Prof. Dr. LEONARDO SILVA DE LIMA, que após terem inquirido a aluna e realizada a avaliação do trabalho, são de parecer pela sua APROVAÇÃO no rito de defesa. A outorga do título de doutora está sujeita à homologação pelo colegiado, ao atendimento de todas as indicações e correções solicitadas pela banca e ao pleno atendimento das demandas regimentais do Programa de Pós-Graduação.

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Dedico este trabalho à minha mãe, que, mesmo não estando mais presente entre nós, é uma luz que me guia e estará sempre viva em meu coração.

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RESUMO

Um grafo G possui um autoespaço simplesmente estruturado se o autoespaço associado a um autovalor da matriz laplaciana admite uma base cujas entradas pertencem ao conjunto $\{-1,0,1\}$. Dizemos que G é simplesmente estruturado se todos os seus autoespaços forem simplesmente estruturados. Neste trabalho, determinamos o número mínimo de vetores em uma base de um autoespaço da matriz laplaciana de um grafo threshold conexo, de modo que essa base seja simplesmente estruturada. Além disso, caracterizamos todos os grafos threshold conexos com n vértices que são simplesmente estruturados e cuja base de autovetores da matriz laplaciana admite uma ordenação tal que vetores não consecutivos sejam ortogonais, os quais chamamos de grafos threshold fracamente Hadamard diagonalizável (WHD). Isso oferece uma resposta parcial ao problema proposto em [2] sobre a determinação de quais cografos são WHD. Também identificamos uma subfamília infinita de grafos em cadeia na qual todos os autovalores inteiros da matriz laplaciana possuem autoespaços simplesmente estruturados, e mostramos que não faz sentido estender as definições de grafos WHD para a matriz laplaciana sem sinal.

Palavras-chave: matriz laplaciana, autoespaço simplesmente estruturado, grafos threshold.

ABSTRACT

A graph G has a simply structured eigenspace if the eigenspace associated with an eigenvalue of the Laplacian matrix admits a basis with all entries in the set $\{-1, 0, 1\}$. We say that G is simply structured if all its eigenspaces are simply structured. In this work, we determine the minimum number of vectors in a basis of an eigenspace of the Laplacian matrix of a connected threshold graph, such that this basis is simply structured. Additionally, we characterize all connected threshold graphs with n vertices that are simply structured and whose Laplacian eigenvector bases admit an ordering in which non-consecutive vectors are orthogonal, which we call threshold *weakly Hadamard diagonalizable* (WHD) graph. This provides a partial answer to the problem posed in [2] with regard to determining which cographs are WHD. We also identify an infinite subfamily of chain graphs in which all integer eigenvalues of the Laplacian matrix have simply structured eigenspaces, and we show that extending the definition of WHD graphs to the signless Laplacian matrix is not appropriate.

Keywords: Laplacian matrix, simply structured eigenspace, threshold graphs.

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Chapter 1

INTRODUCTION

Eigenspaces of matrices associated with graphs have been studied and shown to describe interesting properties of the graph topology. This is the main topic of spectral graph theory, which is an area on the border of linear algebra and graph theory. Eigenvalues can be helpful in understanding the connectivity of a graph [[15], [17]] and eigenvectors can be used to partition the vertex set of the graph, among many other results from the literature, such as [3], [8], [28]. Finding an eigenspace of a matrix related to a graph with a simple and sparse structure has attracted the attention of many researchers since these structures are easy to handle from the computational point of view.

A basis is simply structured if it consists only of vectors with entries in the set $\{-1, 0, 1\}$, [29]. In particular, we found some works characterizing trees and cographs with a simply structured eigenspace basis for the null space [[3], [29]]. Some papers are dedicated to a more complex problem: finding all graphs of a given order such that all eigenspaces bases are simply structured. A pioneer paper in this area is the recent work of Adm *et al.* [2], where the authors found many graphs such that all eigenspaces bases are simply structured. Adm *et al.* considered the eigenvectors of the Laplacian matrix with a given constraint, which we will make more transparent ahead. Even more recent papers on this topic have been published, as we refer to [[22], [26]]. Given the recent development of the topic and its theoretical importance, we state the following problem that will be addressed throughout this work.

Problem A: Given an integer n, determine (if there exists) all graphs G with n vertices for which the eigenspaces bases of the Laplacian matrix of G are simply structured.

Notice that Problem A is very general. Only Laplacian integral graphs can have all simply structured eigenspaces bases for its Laplacian matrix. This makes clear that this is not an easy problem since finding integral Laplacian graphs is by itself a difficult problem, and to solve Problem A, we should find all graphs with simply structured eigenspaces for all eigenvalues among the Laplacian integral graphs. The main results of this work are related to the answer to Problem A in the threshold family of graphs. Therefore, our approach involves studying the following three subproblems that would drive us to answer the more general question.

Problem A.1: Determine the minimum number of vectors in the basis of an eigenspace of Laplacian

matrix of a connected threshold graph G such that the eigenspace basis is simply structured;

Problem A.2: Characterize all threshold graphs that are simply structured.

Problem A.3: Characterize all connected threshold graphs that are simply structured and such that the matrix W, formed by the eigenvectores of L(G), satisfies the condition W^TW is a tridiagonal matrix.

To the best of our knowledge none of the problems above is addressed in the literature. A straightforward result is that connected trees cannot have this special structure in their eigenvectors since it is well-known that every tree (except the star graph) has its second smallest eigenvalue (the algebraic connectivity) less than 0.49. Therefore, any connected tree has algebraic connectivity greater than 0 and less than 0.49, and consequently, there are no connected trees with simply structured eigenspaces.

Motivated by these theoretical results, we developed an algorithm that generates threshold graphs with the desired properties of Problems A.2 and A.3. We also identify an infinite subfamily of chain graphs in which all integer eigenvalues of the Laplacian matrix have simply structured eigenspaces, and we show that extending the definition of weakly Hadamard diagonalizable graph (WHD) to the signless Laplacian matrix is not appropriate.

An interesting question that remains open is to answer Problem A for cographs that are not threshold. We leave this for future work. Our proof techniques are mainly related to the edge principle from Merris in [28], as well as on a recent result from our paper A Laplacian eigenbasis for threshold graphs [24], that states that a star graph and any threshold graph on n vertices share the same Laplacian eigenbasis. We highlight that some results of Chapter 5 have been published in the Special Matrices journal, and another paper with the remaining results is in development.

This work is organized as follows. In Chapter 2, we establish some notations and review basic concepts of linear algebra. We also introduce fundamental notions and terminology of graph theory. The focus of this work is the study of the Laplacian matrix of a graph and its corresponding eigenvalues and eigenvectors. In Chapter 3, we provide a brief literature review regarding Hadamard matrices and weak Hadamard matrices. In Chapter 4, we investigate graphs G for which the Laplacian matrix L can be diagonalized by a matrix P, where P is either the Hadamard matrix H or a weak Hadamard matrix W. In Chapters 5 and 6, we present the main results obtained in the thesis.

Chapter 2

PRELIMINARIES

In this chapter, we establish some notations and explore well-known connections between linear algebra, graphs, and matrices that will be useful later. Only real matrices were considered in this work. We also present the basic notions and terminology of graph theory that are strictly necessary to understand the rest of the work. We finish this chapter by defining chain graphs and presenting a family of chain graphs that have a simple structured eigenspace, and it is the first contribution of this work. The main references used here are [2], [7], [9], [16].

2.1 Graphs and matrices

Throughout the text, we consider G = (V, E) as a finite, simple, undirected, and unweighted graph of order n = |V| and size m = |E|. We define $(i, j) \in E$ as an edge of G if i is adjacent to j, where $i, j \in V$. The graph $G^c = (\overline{V}, \overline{E})$ obtained from G in such a way that $\overline{V} = V$ and $(i, j) \in \overline{E}$ when $(i, j) \notin E$ is called the **graph complement**. Let $N_i(G)$ be the set of vertices adjacent to i, and the degree of $i \in V$ is given by $d_i(G) = |N_i(G)|$. The graph G is r-regular if $d_i(G) = r$ for all i. We denote the star, complete, and path graphs on n vertices as S_n, K_n , and P_n , respectively. The **union** of G and H, denoted by $G \sqcup H$, is the graph that has the vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. For any connected graph G, we write kG for the union of k copies of G. The **join** of G and H, denoted by $G \lor H = (G^c \sqcup H^c)^c$, is the graph on $n_1 + n_2$ vertices obtained from the union of G and H by adding new edges from each vertex of G to every vertex of H. A clique in a graph is a set of pairwise adjacent vertices. A **co-clique** (or *independence set*) in a graph is a set of pairwise nonadjacent vertices.

Several matrices are associated with a graph G. Let $M \in \mathbb{R}^{n \times n}$ be a matrix associated with G. The determinant det $(M - \lambda I)$ is a polynomial in the (complex) variable λ of degree n and is called the **characteristic polynomial** of M. The equation

$$\det(M - \lambda I) = 0$$

is called the **characteristic equation** of M. By the Fundamental Theorem of Algebra, the equation has n complex roots, called the **eigenvalues** of M. The **spectrum** of M is the set of all $\lambda \in \mathbb{C}$ that are eigenvalues of M and the **spectral radius** $\rho(M)$ of A is the maximum modulus of an eigenvalue of M. The eigenvalues might not all be distinct. The number of times an eigenvalue occurs as a root of the characteristic equation is called the **algebraic multiplicity** of the eigenvalue. If λ is an eigenvalue of M, we denote the eigenspace associated with λ by

$$\mathcal{E}_M(\lambda) = \{ \mathbf{x} \in \mathbb{R}^n, \ \mathbf{x} \neq 0 : M\mathbf{x} = \lambda \mathbf{x} \};$$

the vectors $\mathbf{x} \in \mathcal{E}_M(\lambda)$ are called **eigenvectors** of M and (λ, \mathbf{x}) is an **eigenpair** for M. The **geometric multiplicity** of the eigenvalue λ of M is the dimension of the eigenspace $\mathcal{E}_M(\lambda)$. The geometric multiplicity of an eigenvalue does not exceed its algebraic multiplicity.

If M is a symmetric matrix, then its eigenvalues are real, and according to the spectral theorem, there exists an orthogonal matrix P such that

$$PAP^T = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$$

and we say that M is **diagonalized** by P. We are particularly interested when P is a matrix whose entries are only in $\{-1, 0, 1\}$. If M is symmetric, algebraic, and geometric multiplicities of any eigenvalue coincide. In addition, the **rank** of the matrix equals the number of nonzero eigenvalues, counting multiplicities.

The symmetry of a graph reflects in the matrix M associated with G and its eigenvectors and eigenvalues since we can obtain a convenient partition of the vertex set of G. Let $\mathcal{D}: V_1 \cup V_2 \ldots \cup V_k$ be a partition of V. Then the matrix M can be block partitioned as $[M_{ij}]_{k \times k}$, where M_{ij} is the submatrix of M whose rows and columns are induced by V_i and V_j , respectively. The partition \mathcal{D} is called an **equitable partition** if the row-sum of each block is constant. The matrix $B_k = [b_{ij}]$, where b_{ij} is the row-sum of the block M_{ij} , is called the **quotient matrix** or **divisor matrix** of M with respect to \mathcal{D} . The next result will be used later and implies that all eigenvalues of B_k are also eigenvalues of M.

Theorem 2.1 ([12], Theorem 3.9.5). Let M be a real symmetric matrix and \mathcal{D} be an equitable partition of M with quotient matrix B_k . Then, the characteristic polynomial of B_k divides the characteristic polynomial of M.

We will focus on the cases when M is one of the following: the adjacency, the Laplacian, or the signless Laplacian matrices of a graph. The **adjacency matrix** A(G) has entries a_{ij} such that $a_{ij} = 1$ if $\{i, j\} \in E$, and $a_{ij} = 0$ otherwise. Based on the degrees of the vertices, we define the **degree matrix** D(G) where each diagonal entry is equals the degree of vertex i, that is, $D(G) = \text{diag}(d_1(G), \ldots, d_n(G))$. The **Laplacian** and the **signless Laplacian** matrix of G are given by

$$L(G) = D(G) - A(G) \text{ and } Q(G) = D(G) + A(G),$$

respectively. Most of the time in this text, we will work with the Laplacian L(G) of a graph. The celebrated Perron-Frobenius theorem is an important tool of our work.

Theorem 2.2 ([21], Perron-Frobenius). Let $M \in \mathbb{R}^{n \times n}$ with $n \ge 2$ be irreducible and nonnegative. Let $\rho(M)$ be the spectral radius of M. Then

- (*i*) $\rho(M) > 0;$
- (ii) $\rho(M)$ is an eigenvalue of M with algebraic multiplicity 1;
- (iii) there is a unique real positive vector $\mathbf{x} = [x_i]$ such that $M\mathbf{x} = \rho(M)\mathbf{x}$ and $x_1 + \dots + x_n = 1$;
- (iv) there is a unique real positive vector $\mathbf{y} = [y_i]$ such that $\mathbf{y}^T M = \rho(M)\mathbf{y}^T$ and $x_1y_1 + \dots + x_ny_n = 1$.

Theorem 2.2 states that the spectral radius of a matrix M associated with a connected graph equals its largest eigenvalue, and the corresponding eigenvector (Perron vector) has only positive entries. We know that the Perron vector has all entries equal to one for regular graphs. Notice that the Perron-Frobenius theorem does not work for the Laplacian matrix of a graph since it has negative entries.

The **Laplacian spectrum** of G is defined as

$$\operatorname{spec}_{L}(G) = (\mu_{1}, \ \mu_{2}, \dots, \ \mu_{n-1}, \mu_{n}),$$

where $\mu_1 \ge \cdots \ge \mu_{n-1} \ge \mu_n$ are the eigenvalues of L(G) arranged in non-increasing order. Some elementary properties of the Laplacian are summarized next.

Lemma 2.1 ([7], Lemma 4.3). Let G be a graph with $V(G) = \{1, \ldots, n\}$ and $E(G) = \{e_1, \ldots, e_m\}$. Then the following assertions hold.

- (i) L(G) is a symmetric, positive semidefinite matrix.
- (ii) The rank of L(G) equals n k, where k is the number of connected components of G.
- (iii) For any vector $x \in \mathbb{R}^n$,

$$x^T L(G) x = \sum_{i \sim j} (x_i - x_j)^2.$$

- (iv) The row and the column sums of L(G) are zero.
- (v) The cofactors of any two elements of L(G) are equal.

It follows immediately from (iv) that 0 is an eigenvalue of L(G), with the corresponding eigenvector $\mathbb{1}_n$, where $\mathbb{1}_n$ denotes the *n*-entry all-ones vector. Furthermore, the number of connected components of G equals the multiplicity of the eigenvalue 0.

Example 2.1. For the graphs G_1 and G_2 in Figure 2.1, we have $spect_L(G_1) = (6, 4, 4, 4, 2, 2, 2, 0)$ and $spect_L(G_2) = (4, 3, 3, 3, 1, 0, 0, 0)$. Note that the number of connected components of each graph coincides exactly with the multiplicity of the eigenvalue 0, which is the eigenvalue for both.



Figure 2.1: Graphs G_1 and G_2 .

The second smallest eigenvalue of L(G), μ_{n-1} , is called the **algebraic connectivity** of graph G and is denoted by $\alpha(G)$, or simply α . If G is connected, then $\mu_n = 0$ is a simple eigenvalue of L(G), that is, it has algebraic multiplicity 1 and in that case $\alpha > 0$. Conversely if $\alpha = 0$, then G is disconnected. The complete graph K_n which may be regarded as "highly connected" has $\mu_1 = \cdots = \mu_{n-1} = n$.

A graph is called **Laplacian integral** if the eigenvalues of L(G) are all integers. Table 2.1 presents the Laplacian spectrum of certain graphs.

Graph	Notation	Laplacian spectrum
Complete graph	K_n	$(n^{(n-1)}, 0^{(1)})$
Complement graph	G^c	$(n-\mu_{n-1},\ldots,n-\mu_1,0)$
Cycle	C_n	$\left(2-2\cos\left(\frac{2\pi j}{n}\right); \ j=1,\ldots,n\right)$
Complete bipartite graph	$K_{n_{1},n_{2}}$	$((n_1+n_2)^{(1)}, n_1^{(n_2-1)}, n_2^{(n_1-1)}, 0^{(1)})$
Join of graphs G_1 and G_2	$G_1 \vee G_2$	$(n_1+n_2,\lambda_2+n_2,\ldots,\lambda_{n_1}+n_2,$
		$\mu_2 + n_1, \dots, \mu_{n_2} + n_1, 0)$

Table 2.1: Laplacian spectrum of certain types of graphs

Let μ be an eigenvalue of L(G). If $\mathcal{E}_L(\mu)$ admits a simply structured basis B, that is, a basis where all vectors of the basis have entries only from the set $\{-1, 0, 1\}$, we say that $\mathcal{E}_L(\mu)$ is **simply structured**. The vectors in B are **quasi-orthogonal** if there is an ordering of these vectors such that non-consecutive vectors are orthogonal. An **eigenbasis** of L(G) is a basis of \mathbb{R}^n composed of eigenvectors of L(G). A graph G is **simply structured** if L(G) has a simply structured eigenbasis.

We will denote the eigenvalues of signless Laplacian matrix Q(G) by $q_1 \ge q_2 \ge \cdots \ge q_n$. Note that Q(G) is also positive semidefinite, but it is not necessarily singular. This only happens when Gis a bipartite graph ([16], Proposition 5.9). Furthermore, when G is a bipartite graph, the spectrum of the Laplacian matrix is equal to the spectrum of the signless Laplacian matrix, that is, $\mu_i = q_i$, for all $i \in \{1, \ldots, n\}$ ([16], Proposition 5.10). For regular graphs, the spectrum of the signless Laplacian matrix can be determined either from the spectrum of the adjacency matrix or the Laplacian matrix. In this case, all the theory developed for adjacency and Laplacian matrices is also valid for signless Laplacian matrix. We still have that the degrees and the number of connected components of a regular graph can be determined of the characteristic polynomial of the signless Laplacian matrix of the graph, according to next proposition.

Proposition 2.1 ([16], Proposition 5.12). Let G be a graph with n vertices and m edges. Then G is regular if and only if $nq_1 = 4m$ and, in this case, the degrees of its vertices are equal to $\frac{q_1}{2}$ and the number of components is the multiplicity of q_1 .

The following characterizations for regular graphs are also very important.

Proposition 2.2 ([13], Proposition 2.3.2). A graph G is regular if and only if its signless Laplacian has an eigenvector all of whose coordinates are equal to 1.

Proposition 2.3. If G is r-regular graph, then L(G) and Q(G) share the same eigenvectors.

Proof. Let (μ, \mathbf{x}) is an eigenpair for L(G), that is, $L(G)\mathbf{x} = \mu\mathbf{x}$. Note that as L(G) = D(G) - A(G), we obtain Q(G) = D(G) + A(G) = 2D(G) - L(G) and therefore, the eigenvalues of L(G) and the eigenvalues of Q(G) satisfy the following relation $q = 2r - \mu$, where r is the degree of regularity of the graph G. Then,

$$Q(G)\mathbf{x} = (2D(G) - L(G))\mathbf{x} = 2D(G)\mathbf{x} - L(G)\mathbf{x} = 2r\mathbf{x} - \mu\mathbf{x} = (2r - \mu)\mathbf{x} = qx$$

Therefore, (q, \mathbf{x}) is an eigenpair for Q(G).

2.2 Operations on graphs and spectral properties

In this section, we define some operations on graphs that will be useful later. Consider graphs G and H with vertex sets $V(G) = \{u_1, u_2, \ldots, u_{n_1}\}$ and $V(H) = \{v_1, v_2, \ldots, v_{n_2}\}$. Let $\lambda_1, \lambda_2, \ldots, \lambda_{n_1}$ be the eigenvalues of L(G), and $\mu_1, \mu_2, \ldots, \mu_{n_2}$ be the eigenvalues of L(H). Further assume that u_i is an eigenvector of L(G) for eigenvalue λ_i , and v_j an eigenvector of L(H) corresponding to the eigenvalue μ_j .

1. The **Cartesian product** of G and H, denoted by $G \square H$, is the graph with vertex set $V(G) \times V(H)$ and

$$(u_i, v_j) \sim (u_r, v_s)$$
 in $G \square H \iff \begin{cases} u_i = u_r \text{ and } v_j \sim v_s \text{ in } H \\ \text{or} \\ v_j = v_s \text{ and } u_i \sim u_r \text{ in } G \end{cases}$

2. The direct product (or tensor product or Kronecker product) of G and H, denoted by $G \times H$, is the graph with vertex set $V(G) \times V(H)$ and

$$(u_i, v_j) \sim (u_r, v_s)$$
 in $G \times H \iff u_i \sim u_r$ in G and $v_j \sim v_s$ in H

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3. The strong product of G and H, denoted by $G \boxtimes H$, is the graph with vertex set $V(G) \times V(H)$ such that

$$(u_i, v_j) \sim (u_r, v_s) \text{ in } G \boxtimes H \iff \begin{cases} u_i = u_r \text{ and } v_j \sim v_s \text{ in } H \\ \text{or} \\ v_j = v_s \text{ and } u_i \sim u_r \text{ in } G \\ \text{or} \\ u_i \sim u_r \text{ in } G \text{ and } v_j \sim v_s \text{ in } H \end{cases}$$

Note that the strong product is the union of the Cartesian and the tensor product, i.e., $K_{n_1} \boxtimes K_{n_2} = K_{n_1 n_2}$.

4. The lexicographic product of G with H, denoted by $G \circ H$, is the graph with vertex set $V(G) \times V(H)$ such that

$$(u_i, v_j) \sim (u_r, v_s) \text{ in } G \circ H \iff \begin{cases} u_i \sim u_r \text{ in } G \text{ and } v_j = v_s \\ \text{or} \\ u_i \sim u_r \text{ in } G \text{ and } v_j \sim v_s \text{ in } H \\ \text{or} \\ u_i \sim u_r \text{ in } G \text{ and } v_j \neq v_s \text{ in } H \end{cases} \iff \begin{cases} u_i \sim u_r \text{ in } G \\ \text{or} \\ u_i = u_r \text{ and } v_j \sim v_s \text{ in } H \\ \text{or} \\ u_i = u_r \text{ and } v_j \sim v_s \text{ in } H \end{cases}$$

Let $\star \in \{\Box, \times, \boxtimes, \circ\}$, where \Box denotes the Cartesian product, \times the direct product, \boxtimes the strong product, and \circ the lexicographic product. For each of these products, if the graphs G and H are regular of regularities s and r, respectively, then the product $G \star H$ is also regular, and its degree can be easily calculated. Moreover, the eigenvectors of the Laplacian matrix of each of these products can be computed from the eigenvectors of the Laplacian matrix of the constituent graphs. We have:

Graph	Notation	Laplacian spectrum
Cartesian product	$G \square H$	$\lambda_i+\mu_j;\ 1\leq i\leq n_1,\ 1\leq j\leq n_2$
Direct product	$G \times H$	$r\lambda_i + s\mu_j - \lambda_i\mu_j; \ 1 \le i \le n_1, \ 1 \le j \le n_2$
Strong product	$G\boxtimes H$	$(1+r)\lambda_i + (1+s)\mu_j - \lambda_i\mu_j; \ 1 \le i \le n_1, \ 1 \le j \le n_2$
Lexicograph product	$G \circ H$	$\lambda_i n_2, \ \mu_j + d_{u_i} n_2; \ 1 \le i \le n_1, \ 2 \le j \le n_2$

Table 2.2: Laplacian spectrum of graph products

5. The operation of adding or removing an edge $e = \{u_i, u_j\}$ to or from a graph G is called **edge** addition or edge removal, respectively. In edge addition, if e is not already an edge in G, the resulting graph G' = G + e will include e along with all the original edges of G. Conversely, in edge removal, if e is an existing edge in G, the resulting graph $G' = G \setminus e$ will exclude e but retain all the other original edges of G. Let $G = K_n \setminus pK_2$ be a complete graph minus a matching of size p. The Laplacian spectrum of G is spec_L $(G) = (n^{(n-p-1)}, (n-2)^{(p)}, 0^{(1)})$.

The *Interlacing Theorem for the Laplacian Matrix* provides a relationship between the eigenvalues of a graph and the eigenvalues of the graph obtained by adding an edge.

Theorem 2.3 ([16], Theorem 4.1). Let G = (V, E) be a graph with n vertices, and let $e \in E$. If G' = G + e, then

$$\mu_j(G) \le \mu_j(G') \le \mu_{j+1}(G), \text{ for all } j \in \{1, 2, \dots, n-1\}.$$
(2.1)

Noting that tr(L(G)) = 2m, we obtain $\sum_{i=1}^{n} (\mu_i(G') - \mu_i(G)) = 2m + 2 - 2m = 2$. Therefore, at least one of the inequalities in (2.1) must be strict.

The next results establish that an appropriate change in a graph G by adding or removing edges yields a new graph G' such that an eigenvector \mathbf{x} to L(G) is also still an eigenvector to L(G') under some conditions. In [28], Merris proved that this is true when the entries \mathbf{x}_i and \mathbf{x}_j of the eigenvector \mathbf{x} corresponding to the edge $\{i, j\} \in E$ are equal.

Theorem 2.4 ([28], Edge Principle). Let μ be an eigenvalue of L(G) associated with eigenvector \mathbf{x} . If $\mathbf{x}_i = \mathbf{x}_j$, then μ is an eigenvalue of L(G') associated with \mathbf{x} , where G' is obtained from G by deleting or adding an edge $e = \{i, j\}$ depending on whether or not it is an edge of G.

The results of [24] show that we can even go beyond the Edge Principle. The authors show that it is possible to add or remove an edge $\{i, j\}$ from G where the corresponding entries \mathbf{x}_i and \mathbf{x}_j are not equal and still guarantee that \mathbf{x} is also an eigenvector to the Laplacian matrix of the new graph G'. It turns out that the results stated in Lemmas 2.2 and 2.3 are very important tools for proving the main results presented in Chapter 5

Lemma 2.2 ([24], Lemma 2.2). Let G = (V, E) be a graph on n vertices and $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k, 0, \dots, 0)$ is an eigenvector of L(G) associated with eigenvalue μ , in a way that $\sum_{l=1}^k \mathbf{x}_l = 0$ and $\mathbf{x}_l \neq 0$, for all $l \in \{1, \dots, k\}$. Take the vertex partition $W_1 = \{1, \dots, k\}$ and $W_2 = \{k + 1, \dots, n\}$. If $i \in W_2$ and $e_l = \{i, l\} \notin E$, for $l = 1, \dots, k$, then \mathbf{x} is an eigenvector of L(G'), where $G' = G + e_1 + \dots + e_k$, associated with eigenvalue $\mu + 1$.

Lemma 2.3 ([24], Lemma 2.3). Let G = (V, E) be a graph on n vertices and suppose that $\mathbf{x} = \mathbf{x}^{n-k} = (1, 1, \dots, 1, -n + k, \underbrace{0, 0, \dots, 0})$ is an eigenvector of L(G) associated with eigenvalue μ . Let $G' = G + e_1 + e_2 + \dots + e_{n-k}$, where $e_l = \{l, n-k+1\} \notin E(G)$, for $l = 1, \dots, n-k$. Then, \mathbf{x} is an eigenvector of L(G') associated with eigenvalue $\mu + (n-k) + 1$.

Notice that the previous results hold for any graph, but we will usually apply them to the family of threshold graphs.

2.3 Cograph and threshold graphs

The family of *complement reducible graphs* (or *cographs* for short) is much studied. The literature presents several definitions that characterize these graphs, for example, [1], [6], [7] and [11]. One way to define these graphs is through a recursive process.

Definition 2.1. A graph G is called a **cograph** if it is constructed using the following rules:

- 1) K_1 is a cograph.
- 2) The union of two cographs is a cograph.
- 3) The complement of a cograph is a cograph.

Note that Definition 2.1 provides a recursive procedure for constructing a cograph. The operations of disjoint union and join can also be used to build cographs. The rule number 3) in Definition 2.1 can be replaced by

3') The join of two cographs is a cograph.

Equivalently, the authors in [11] showed that:

Proposition 2.4. A graph G is a cograph if and only if G does not contain P_4 , as an induced subgraph.

It follows that if G is a cograph, then every induced subgraph of G is a cograph, and every component of G is a cograph. Examples of cographs include every complete graph K_n is a cograph; every complete bipartite graph K_{n_1,n_2} is a cograph; no cycle of length greater than four is a cograph, as C_n with $n \ge 5$ has an induced P_4 .

Let G_1 and G_2 be two cographs on n_1 and n_2 vertices, respectively. Let $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n_1}$ be the eigenvalues of $L(G_1)$ and $0 = \mu_1 \leq \mu_2 \leq \cdots \leq \mu_{n_2}$ be the eigenvalues of $L(G_2)$. It follows from Definition 2.1 that any connected cograph can be written as $G_1 \vee G_2$, and any disconnected cograph can be written as $G_1 \sqcup G_2$. Therefore, the spectrum of connected and disconnected cographs are, respectively:

$$\operatorname{spect}_{L}(G_{1} \lor G_{2}) = (n_{1} + n_{2}, \lambda_{2} + n_{2}, \dots, \lambda_{n_{1}} + n_{2}, \mu_{2} + n_{1}, \mu_{n_{2}} + n_{1}, 0) \text{ and}$$
$$\operatorname{spect}_{L}(G_{1} \sqcup G_{2}) = (\lambda_{2}, \dots, \lambda_{n_{1}}, \mu_{2}, \dots, \mu_{n_{2}}, 0, 0)$$

Thus the eigenvalues of cographs are always integers, that is, cographs are Laplacian integral.

Note that there are other Laplacian integral graphs that are not cographs. For example, the graph $G = K_2 \Box K_3$ (see Figure 2.2) is a Laplacian integral graph, as spect_L(G) = (5,5,3,3,2,0), but

G is not a cograph since it contains an induced subgraph (for example, the 4-vertex path given by $(1,4) \sim (2,4) \sim (2,5) \sim (1,5)$) isomorphic to P_4 .



Figure 2.2: Cartesian product of $G = K_2$ and $H = K_3$.

Although some Laplacian integral graphs are not cographs, we have the following characterization of cographs.

Proposition 2.5 ([1], Proposition 2.12). A graph G is a cograph if and only if every induced subgraph of G is Laplacian integral.

The authors state in [8] that the eigenvectors of the Laplacian matrix of a cograph can be chosen to have a simple structure, with most entries being zero.

Theorem 2.5 ([8], Theorem 11). Let G be a cograph. Then there exists a basis B of eigenvectors of L(G) such that each vector of B has at most two distinct nonzero entries.

This theorem is important because it provides a characterization of the eigenvectors of cographs, which simplifies their analysis and interpretation. The converse of Theorem 2.5 fails in general. For example, the graph $K_3 \square K_2$ (see Figure 2.2) has a basis $B = \{(1,1,1,-1,-1,-1), (1,1,1,1,1,1), (1,0,-1,1,0,-1), (0,1,-1,1,-1,0), (1,0,-1,-1,0,1), (0,1,-1,-1,1,0)\}$ of eigenvectors of L(G) such that each vector in the basis B has at most two distinct nonzero entries, but $K_3 \square K_2$ is not a cograph since it contains an induced subgraph isomorphic to P_4 . More generally, we have:

Lemma 2.4 ([8], Lemma 12). If G is a connected graph with $n \ge 3$ vertices, then $G \square K_2$ is not a cograph.

There are several different ways to define a *threshold graph*, as can be seen in [25]. We use the characterization by a binary generating sequence as follows.

Definition 2.2. Given a sequence $\{b_i\}$ of 0's and 1's with n elements, the **threshold** graph associated with the binary sequence $\{b_i\}$ is the graph on n vertices constructed recursively, starting with an empty graph, and for i = 1, ..., n

(i) add the isolated vertex i if $b_i = 0$,

(ii) add the vertex i adjacent to all vertices with label less than i if $b_i = 1$.

A vertex *i* is an *isolated vertex* if $b_i = 0$ and a *dominating vertex* if $b_i = 1$. For example, the star $K_{1,n-1}$ of order *n* is a threshold graph with exactly one dominating vertex and can be represented by the binary sequence (0, 0, ..., 0, 1). The graphs G_1 and G_2 in Figure 2.3 are also threshold graphs and can be represented by the binary sequences (0, 0, ..., 0, 1).



Figure 2.3: Threshold graphs G_1 and G_2 with 5 and 6 vertices, respectively.

In the case where G is a connected threshold graph, by Definition 2.2, the last entry in the binary sequence representing it will be equal to 1, meaning the last vertex will necessarily be a dominating vertex. As a result, all connected threshold graphs have a diameter of at most 2. Furthermore, every connected threshold graph G on n vertices has a star S_n as a subgraph. In the case where G is a disconnected threshold graph, by Definition 2.2, for some vertex i, we have $b_i = 1$ and $b_j = 0$ for all j > i. Thus, every disconnected threshold graph on n vertices can be constructed by taking the disjoint union of a star graph of order n - p with pK_1 , where p is the number of isolated vertices in G. In this way, G will have p + 1 connected components.

Threshold graphs also have a minimal forbidden subgraph characterization, as demonstrated by the authors in [10].

Proposition 2.6. A graph G is a threshold graph if and only if G does not contain P_4 , C_4 or $2K_2$ as induced subgraphs.

Note that this characterization implies that every threshold is a cograph. However, the converse is not true. For example, the cycle C_4 is a cograph but not a threshold graph.

Since cographs are Laplacian integral, threshold graphs are also integral. The computation of the eigenvalues of the Laplacian matrix of threshold graphs, based on their vertex degrees, is well-known [27]. More specifically, let G be a threshold graph on n vertices defined by the binary sequence (b_1, b_2, \ldots, b_n) , with degree sequence $d = (d_1, d_2, \ldots, d_n)$, where $d_1 \ge d_2 \ge \ldots \ge d_n$, and $\operatorname{tr}(G) = \sum_{i=1}^n b_i$.

Then, the eigenvalues of L(G), denoted as μ_i for each $i \in \{1, 2, ..., n\}$, are given by:

$$\mu_{i} = \begin{cases} d_{i} + 1, & \text{if } 1 \leq i \leq \operatorname{tr}(G), \\ d_{i+1}, & \text{if } \operatorname{tr}(G) + 1 \leq i \leq n-1, \\ 0, & \text{if } i = n, \end{cases}$$
(2.2)

It is worth highlighting that the threshold graphs are determined by the Laplacian spectrum; that is, no two threshold graphs on n vertices have the same spectrum unless they are isomorphic.

2.4 Chain graphs

Several authors have studied the eigenvalues of the Laplacian matrix of chain graphs, among which we can mention the recent work by Milica *et al.* [5], but little has been explored in the literature regarding the eigenspaces of this family of graphs. Our interest in chain graphs is related to the fact that any threshold graph can be obtained from a chain graph. It is known that every chain graph is bipartite, with parts denoted as A and B, and the neighbors of vertices in each partition form a chain with respect to inclusion. Parts A and B are organized into h non-empty cells denoted by $A = \bigcup_{i=1}^{h} U_i$ and $B = \bigcup_{i=1}^{h} V_i$. The edges present in the chain graph are such that all vertices in U_s are connected to all vertices in $\bigcup_{k=1}^{h+1-s} V_k$, for $1 \le s \le h$. From this connection structure, it is possible to observe that all vertices in a cell U_i share the same set of neighbors, as do the vertices in V_i for every $i = 1, \ldots, h$. This fact means that all vertices within the same cell have the same neighbors; that is, they are **twin vertices**. We denote the chain graph G as $C(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$, where $m_i = |U_i|$ and $n_i = |V_i|$, for $1 \le i \le h$. A general idea of a chain graph is presented in Figure 2.4. Since $C(m_1, \ldots, m_h; n_1, \ldots, n_h)$ and $C(n_1, n_2, \ldots, n_h; m_1, m_2, \ldots, m_h)$ are isomorphic, in all forthcoming considerations we will only mention one of the corresponding isomorphic pair.



Figure 2.4: The chain graph $G = C(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$.

For i = 1, ..., h the degree of each vertex in U_i is equal to

$$d_i = \sum_{k=1}^{h+1-i} n_k,$$

while each vertex of V_i has degree equal to

$$d_i^* = \sum_{k=1}^{h+1-i} m_k.$$

By using this structure of a chain graph, it is possible to prove that any threshold graph can be obtained from a chain graph by adding all edges to one co-clique or, in the other direction, by deleting edges from the clique [5]. Chain graphs can also be characterized by forbidden subgraphs: they are precisely the graphs that are $\{C_3, C_5, 2K_2\}$ -free.

The subsets U_i and V_i of V(G) induce an equitable partition of the Laplacian matrix of the chain graph. We denote by $\mathcal{D}(G)$ the quotient matrix of order 2*h* corresponding to the partition $\mathcal{D}: \left(\bigcup_{i=1}^{h} U_i\right) \cup \left(\bigcup_{i=1}^{h} V_i\right)$, i.e.,

$$\mathcal{D}(G) = \begin{bmatrix} d_1 & & & -n_1 & \cdots & -n_{h-1} & -n_h \\ & d_2 & & & -n_1 & \cdots & -n_{h-1} \\ & & \ddots & & \vdots & \ddots & & \\ & & & d_h & -n_1 & & \\ \hline -m_1 & \cdots & -m_{h-1} & -m_h & d_1^* & & \\ & -m_1 & \cdots & -m_{h-1} & & d_2^* & & \\ & & & \ddots & & \\ -m_1 & & & & & d_h^* \end{bmatrix}.$$
(2.3)

The following result gives a formula for the characteristic polynomial of the Laplacian matrix of a chain graph.

Theorem 2.6 ([5], Lemma 3.4). Let $G = C(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ be a chain graph, $d_i = \sum_{k=1}^{h+1-i} n_k$, $d_i^* = \sum_{k=1}^{h+1-i} m_k$, $p_j = (d_j^* - \lambda)(\lambda - d_{h+1-j})$, for $j = 1 \ldots h$, and $\mathcal{D}(G)$ its quotient matrix defined in (2.3). Then the characteristic Laplacian polynomial $\phi(L(G), \lambda)$ of G is given by

$$\phi(L(G),\lambda) = \prod_{i=1}^{h} (\lambda - d_i)^{m_i - 1} (\lambda - d_i^*)^{n_i - 1} \phi(D(G),\lambda),$$

where

$$\phi(\mathcal{D}(G),\lambda) = (-1)^h \lambda \prod_{j=1}^h p_j \left(\frac{n_1}{p_1} + \lambda \sum_{j=2}^h \frac{n_j}{(\lambda - d_{h+2-j})p_j} + \frac{1}{\lambda - d_1} \right),$$

denotes the characteristic polynomial of $\mathcal{D}(G)$.

The interchange of the roles of n_i 's and m_i 's and d_i 's and d_i 's yields another formula for the characteristic polynomial of $\mathcal{D}(G)$, that is,

$$\phi(\mathcal{D}(G),\lambda) = (-1)^h \lambda \prod_{j=1}^h p_j \left(\frac{m_1}{p_h} + \lambda \sum_{j=2}^h \frac{m_j}{(\lambda - d_{h+2-j}^*)p_{h+1-j}} + \frac{1}{\lambda - d_1^*} \right)$$

From Theorem 2.6, every eigenvalue of $\mathcal{D}(G)$ is an eigenvalue to L(G). The following theorem collects some properties of the eigenvalues of chain graphs.

- **Theorem 2.7** ([4], [5]). Let $G = C(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph, $d_i = \sum_{k=1}^{h+1-i} n_k$, $d_i^* = \sum_{k=1}^{h+1-i} m_k$ and $\mathcal{D}(G)$ its divisor matrix defined in (2.3). The following items hold true.
 - (i) all the eigenvalues of the divisor matrix $\mathcal{D}(G)$ are simple. Furthermore, 0 is always an eigenvalue of $\mathcal{D}(G)$.
 - (ii) If $m_i \ge 2$, then d_i is an L-eigenvalue with multiplicity at least $m_i 1$ and the corresponding eigenvectors of L(G) have the form

$$x_{k} = (0, \dots, 0, \underbrace{1}_{\substack{k-th \\ coordinate}}, 0, \dots, 0, \underbrace{-1}_{\substack{k+i-th \\ coordinate}}, 0, \dots, 0)^{T},$$
(2.4)

for $1 \le k \le m_i - 1$, as it can be seen at [14]. Similarly for $n_i \ge 2$, with d_i^* in the role of d_i . The remaining 2h L-eigenvalues are the eigenvalues of $\mathcal{D}(G)$.

(iii) A vertex degree d is an eigenvalue of $\mathcal{D}(G)$ if and only if $d = d_i = d_j^*$, for some $i, j \in \{1, 2, ..., h\}$ such that $i + j \notin \{h + 1, h + 2\}$.

We obtain the first result of this work by determining $G = C(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ in which all integer eigenvalues of L(G) have simply structured eigenspaces. Specifically, we aim to construct chain graphs of order n such that $d = d_i = d_j^*$ is not an eigenvalue of the quotient matrix $\mathcal{D}(G)$, because if d is an eigenvalue of the quotient matrix $\mathcal{D}(G)$ defined in (2.3), we cannot ensure that the corresponding eigenvector will have all its entries in $\{-1, 0, 1\}$. Thus, according to condition (*iii*) of Theorem 2.7, we permit $d = d_i = d_j^*$ if and only if $i + j \in \{h + 1, h + 2\}$ ensuring that $d = d_i = d_j^*$ will not be an eigenvalue of $\mathcal{D}(G)$. We have that if i = 1 and j = h, then $i + j \in \{h + 1, h + 2\}$. Thus, $d_1 = d_h^*$ if and only if $\sum_{k=1}^{h} n_k = m_1$. In this case, m_2, \ldots, m_h can be any natural numbers greater than or equal to 2. Similarly, if i = h and j = 1, then $i + j \in \{h + 1, h + 2\}$, and $d_h = d_1^*$ if and only if $n_1 = \sum_{k=1}^{h} m_k$, where n_2, \ldots, n_h can be any natural numbers greater than or equal to 2. As the sequences (m_1, \ldots, m_h) and (n_1, \ldots, n_h) correspond to the sizes of cells U_1, \ldots, U_h and V_1, \ldots, V_h , respectively, we obtain an infinite subfamily of chain graphs G in which all integer eigenvalues of L(G) have simply structured eigenspaces. **Proposition 2.7.** Let $G = C(m_1, \ldots, m_h; n_1, \ldots, n_h)$ be a chain graph such that $m_i \ge 2$ and $n_i \ge 2$, for $i \in \{1, \ldots, h\}$. If $m_1 = \sum_{k=1}^h n_k$, then all integer eigenvalues of L(G) have simply structured eigenspaces. Proof. Given that $m_i \ge 2$ and $n_i \ge 2$, for $i = 1, \ldots, h$, we apply item (*ii*) of Theorem 2.7 to conclude that d_i and d_i^* are eigenvalues of L(G) with multiplicity at least $m_i - 1$ and $n_i - 1$, respectively. Moreover, the corresponding eigenvectors given in (2.4) have all their entries in $\{-1, 0, 1\}$. Let $\mathcal{D}(G)$ be the quotient matrix of L(G) with respect to the partition $\mathcal{D} : (\bigcup_{i=1}^h U_i) \cup (\bigcup_{i=1}^h V_i)$. By items (*i*) and (*iii*) of Theorem 2.7, all eigenvalues of $\mathcal{D}(G)$ are simple, and a vertex degree d is an eigenvalue of $\mathcal{D}(G)$ if and only if $d = d_i = d_j^*$ for some $i, j \in \{1, 2, \ldots, h\}$ such that $i + j \notin \{h + 1, h + 2\}$. By hypothesis, we have $d_h^* = d_1$. In this case, $i + j \in \{h + 1, h + 2\}$, and therefore by item (*iii*) of Theorem 2.7, $d = d_h^* = d_1$ will not be an eigenvalue of $\mathcal{D}(G)$. Consequently, all integer eigenvalues of L(G) have simply structured eigenspaces.

From Proposition 2.7, we can prove that if we exchange $m_1 = \sum_{k=1}^{h} n_k$ for $n_1 = \sum_{k=1}^{h} m_k$ the same result is valid.

Chapter 3

CONSTRUCTIONS AND PROPERTIES OF HADAMARD AND WEAK HADAMARD MATRICES

In this chapter, we present a short literature review of the Hadamard matrix, denoted by H, and a weak Hadamard matrix denoted by W. Those matrices have entries only in a specific set S and satisfying an additional property. More specifically:

- 1. $S = \{-1, 1\}$ and H satisfies $HH^T = nI$.
- 2. $S = \{-1, 0, 1\}$ and W satisfies $W^T W$ is a tridiagonal matrix.

3.1 Hadamard Matrices

Hadamard matrices have been a subject of interest for almost 150 years, ever since Sylvester published the first examples in 1867 [30]. They have a wide range of applications, including in signal processing, coding theory, and cryptography [20].

Definition 3.1. A (real) Hadamard matrix of order n is an $n \times n$ matrix H with all entries in the set $S = \{-1, 1\}$ and with the property that

$$HH^T = nI; (3.1)$$

that is, the inner product of two distinct rows is 0 and the inner product of a row with itself is n.

Examples for the orders n = 1, 2 and 4 are

Sylvester also noted that if H is a Hadamard matrix, so is

$$\left[\begin{array}{cc} H & H \\ H & -H \end{array}\right]. \tag{3.2}$$

Then, in 1893, Hadamard [18] published examples of orders 12 and 20, showing that the matrices which have come to bear his name could exist in orders other than the powers 2^k previously demonstrated by Sylvester. Hadamard was interested in finding the maximal determinant of square matrices with entries from the unit disc, and he showed in [18] that this maximal determinant $n^{n/2}$ was achieved by matrices with entries $\{-1,1\}$ if and only if they satisfied (3.1). So Hadamard matrices are extremal solutions of a problem in real analysis.

These matrices have been extensively studied, and it is known that a necessary condition for the existence of such a matrix is that n = 1, 2, or is a multiple of 4. A well-known and still open problem concerns the question of whether this is sufficient.

Conjecture 3.1 (Hadamard). Hadamard matrices exist for all orders n of the form n = 4k.

The Hadamard conjecture is one of the longest-standing open problems in mathematics. We will present the four major families of Hadamard matrices that have been discovered over the past century: 1) Sylvester, 2) Paley, 3) Hadarmard Design and 4) Williamson. These families include different construction methods, each with its own specific characteristics and properties.

3.1.1 Classical constructions

The *tensor product* is the basis of techniques for constructing Hadamard matrices, allowing for the systematic generation of new matrices from existing ones.

Definition 3.2. Let A and B be matrices of order $m \times n$ and $p \times q$, respectively. The **tensor product** (also called **Kronecker product** or **direct product**), denoted $A \otimes B$, is a matrix of order $mp \times nq$ defined by

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1m}B \\ a_{21}B & a_{22}B & \dots & a_{2m}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mm}B \end{bmatrix}$$
(3.3)

or $A \otimes B = [a_{ij}B]$.

It can be verified from the definition that

$$(A \otimes B)(C \otimes D) = AC \otimes BD. \tag{3.4}$$

Some elementary constructions of Hadamard matrices follow easily from (3.1), (3.2) and (3.3).

Lemma 3.1 ([20], Lemma 2.2). Let H be a Hadamard matrix of order n, so by (3.1) it is invertible over \mathbb{Q} , with $H^{-1} = n^{-1}H^T$. Set $H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$. Then

- i) the negation -H of H is a Hadamard matrix;
- ii) the transpose H^T of H is a Hadamard matrix;
- iii) if H' is a Hadamard matrix of order n', the tensor product $H' \otimes H$ is a Hadamard matrix of order n'n;
- iv) for $k \ge 1$, $(\otimes^k H_1) \otimes H$ is a Hadamard matrix of order $2^k n$.

Next, we present the four well-known ways of constructing Hadamard matrices.

1) Sylvester Hadamard matrices

The earliest known, and still by far the most significant, family of Hadamard matrices are those of order 2^k for $k \ge 1$, due to Sylvester. They are constructed by iterating the tensor product of H_1 with itself (that is, by setting H = [1] in Lemma 3.1). These matrices are all symmetric.

The Sylvester Hadamard matrices are the matrices in the family

$$\{H_k = \otimes^k H_1; \ k \ge 1\}.$$

In other words, by defining $H_0 = [1]$, we have

$$H_{k+1} = \left[\begin{array}{cc} H_k & H_k \\ H_k & -H_k \end{array} \right], \text{ for } k \ge 0.$$

For k = 0 and k = 1, we get

2) Paley Hadamard matrices

This method is due to Paley [23] and it uses the quadratic residues in a finite field GF(q) of odd order. An integer g is called a **quadratic residue modulo** q if it is congruent to a perfect square modulo q, i.e., if there exists an integer x such that $x^2 \equiv g \pmod{q}$. The **quadratic character** \mathcal{X} on the cyclic group $GF(q)^* = GR(q) \setminus \{0\}$, defined by

$$\mathcal{X}(g) = \begin{cases} 1, & \text{if } g \text{ is a quadratic residue in } GF(q) \\ -1, & \text{if } g \text{ is a quadratic nonresidue in } GF(q) \end{cases}$$

is extended to GF(q) by setting $\mathcal{X}(0) = 0$. The version of Paley's constructions given here, and a more accessible proof, may be found in [19].

Lemma 3.2 ([20], Lemma 2.4). For q an odd prime power, and an ordering $\{g_0 = 0, g_1, \dots, g_{q-1}\}$ of GF(q), set $Q = [\mathcal{X}(g_i - g_j)]_{0 \le i,j < q}$. Let R be the $(q+1) \times (q+1)$ matrix $R = \begin{bmatrix} 0 & \mathbb{1}_q \\ \mathbb{1}_q^T & Q \end{bmatrix}$.

i) Paley Type I Hadamard matrix - If $q \equiv 3 \pmod{4}$, then

$$P_q = \left[\begin{array}{c|c} 1 & -\mathbb{1}_q \\ \hline \mathbb{1}_q^T & Q + I_q \end{array} \right]$$

is a Hadamard matrix of order q + 1.

ii) Paley Type II Hadamard matrix - If $q \equiv 1 \pmod{4}$, then

$$P'_{q} = \left[\begin{array}{c|c} R + I_{q+1} & R - I_{q+1} \\ \hline R - I_{q+1} & -R - I_{q+1} \end{array} \right]$$

is a Hadamard matrix of order 2(q+1).

Note that Q is skew-symmetric when $q \equiv 3 \pmod{4}$ and symmetric when $q \equiv 1 \pmod{4}$.

Example 3.1. If q = 7, so the quadratic residues in GF(7) are 1,2,4, and the Paley Type I Hadamard matrix P_7 of order 8 is

Now, if q = 5, so the quadratic residues in GF(5) are 1, 4, and the Paley Type II Hadamard matrix

 P_5 of order 12 is

. 1	1	1	1	1	1	-1	1	1	1	1	1		
1	1	1	-1	-1	1	1	-1	1	-1	-1	1		
1	1	1	1	-1	-1	1	1	-1	1	-1	-1		
1	-1	1	1	1	-1	1	-1	1	-1	1	-1		
1	-1	-1	1	1	1	1	-1	-1	1	-1	1		
1	1	-1	-1	1	1	1	1	-1	-1	1	-1	(3.6)
-1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	(3.0)
1	-1	1	-1	-1	1	-1	-1	-1	1	1	-1		
1	1	-1	1	-1	-1	-1	-1	-1	-1	1	1		
1	-1	1	-1	1	-1	-1	1	-1	-1	-1	1		
1	-1	-1	1	-1	1	-1	1	1	-1	-1	-1		
1	1	-1	-1	1	-1	-1	-1	1	1	-1	-1		

Combining these constructions using tensor products (Lemma 3.1) gives a very large family of Hadamard matrices, but, as always, the tensor product increases the 2-power factor in the order.

Definition 3.3. Let $\{q_i; i \in I\}$ $e \{q'_j; j \in J\}$ be finite sets of prime powers congruent to $3 \pmod{4}$ and $1 \pmod{4}$, respectively. A matrix of the form

$$\left(\bigotimes_{i\in I} P_{q_i}\right) \bigotimes \left(\bigotimes_{j\in J} P'_{q'_j}\right),$$

which is a Hadamard matrix of order $\prod_{i \in I} (q_i+1) \prod_{j \in J} 2(q'_j+1)$, is called a **Paley Hadamard matrix**.

3) Hadamard designs

The Paley Type I Hadamard matrices form one of three main known families of Hadamard matrices which may be constructed directly from square block designs, so a little combinatorial design theory is now introduced.

Definition 3.4. A (square) (v, k, λ) -design is a pair $\mathcal{D} = (P, B)$ consisting of a set $P = \{p_1, p_2, \dots, p_v\}$ of v points and a set $B = \{B_1, B_2, \dots, B_v\}$ of v blocks each containing k points (1 < k < v), such that each pair of distinct points is contained in exactly λ blocks.

An incidence matrix $A = [a_{ij}] de \mathcal{D}$ is a $v \times v$ matrix with entries 0,1, having

$$a_{ij} = 1$$
 if and only if $p_j \in B_i$.

It follows that a $v \times v$ matrix A with entries 0,1 is a incidence matrix of a (v, k, λ) -design if and only if

$$AA^{T} = (k - \lambda)I + \lambda J, \quad AJ = kJ, \tag{3.7}$$

For proof, see, for example, [31].

Definition 3.5. A normalised matrix is a matrix whose first row and first column consist entirely of 1's. The submatrix excluding the first row and column of a normalised matrix is called its core.

In general, the formula (3.7) allows us to equate the core of a normalised Hadamard matrix of order 4n and the $\{-1,1\}$ version of an incidence matrix of a (4n-1, 2n-1, n-1)-design. That is, if A' = 2A - J is the $\{-1,1\}$ matrix obtained from incidence matrix A by replacing 0 by -1, then

$$H = \begin{bmatrix} 1 & 1 \\ 1^T & A' \end{bmatrix}$$
(3.8)

is the corresponding Hadamard matrix of order 4n, and vice versa.

Example 3.2. Consider the Paley Type I Hadamard matrix P_7 , defined in (3.5). Multiplying each column except the first by -1 gives a normalised Hadamard matrix of the form

The $\{0,1\}$ version of the core $-(Q + I_7)$ of the normalised P_7 in (3.9) is

$$A = \frac{1}{2}(J - (Q + I_7)) = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$
(3.10)

Then $AA^T = 2I + J$, AJ = 3J and A is the incidence matrix of a (7,3,1)-design.

Lemma 3.3 ([20], Lemma 2.7). There exists a Hadamard matrix of order 4n if and only if there exists a square (4n - 1, 2n - 1, n - 1)-design.

For obvious reasons, a square (4n-1, 2n-1, n-1)-design is called a **Hadamard design**. Hadamard designs are doubly valuable because, by adjoining one point and suitably redefining blocks, an extended design is obtained in which every block is incident with 2n points, with the stronger incidence property that every 3 distinct points, not just every 2, are together incident with exactly n-1 blocks. Such a 3-(4n, 2n, n-1)-design is called a *Hadamard 3-design*, and conversely, every 3-(4n, 2n, n-1)-design is the unique extension (up to isomorphism) of a Hadamard design. For more details, we refer the reader to [5].

4) Williamson Hadamard matrices

The Williamson construction is the simplest of many powerful 'plug-in' methods for finding Hadamard matrices. These techniques essentially capitalise on the success of tensoring as a generator of Hadamard matrices, by allowing judicious replacement of a matrix B_i in definition

-

$$A \otimes [B_1, B_2, \dots, B_m] = \begin{bmatrix} a_{11}B_1 & a_{12}B_1 & \dots & a_{1m}B_1 \\ a_{21}B_2 & a_{22}B_2 & \dots & a_{2m}B_2 \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B_m & a_{m2}B_m & \dots & a_{mm}B_m \end{bmatrix}$$
(3.11)

by several different matrices, which do not have to be Hadamard. We will vary Williamson's original template [32], by taking the overlying matrix A in (3.11) to be the Hadamard matrix

Lemma 3.4 ([20], Lemma 2.10). If there exist $\{-1,1\}$ matrices A, B, C, D of order n which satisfy both

$$XY^T = YX^T$$
, for $X \neq Y \in \{A, B, C, D\}$

and

$$AA^T + BB^T + CC^T + DD^T = 4nI_n,$$

then

$$\left[\begin{array}{cccc} A & B & C & D \\ B & -A & D & -C \\ C & -D & -A & B \\ D & C & -B & -A \end{array} \right]$$

is a Hadamard matrix of order 4n.

Definition 3.6. The Williamson Hadamard matrices are the Hadamard matrices constructed in Lemma 3.4.

Next, we give an example of obtaining a Hadarmard matrix of order 12 by using the Williamson Hadamard process.

Example 3.3. The matrices

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad B = C = D = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix},$$

satisfy the relations of the Lemma 3.4. Then,

1	1	1	1	-1	-1	1	-1	-1	1	-1	-1
1	1	1	-1	1	-1	-1	1	-1	-1	1	-1
1	1	1	-1	-1	1	-1	-1	1	-1	-1	1
1	-1	-1	-1	-1	-1	1	-1	-1	-1	1	1
-1	1	-1	-1	-1	-1	-1	1	-1	1	-1	1
-1	-1	1	-1	-1	-1	-1	-1	1	1	1	-1
1	-1	-1	-1	1	1	-1	-1	-1	1	-1	-1
-1	1	-1	1	-1	1	-1	-1	-1	-1	1	-1
-1	-1	1	1	1	-1	-1	-1	-1	-1	-1	1
1	-1	-1	1	-1	-1	-1	1	1	-1	-1	-1
-1	1	-1	-1	1	-1	1	-1	1	-1	-1	-1
-1	-1	1	-1	-1	1	1	1	-1	-1	-1	-1

is a Hadamard matrix of order 12.

3.1.2 Equivalency of Hadamard matrices

The notion of equivalent Hadamard matrices is basic to our understanding. Most often, it is sufficient to demonstrate any proof or property for Hadamard matrices up to membership of an equivalence class.

Definition 3.7. Two $\{-1,1\}$ $n \times n$ matrices H and H' are (Hadamard) equivalent, written $H \sim H'$, if one can be obtained from the other by performing a finite sequence of the following operations:

- 1. permute the rows or the columns;
- 2. multiply a row or a column by -1.

In particular, any equivalence class of $n \times n$ matrices with entries from $\{-1, 1\}$ will contain at least one normalized representative. Any equivalence operations applied to a Hadamard matrix give a Hadamard matrix, so the Hadamard matrices of order n partition naturally into equivalence classes, each containing normalized Hadamard matrices. Of the elementary constructions in Lemma 3.1, $H \sim -H$ e $H \otimes H' \sim H' \otimes H$, but often $H \neq H^T$; the first examples of inequivalent transposes occur at order 16. In Table 3.1 we display the number of non-equivalent Hadamard matrices up to order 32. The number of non-equivalent Hadamard matrices (H. matrices) of order 36 is still unknown.

Order	H. matrices
4	1
8	1
12	1
16	5
20	3
24	60
28	487
32	13.710.027
36	(unknown)

Table 3.1: The order and the number of Hadamard matrices (H. matrices).

3.2 Weak Hadamard matrices

Adm *et al.* in [2] generalized the notion of Hadamard matrices and introduced a new family of matrices whose entries are all in the set $S = \{-1, 0, 1\}$ and satisfy the condition that the product of the matrix with its transpose is a tridiagonal matrix. Later, Hermie, Plosker and McLaren in [26] studied some constructions and properties of these matrices.

Definition 3.8. A matrix W is called weak Hadamard if it satisfies the following two properties:

- 1) the entries of the matrix are from the set $S = \{-1, 0, 1\}$;
- 2) there is an ordering of the columns of the matrix so that the non-consecutive columns are orthogonal. The consecutive columns can be either orthogonal or not orthogonal. The second condition implies that the product of any such matrix with its transpose is a tridiagonal matrix, that is, W^TW is a tridiagonal matrix.
For example,
$$W = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$
 is a weak Hadamard matrix.

If W is a weak Hadamard matrix, the operations of permuting the rows or columns of W and multiplying a row or column of W by -1 used to produce an equivalent matrix W' can affect the quasi-orthogonality of the columns. Note also that not all weak Hadamard matrices can be normalized.

Example 3.4. Let

Note that all entries of W are in the set $S = \{-1,0,1\}$ and that

$$W^{T}W = \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

it is a tridiagonal matrix. Therefore, W is a weak Hadamard matrix of order n = 5. Now, consider the matrix

 $equivalent \ to \ W.$ Note that

$$(W')^T W' = \begin{bmatrix} 2 & 0 & -1 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 \\ -1 & 0 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}.$$

Therefore, W' is not a weak Hadamard matrix. Also, note that it is not possible to normalize the matrix W, i.e., it is not possible to perform a finite sequence of row and column permutation operations on W and multiply its rows and columns by -1 to obtain a matrix whose first row and first column are entirely composed of 1's.

We know that a necessary condition for the existence of a Hadamard matrix H is that the order of H is 1, 2, or a multiple of 4. In [26], the authors presented sufficient conditions for when the same holds for weak Hadamard matrices.

Theorem 3.1. Let W be a weak Hadamard matrix of order n with two columns \mathbf{x} and \mathbf{z} that are orthogonal to $\mathbb{1}_n$. Then the following statements hold:

- 1. The vector \mathbf{x} has an even number of non-zero entries, exactly half of which are 1's.
- 2. If **x** has k number of 1's and r number of 0's, then r = n 2k. If k is even, then $n \equiv r \pmod{4}$.
- 3. If **x** has all entries non-zero, then n = 2k. Moreover, k is even if and only if $n \equiv 0 \pmod{4}$.
- 4. If (i) k is even and $r \equiv 0 \pmod{4}$ or (ii) all entries of both x and z are non-zero, then $n \equiv 0 \pmod{4}$.

When W is a normalized weak Hadamard matrix of odd order $(n = 2k + 1, \text{ for } k \ge 1)$ with pairwise orthogonal columns, then each column of W (other than $\mathbb{1}_n$) has three or more zero entries (Corollary 1, [26]. A consequence of this result is that there is no normalized weak Hadamard matrix of order 5 that has pairwise orthogonal columns (Corollary 2 in [26]).

3.2.1 Constructions of weak Hadamard matrices

In [26], the authors also explored the idea of constructing weak Hadamard matrices analogously to the classical constructions of Hadamard matrices.

- 1) Sylvester: The tensor product $A \otimes B$ of two weak Hadamard matrices A and B, where B is not equal to the all-zeros matrix, is a weak Hadamard matrix if and only if the columns of A are all pairwise orthogonal (Proposition 1, in [26]). It follows that the tensor product of a Hadamard matrix with a weak Hadamard matrix is a weak Hadamard matrix (Proposition 3.3, in [2]).
- 2) Invertible weak Hadamard matrices: Take any orthogonal vectors a, b, c, ..., with components in {-1,0,1}. Construct the matrix having two copies of each vector side by side as columns: W = [a, a, b, b, c, c, ...]. Such a matrix is a weak Hadamard matrix with W^TW having non-zero entries only on the diagonal and super-diagonal.

For n = 2k (even), partition \mathbb{R}^n into k orthogonal subspaces S_1, S_2, \ldots, S_k . From each partition select any two independent vectors $\mathbf{a}_1, \mathbf{a}_2 \in S_1$, $\mathbf{b}_1, \mathbf{b}_2 \in S_2$ etc., while ensuring the vectors have components in $\{-1, 0, 1\}$. Then the matrix $W = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{b}_1, \mathbf{b}_2, \ldots]$ is an invertible weak Hadamard matrix.

This construction works for any n > 1, because we can decompose \mathbb{R}^n as the direct sum of the orthogonal subspaces S_1, S_2, \ldots, S_k , where $\sum_{i=1}^k \dim(S_i) = n$.

3) Williamson: A matrix

$$W = \begin{bmatrix} A & B & C & D \\ -B & A & -D & C \\ -C & D & A & -B \\ -D & -C & B & A \end{bmatrix}$$

is weak Hadamard if the matrices A, B, C, D has all entries in the set $\{-1, 0, 1\}$ and satisfy

$$X^T Y = Y^T X$$
, para $X, Y \in \{A, B, C, D\}$

and

$$A^{T}A + B^{T}B + C^{T}C + D^{T}D$$
 is tridiagonal.

- 4) Weak Hadamard matrices of higher order: Can be constructed in two ways.
 - i) Let G and H be matrices with entries in $\{-1, 0, 1\}$. If $H^T H + G^T G$ is tridiagonal and $H^T G G^T H = 0$, then $W = \begin{bmatrix} H & G \\ G & -H \end{bmatrix}$ is a weak Hadamard matrix.
 - ii) Let G and H be weak Hadamard matrices of order n such that **x** is the first column of both matrices, and, moreover, that **x** is orthogonal to every other column in G and H. Then the block matrix $W = \begin{bmatrix} H & X \\ X & -G \end{bmatrix}$, with X the matrix with first column **x** and all others 0, is a weak Hadamard matrix. Furthermore, if G and H have pairwise orthogonal columns, then so too does W.
- 5) **Paley:** Let \mathbb{Z}_q be the integers mod q, where q is a power of an odd prime. Define

$$\mathcal{X}(a) = \begin{cases} 0, & \text{if } a \equiv 0 \\ 1, & \text{if } a \equiv b^2, \text{ for some non-zero } b \in \mathbb{Z}_q \\ -1, & \text{otherwise} \end{cases}$$

Construct the circulant matrix $C = [c_{ij}]$, where $c_{ij} = \mathcal{X}(i-j)$. Then the matrix $W = \begin{bmatrix} 0 & \mathbb{1}_q^T \\ \hline \mathbb{1}_q & C^T \end{bmatrix}$ is a weak Hadamard matrix of order $(q+1) \times (q+1)$ with pairwise orthogonal columns.

6) Weak Hadamard matrices of order 2^n : For $n, k \in \mathbb{N}$ with $k \leq n$, define the sets X_{2^k} consisting of 2^{n-k} vectors $\{\mathbf{x}_j\}_{j \in \mathbb{Z}_{2^{n-k}}}$ of dimension 2^n , where the *i*-th component of the vector \mathbf{x}_j is given by:

$$\mathbf{x}_{j}(i) = \begin{cases} 1, & \text{if } i \in \{2^{k}j + 1, \dots, 2^{k}j + 2^{k-1}\}, \\ -1, & \text{if } i \in \{2^{k}j + 2^{k-1} + 1, \dots, 2^{k}j + 2^{k}\}, \\ 0, & \text{otherwise.} \end{cases}$$

Note that each vector \mathbf{x}_j will have 2^k non-zero consequent entries, with an equal number of 1's and -1's. Furthermore, each set X_{2^k} consists of 2^{n-k} mutually orthogonal vectors, all of which are orthogonal to 1. The set $X = \bigcup_{1 \le k \le n} X_{2^k}$ combined with 1 gives a collection of 2^n mutually orthogonal vectors. Consequently, for any $n \in \mathbb{N}$ there exists a weak Hadamard matrix W of order 2^n , such that W has pairwise orthogonal columns and contains 1 as a column, but where W is not a Hadamard matrix.

3.2.2 Equivalency of weak Hadamard matrices

For a weak Hadamard W, let a_W be the number of blocks of any size in the block digonal form of $W^T W$, b_W be the number of blocks of size greater than or equal to 2, and c_W is the number of pairs of identical columns in W. With these definitions, the authors in [26] showed that the number of equivalent weak Hadamard matrices to W attained by permuting of the columns of W is given by

$$2^{b_W/c_W} a_W!$$
 (3.12)

(Theorem 2, in [26]).

Example 3.5. Let

$$W = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 1 & 1 & 1 & 0 \\ 1 & -1 & -1 & 0 \end{bmatrix}$$

be a weak Hadamard matrix. We have that

$$W^{T}W = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \quad a_{W} = 3 \quad e \quad b_{W} = c_{W} = 1.$$

Therefore, it follows from (3.12) that the number of weak Hadamard matrices equivalent to W is equal to 12.

Chapter 4

HADAMARD AND WEAK HADAMARD DIAGONALIZABLE GRAPHS

In this chapter, we will present some results from the literature on graphs G for which the Laplacian matrix L(G) can be diagonalized by a matrix P, where P is either a Hadamard matrix H or a weak Hadamard matrix W. Specifically, this means that L(G) can be written as $L(G) = P\Lambda P^T$, where $\Lambda = \text{diag}(\mu_1, \mu_2, \ldots, \mu_n)$. The main focus of this work is to study and characterize graphs G such that L(G) can be diagonalized by a weak Hadamard matrix W.

4.1 Hadamard diagonalizable graphs

One of the interesting questions in the spectral graph theory is about the structure of the eigenvectors of matrices associated with graphs. Barik, Fallat and Kirkland in [8] studied graphs for which their Laplacian matrix can be diagonalized by a Hadamard matrix H.

Definition 4.1. We say that a graph G is **Hadamard diagonalizable** and denoted by HD if an H Hadamard matrix exists such that

$$\frac{1}{n}H^T L(G)H = \Lambda,$$

or equivalently,

$$L(G) = \frac{1}{n} H \Lambda H^T,$$

where Λ is the diagonal matrix consisting of the eigenvalues of L(G).

This class of graphs corresponds to graphs on n vertices such that their Laplacian matrix has n orthogonal eigenvectors with entries only from the set $\{-1, 1\}$. The absence of definitive knowledge about the existence of Hadamard matrices makes characterizing graphs that are Hadamard diagonalizable challenging. In fact, a complete graph on n vertices is Hadamard diagonalizable if and only if a Hadamard matrix of order n exists [8]. This means that determining which complete graphs are Hadamard diagonalizable requires first demonstrating that a Hadamard matrix of a given order n exists, and hence resolving the Hadamard conjecture 3.1. In [8], the authors investigate the following question:

Which graphs are Hadamard diagonalizable?

Firstly, they demonstrated that a graph G is Hadamard diagonalizable if and only if there is a normalized Hadamard matrix that diagonalizes L(G) (Lemma 4 in [8]). They also observed and demonstrated that given any Hadamard matrix H of order $n = 4k, k \ge 1$, the complete graph K_n is diagonalizable by H (Observation 1 in [8]) and there is a permutation matrix P such that the complete bipartite graph $K_{n/2,n/2}$ is diagonalizable by the Hadamard matrix PH (Observation 2 in [8]).

Two important features of diagonalizable Hadamard graphs are stated in the following theorem.

Theorem 4.1 ([8]). Let G be a graph of order n which is Hadamard diagonalizable. Then G is regular and all its Laplacian eigenvalues are even integers.

However, regularity and even integer eigenvalues are not sufficient conditions for a graph to be Hadamard diagonalizable. In other words, even if a graph is regular or has even integer eigenvalues, it may not satisfy the additional condition of having an orthogonal basis of eigenvectors with all entries in $\{-1, +1\}$, which is necessary for a graph to be Hadamard diagonalizable. For example, the cycle C_8 is regular but is not Hadamard diagonalizable, and the complete graph K_8 minus one edge e, i.e., $G = K_8 \setminus e$ has all its eigenvalues as even integers, but is also not Hadamard diagonalizable.

Also, note that if G is a Hadamard diagonalizable graph by a Hadamard matrix, say H, since the eigenspaces for the Laplacian matrix of G and its complement graph G^c are the same (although the eigenvalues are different), it follows that G^c is a Hadamard diagonalizable graph by the same Hadamard matrix H (Lemma 7 in [8]).

The union and join operations of Hadamard diagonalizable graphs were also characterized. Let G_1 and G_2 be two graphs. If $G_1 \sqcup G_2$ is Hadamard diagonalizable, then G_1 and G_2 satisfy the following properties: both are regular graphs of the same order and same regularity, both have even eigenvalues and share the same eigenvalues (Lemma 6 in [8]). It follows that if G is a Hadamard diagonalizable graph by a Hadamard matrix H, then $G \sqcup G$ and $G \lor G$ are also Hadamard diagonalizable graphs (Lemma 7 in [8]), both diagonalizable by the same Hadamard matrix $\begin{bmatrix} H & H \\ H & -H \end{bmatrix}$.

Observation 4.1. If $G \sqcup G$ and $G \lor G$ are Hadamard diagonalizable graphs, it is not always true that G is Hadamard diagonalizable. For example, consider $G = K_6$. Both $K_6 \sqcup K_6$ and $K_6 \lor K_6$ are diagonalizable by a Hadamard matrix of order 12, but since there does not exists any Hadamard matrix of order 6, K_6 is not Hadamard diagonalizable.

Let $\star \in \{\Box, \times, \boxtimes\}$, where \Box denotes the Cartesian product of graphs, \times the direct product, and \boxtimes the strong product. We have already seen that the eigenvectors for the Laplacian matrix of each of these products can be computed from the eigenvectors of the constituent graphs. Thus, knowing the eigenvectors for each of these graph products shows that if the constituent graphs are Hadamard diagonalizable, then the product graph is also Hadamard diagonalizable.

Theorem 4.2 ([2], Theorem 3.2). If G_1 and G_2 are both Hadamard diagonalizable graphs on n_1 and n_2 vertices, respectively, then $G_1 \star G_2$ is Hadamard diagonalizable for $\star \in \{\Box, \times, \boxtimes\}$.

In [9], it was also shown that the lexicographic product of $G_1 \circ G_2$ of two diagonalizable Hadamard graphs G_1 and G_2 is a Hadamard diagonalizable graph. The proof from the results about the product of Hadamard diagonalizable graphs still being a Hadamard diagonalizable graph is straightforward. If H_1 and H_2 are Hadamard matrices that diagonalize G_1 and G_2 , respectively, then $H_1 \otimes H_2$ is also a Hadamard matrix and it diagonalizes $G_1 \star G_2$, for $\star \in \{\Box, \times, \boxtimes, \circ\}$.

In the paper [9], the authors developed further tools to determine the Hadamard diagonalizable graphs of a given order and listed all Hadamard diagonalizable graphs up to order n = 36. It is important to mention that the number of non-equivalent Hadamard matrices is still unknown. They proved that if n = 8k + 4, there are only four Hadamard diagonalizable graphs of order n.

Theorem 4.3 ([9], Theorem 5). Let G be a graph of order n. If n = 8k + 4 and G is Hadamard diagonalizable, then $G \in \{K_n, K_{n/2}, n/2, 2K_{n/2}, nK_1\}$.

Moreover, the graphs K_n , $K_{n/2,n/2}$, nK_1 , and $2K_{n/2}$ are Hadamard diagonalizable, and they are diagonalizable by any normalized Hadamard matrix H of order $n \ge 4$ (Proposition 6 in [9]). Note that it doesn't matter which matrix H is used; it simply needs to be normalized so that these four graphs are diagonalized by H. In other words, any normalized Hadamard matrix will always diagonalize at least four graphs.

In [9] the authors also developed computational tools to search for all possible Hadamard diagonalizable graphs of small order. In particular, given a Hadamard matrix H, an algorithm was presented by which all graphs which are diagonalized by H are produced. The algorithm proposed by the authors is based on the following result.

Proposition 4.1 ([9], Proposition 8). Let G be a Hadamard diagonalizable graph with its Laplacian matrix L. Let H be a normalized Hadamard matrix diagonalizing L. Let Λ be the diagonal matrix with its diagonal entries $\lambda_1 = 0, \lambda_2, \dots, \lambda_n$, the eigenvalues of L corresponding to the columns of H as their associated eigenvectors. Then the entries L_{12}, \dots, L_{1n} uniquely determine $\lambda_2, \dots, \lambda_n$.

To conclude this section, we summarize in Table 4.1 the number of Hadamard diagonalizable graphs (H. graphs) up to order 36.

Order	H.graphs
4	4
8	10
12	4
16	50
20	4
24	26
28	4
32	10.196
36	4

Table 4.1: The number of Hadamard diagonalizable graphs (H. graphs) up to 36 vertices.

4.2 Weakly Hadamard diagonalizable graphs

The determination of graphs whose Laplacian matrix can be diagonalized by a weak Hadamard matrix W is quite recent and first appeared in the article of Adm et al. [2]. In this article, the authors introduced the subject and determined several families of graphs that are WHD.

Definition 4.2. A graph G is weakly Hadamard diagonalizable and denoted by WHD if its Laplacian matrix L(G) can be diagonalized with a weak Hadamard matrix W, that is,

$$L(G) = W\Lambda W^{-1}$$

where Λ is the diagonal matrix consisting of the eigenvalues of L(G) and W has all entries from the set $\{-1, 0, 1\}$ and W^TW is tridiagonal.

Note that any Hadamard diagonalizable graph is also weakly Hadamard diagonalizable. However, the converse need not hold in general. The following example illustrates these facts.

Example 4.1. Let G be the complete graph K_4 minus one edge e, i.e., $G = K_4 \setminus e$. Without loss of generality, suppose that $e = \{1, 2\}$. We have that:

$$L(G) = \begin{bmatrix} 2 & 0 & -1 & -1 \\ 0 & 2 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix},$$

and the vectors (1,1,1,1), (1,-1,0,0), (1,1,-1,-1), (0,0,1,-1) form an ordered basis of \mathbb{R}^4 composed of eigenvectors of L(G) associated with eigenvalues 0, 2, and 4 of multiplicities 1, 1, and 2, respectively. Thus, if we form the matrix W where each column is an eigenvector of L(G), and the diagonal matrix Λ consisting of the eigenvalues of L(G), that is,

	1	1	1	0			0	0	0	0	
W =	1	-1	1	0	and	Λ -	0	2	0	0	
	1	0	-1	1	unu	Λ =	0	0	4	0	
	1	0	-1	-1			0	0	0	4	

it follows that $W^T W$ is tridiagonal, and $L(G) = W \Lambda W^{-1}$. Therefore, G is a WHD graph. However, by Theorem 4.1, G is not Hadamard diagonalizable graph as it is not a regular graph.

Example 4.1 shows that the Theorem 4.1 need not hold in general for WHD graphs, that is, WHD graphs may not be regular.

In the article [2] the authors extended some of the existing results on Hadamard diagonalizable graphs to weakly Hadamard diagonalizable graphs. First, they showed that the complete graph K_n is WHD for every value of $n \ge 1$ (Lemma 1.5 in [2]). Note that this is not the case in the usual Hadamard diagonalizable graphs, as a necessary condition for a graph to be Hadamard diagonalizable is that it has an order of n = 1, 2, or 4k (as Hadamard matrices only exist for these orders). Unlike Hadamard matrices, there is a weak Hadamard matrix of order n for every $n \ge 1$.

Furthermore, a graph G that is WHD can have odd eigenvalues for its Laplacian matrix. More precisely, the authors showed that if G is WHD, then all the eigenvalues of L(G) are integers (Lemma 2.2 in [2]).

Example 4.2. The complete graph K_3 is WHD (since K_n is WHD for all $n \ge 1$) and the eigenvalues of L(G) are 0 and 3, with multiplicities 1 and 2, respectively. Therefore, this is an example of a graph G that is WHD and has an odd integer as an eigenvalue of L(G).

Union, join and products operations for WHD graphs were also characterized. For the union of WHD graphs, a more general result of the union of Hadamard diagonalizable graphs holds. We have that $G_1 \sqcup G_2$ is a WHD graph if G_1 and G_2 are WHD graphs (Lemma 2.3 in [2]).

Example 4.3. Since K_4 and K_8 are WHD graphs it follows that the graph $K_4 \sqcup K_8$ is also WHD. Note that the graphs K_4 and K_8 are also Hadamard diagonalizable. However, by Theorem 4.3, we know that the only disconnected graphs of order 12 that are Hadamard diagonalizable are K_{12}^c and $K_6 \sqcup K_6$. Therefore, the disconnected graph $K_4 \sqcup K_8$ is not Hadamard diagonalizable.

Conditions for the complement of a WHD graph to also be WHD were presented. The cases when G is a connected WHD graph and when G is a disconnected WHD graph were considered separately. If G is a connected WHD graph, then G^c is also a WHD graph (Lemma 2.4 in [2]). If G is disconnected and WHD, then G^c is not necessarily a WHD graph.

Example 4.4. Consider the disconnected graph $G = K_1 \sqcup K_2$. We can conclude that G is a WHD graph since it is the union of two WHD graphs. Note that $G^c = K_{1,2}$ and the eigenvalues of $L(G^c)$ are 0, 1, and 3. Since $\mathcal{E}_L(3) = \text{span } \{(1,1,-2)\}$, it follows that $L(G^c)$ cannot be diagonalized by a weak Hadamard matrix.

The complement G^c of a disconnected WHD graph G on n vertices is also a WHD graph if G is regular and its components are of equal size (Lemma 2.5 in [2]).

Example 4.5. The graph $K_{n,n} = (K_n \sqcup K_n)^c$ is WHD. In fact, we know that K_n is WHD, for all $n \ge 1$, and that $K_n \sqcup K_n$ is WHD, since it is the union of graphs WHD. Furthermore, $K_n \sqcup K_n$ is disconnected, regular and its connected components have the same size, so by Lemma 2.5 in [2], we conclude that $K_{n,n} = (K_n \sqcup K_n)^c$ is WHD.

In Example 4.5 the bipartite graph $K_{n,n}$ is WHD. In fact, this is the only bipartite graph that is WHD. More precisely, the graph K_{n_1,n_2} is WHD if and only if $n_1 = n_2$ (Lemma 2.6 in [2]). Additionally, the authors in [2] investigated the conditions under which the cycles are WHD. They showed that the cycle C_n is WHD if and only if n = 3, 4 or 6 (Proposition 2.7 in [2]).

To analyze the product of WHD graphs, we begin with the following observation: if W_1 and W_2 are two weak Hadamard matrices that diagonalize the graphs G_1 and G_2 , respectively, then $W_1 \otimes W_2$ will diagonalize the graph $G_1 \star G_2$, for $\star \in \{\Box, \times, \boxtimes\}$. However, it is important to note that $W_1 \otimes W_2$ is not necessarily tridiagonal. So an extra condition is required to guarantee that the graph products produce WHD graphs.

Proposition 4.2 ([2], Proposition 3.3). Suppose graphs G_1 and G_2 are WHD with the matrix of eigenvectors W_1 and W_2 , respectively, such that $W_1^T W_1$ is a diagonal matrix. Then $G_1 \star G_2$ is WHD for any $\star \in \{\Box, \times, \boxtimes\}$.

As a consequence of the Proposition 4.2 if G_1 is Hadamard diagonalizable and G_2 is a WHD graph, then $G_1 \star G_2$ is WHD for any $\star \in \{\Box, \times, \boxtimes\}$ (Corollary 3.4 in [2]). Note that Proposition 4.2 does not characterize the products of graphs that are WHD. For example we know that $K_{n_1n_2} = K_{n_1} \boxtimes K_{n_2}$ is WHD, but this graph is not included in Proposition 4.2. In particular, the matrix $W = W_1 \otimes W_2$, where W_1 and W_2 are weak Hadamard matrices que diagonalize the graphs $K_{n_1} \in K_{n_2}$, respectively, has entries only from the set $\{0, -1, 1\}$ and it diagonalizes $K_{n_1n_2}$, but $W^T W$ is not a tridiagonal matrix. So this natural construction of eigenvectors with entries from $\{0, -1, 1\}$ for the product graph may not give a quasi-orthogonal basis of eigenvectors.

The join of WHD graphs can be improved compared to the case of Hadamard diagonalizable graphs.

Definition 4.3. An integer partition of an integer n to be recursively balanced partition if it satisfies the following. The partition with only one part, i.e. P = [n], is defined to be a recursively

balanced partition. A partition $P = [n_1, n_2, ..., n_k], k \ge 2$ is called a recursively balanced partition if there is a partition $Q = [Q_1, Q_2, ..., Q_l]$ of the parts of P with $Q_i = [n_{i_1}, ..., n_{i_{k_i}}]$ such that

(1) for any $i, j \in \{1, ..., l\}$

$$n_{i_1} + n_{i_2} + \dots + n_{i_{k_i}} = n_{j_1} + n_{j_2} + \dots + n_{j_k}$$

and

(2) each sub-partition Q_i is also a recursively balanced partition.

For example, the recursively balanced partitions of 8 are:

$$[8], [4,4], [4,2,2], [4,2,1,1], [4,1,1,1,1], [2,2,2,2], [2,2,2,1,1], \\ [2,2,1,1,1,1], [2,1,1,1,1,1], [1,1,1,1,1,1].$$

With the previous definition, it can be shown that the join of k connected WHD graphs X_i on n_i vertices, is a WHD graph if $[n_1, n_2, \ldots, n_k]$ is a recursively balanced partition (Lemma 4.3 in [2]). This result can be applied to complete multipartite graphs, since they are joins of empty graphs, that is, the complete multipartite graph K_{n_1,n_2,\ldots,n_k} is WHD if $[n_1, n_2, \ldots, n_k]$ is a recursively balanced partition (Corollary 4.4 in [2]). However, this condition does not characterize complete multipartite graphs that are WHD.

Example 4.6. $K_{3,2,2,1}$ is a WHD graph with 8 vertices, but [3,2,2,1] is not a recursively balanced partition of 8.

The graph $G = K_k^c \vee K_n$ can be represented as a complete multipartite graph by the partition [1, 1, ..., 1, k]. By Corollary 4.4 in [2] see that if n = k, then the graph G will have a recursively balanced partition given by [1, ..., 1, k] and therefore G will be WHD.

Lemma 4.1 ([2], Lemma 4.6). Let $G = K_k^c \vee K_n$. If $n - k \in \{0, 1, 2\}$, then G is a WHD graph.

Furthermore,

Lemma 4.2 ([2], Lemma 4.7). Let $G = H \lor K_n$ where H is a WHD connected graph on k vertices. If $n - k \in \{0, 1, 2\}$, then G is a WHD graph.

We note that $G = H \vee K_n = K_{n+k} \setminus H^c$, where $k \in \{n, n-1, n-2\}$. In other words, $G = K_{2n-i} \setminus H^c$ with $i \in \{0, 1, 2\}$. Therefore, the previous result can be seen as a result about the join of two graphs or a result about removing a subgraph from a complete graph.

Other examples of the join of graphs that is WHD are presented below; in these examples one of the graphs is disconnected. The following two results show that K_n minus matching is WHD for $n \ge 4$. Note that if n = 3, then K_3 minus one edge is P_3 , which is not WHD (see Example 4.4). **Lemma 4.3** ([2], Lemma 4.8). For $n \ge 4$, the graph G obtained from K_n minus an edge is WHD.

Corollary 4.1 ([2], Corollary 4.9). For $n \ge 4$, a complete graph K_n minus a matching of size p with $p \le \frac{n}{2}$ is WHD.

Let $A = \{K_4, C_4, K_4 \setminus e, K_4^c, K_2 \sqcup K_2, K_2^c \sqcup K_2\}$ be the set of all 6 graphs (both connected and disconnected) with 4 vertices that are WHD. Consider $X_{(k)} = \bigsqcup_{j=1}^k X_j$ and $Z_{(k)} = X \lor X \lor \cdots \lor X$, where $X_j, X \in A$. In the paper of McLaren, Monterde and Plosker [26], they showed (Corollary 6) that if X is WHD and P_X has pairwise orthogonal columns, then $Z_{(k)}$ is WHD if $k = 2^l$, $l \ge 1$. In particular, if $X \in \{K_4 \smallsetminus e, K_2^c \sqcup K_2\}$ then $\mathcal{F}_1 = \{Z_{(k)} : k = 2^l, l \ge 1\}$ is an infinite family of WHD graphs, and $P_{Z_{(k)}}$ has pairwise orthogonal columns. They also showed that $\mathcal{F}_2 = \{X_{(k)} : k = 2^l, l \ge 1\}$ is an infinite family of disconnected non-regular WHD graphs, where at least two of the X_j 's are distinct, and each $X_{(k)}^c$ is also WHD, with $P_{X_{(k)}} = P_{X_{(k)c}}$ having pairwise orthogonal columns. Furthermore, they presented the conditions under which these families exhibit perfect state transfer (PST).

We conclude this section by presenting Tables 4.2 and 4.3 where we summarize some of the differences and similarities between HD and WHD graphs.

HD Graphs	WHD Graphs
K_n is HD if, and only if, there exists	K_n is WHD, for all $n \ge 1$.
a Hadamard matrix of order n .	
G is regular	${\cal G}$ does not need to be regular.
All Laplacian eigenvalues are even	All Laplacian eigenvalues are
integers.	integers.
If G is HD, then $G \sqcup G$ is HD.	If G_1 and G_2 are WHD, then $G_1 \sqcup G_2$
	is also WHD.
If G is HD, then G^c is HD.	 If G is connected and WHD, then G^c is WHD. If G is disconnected and WHD, G is regular and all its connected components have the same size, then G^c is WHD.
If H_1 diagonalizes G_1 , H_2 diagonalizes G_2 , and both H_1 and H_2 are HD, then $H_1 \otimes H_2$ diagonalizes $X \star Y$, and it is HD, with $\star \in \{\Box, \times, \boxtimes, \circ\}$.	If W_1 diagonalizes G_1 , W_2 diagonalizes G_2 , and both W_1 and W_2 are both weak Hadamard, then $W_1 \otimes W_2$ diagonalizes $G_1 \star G_2$, with $\star \in \{\Box, \times, \boxtimes\}$, but $W_1 \otimes W_2$ is not necessarily weak Hadamard.
If both G_1 and G_2 are HD, then $G_1 \star$	If G_1 is WHD with W_1 , G_2 is WHD
G_2 is also HD, with $\star \in \{\Box, \times, \boxtimes, \circ\}$.	with W_2 , and $W_1^T W_1$ is diagonal,
	then $G_1 \star G_2$ is also WHD, with
	$\star \in \{\Box, \times, \boxtimes\}$. In particular, if G_1
	is a HD graph and G_2 is a WHD
	graph, then $G_1 \star G_2$ is WHD, for any
	$\star \in \{\Box, \times, \boxtimes\}.$

Table 4.2: Comparison between HD and WHD graphs

If there exists a Hadamard matrix of	K_{n_1,n_2} is WHD if, and only if, $n_1 =$
order n , then $K_{n/2,n/2}$ is HD.	n_2 .
	The multipartite graph K_{n_1,n_2,\ldots,n_k}
	is WHD if $[n_1, n_2, \ldots, n_k]$ is a
	recursively balanced partition.
If G is HD, then $G \lor G$ is also HD.	If G_i , $i = 1, 2, \dots, k$, are connected
	and WHD graphs with n_i vertices,
	and $[n_1, n_2, \cdots, n_k]$ is a recursively
	balanced partition, then $\bigvee_{i=1}^{k} G_i$ is
	a WHD graph.
	If $n - k \in \{0, 1, 2\}$, then $K_k^C \vee K_n$ is
	WHD.
	Let $G = H \vee K_n$, where H is a
	connected and WHD graph with k
	vertices. If $n - k \in \{0, 1, 2\}$, then G
	is WHD.
	$G = K_n \smallsetminus e$ is WHD for $n \ge 4$.
	$G = K_n$ minus a matching of size p
	is WHD for $n \ge 4$ and $p \le \frac{n}{2}$.

Table 4.3: Comparison between HD and WHD graphs

Chapter 5

THRESHOLD GRAPHS THAT ARE SIMPLY STRUCTURED

The main results of this work address the following problems: A.1) Determine the minimum number of vectors in the basis of an eigenspace of Laplacian matrix of a connected threshold graph G such that the eigenspace basis is simply structured; A.2) Characterize all threshold graphs that are simply structured; A.3) Characterize all connected threshold graphs that are WHD. Additionally, we show that it does not make sense to extend the definitions of HD and WHD graphs to the signless Laplacian matrix.

Our motivations are related to (i) showing the relevance of our very recent result of [24], have been published in the Special Matrices journal, by obtaining all threshold graphs that are WHD since those graphs are not easy to find; (ii) the fact that it could be useful to create new graphs with Laplacian perfect state transfer among those threshold graphs WHD since the eigenvectors are known for a given order and the eigenvalues are easily obtained from the degree sequence. Related works in this subject include recent studies by McLaren, Hermie, and Plosker [26], as well as Johnston et al. [22]; (iii) the authors of [2] raised an interesting problem of determining all cographs that are WHD. While completely solving this problem seems to be a difficult task, we give a step forward to find all threshold graphs that are WHD and partially answer the question.

5.1 Structural tools

In this section, we present a specific eigenbasis $\{\mathbf{x}^1, \ldots, \mathbf{x}^n\}$ of $L(S_n)$ and we will see that when G is any threshold graph on n vertices, we can obtain a Laplacian eigenbasis for G from $\{\mathbf{x}^1, \ldots, \mathbf{x}^n\}$. This result serves as an important structural tool for addressing Problems A.1, A.2, and A.3 in the following sections.

Let S_n be a star graph on n vertices. For $1 \le k < n$, it is easy to see that each \mathbf{x}^k satisfying

$$\mathbf{x}_{i}^{k} = \begin{cases} 1, & \text{if } i < k+1, \\ -k, & \text{if } i = k+1, \\ 0, & \text{if } k+1 < i \le n, \end{cases}$$
(5.1)

and $\mathbf{x}^n = \mathbb{1}_n = (1, 1, \dots, 1)^T$ are pairwise orthogonal eigenvectors of $L(S_n)$ associated with eigenvalues 1,

n and 0 of multiplicities n-2, 1 and 1, respectively. So, $\{\mathbf{x}^1, \ldots, \mathbf{x}^n\}$ is an eigenbasis $L(S_n)$. Macharete et al. in [24] proved that any threshold graph of a given order can be recognized from a specific Laplacian eigenbasis, which is a spectral characterization of a threshold graph. In this sense, they proved that L(G) and $L(S_n)$ share the same eigenvectors when G is a connected threshold graph on n vertices, as stated in Theorem 5.1.

Theorem 5.1 ([24], Theorem A). Let G be a connected graph on n vertices. Then, G is a threshold graph if and only if $\{\mathbf{x}^1, \ldots, \mathbf{x}^n\}$ is an eigenbasis of the Laplacian matrix of G.

Lemmas 2.2 and 2.3 and Edge Principle 2.4 are applied in the context of threshold graphs and are important structural tools to prove the Theorema 5.1. Interestingly, the result implies that the knowledge of the eigenvectors is sufficient to identify whether the graph is a threshold graph. However, notice that the eigenspaces associated with the eigenvalues of L(G) can be different from the eigenspaces of $L(S_n)$. The next example illustrate Theorem 5.1.

Example 5.1. Let G_1 be the threshold graph of Figure 5.1. Its binary sequence is given by $b^1 = (0, 0, 0, 1, 0, 1)$.



Figure 5.1: Graph G_1 .

Note that G_1 has the graph S_6 as a subgraph. In other words, we have that $G_1 = S_6 + \{1, 4\} + \{2, 4\} + \{3, 4\}$. The eigenvalues of $L(S_6)$ are 1, 6, and 0 of multiplicities 4, 1, and 1, respectively. An eigenbasis of $L(S_6)$ is given by $B = \{\mathbf{x}^1, \mathbf{x}^2, \mathbf{x}^3, \mathbf{x}^4, \mathbf{x}^5, \mathbf{x}^6\}$, where $\mathbf{x}^1 = (1, -1, 0, 0, 0, 0)$, $\mathbf{x}^2 = (1, 1, -2, 0, 0, 0), \mathbf{x}^3 = (1, 1, 1, -3, 0, 0), \mathbf{x}^4 = (1, 1, 1, 1, 1, -4, 0), \mathbf{x}^5 = (1, 1, 1, 1, 1, 1, -5), and$ $<math>\mathbf{x}^6 = (1, 1, 1, 1, 1, 1)$. Moreover, the vectors $\mathbf{x}^1, \mathbf{x}^2, \mathbf{x}^3$ and \mathbf{x}^4 are associated with eigenvalue 1, the eigenvector \mathbf{x}^5 is associated with eigenvalue 6, and the eigenvector \mathbf{x}^6 is associated with eigenvalue 0. Note that b_4 is the first entry equal to one in b^1 . Then, by Lemma 2.2 we add one unit to the eigenvalue 1 for $1 \le k \le i - 2 = 2$, and we obtain that $(2, \mathbf{x}^1)$ and $(2, \mathbf{x}^2)$ are eigenpair for $L(G_1)$. When k = 3, that is, k = i - 1, by Lemma 2.2 we add 1 + k to the eigenvalue 1 and hence we have that $(5, \mathbf{x}^3)$ is the eigenpair for $L(G_1)$. Finally, by Theorem 2.4 (Edge Principle), we obtain that the eigenpairs $(1, \mathbf{x}^4), (6, \mathbf{x}^5)$ and $(0, \mathbf{x}^6)$ are preserved in the graph G_1 . Therefore, the eigenbasis B of $L(S_6)$ is also an eigenbasis of $L(G_1)$. Table 5.1 summarizes the result.

Figure of I	Eigenvalue of L					
Eigenvector of L	For $L(S_6)$	For $L(G_1)$				
\mathbf{x}^1	1	2				
\mathbf{x}^2	1	2				
\mathbf{x}^3	1	5				
\mathbf{x}^4	1	1				
\mathbf{x}^5	6	6				
\mathbf{x}^{6}	0	0				

Table 5.1: Eigenvectors and eigenvalues for the Laplacian matrix of the connected threshold graphs S_6 and G_1 .

We also extended the result of Theorem 5.1 to disconnected threshold graphs as presented in Macharete *et al.*, [24]. Consider now that G is a disconnected threshold graph on n vertices and can be written as $G = H \sqcup pK_1$, where H is a connected threshold graph with n - p vertices, and p is the number of isolated vertices. For $1 \le k \le n - p$, let \mathbf{y}^k be the n-vector with entries:

$$\mathbf{y}_{j}^{k} = \begin{cases} \mathbf{x}_{j}^{k}, & \text{if } 1 \le j \le n - p, \\ 0, & \text{otherwise,} \end{cases}$$
(5.2)

where the \mathbf{x}_{j}^{k} are given in Equation (5.1). For $1 \leq l \leq p$, define

$$\mathbf{y}_{j}^{n-p+l} = \begin{cases} 1, & \text{if } j = n-p+l, \\ 0, & \text{otherwise.} \end{cases}$$
(5.3)

The next theorem establishes that the eigenvectors of L(G) are the same as those of $L(S_{n-p} \sqcup pK_1)$, where $p \ge 1$ is the number of isolated vertices. In other words, it means that n-p eigenvectors of L(G) can be obtained from the eigenvectors of $L(S_{n-p})$ by adding p entries equal to 0 and the remaining p eigenvectors are the standard vectors e_j for a convenient j. More precisely, we have that:

Theorem 5.2 ([24], Theorem 3.6). Let G be a disconnected graph on n vertices. Then, G is threshold if and only if $\{\mathbf{y}^1, \mathbf{y}^2, \dots, \mathbf{y}^n\}$ is an eigenbasis of L(G).

The next example illustrates Theorem 5.2.

Example 5.2. Consider the disconnected threshold graphs $G = S_6 \sqcup 3K_1$ and $H = G_1 \sqcup 3K_1$, where G_1 is the graph given in the Example 5.1. Since the Laplacian spectrum of the union is the union of the spectra of the connected components (and multiplicities are added), it follows that

 $spect_L(G) = (6, 1, 1, 1, 1, 0, 0, 0, 0)$ and $spect_L(H) = (6, 5, 2, 2, 1, 0, 0, 0, 0).$

By Theorem, 5.2 the basis $B' = \{y^1, y^2, y^3, y^4, y^5, y^6, y^7, y^8, y^9\}$, where $y^1 = (1, -1, 0, 0, 0, 0, 0, 0, 0)$, $y^2 = (1, 1, -2, 0, 0, 0, 0, 0, 0), y^3 = (1, 1, 1, -3, 0, 0, 0, 0, 0), y^4 = (1, 1, 1, 1, -4, 0, 0, 0, 0), y^5 = (1, 1, 1, 1, 1, -5, 0, 0, 0),$ $y^6 = (1, 1, 1, 1, 1, 1, 0, 0, 0), y^7 = (0, 0, 0, 0, 0, 0, 1, 0, 0), y^8 = (0, 0, 0, 0, 0, 0, 0, 1, 0), y^9 = (0, 0, 0, 0, 0, 0, 0, 0, 1)\}$ is an eigenbasis of L(G) and L(H). In Table 5.2, we show the eigenvalues and their corresponding eigenspaces for the graphs G and H.

Figure at an of I	Eigenvalue of L					
Eigenvector of L	For $L(G)$	For $L(H)$				
\mathbf{y}^1	1	2				
\mathbf{y}^2	1	2				
\mathbf{y}^3	1	5				
\mathbf{y}^4	1	1				
\mathbf{y}^5	6	6				
\mathbf{y}^{6}	0	0				
\mathbf{y}^7	0	0				
y ⁸	0	0				
\mathbf{y}^9	0	0				

Table 5.2: Eigenvectors and eigenvalues for the Laplacian matrix of the disconnected threshold graphs G and H.

Similarly to the case of connected threshold graphs, the eigenvectors of L(G) and L(H) are the same but they are associated with different eigenvalues.

5.2 Minimum number of eigenvectors in certain eigenspaces

In this section, we investigate the answer to problem A.1, which we state again next, but considering our analysis when G is a connected threshold graph.

Problem A.1: Determine the minimum number of vectors on the basis of an eigenspace of the Laplacian matrix of a connected threshold graph G such that the eigenspace basis is simply structured.

In Section 5.1, we see that L(G) and $L(S_n)$ share the same eigenvectors when G is a connected threshold graph on n vertices ([24], Theorem A). The eigenvectors \mathbf{x}^1 and \mathbf{x}^n are the only ones in the eigenbasis $B = {\mathbf{x}^1, \ldots, \mathbf{x}^n}$ of L(G) with all the entries in the set $\{-1, 0, 1\}$. We also know that the eigenbasis B is not unique, and that any other eigenbasis \mathcal{B} for L(G) can be obtained from B through a linear combination. We know that 0 is an eigenvalue of L(G) with multiplicity 1 and $\mathcal{E}_L(0) = \text{span} \{\mathbf{x}^n\}$, where $\mathbf{x}^n = (1, 1, ..., 1)$. Therefore, $\mathcal{E}_L(0)$ is simply structured. We also know that the largest eigenvalue of L(G) is equal to n. In this section, we determine the minimum dimension of the eigenspace of the eigenvalue n, that is, we proved that $\dim(\mathcal{E}_L(n)) \ge \lfloor n/2 \rfloor$ when G is threshold and simply structured, which is the result of Proposition 5.1. Also, assuming the result of Proposition 5.1, we easily see that n - k is an eigenvalue to L(G) and prove that $\dim(\mathcal{E}_L(n-k)) \ge k$, for $k \ge \lfloor n/4 \rfloor$, which is the result of Proposition 5.2. These results solve Problem A.1 to Laplacian eigenvalues n and n - k, but when applied recursively enabled us to generate all connected threshold graphs of a given order n with simply structured eigenspaces. Therefore, we finish this chapter by presenting a recursive algorithm that generates all connected threshold graphs of a given order n with simply structured eigenspaces.

Proposition 5.1. Let G be a connected threshold graph on n vertices defined by the binary sequence $b = (b_1, b_2, \ldots, b_k, b_{k+1}, \ldots, b_{n-1}, b_n)$, and let $k \in \{1, \ldots, n-1\}$ be such that $b_{k+1} = \cdots = b_n$ and $b_k \neq b_{k+1}$. Then, $\mathcal{E}_L(n)$ is simply structured if and only if $1 \le k \le \lfloor \frac{n}{2} \rfloor$.

Proof. By Theorem 5.1, L(G) and $L(S_n)$ share the same eigenvectors. Let $k \in \{1, \ldots, n-1\}$ such that $b_{k+1} = \ldots = b_n$ and $b_k \neq b_{k+1}$. By hypothesis, G is connected, so $b_n = 1$. Thus, we obtain $b_{k+1} = \ldots = b_n = 1$ and $b_k = 0$. By Theorem 5.1 ([24], Theorem A) we have that

$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{x}^k, \dots, \mathbf{x}^{n-1} \}$$
 e $\dim(\mathcal{E}_L(n)) = n - k.$

Suppose that $\mathcal{E}_L(n)$ is simply structured. Then, by hypothesis, there is a basis $B = {\mathbf{v}^{k+1}, \dots, \mathbf{v}^{n-1}, \mathbf{v}'}$ such that

$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{x}^k, \dots, \mathbf{x}^{n-1} \} = \operatorname{span} \{ \mathbf{v}^{k+1}, \dots, \mathbf{v}^{n-1}, \mathbf{v}' \},\$$

where each vector $\mathbf{v} \in B$ has entries only in the set $\{-1, 0, 1\}$. Take $\mathbf{v} = [v_1, \dots, v_n] \in B$ and determining it from the vectors \mathbf{x}^i corresponds to finding coefficients $a = [a_k, a_{k+1}, \dots, a_{n-1}]^T$ such that

$$Xa = \mathbf{v},\tag{5.4}$$

where

$$X = \begin{bmatrix} 1 & 1 & \dots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \dots & 1 & 1 \\ -k & 1 & \dots & 1 & 1 \\ 0 & -(k+1) & \dots & 1 & 1 \\ 0 & 0 & \dots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 1 \\ 0 & 0 & \dots & -(n-2) & 1 \\ 0 & 0 & \dots & 0 & -(n-1) \end{bmatrix},$$

and each column of X is a vector \mathbf{x}^i for i = k, ..., n-1. Note that \mathbf{v} must have the same number of -1's and 1's since it is orthogonal to the vector $\mathbf{x}^n = (1, 1, ..., 1)$. Observe that the first k equations of (5.4) are all identical, and therefore $v_1 = v_2 = \cdots = v_k$. The other n - k equations are given by

$$\begin{cases}
-k a_{k} + a_{k+1} + \dots + a_{n-2} + a_{n-1} = v_{k+1} \\
-(k+1) a_{k+1} + \dots + a_{n-2} + a_{n-1} = v_{k+2} \\
\vdots & \vdots & \vdots \\
-(n-2) a_{n-2} + a_{n-1} = v_{n-1} \\
-(n-1) a_{n-1} = v_{n}
\end{cases}$$
(5.5)

Let us analyze the cases where $v_1 = \cdots = v_k = 0$ or $v_1 = \cdots = v_k = 1$. Note that the case where $v_1 = \cdots = v_k = -1$ is analogous to the previous case, except for a change of sign. Initially, suppose that $v_1 = \cdots = v_k = 0$. Since the number of 1's and -1's must be equal, for each $i \in \{k + 1, \dots, n - 1\}$, take $v_i = 1, v_{i+1} = -1$ and $v_j = 0$ for all $j \neq \{i, i + 1\}$. The solution to the system (5.4) is unique and is given by

$$a_i = \frac{1}{i}, \ a_{i+1} = -\frac{1}{i} \in a_j = 0, \text{ para } j \in \{k+1, \dots, n-1\} \setminus \{i, i+1\}.$$

This shows that it is possible to combine the vectors $\mathbf{x}^{k+1}, \ldots, \mathbf{x}^{n-1}$ to obtain n - k - 1 eigenvectors of L(G) that are linearly independent with entries in $\{-1, 0, 1\}$. These vectors are

$$\mathbf{v}^{i} = \frac{1}{i}\mathbf{x}^{i} - \frac{1}{i}\mathbf{x}^{i-1} = e_{i} - e_{i+1}$$
(5.6)

for each $i \in \{k+1, \ldots, n-1\}$. Furthermore, in the other cases where there are two or more 1's and -1's, the vectors obtained are a linear combination of the vectors \mathbf{v}^i obtained in (5.6).

Now, suppose that $v_1 = \cdots = v_k = 1$. In this case, we must have at least k entries equal to -1 among v_{k+1}, \ldots, v_n in the n-k equations in (5.5). Hence, we must have $n-k \ge k$, which implies that $1 \le k \le \lfloor \frac{n}{2} \rfloor$. Suppose that $v_{k+1} = \cdots = v_{2k} = -1$ and let $\mathbf{v} = \sum_{i=1}^{k} e_i - \sum_{i=k+1}^{2k} e_i$. The solution to the system (5.4) is unique and is given by

$$a_i = \frac{2k}{i(i+1)}$$
, for $i = k, \dots, 2k-1$ and $a_i = 0$, for $i = 2k, \dots, n-1$

Thus, it is possible to combine the vectors $\mathbf{x}^k, \dots, \mathbf{x}^{2k-1}$ to obtain an eigenvector of L(G) with entries in $\{-1, 0, 1\}$ given by

$$\mathbf{v}' = \frac{2k}{k(k+1)} \mathbf{x}^k + \ldots + \frac{2k}{(2k-2)(2k-1)} \mathbf{x}^{2k-2} + \frac{1}{2k-1} \mathbf{x}^{2k-1}$$
(5.7)

Note that \mathbf{v}' in (5.7) is not a linear combination of the vectors $\mathbf{v}^{k+1}, \ldots, \mathbf{v}^{n-1}$ in (5.6), since the first k coordinates of \mathbf{v}' are equal to 1, while the first k coordinates of $\mathbf{v}^{k+1}, \ldots, \mathbf{v}^{n-1}$ are equal to 0. Therefore, the vectors $\{\mathbf{v}^{k+1}, \ldots, \mathbf{v}^{n-1}, \mathbf{v}'\}$ are linearly independent. Thus, if $\mathcal{E}_L(n)$ is simply structured, then $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

On the other hand, suppose that $1 \le k \le \lfloor \frac{n}{2} \rfloor$ and that $b_{k+1} = \ldots = b_n = 1$ and $b_k = 0$. Then,

$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{x}^k, \dots, \mathbf{x}^{n-1} \}$$
 e $\left\lceil \frac{n}{2} \right\rceil \le \dim(\mathcal{E}_L(n)) \le n-1$

Since $k \in \{1, \ldots, \lfloor \frac{n}{2} \rfloor\}$, it is possible to combine the vectors $\mathbf{x}^k, \ldots, \mathbf{x}^{n-1}$ that are in the basis of $\mathcal{E}_L(n)$ to obtain a new basis for $\mathcal{E}_L(n)$ formed by the vectors $\mathbf{v}^{k+1}, \ldots, \mathbf{v}^{n-1}, \mathbf{v}'$ with entries only in $\{-1, 0, 1\}$, where the vectors \mathbf{v}^i , para $i = k + 1, \ldots, n - 1$ are given in (5.6) and the vector \mathbf{v}' is given in (5.7). Therefore, if $1 \le k \le \lfloor \frac{n}{2} \rfloor$, then $\mathcal{E}_L(n)$ is simply structured.

From Proposition 5.1, we conclude that the minimum number of vectors in the basis of $\mathcal{E}_L(n)$ is $\left\lceil \frac{n}{2} \right\rceil$. This result provides the answer to Problem A.1 for $\mathcal{E}_L(n)$. Assuming that G is a connected threshold graph with binary sequence such that $b_{k+1} = \cdots = b_n = 1$ and $b_k = 0$, for some $k \in \{2, \ldots, n-1\}$, we always obtain n - k as an eigenvalue of L(G). For that reason, from now on, we will focus on addressing Problem A.1 for the eigenspace of the eigenvalue n - k.

Proposition 5.2. Let G be a connected threshold graph on n vertices defined by the binary sequence $b = (b_1, b_2, b_3, \ldots, b_k, b_{k+1}, \ldots, b_n)$ such that $b_k = 0$ and $b_{k+1} = \ldots = b_n = 1$, for some $k \in \{2, \ldots, n-1\}$. Let $l \in \{1, \ldots, k-1\}$ such that $b_{l+1} = \ldots = b_k$ and, if $l \ge 2$, then $b_l \ne b_{l+1}$. Then, $\mathcal{E}_L(n-k)$ is simply structured if and only if $1 \le l \le \lfloor \frac{k}{2} \rfloor$.

Proof. By Theorem 5.1 ([24], Theorem A), L(G) and $L(S_n)$ share the same eigenvectors. By hypothesis, we have $b_k = 0$ and $b_{k+1} = \ldots = b_n = 1$, for some $k \in \{2, \ldots, n-1\}$. Let $l \in \{1, \ldots, k-1\}$ be such that $b_{l+1} = \ldots = b_k = 0$ and, if $l \ge 2$, then $b_l = 1$. Under these conditions, n - k is an eigenvalue of L(G), and by Theorem 5.1 ([24], Theorem A) we have that

$$\mathcal{E}_L(n-k) = \operatorname{span} \{\mathbf{x}^l, \dots, \mathbf{x}^{k-1}\}$$
 and $\dim(\mathcal{E}_L(\mu)) = k - l$.

Suppose that $\mathcal{E}_L(n-k)$ is simply structured. Then, by hypothesis, there is a basis $B = {\mathbf{u}^{l+1}, \dots, \mathbf{u}^{k-1}, \mathbf{u}'}$ such that

$$\mathcal{E}_L(n-k) = \operatorname{span} \{\mathbf{x}^l, \dots, \mathbf{x}^{k-1}\} = \operatorname{span} \{\mathbf{u}^{l+1}, \dots, \mathbf{u}^{k-1}, \mathbf{u}'\}$$

where each vector $\mathbf{u} \in B$ has entries only in the set $\{-1, 0, 1\}$. Tome $\mathbf{u} = [u_1, \dots, u_n] \in B$ and determining it from the vectors \mathbf{x}^i corresponds to finding coefficients $a = [a_l, a_{l+1}, \dots, a_{k-1}]^T$ such that

$$Xa = \mathbf{u},\tag{5.8}$$

where

$$X = \begin{bmatrix} 1 & 1 & \dots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \dots & 1 & 1 \\ -l & 1 & \dots & 1 & 1 \\ 0 & -(l+1) & \dots & 1 & 1 \\ 0 & 0 & \dots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 1 \\ 0 & 0 & \dots & -(k-2) & 1 \\ 0 & 0 & \dots & 0 & -(k-1) \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \end{bmatrix}$$

where each column of X is a vector \mathbf{x}^i for i = l, ..., k - 1. Note that **u** must have same number of -1's and 1's since it is orthogonal to vector $\mathbf{x}^n = (1, 1, ..., 1)$. Observe that the first l equations of (5.8) are all identical, and therefore $u_1 = u_2 = \cdots = u_l$. The other k - l equations are given by

$$\begin{cases}
-l a_{l} + a_{l+1} + \dots + a_{k-2} + a_{k-1} = u_{l+1} \\
-(l+1) a_{l+1} + \dots + a_{k-2} + a_{k-1} = u_{l+2} \\
\vdots & \vdots & \vdots \\
-(k-2) a_{k-2} + a_{k-1} = u_{k-1} \\
-(k-1) a_{k-1} = u_{k}
\end{cases}$$
(5.9)

and the remaining t equations from (5.8) are all equal to 0, and therefore $u_{n-t+1} = \cdots = u_n = 0$. Let us analyze the cases where $u_1 = \cdots = u_l = 0$ or $u_1 = \cdots = u_l = 1$. Note that the case where $u_1 = \cdots = u_l = -1$ is analogous to the previous case, except for the change of sign. Initially, suppose that $u_1 = \cdots = u_l = 0$. Since the number of 1's and -1's must be equal, for each $i \in \{l+1, \ldots, n-t-1\}$, take $u_i = 1, u_{i+1} = -1$ and $u_j = 0$ for all $j \neq \{i, i+1\}$. The solution to the system (5.8) is unique and given by

$$a_i = \frac{1}{i}, \ a_{i+1} = -\frac{1}{i} \text{ and } a_j = 0, \text{ for } j \in \{l+1, \dots, k-1\} \setminus \{i, i+1\}$$

This shows that is possible to combine the vectors $\mathbf{x}^{l+1}, \ldots, \mathbf{x}^{k-1}$ to obtain k-l-1 eigenvectors of L(G) that are linearly independent with entries in $\{-1, 0, 1\}$. These vectors are

$$\mathbf{u}^{i} = \frac{1}{i}\mathbf{x}^{i} - \frac{1}{i}\mathbf{x}^{i-1} = e_{i} - e_{i+1}$$
(5.10)

for each $i \in \{l + 1, ..., k - 1\}$. Furthermore, in the other cases where are two or more 1's and -1's, the vectors obtained are a linear combination of the vectors \mathbf{u}^i obtained in 5.10.

Now, suppose that $u_1 = \cdots = u_l = 1$. In this case, we must have at least l entries equal to -1 among u_{l+1}, \ldots, u_k in the k - l equations in (5.9). Hence, we have must $k \ge 2l$, which implies that $1 \le l \le \lfloor \frac{k}{2} \rfloor$. Suppose that $u_{l+1} = \cdots = u_{2l} = -1$ and let $\mathbf{u} = \sum_{i=1}^{l} e_i - \sum_{i=l+1}^{2l} e_i$. The solution to the system (5.8) is unique and is given by

$$a_i = \frac{2l}{i(i+1)}$$
, for $i = l, \dots, 2l-1$ and $a_i = 0$, for $i = 2l, \dots, k-1$.

Thus, it is possible to combine the vectors $\mathbf{x}^{l}, \ldots, \mathbf{x}^{2l-1}$ to obtain 1 eigenvector of L(G) with entries in $\{-1, 0, 1\}$ given by

$$\mathbf{u}' = \frac{2l}{l(l+1)} \,\mathbf{x}^l + \ldots + \frac{2l}{(2l-2)(2l-1)} \,\mathbf{x}^{2l-2} + \frac{1}{2l-1} \,\mathbf{x}^{2l-1}$$
(5.11)

Note that \mathbf{u}' in (5.11) is not a linear combination of the vectors $\mathbf{u}^{l+1}, \ldots, \mathbf{u}^{k-1}$ in (5.10), since the first l coordinates of \mathbf{u}' are equal to 1, while the first l coordinates of $\mathbf{u}^{l+1}, \ldots, \mathbf{u}^{k-1}$ are equal to 0. Therefore, the vectors $\{\mathbf{u}^{l+1}, \ldots, \mathbf{u}^{k-1}, \mathbf{u}'\}$ are linearly independent. Thus, if $\mathcal{E}_L(n-k)$ is simply structured, then $1 \leq l \leq \lfloor \frac{k}{2} \rfloor$.

On the other hand, suppose that $1 \le l \le \lfloor \frac{k}{2} \rfloor$ and that $b_{l+1} = \ldots = b_k = 0$ and, if $l \ge 2$, then $b_l = 1$. So,

$$\mathcal{E}_L(n-k) = \operatorname{span} \{\mathbf{x}^l, \dots, \mathbf{x}^{k-1}\}$$
 and $\left\lceil \frac{k}{2} \right\rceil \leq \dim(\mathcal{E}_L(n-k)) \leq k-1$

Since $l \in \{1, \ldots, \lfloor \frac{k}{2} \rfloor\}$, it is possible to combine the vectors $\mathbf{x}^{l}, \ldots, \mathbf{x}^{k-1}$ that are in the basis of $\mathcal{E}_{L}(\mu)$ to obtain a new basis for $\mathcal{E}_{L}(\mu)$ formed by the vectors $\mathbf{u}^{l+1}, \ldots, \mathbf{u}^{k-1}, \mathbf{u}'$ with entries only in $\{-1, 0, 1\}$, where the vectors \mathbf{u}^{i} , for $i = l + 1, \ldots, k - 1$ are given in (5.10) and the vector \mathbf{u}' is given in (5.11). Threfore, if $1 \leq l \leq \lfloor \frac{k}{2} \rfloor$, then $\mathcal{E}_{L}(n-k)$ is simply structured.

From Proposition 5.2, we conclude that the minimum number of vectors in the basis of $\mathcal{E}_L(n-k)$ is $\left\lceil \frac{k}{2} \right\rceil$. This result provides the answer to Problem A.1 for $\mathcal{E}_L(n-k)$. Assuming that G is a connected threshold graph with binary sequence such that $b_{l+1} = \cdots = b_k = 0$ and $b_{k+1} = \cdots = b_n = 1$, for some $k \in \{2, \ldots, \lfloor \frac{n}{2} \rfloor\}$ and $l \in \{1, \ldots, \lfloor \frac{k}{2} \rfloor\}$, we always have $\mathcal{E}_L(n)$ and $\mathcal{E}_L(n-k)$ as simply structured, regardless of what happens in the other positions of the binary sequence. Therefore, propositions 5.1 and 5.2 provide an important starting point to determine the threshold graphs that are simply structured. Applying those results recursively, we can generate all simply structured threshold graphs of order n. This idea will be detailed in the next section.

5.3 Algorithm

Based on the theoretical results of the previous section, we build an algorithm to generate all connected threshold graphs on n vertices that are simply structured.

Let G be a connected threshold graph on n vertices defined by binary sequence $b = (b_1, b_2, \ldots, b_k, b_{k+1}, \ldots, b_n)$. Propositions 5.1 and 5.2 allow us to address Problem A.1 for the eigenspaces associated with the eigenvalues n and n - k, respectively. From now on, we will see that by recursively applying the same ideas used in the proofs of the Propositions 5.1 and 5.2 we can solve Problem A.1 for all the eigenspaces of L(G). In other words, we solve Problem A.2, which states:

Problem A.2: Characterize all threshold graphs that are simply structured.

Problem A.2 will be solved in the steps of Algorithms 1 and 2. We designed Algorithm 1 to generate all possible partitions of an integer n, that is, the order of the threshold graph. The idea of Algorithm 1 is explained below.

Algorithm 1: We start by letting P = [n] be the first partition, and make LP containing P. In general, let $P = [P(1), P(2), \ldots, P(m)]$ be a partition of the integer n with length m, where $m \ge 1$. We want to determine a list LP that contains all possible non-decreasing partitions. We refer to the length of a given partition P, which is equal to its number of parts, as the *level* of its partition. All other partitions in the list LP will be obtained through a procedure that we will call *expansion*. This procedure consists of obtaining a new partition P' of level m + 1 from P, and it can occur in two ways, depending on the parity of level m:

- 1.1) If level *m* is odd: for each $j \in \{1, \dots, \left\lfloor \frac{P(1)}{2} \right\rfloor\}$, construct a partition $P' = [j, P(1) j, P(2), \dots, P(m)]$ and then add P' to the list LP.
- 1.2) If level *m* is even: for each $j \in \{2, \dots, \lfloor \frac{P(1)}{2} \rfloor\}$, construct a partition $P' = [j, P(1) j, P(2), \dots, P(m)]$ and then add P' to the list *LP*.

The expansion will be performed recursively for each partition P obtained in substeps 1.1 and 1.2, and that were added to the list LP. We continue to apply the expansion procedure until $\left\lfloor \frac{P(1)}{2} \right\rfloor \leq 3$. Note that the criterion for applying the expansion procedure is the same as the one used in Propositions 5.1 and 5.2. We represent the Step 1 procedure in Figure 5.2.



Figure 5.2: Diagram to represent the expansion procedure.

According to the ideas above, Algorithm 1 is presented next.

Algorithm 1 - Partition1(P)

Input : Partition P=[n], $LP = \emptyset$ **Output:** List of partitions *LP* 1. $LP = LP \cup [P]$ **2.** Let x = P(1)3. Let level = len(P) // len(P) is the length of P 4. if level is odd then 5. $j_0 = 1$ 6. else 7. *j*₀ = 2 s. end if 9. for $j = j_0$ to $|\frac{x}{2}|$ do Set $P' = [j, x - j, P(2), \dots, P(m)]$ 10. Partition1(P') // Call Algorithm 1 recursively for P' and put all of the 11. results into LP12. end for

Algorithm 2 consists of generating the binary sequence of all threshold graphs that are simply structured from partitions obtained from Algorithm 1. The main ideas of this algorithm are described in the following steps below.

Step 1: It consists of removing all partitions of odd length from the list LP since only partitions of even length can guarantee the construction of a binary sequence b that alternates 0's and 1's, where the first P(1) positions are 0's and the last P(m) positions of b are 1's. We will denote by LP' the list that contains all the non-decreasing partitions P of even length from n obtained in Algorithm 1.

Step 2: For each partition $P \in LP'$, we construct the corresponding binary sequence b, that is, if $P = [P(1), P(2), \ldots, P(m)]$, then $b_1 = \ldots = b_{P(1)} = 0$ and for $i \in \{2, \ldots, m\}$, we have that $b_{\sum_{j=1}^{i-1} P(j)+1} = \ldots = b_{\sum_{j=1}^{i} P(j)}$ is equal to 0 or 1, depending on whether i is odd or even, respectively. Since the number of elements in each part P(i), for $i \in \{1, \ldots, m\}$, was obtained using the same criteria as in Propositions 5.1 and 5.2 (given by $\lfloor P(1)/2 \rfloor$), we can ensure a simply structured basis for the eigenspace associated with each eigenvalue of the graph. Therefore, the threshold graphs defined by these binary sequences are simply structured.

Algorithm 2 is presented below.

Algorithm 2 - Algorithm for determining threshold graphs that are simply

```
structured
    Input : n (order of the graph); BS = \emptyset
    Output: BS (list of a binary sequence)
 1. LP = Algorithm1(P=[n])
 2. LP' = \text{remove\_odd}(LP) // Remove all partitions of odd length
 3. for P \in LP' do
        b = \emptyset // Empty list of length n
 4.
        b_1 = \dots = b_{P(1)} = 0
 5.
        for i = 2 to len(P) do
 6.
            if i is odd then
 7.
                b_{\sum_{j=1}^{i-1} P(j)+1} = \dots = b_{\sum_{j=1}^{i} P(j)} = 0
 8.
            else
 9.
                b_{\sum_{j=1}^{i-1} P(j)+1} = \dots = b_{\sum_{j=1}^{i} P(j)} = 1
10.
            end if
11.
        end for
12.
        \mathrm{BS}=\mathrm{BS}\cup\mathrm{b} // Append b to the binary sequence list
13.
14. end for
```

Next, we present an example that illustrates the functioning of Algorithms 1 and 2.

Example 5.3. Let us characterize all connected threshold graphs with n = 9 vertices that are simply structured. Initially, we will determine all extensions according to Step 1.

Level 1	Level 2	Level 3	Level 4
9	1,8		
	2,7		
	3,6		
	4,5	2,2,5	$1,\!1,\!2,\!5$

Next, we remove all partitions of odd length generated by the expansion procedure. With the remaining partitions, we construct the corresponding binary sequences b and represent the graph defined by b as shown in the Table 5.3.

Partitions of even length	Binary sequence	Graph
1,8	(0,1,1,1,1,1,1,1,1)	$K_1^c \lor K_8 \cong K_9$
2,7	(0,0,1,1,1,1,1,1,1)	$K_2^c \lor K_7 \cong K_9 - (1,2)$
$3,\!6$	(0,0,0,1,1,1,1,1,1)	$K_3^c \lor K_6$
4,5	(0,0,0,0,1,1,1,1,1)	$K_4^c \lor K_5$
$1,\!1,\!2,\!5$	(0,1,0,0,1,1,1,1,1)	$(K_2 \sqcup K_2^c) \lor K_5 \cong K_4^c \lor K_5 + (1,2)$

Table 5.3: Connected threshold graphs on 9 vertices that are simply structured.

In Appendix A, we present all connected threshold graphs with order $n \in \{3, 4, ..., 18\}$ generated by Algorithm 2.

Chapter 6

THRESHOLD GRAPHS THAT ARE WHD

In the previous chapter we characterized all connected thresholds that are simply structured. In this chapter, we are interested in exploring the connection between weak Hadamard matrices and thresholds. It is worth mentioning that not all graphs obtained from Algorithm 2 are WHD. Here, we present results that identify certain families of threshold graphs that are WHD. These theoretical results were crucial in the development of an algorithm through which we characterize all connected threshold on n vertices that are WHD.

6.1 Introduction

In Example 5.3, we obtained that K_9 , $K_9 - (1, 2)$, $K_3^c \vee K_6$, $K_4^c \vee K_5$ and $K_4^c \vee K_5 + (1, 2)$ are the only graphs with 9 vertices having a simply structured eigenbasis. Consider the graph $G = K_3^c \vee K_6$. By Proposition 5.1, $\mathcal{E}_L(9) = \text{span} \{\mathbf{v}^4, \mathbf{v}^5, \mathbf{v}^6, \mathbf{v}^7, \mathbf{v}^8, \mathbf{v}'\}$, and by Proposition 5.2, $\mathcal{E}_L(6) = \text{span} \{\mathbf{u}', \mathbf{u}^2\}$, where $\mathbf{v}^4 = e_4 - e_5$, $\mathbf{v}^5 = e_5 - e_5$, $\mathbf{v}^6 = e_6 - e_7$, $\mathbf{v}^7 = e_7 - e_8$, $\mathbf{v}^8 = e_8 - e_9$, $\mathbf{v}' = (e_1 + e_2 + e_3) - (e_4 + e_5 + e_6)$, $\mathbf{u}' = e_1 - e_2$, $\mathbf{u}^2 = e_2 - e_3$. Moreover, we know that $\mathcal{E}_L(0) = \text{span} \{\mathbf{x}^9\}$, where $\mathbf{x}^9 = \mathbb{1}_9$. Therefore, $B = \{\mathbf{u}', \mathbf{u}^2, \mathbf{v}^4, \mathbf{v}^5, \mathbf{v}^6, \mathbf{v}^7, \mathbf{v}^8, \mathbf{v}', \mathbf{x}^9\}$ is a simply structured eigenbasis of L(G). If we form the matrix

$$W = \left[(\mathbf{u}')^T, (\mathbf{u}^2)^T \mid (\mathbf{v}^4)^T, (\mathbf{v}^5)^T, (\mathbf{v}^6)^T, (\mathbf{v}^7)^T, (\mathbf{v}^8)^T, (\mathbf{v}')^T \mid (\mathbf{x}^9)^T \right],$$

that is,

$$W = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix}$$

we obtain that

	2	-1	0	0	0	0	0	0	0	
	-1	2	0	0	0	0	0	0	0	
	0	0	2	-1	0	0	0	0	0	
	0	0	-1	2	-1	0	0	0	0	
$W^TW =$	0	0	0	-1	2	-1	0	-1	0	
	0	0	0	0	-1	2	-1	0	0	
	0	0	0	0	0	-1	2	0	0	
	0	0	0	0	-1	0	0	6	0	
	0	0	0	0	0	0	0	0	9	

is not tridiagonal. Since the vector \mathbf{v}^6 is not orthogonal to the vectors \mathbf{v}^5 , \mathbf{v}^7 , and \mathbf{v}' , any other matrix W' formed by the vectors in the eigenbasis B will result in $W'^T W'$ not being tridiagonal. Therefore, the graph $G_3 = K_3^c \vee K_6$ is not WHD for the given basis. This implies that not all threshold graphs that are simply structured are necessarily WHD. Motivated by this fact, we developed procedures based on some theoretical results that together with the results of Chapter 5 helped us to determine all threshold WHD graphs.

6.2 Theoretical results

Some families of threshold graphs that are WHD have already been studied. Recently, Adm et al. in [2], showed that the threshold graphs $G = K_k^c \vee K_{n-k}$ are WHD under certain conditions on nand k. For instance, if k = 1 and $n \ge 2$, then $G \cong K_n$ and G are WHD according to Lemma 1.5, ([2], Lemma 1.5). If k = 2 and $n \ge 4$, then $G \cong K_n - e$, that is, G is the complete graph minus an edge, and G is WHD according to Lemma 4.8 ([2], Lemma 4.8). If $k \ge 3$ and $n \in \{2k, 2k + 1, 2k + 2\}$, then G is WHD according to Lemma 4.6 ([2], Lemma 4.6). Macharete *et al.* in [24] presented an alternative and more complete proof of Lemma 4.6, since they showed that the matrix W of eigenvectors satisfies the additional property that $W^T W$ is tridiagonal, in such a way that it is clearer than in the proof provided by the authors in [2]. This new proof is in Proposition 6.1. Besides, it shows the power of the structure tools developed in Lemmas 2.2 and 2.3.

Proposition 6.1. ([24], Proposition 4.1) Let $G = K_k^c \vee K_{n-k}$, with $k \ge 3$. If $n - 2k \in \{0, 1, 2\}$, then G is a WHD graph.

Proof. Note that $G = K_k^c \vee K_{n-k}$ is a threshold graph on n vertices and binary sequence $b = (\underbrace{0, 0, \ldots, 0}_{k}, \underbrace{1, 1, \ldots, 1}_{n-k})$. The eigenvalues of L(G) are n - k, n, and 0 with multiplicities k - 1, n - k,

and 1, respectively. We arrange the vertices of G so that the first k vertices are the vertices of K_k^c . From Theorem 5.1, L(G) and $L(S_n)$ share the same eigenvectors and we obtain that the eigenspaces associated with eigenvalues n - k, n and 0 of L(G) are given by

$$\mathcal{E}_L(n-k) = \operatorname{span} \{ \mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^{k-1} \},$$
$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{x}^k, \dots, \mathbf{x}^{n-1} \},$$
$$\mathcal{E}_L(0) = \operatorname{span} \{ \mathbf{x}^n \}.$$

Now, we are going to obtain linear combinations of those vectors to obtain vectors with entries in the set $\{-1, 0, 1\}$. Consider a convenient linear combination given by

$$\mathbf{u}^{1} = \mathbf{x}^{1}$$
 and $\mathbf{u}^{i} = \frac{\mathbf{x}^{i} - \mathbf{x}^{i-1}}{i}$, for $i = 2, ..., k - 1$,

that is,

$$\mathbf{u}^{i} = e_{i} - e_{i+1}, \text{ for } i = 1, \dots, k-1.$$

Hence we obtain

$$\mathcal{E}_L(n) = \operatorname{span} \{\mathbf{u}^1, \mathbf{u}^2, \dots, \mathbf{u}^{k-1}\}$$

and each entry of \mathbf{u}^i , for i = 1, ..., k - 1 is equal to -1, 0 or 1. Similarly, consider a convenient linear combination given by

$$\mathbf{v}^{i} = \frac{\mathbf{x}^{i} - \mathbf{x}^{i-1}}{i}, \text{ for } i = k+1, \dots, n-1,$$
 (6.1)

that is,

$$\mathbf{v}^{i} = e_{i} - e_{i+1}$$
, for $i = k+1, \dots, n-1$.

Hence we obtain n-1 vectors that belong to $\mathcal{E}_L(n)$, and each entry of \mathbf{v}^i is equal to -1,0 or 1. Since $\dim(\mathcal{E}_L(n)) = n-k$ we need another vector \mathbf{v} to complete the eigenspace related to the eigenvalue n+k of L(G). Since

	n-k	0	0		0	-1	-1	-1		-1
	0	n-k	0		0	-1	-1	-1		-1
	÷	÷	:	·.	÷	÷	÷	÷	·.	÷
L(C) =	0	0	0		n-k	-1	-1	-1		-1
<i>L</i> (G) –	-1	-1	-1		-1	n-1	-1	-1		-1
	-1	-1	-1		-1	-1	n-1	-1		-1
	÷	÷	÷	·.	÷	÷	÷	÷	·.	÷
	-1	-1	-1		-1	-1	-1	-1		n – 1

notice that $\mathbf{v} = (\underbrace{1, 1, \dots, 1}_{k}, \underbrace{-1, -1, \dots, -1}_{n-k-1}, \underbrace{n-2k-1}_{1})$ is an eigenvector of L(G) associated with eigenvalue n+k. Moreover, if $n-2k \in \{0, 1, 2\}$, then the eigenvector v of L(G) has entries from $\{-1, 0, 1\}$. Besides,

n + k. Moreover, if $n - 2k \in \{0, 1, 2\}$, then the eigenvector v of L(G) has entries from $\{-1, 0, 1\}$. Besides, \mathbf{v} is not a linear combination of the set $\{\mathbf{v}^{k+1}, \dots, \mathbf{v}^{n-1}\}$ since the first k entries of each \mathbf{v}^i are equal to zero. Then, we obtain that

$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{v}^{k+1}, \dots, \mathbf{v}^{n-1}, \mathbf{v} \}$$

and each entry of \mathbf{v}^i , for $i = k + 1, \dots, n - 1$ and \mathbf{v} are equal to -1, 0 or 1.

Let

$$\beta = \{\mathbf{u}^1, \mathbf{u}^2, \dots, \mathbf{u}^{k-1}, \mathbf{v}^{k+1}, \mathbf{v}^{k+2}, \dots, \mathbf{v}^{n-1}, \mathbf{v}, \mathbf{x}^n\}$$
(6.2)

an eigenbasis of L(G). Note that \mathbf{u}^1 is orthogonal to all vectors in β , except for the vector \mathbf{u}^2 ; \mathbf{u}^i , for i = 2, 3, ..., k - 2, is orthogonal to all vectors in β , except for the vectors \mathbf{u}^{i-1} and \mathbf{u}^{i+1} ; \mathbf{u}^{k-1} is orthogonal to all vectors in β , except for the vector \mathbf{u}^{k-2} ; \mathbf{v}^{k+1} is orthogonal to all vectors in β , except for the vector \mathbf{v}^{k+2} ; \mathbf{v}^i , for i = k + 2, k + 3, ..., n - 2, is orthogonal to all vectors in β , except for the vectors \mathbf{v}^{i-1} and \mathbf{v}^{i+1} ; \mathbf{v}^{n-1} is orthogonal to all vectors in β , except for the vector \mathbf{v}^{n-2} ; \mathbf{v} and \mathbf{x}^n are orthogonal to all vectors in β .

In this case, if we form the matrix W where the first k - 1 columns are the eigenvectors of $\mathcal{E}_L(n-k)$, the next n-k columns are the eigenvectors of $\mathcal{E}_L(n)$, and the last column is given by the eigenvector of $\mathcal{E}_L(0)$, then we have

$$W = [(\mathbf{u}^{1})^{T}, \ldots, (\mathbf{u}^{k-1})^{T} | (\mathbf{v}^{k+1})^{T}, \ldots, (\mathbf{v}^{n-1})^{T}, (\mathbf{v})^{T} | \mathbf{x}^{n}],$$

and therefore, it follows that $W^T W$ is tridiagonal, and the proof is complete.

Let $G = H \vee K_{n-k}$ be a graph, where $H = K_l^c \vee K_{k-l}$ is a connected on k vertices. By Proposition 6.1, H is a WHD graph, if $l \ge 3$ and $k - 2l \in \{0, 1, 2\}$. Lemma 4.7 ([2], Lemma 4.7) ensures that G is a WHD graph if $n - 2k \in \{0, 1, 2\}$. Therefore, the thereshold graphs $G = K_l^c \vee K_{k-l} \vee K_{n-k} \cong K_l^c \vee K_{n-l}$ are WHD if $k - 2l \in \{0, 1, 2\}$ and $n - 2k \in \{0, 1, 2\}$. However, in the proof of Lemma 4.7 presented in [2], we identified some inaccuracies, which motivated us to rewrite the proof of this result as Proposition 6.2 of this thesis.

Proposition 6.2. Let $G = H \lor K_n$ where H is a WHD connected graph on $k \ge 2$ vertices. If $n - k \in \{0, 1, 2\}$, then G is a WHD graph.

Proof. Let spec_L(H) = { $\mu_1^{(n_1)}, \ \mu_2^{(n_2)}, \dots, \ \mu_l^{(n_l)}, \ 0^{(1)}$ }, then

$$\operatorname{spec}_{L}(G) = \{ (n+k)^{(n)}, (n+\mu_{1})^{(n_{1})}, (n+\mu_{2})^{(n_{2})}, \dots, (n+\mu_{l})^{(n_{l})}, 0^{(1)} \}$$

The all ones vector, denoted by $\mathbb{1}_{n+k}$, is an eigenvector of L(G) associated with eigenvalue 0. We arrange the vertices of G so that the first k vertices are the vertices of H. Denote by u_{i_j} the eigenvectors of L(H) associated with eigenvalues μ_i . Since H is WHD, the vectors u_{i_j} form a weak Hadamard matrix which diagonalizes L(H). Moreover, the vectors u_{i_j} concatenated with n zeros, denoted by U_{i_j} , form suitable eigenvectors for the eigenspace associated with $n + \mu_i$.

Similarly, the vectors $\mathbf{v}_i = e_i - e_{i+1}$, with $i = k+1, \ldots, n+k-1$ are n-1 suitable eigenvectors of L(G) for the eigenspace associated with n+k. The vector $\mathbf{v} = (\underbrace{1, 1, \ldots, 1}_{k}, \underbrace{-1, -1, \ldots, -1}_{n-1}, \underbrace{n-k-1}_{1})$ is an eigenvector of L(G) associated with eigenvalue n+k. Moreover, if $n-k \in \{0, 1, 2\}$, then the eigenvector \mathbf{v} of L(G) has entries from $\{-1, 0, 1\}$. Besides, \mathbf{v} is not a linear combination of the set $\{\mathbf{v}_{k+1}, \ldots, \mathbf{v}_{n+k-1}\}$ since the k first entries of each \mathbf{v}_i is equal to zero.

If we form the matrix W where the first k-1 columns are the eigenvectors U_{i_j} of L(G)associated with eigenvalues $n + \mu_i$, the next n columns are the eigenvectors $\mathbf{v}_{k+1}, \ldots, \mathbf{v}_{n+k-1}, \mathbf{v}$ of L(G)associated with eigenvalues n+k, and the last column is given by the eigenvector $\mathbb{1}_{n+k}$ of L(G) associated with eigenvalue 0, then we have that $W^T W$ is tridiagonal, and the proof is complete.

We proved that it is possible to extend Proposition 6.1 and that the graphs obtained from $K_k^c \vee K_{n-k}$ by adding a single edge preserves the properties of being threshold and WHD. Hence, this results in a new infinite family of threshold graphs that are WHD, and it was published in Macharete *et al.*, [24].

Proposition 6.3. Let $G = K_k^c \vee K_{n-k}$ such that $n - 2k \in \{0, 1, 2\}$ and $k \ge 4$. Then, G' = G + e is a WHD threshold graph.

Proof. From Proposition 6.1, $G = K_k^c \vee K_{n-k}$ is WHD. Let G' = G + e. Without loss of generality, take $e = \{1, 2\}$. Hence, G' can be represented by the binary sequence $b = (0, 1, \underbrace{0, 0, \ldots, 0}_{k-2}, \underbrace{1, 1, \ldots, 1}_{n-k})$. So, G' is a threshold graph on n + k vertices. The eigenvalues of L(G') are n - k + 2, n - k, n and 0 with multiplicities 1, k - 2, n - k, and 1, respectively. From Theorem 5.1, L(G') and $L(S_n)$ share the same

eigenvectors. Also,

$$\mathcal{E}_L(n-k+2) = \operatorname{span} \{\mathbf{x}^1\},$$
$$\mathcal{E}_L(n-k) = \operatorname{span} \{\mathbf{x}^2, \dots, \mathbf{x}^{k-1}\},$$
$$\mathcal{E}_L(n) = \operatorname{span} \{\mathbf{x}^k, \dots, \mathbf{x}^{n-1}\},$$
$$\mathcal{E}_L(0) = \operatorname{span} \{\mathbf{x}^n\}.$$

We have that $\mathcal{E}_L(n) = \text{span} \{ \mathbf{v}^{k+1}, \dots, \mathbf{v}^{n-1}, \mathbf{v} \}$, where the vectors $\mathbf{v}^{k+1}, \dots, \mathbf{v}^{n-1}$ are given in (6.1) and

$$\mathbf{v} = (\underbrace{1, 1, \dots, 1}_{k}, \underbrace{-1, -1, \dots, -1}_{n-k-1}, \underbrace{n-2k-1}_{1}).$$

If k is even, we can make the appropriate linear combination of the vectors $\mathbf{x}^2, \ldots, \mathbf{x}^{k-1}$ to obtain the vectors \mathbf{w}^j and \mathbf{z}^j , for $j = 1, \ldots, \frac{k}{2} - 1$, where

$$\begin{cases} \mathbf{w}^{j} = -\frac{1}{2j-1} \mathbf{x}^{2j-2} - \frac{(j-1)}{j(2j-1)} \mathbf{x}^{2j-1} + \frac{(j+1)}{j(2j+1)} \mathbf{x}^{2j} + \frac{1}{2j+1} \mathbf{x}^{2j+1} \\ \mathbf{z}^{j} = \frac{1}{2j+1} (\mathbf{x}^{2j+1} - \mathbf{x}^{2j}) \end{cases}$$
(6.3)

that is,

and

Therefore,

$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{w}^1, \dots, \mathbf{w}^j, \mathbf{z}^1, \dots, \mathbf{z}^j \}.$$

Notice that each entry of \mathbf{w}^{j} and \mathbf{z}^{j} , for $j = 1, \ldots, \frac{k}{2} - 1$, is equal to -1, 0 or 1. Moreover, $\{\mathbf{z}^{1}, \mathbf{z}^{2}, \ldots, \mathbf{z}^{j}\}$ forms a mutually orthogonal set and \mathbf{w}^{i} is orthogonal to $\{\mathbf{w}^{i+2}, \mathbf{w}^{i+3}, \ldots, \mathbf{w}^{j}\}$, for $i = 1, \ldots, j-2$. Finally, observe that \mathbf{w}^{i} is orthogonal to \mathbf{z}^{k} for any i, k. Hence, if we form the matrix

$$W = \left[(\mathbf{x}^{1})^{T} \mid (\mathbf{w}^{1})^{T}, \dots, (\mathbf{w}^{j})^{T}, (\mathbf{z}^{1})^{T}, \dots, (\mathbf{z}^{j})^{T} \mid (\mathbf{v}^{k+1})^{T}, \dots, (\mathbf{v}^{n+k-1})^{T}, (\mathbf{v})^{T} \mid (\mathbf{x}^{n+k})^{T} \right]$$

then it follows that W^TW is a tridiagonal matrix.

If k is odd, consider the appropriate linear combination of the vectors $\mathbf{x}^2, \ldots, \mathbf{x}^{k-1}$ to obtain the vectors \mathbf{w}^j , \mathbf{z}^j and \mathbf{z} , for $j = 1, \ldots, \frac{k-1}{2} - 1$, where

$$\begin{cases} \mathbf{w}^{j} = -\frac{1}{2j-1} \mathbf{x}^{2j-2} - \frac{(j-1)}{j(2j-1)} \mathbf{x}^{2j-1} + \frac{(j+1)}{j(2j+1)} \mathbf{x}^{2j} + \frac{1}{2j+1} \mathbf{x}^{2j+1} \\ \mathbf{z}^{j} = \frac{1}{2j+1} (\mathbf{x}^{2j+1} - \mathbf{x}^{2j}) \\ \mathbf{z} = \frac{1}{n-1} (\mathbf{x}^{n-1} - \mathbf{x}^{n-2}) \end{cases}$$

$$(6.4)$$

that is,

and

Therefore,

$$\mathcal{E}_L(n) = \operatorname{span} \{ \mathbf{w}^1, \dots, \mathbf{w}^j, \mathbf{z}^1, \dots, \mathbf{z}^j, \mathbf{z} \}.$$

Observe that each entry of \mathbf{w}^{j} , \mathbf{z}^{j} , for $j = 1, \ldots, \frac{k-1}{2} - 1$, and \mathbf{z} is equal to -1, 0 or 1. Moreover, $\{\mathbf{z}^{1}, \mathbf{z}^{2}, \ldots, \mathbf{z}^{j}\}$ forms a mutually orthogonal set and \mathbf{w}^{i} is orthogonal to $\{\mathbf{w}^{i+2}, \mathbf{w}^{i+3}, \ldots, \mathbf{w}^{j}\}$, for $i = 1, \ldots, j-2$, and \mathbf{w}^{i} is orthogonal to \mathbf{z}^{k} for any i, k. Finally, note that \mathbf{z} is orthogonal to $\{\mathbf{w}^{1}, \mathbf{w}^{2}, \ldots, \mathbf{w}^{j-1}, \mathbf{z}^{1}, \mathbf{z}^{2}, \ldots, \mathbf{z}^{j-1}\}$, but \mathbf{z} is not orthogonal to neither \mathbf{w}^{j} nor \mathbf{z}^{j} . In this case, we form the matrix

$$W = \left[(\mathbf{x}^{1})^{T} | (\mathbf{w}^{1})^{T}, \dots, (\mathbf{w}^{j-1})^{T} | (\mathbf{w}^{j})^{T}, (\mathbf{z})^{T}, (\mathbf{z}^{j})^{T} | (\mathbf{z}^{1})^{T}, \dots, (\mathbf{z}^{j-1})^{T} | (\mathbf{v}^{k+1})^{T}, \dots, (\mathbf{v}^{n-1})^{T}, (\mathbf{v})^{T} | (\mathbf{x}^{n})^{T} \right]$$

and it follows that $W^T W$ is a tridiagonal matrix. So G' is WHD and the proof is complete.

In the paper of McLaren, Monterde and Plosker [26], they build an infinite family of threshold graphs that are WHD of order 2^l for $l \ge 1$. Proposition 6.3 we build an infinite family of threshold graphs that are WHD and are not completely described by their work. For instance, the graph $(K_2 \sqcup K_6^c) \lor K_8$ belongs to the family we build but does not belong to the families defined in [26]. In addition, we are able to generate threshold WHD graphs for any number of vertices, and we are not restricted to threshold graphs of order $n = 2^l$ for $l \ge 1$. These facts make the graphs obtained from Proposition 6.3 interesting.

We conclude this section by using Theorem 5.2 to show that the disconnected threshold graph $G = H \sqcup pK_1$ is WHD if H is WHD.
Corollary 6.1. Let $G = H \sqcup pK_1$ be a disconnected threshold graph, where H is a connected threshold graph with n - p vertices and p is the number of isolated vertices. If H is a WHD graph, then G is also a WHD graph.

Proof. Consider the disconnected threshold graph $G = H \sqcup pK_1$, where H is a connected threshold graph with n - p vertices and p is the number of isolated vertices. By Theorem 5.1, the L(H) and $L(K_{1,n-p-1})$ share the same eigenvectors. Assuming that H is WHD, we can reconfigure the eigenvectors of $L(K_{1,n-p-1})$ to obtain an eigenbasis \mathcal{B} for L(H) that is simply structured. Furthermore, the matrix W, formed by the vectors in \mathcal{B} , results in W^TW being a tridiagonal matrix. By Theorem 5.2, the eigenvectors of L(G) are the same as those in the basis $B' = \{\mathbf{y}^1, \mathbf{y}^2, \dots, \mathbf{y}^n\}$, defined in (5.2) and (5.3). Thus, L(G) has a simply structured eigenbasis and the matrix $W' = [\mathbf{y}^1, \mathbf{y}^2, \dots, \mathbf{y}^n]$ satisfies the condition that W'^TW' is a tridiagonal matrix. Therefore, we conclude that the graph G is also WHD. □

6.3 Algorithm

Let P = [P(1), P(2), ..., P(m)] be a partition of n and let $b = (b_1, b_2, ..., b_n)$ be a binary sequence that defines a connected threshold graph G. In the families of connected threshold WHD graphs that have been studied, we can observe that the binary sequence b follows the following pattern:

$$b_1 = \dots = b_{P(1)} = 0$$

$$b_{\sum_{j=1}^{i-1} P(j)+1} = \dots = b_{\sum_{j=1}^{i} P(j)}, \text{ for } i \in \{2, \dots, m\}$$

such that the following conditions hold:

$$P(i+1) - 2P(i) \in \{0, 1, 2\}, \text{ for } \in \{1, \dots, m-1\}$$
(6.5)

This observation led us to conclude that, to identify all WHD threshold graphs on n vertices, we need to determine all partitions of n that satisfy the conditions in (6.5). In this way, we will be able to address Problem A.3, which states:

Problem A.3: Characterize all connected threshold graphs on n vertices that are WHD.

We completely solve Problem A.3 by using the following three steps.

Step 1: To determine a list S that contains all non-decreasing partitions P = [P(1), P(2), ..., P(m)] of length m of n that satisfy (6.5). Note that P = [P(1)], where P(1) = n, is a partition of n of length 1, and this is the first element of S. All other partitions in the list S will be obtained through two procedures that we will call *expansion* and *reduction*, respectively, which will be defined below.

Substep 1.1 (Expansion) : this procedure consists of obtaining a new partition P' of length m + 1 from P, and it can occur in two ways.

- Criterion (1): We determine all positive integers k that are solutions to equation P(1) 2k ∈ {0,1,2}. If P(1) is even, k ∈ {P(1)/2/2}, P(1)-2/2 ≥ . If P(1) is odd, k ∈ {P(1)-1/2}. For each of these solutions, we construct the partition P' = [k, P(1) k, P(2), ..., P(m)] and then add P' to the list S. The Criterion (1) will be performed recursively for each partition P obtained. We continue to apply the expansion procedure until P(1) = 1. Note that Criterion (1) for applying the expansion procedure is the same as the one used in Proposition 6.1.
- Criterion (2): If $P(1) \ge 7$ and is odd, then we construct the partition $P' = [2, P(1) 2, P(2), \dots, P(m)]$ and add P' to the list S. Criterion (2) will be performed recursively for each partition P obtained. We continue to apply the expansion procedure until P(1) < 7. Note that Criterion (2) for applying the expansion procedure is the same as the one used in Lemma 4.8 [2].

Substep 1.2 (Reduction) : Let $P \in S$ be a partition of length $m \ge 3$. The reduction procedure consists of obtaining a new partition P' of length m - 1 from P by adding the number of elements in parts $P(2) \in P(3)$. Specifically, we construct $P' = [P(1), P(2) + P(3), P(4), \dots, P(m)]$ and then add P'to the list S. The reduction will be performed recursively for each partition P obtained. We continue to apply the reduction procedure until m = 2. Note that the criterion for applying the reduction procedure is the same as the one used in Proposição 6.2.

Figure 6.1 captures the expansion and reduction procedures described above.



Figure 6.1: Diagram to represent the expansion and reduction procedures.

Step 2: Consists of removing all partitions of odd length from the list S, as only with partitions of even length we can guarantee the construction of a binary sequence b that alternates 0's and 1's, where the first P(1) positions are 0's and the last P(m) positions of b are 1's. We will denote by S' the list that contains all the non-decreasing partitions P of even length from n obtained in **Step 1**.

Step 3: For each partition $P \in S'$, we construct the corresponding binary sequence *b*. Specifically, if $P = [P(1), P(2), \ldots, P(m)]$, then $b_1 = \cdots = b_{P(1)} = 0$ and for $i \in \{2, \ldots, m\}$, we have that $b_{\sum_{j=1}^{i-1} P(j)+1} = \cdots = b_{\sum_{j=1}^{i} P(j)}$ is equal to 0 or 1, depending on whether *i* is odd or even, respectively. Since the number of elements in each part P(i), for $i \in \{1, \ldots, m\}$ was obtained using the same criteria as in Propositions 6.1, 6.2 and Lemma 4.6 [2]), we can ensure that the threshold graphs defined by these binary sequences are WHD.

The following example illustrates the procedures described above.

Example 6.1. Let's determine all connected threshold graphs with n = 9 vertices that are WHD. Figure shows all the partitions of n = 9 obtained through the extensions and reductions described in Step 1.



Figure 6.2: All partitions of n = 9 obtained through the extensions and reductions procedures described in Step 1

Next, we remove all partitions of odd length generated by the expansion and reduction procedures. With the remaining partitions, we construct the corresponding binary sequences b and represent the graph defined by b as shown in the Table 6.1.

Partitions of even lenght	Binary sequence	Graph
1,8	(0, 1, 1, 1, 1, 1, 1, 1, 1)	$K_1^c \lor K_8 \cong K_9$
2,7	(0, 0, 1, 1, 1, 1, 1, 1, 1, 1)	$K_2^c \lor K_7 \cong K_9 - (1,2)$
4,5	(0, 0, 0, 0, 1, 1, 1, 1, 1)	$K_4^c \lor K_5$
$1,\!1,\!2,\!5$	(0, 1, 0, 0, 1, 1, 1, 1, 1)	$(K_2 \sqcup K_2^c) \lor K_5 \cong K_4^c \lor K_5 + (1,2)$

Table 6.1: Threshold graphs on 9 vertices that are WHD.

Note that among all the simply structured graphs obtained in Example 5.3 only the graph $K_3^c \vee K_6$ is not WHD.

Algorithms 3 and 4 capture the processes described in Steps 1,2 e 3 e are able to generate all connected threshold graphs on n vertices that are WHD.

Algorithm 3 - Partition2(P)

Input : Partition $P = [n], S = \emptyset$

Output: S (set of resulting partitions)

- 1. if $P \in S$ then
- 2. return
- 3. end if
- 4. n = P[1]
- 5. Add P into S
- 6. for k positive integer in solutions to $n 2k \in \{0, 1, 2\}$ do

7. $P' = [k, n - k, P(2), \dots, P(m)]$

8. Invoke Algorithm 3 recursively with P' and S

9. end for

10. if $n \ge 7$ and n odd then

11. $P' = [2, n - 2, P(2), \dots, P(m)]$

12. Invoke Algorithm 3 recursively with P' and S

13. end if

14. if $len(P) \ge 3$ then

15. $P' = [P(1), P(2) + P(3), P(4), \dots, P(m)]$

16. Partition2(P') // Recursive call

17. end if

Algorithm 4 - Algorithm for determining threshold graphs that are WHD

Input : n

Output: BS: list of binary sequences

```
1. S = \text{Algorithm3}(P=[n])
 2. S' = \text{remove\_odd}(S)
 3. for P in S' do
         b = \emptyset // Empty list of length n
 4.
        b_1 = \ldots = b_{P(1)} = 0
 5.
         for i = 2 to len(P) do
 6.
             if i is odd then
 7.
                 b_{\sum_{j=1}^{i-1} P(j)+1} = \dots = b_{\sum_{j=1}^{i} P(j)} = 0
 8.
             else
 9.
                b_{\sum_{j=1}^{i-1} P(j)+1} = \dots = b_{\sum_{j=1}^{i} P(j)} = 1
10.
             end if
11.
         end for
12.
         BS = BS \cup b // Append b to BS
13.
14. end for
```

In Appendix B, we present all threshold graphs of order $n \in \{3, 4, ..., 18\}$ generated by Algorithm 4. Table 6.2 compares the number of graphs generated by Algorithm 2 and Algorithm 4. Note that up to n = 8, all graphs with a simply structured eigenbasis are also WHD. Also, note that from n = 18, the number of graphs with a simply structured eigenbasis is significantly greater than the number of WHD graphs.

n	Algorithm 2	Algorithms 4
3	1	1
4	2	2
5	2	2
6	3	3
7	3	3
8	5	5
9	5	4
10	7	6
11	7	4
12	10	8
13	10	6
14	13	9
15	13	6
16	18	13
17	18	10
18	23	14
19	23	8
20	30	16
21	30	12
22	37	16
23	37	8
24	47	20
25	47	16
26	57	22
27	57	12
28	70	24
29	70	18
30	83	24
31	83	12

Table 6.2: Number of threshold graphs with simply structured generated from Algorithm 2 and WHD graphs generated from Algorithm 4.

Adm et al. in [2], raised the following problem: Which cographs are WHD? While solving this

problem completely may be challenging, we have made significant progress by determining all threshold graphs that are WHD. It is important to note that this result contributes to the broader question, as every threshold graph is a cograph. An interesting question that remains open is to answer Problem A for cographs that are no threshold. We left it for future work. Since we have characterized all threshold graphs that are WHD, this provides a useful foundation for the authors in [26] to study WHD threshold graphs that exhibit perfect state transfer with arbitrary order.

6.4 Q-WHD graphs

In this section, we aim to address the following question: Given a graph G with n vertices, does it make sense to think of the weak Hadamard matrix W that diagonalizes the signless Laplacian matrix Q? We will treat separately the cases in which G is a connected and disconnected graph and we will show that in both cases the study of graphs whose signless Laplacian matrix Q can be diagonalized by weak Hadamard matrix W is reduced to the study of WHD graphs.

First, let's suppose that G is a connected graph on n vertices. We will show that only regular graphs can have their matrix Q diagonalized by W.

Proposition 6.4. Let G be a connected graph on n vertices. If the signless Laplacian matrix Q associated to a graph G is diagonalized by a weak Hadamard matrix W, then G is regular.

Proof. If G is connected, the signless Laplacian matrix Q = D + A is irreducible, and by the Theorem 2.2, $\rho(Q)$ is an eigenvalue of Q with algebraic multiplicity 1 and has a unique positive unit eigenvector associated **x**. By hypothesis, Q is diagonalized by W, therefore **x** is a column of W and as all the entries of W are from $\{-1, 0, 1\}$ it follows that $\mathbf{x} = \mathbb{1}_n$. By Proposition 2.2, we have that G is regular.

Next, we show that if G is r-regular and WHD, then the signless Laplacian Q(G) is diagonalizable by a weak Hadamard matrix W.

Proposition 6.5. Let G be a connected graph on n vertices. If G is r-regular and WHD, then the signless Laplacian matrix Q associated to a graph G is diagonalized by a weak Hadamard matrix W.

Proof. Since G is WHD we have the Laplacian matrix L is diagonalized by a weak Hadamard matrix W. By hypotesis, G is r-regular then from Proposition 2.3 we have that if (μ, \mathbf{x}) is an eigenpair of L(G) then (q, \mathbf{x}) is an eigenpair of Q, where the eigenvalues of L and Q satisfy the following relation $q = 2r - \mu$, for all L-autovalor μ . Therefore it follows that matrix Q associated with the graph G is diagonalized by the same weak Hadamard matrix W that diagonalizes L.

Now, let us consider that G is a disconnected graph. We will show that the matrix Q is diagonalized by weak Hadamard matrix W if and only if the connected components of G are regulars and WHD. **Proposition 6.6.** Let $G = G_1 \sqcup \ldots \sqcup G_k$ be a disconnected graph on *n* vertices, where the order of $G_i = n_i$, for $1 \le i \le k$. The signless Laplacian matrix Q associated to a graph G is diagonalized by a weak Hadamard matrix W if and only if the connected components G_i , for all $i = 1, \ldots, k$, are regular and WHD.

Proof. Note that the matrices L and Q of graph G are block matrices. Since the connected components G_i are WHD we have the Laplacian matrix $L(G_i)$ are diagonalized by a weak Hadamard matrix W_i , for i = 1, ..., k. Moreover, we have that $\operatorname{spect}_Q(G) = \operatorname{spect}_Q(G_1) \cup ... \cup \operatorname{spect}_Q(G_k)$. Since the connected components of G are regulares, from Proposition 2.3 we have that for each block of Q if (μ_i, \mathbf{x}) is an eigenpair of $L(G_i)$ then (q_i, \mathbf{x}) is an eigenpair of $Q(G_i)$, where $q_i = 2r - \mu_i$ for i = 1...k and $\mathbf{x} = [x_j]$ for $j = 1...n_i$. Therefore, it follows the matrix $Q(G_i)$ is diagonalized by the same weak Hadamard matrix W_i that diagonalizes $L(G_i)$, for i = 1, ..., k. Let

	W_1	0		0]
W -	0	W_2		:	
<i>vv</i> –	:	:	·	0	,
	0		0	W_k	

a matrix where W_1, W_2, \ldots, W_k are matrices weak Hadamard that diagonalized the connected components G_1, G_2, \ldots, G_k of G, respectively, that is, the columns of W are given by

$$\mathbf{x}' = (\mathbf{x}'_j) = \begin{cases} x_j, & 1 \le j \le n_i, \\ 0, & n_i + 1 \le j \le n. \end{cases}$$

where $\mathbf{x} = [x_j]$, for $j = 1, ..., n_i$ are the eigenvectors of $L(G_i)$, for i = 1, ..., k. Since all entries of W are in $\{-1, 0, 1\}$ and $W^T W$ is a tridiagonal matrix, it follows that the matrix Q is diagonalized by matrix W. The converse follows from applying Theorem 2.2 for each block.

CONCLUDING REMARKS AND FUTURE WORK

In this work, we study the eigenspaces of the Laplacian matrix associated with threshold and chain graphs. It has been shown in the literature, mainly in the spectral graph theory area, that eigenvalues and eigenvectors are related to combinatorial invariants of graphs and can encode nice properties of the graph. In particular, we are interested in describing which threshold and chain graphs have eigenspaces where all vectors on the basis have entries only from the set $\{-1, 0, 1\}$. If an eigenspace has all vectors with entries from the set $\{-1, 0, 1\}$ we say that this eigenspace is simply structured.

We studied the chain graphs because every threshold graph can be obtained from a chain graph. We obtained a subfamily of the chain graphs (graphs where all cells have at least two vertices and other constraints) where the integer eigenvalues have simply structured eigenspaces, but we could not guarantee that all eigenvalues are integer. So, we could not find Laplacian integral chain graphs, and that is the reason why we did not make much progress in finding WHD chain graphs.

We addressed the problem of determining all threshold graphs of a given order with a simply structured eigenspace for all eigenvalues of the Laplacian matrix. Besides, we determined all thresholds WHD graphs. Our approach consisted of determining the minimum number of vectors in the basis of an eigenspace of the Laplacian matrix of a connected threshold graph so that this basis is simply structured, as it can be seen in Propositions 5.1 and 5.2. We solved this question for the eigenvalues n and n-k, and observed that the same ideas used for these two eigenvalues can be applied recursively in such a way that we can guarantee the minimum number of eigenvectors to generate simply structured eigenspace for all eigenvalues. This allowed us to develop the Algorithm 2 that generates all connected threshold graphs of order n that are simply structured. For these graphs, we went a step further and identified those whose basis of L(G) has an ordering in which nonconsecutive vectors are orthogonal. As a consequence, we partially answered the problem proposed in [2], which aims to determine which cographs are WHD by characterizing all threshold graphs that are WHD for the development of Algorithm 4.

We also investigated unicyclic graphs, that is, connected graphs in which the number of vertices is exactly equal to the number of edges, that are WHD. In this context, we have that if G is a unicyclic graph of order $n \ (n \ge 3)$, then G is Laplacian integral if and only if $G \cong S_n + e$ or $G \cong C_3$ or $G \cong C_4$ or $G \cong C_6$ (Theorem 3.2., [23]). By Proposition 2.7 in [2], the graphs C_3, C_4 and C_6 are WHD. Note that Sn + e is a threshold graph and $\operatorname{spec}_L(S_n + e) = \{(k+3)^{(1)}, 3^{(1)}, 1^{(k)}, 0^{(1)}\}$, where k is the number of pendant vertices. Since $\mathcal{E}_L(k+3) = \operatorname{span}\{(1, 1, \dots, 1, -(k+2))\}$, it follows that for all $k \ge 1$, the unicyclic graph $S_n + e$ is not WHD. Thus, we conclude that the only unicyclic graphs that are WHD are C_3, C_4 and C_6 . As a future work, we consider the following problem:

Problem 1: Let \mathcal{G}_n be the family of all cographs on n vertices such that for each $G \in \mathcal{G}_n$, G is not threshold. Find all WHD graphs in \mathcal{G}_n .

In this sense, note that the complete bipartite graph $K_{k,k}$ is cograph but not threshold. Adm et al. in [2] proved that those graphs are WHD. Also, we can prove that there are graphs of type $G = K_{k,k} \vee K_n$ that is a WHD cograph if $n - 2k \in \{0, 1, 2\}$ and is not a threshold. However, determining all graphs of the family \mathcal{G}_n remains an open problem.

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Appendix A

THRESHOLD GRAPHS THAT ARE SIMPLY STRUCTURED

n = 3	
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Binary Sequence	Graph
011	K_3
Number of Graphs: 1	

n = 4

r

Binary Sequence	Graph
0111	K_4
0011	$K_2^c \vee K_2$

Number of Graphs: 2

<i>n</i> = 5	
Binary	Sequence
01111	

01111	K_5
00111	$K_2^c \vee K_3$

Number of Graphs: 2

Graph

<i>n</i> = 6	
Binary Sequence	Graph
011111	K_6
001111	$K_2^c \vee K_4$
Continued on next page	

Binary Sequence	Graph
000111	$K_3^c \vee K_3$
Number of C	Graphs: 3

<i>n</i> = 7	
Binary Sequence	Graph
0111111	K_7
0011111	$K_2^c \lor K_5$
0001111	$K_3^c \vee K_4$
Number of G	Graphs: 3

<i>n</i> =	8	

Binary S	equence	Graph
01111111		K_8
00111111		$K_2^c \vee K_6$
00011111		$K_3^c \vee K_5$
00001111		$K_4^c \vee K_4$
01001111		$K_2 \sqcup K_2^c \vee K_4$
Number of Graphs: 5		

<i>n</i> = 9	
Binary Sequence	Graph
011111111	K_9
001111111	$K_2^c \lor K_7$
000111111	$K_3^c \lor K_6$
000011111	$K_4^c \lor K_5$
010011111	$K_2 \sqcup K_2^c \lor K_5$
Number of Graphs: 5	

n	=	10
10	_	10

Binary Sequence	Graph
0111111111	K_{10}
0011111111	$K_2^c \vee K_8$
0001111111	$K_3^c \lor K_7$
0000111111	$K_4^c \lor K_6$
0000011111	$K_5^c \lor K_5$
0100111111	$K_2 \sqcup K_2^c \lor K_6$
0100011111	$K_2 \sqcup K_3^c \vee K_5$
Number of Graphs: 7	

		11
n	=	11

Binary Sequence	Graph	
01111111111	K_{11}	
00111111111	$K_2^c \lor K_9$	
00011111111	$K_3^c \vee K_8$	
00001111111	$K_4^c \lor K_7$	
00000111111	$K_5^c \vee K_6$	
01001111111	$K_2 \sqcup K_2^c \vee K_7$	
01000111111	$K_2 \sqcup K_3^c \vee K_6$	
Number of Graphs: 7		

<i>n</i> = 12		
Binary	Sequence	Graph
0111111	11111	K_{12}
0011111	111111	$K_2^c \lor K_{10}$
0001111	11111	$K_3^c \vee K_9$
0000111	111111	$K_4^c \vee K_8$
0000011	111111	$K_5^c \vee K_7$
0000001	11111	$K_6^c \vee K_6$
	Continue	ed on next page

Binary Sequence	Graph	
010011111111	$K_2 \sqcup K_2^c \lor K_8$	
010001111111	$K_2 \sqcup K_3^c \lor K_7$	
010000111111	$K_2 \sqcup K_4^c \vee K_6$	
011000111111	$K_3 \sqcup K_3^c \vee K_6$	
Number of Graphs: 10		

<i>n</i> =	13
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Binary Sequence	Graph
0111111111111	K_{13}
0011111111111	$K_2^c \vee K_{11}$
0001111111111	$K_3^c \vee K_{10}$
0000111111111	$K_4^c \lor K_9$
0000011111111	$K_5^c \lor K_8$
0000001111111	$K_6^c \vee K_7$
0100111111111	$K_2 \sqcup K_2^c \vee K_9$
0100011111111	$K_2 \sqcup K_3^c \vee K_8$
0100001111111	$K_2 \sqcup K_4^c \vee K_7$
0110001111111	$K_3 \sqcup K_3^c \vee K_7$

<i>n</i> = 14	
Binary Sequence	Graph
011111111111111	K_{14}
00111111111111	$K_2^c \vee K_{12}$
00011111111111	$K_3^c \lor K_{11}$
00001111111111	$K_4^c \vee K_{10}$
00000111111111	$K_5^c \vee K_9$
00000011111111	$K_6^c \vee K_8$
00000001111111	$K_7^c \lor K_7$
Continued on next page	

Binary Sequence	Graph	
01001111111111	$K_2 \sqcup K_2^c \lor K_{10}$	
01000111111111	$K_2 \sqcup K_3^c \lor K_9$	
01000011111111	$K_2 \sqcup K_4^c \vee K_8$	
01100011111111	$K_3 \sqcup K_3^c \vee K_8$	
01000001111111	$K_2 \sqcup K_5^c \lor K_7$	
01100001111111	$K_3 \sqcup K_4^c \vee K_7$	
Number of Graphs: 13		

<i>n</i> =	15
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Binary Sequence	Graph	
0111111111111111	K_{15}	
0011111111111111	$K_2^c \vee K_{13}$	
0001111111111111	$K_3^c \lor K_{12}$	
000011111111111	$K_4^c \vee K_{11}$	
000001111111111	$K_5^c \vee K_{10}$	
000000111111111	$K_6^c \vee K_9$	
000000011111111	$K_7^c \vee K_8$	
010011111111111	$K_2 \sqcup K_2^c \vee K_{11}$	
010001111111111	$K_2 \sqcup K_3^c \vee K_{10}$	
010000111111111	$K_2 \sqcup K_4^c \lor K_9$	
011000111111111	$K_3 \sqcup K_3^c \lor K_9$	
010000011111111	$K_2 \sqcup K_5^c \vee K_8$	
011000011111111	$K_3 \sqcup K_4^c \vee K_8$	
Number of Graphs: 13		

n	=	16
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Binary Sequence	Graph
011111111111111111	K_{16}
001111111111111111	$K_2^c \vee K_{14}$

Continued on next page

Binary Sequence	Graph	
00011111111111111	$K_3^c \lor K_{13}$	
00001111111111111	$K_4^c \lor K_{12}$	
0000011111111111	$K_5^c \vee K_{11}$	
0000001111111111	$K_6^c \lor K_{10}$	
0000000111111111	$K_7^c \lor K_9$	
0000000011111111	$K_8^c \vee K_8$	
01001111111111111	$K_2 \sqcup K_2^c \vee K_{12}$	
0100011111111111	$K_2 \sqcup K_3^c \vee K_{11}$	
0100001111111111	$K_2 \sqcup K_4^c \vee K_{10}$	
0110001111111111	$K_3 \sqcup K_3^c \vee K_{10}$	
0100000111111111	$K_2 \sqcup K_5^c \lor K_9$	
0110000111111111	$K_3 \sqcup K_4^c \vee K_9$	
0100000011111111	$K_2 \sqcup K_6^c \vee K_8$	
0110000011111111	$K_3 \sqcup K_5^c \vee K_8$	
0111000011111111	$K_4 \sqcup K_4^c \vee K_8$	
0011000011111111	$K_2^c \vee K_2 \sqcup K_4^c \vee K_8$	
Number of Graphs: 18		

N	um	ber	of	Grap	hs:	18
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<i>n</i> =	: 17
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Binary Sequence	Graph	
0111111111111111111	K_{17}	
0011111111111111111	$K_2^c \vee K_{15}$	
0001111111111111111	$K_3^c \vee K_{14}$	
0000111111111111111	$K_4^c \vee K_{13}$	
000001111111111111	$K_5^c \lor K_{12}$	
000000111111111111	$K_6^c \vee K_{11}$	
00000001111111111	$K_7^c \lor K_{10}$	
00000000111111111	$K_8^c \lor K_9$	
010011111111111111	$K_2 \sqcup K_2^c \lor K_{13}$	
010001111111111111	$K_2 \sqcup K_3^c \lor K_{12}$	
Continued on next page		

Binary Sequence	Graph
01000011111111111	$K_2 \sqcup K_4^c \lor K_{11}$
011000111111111111	$K_3 \sqcup K_3^c \vee K_{11}$
01000001111111111	$K_2 \sqcup K_5^c \vee K_{10}$
01100001111111111	$K_3 \sqcup K_4^c \vee K_{10}$
01000000111111111	$K_2 \sqcup K_6^c \vee K_9$
01100000111111111	$K_3 \sqcup K_5^c \vee K_9$
01110000111111111	$K_4 \sqcup K_4^c \vee K_9$
00110000111111111	$K_2^c \lor K_2 \sqcup K_4^c \lor K_9$

Number of Graphs: 18

<i>n</i> =	18
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Binary Sequence	Graph
01111111111111111111	K_{18}
00111111111111111111	$K_2^c \vee K_{16}$
00011111111111111111	$K_3^c \vee K_{15}$
00001111111111111111	$K_4^c \vee K_{14}$
0000011111111111111	$K_5^c \vee K_{13}$
0000001111111111111	$K_6^c \vee K_{12}$
000000011111111111	$K_7^c \vee K_{11}$
000000001111111111	$K_8^c \vee K_{10}$
000000000111111111	$K_9^c \lor K_9$
01001111111111111111	$K_2 \sqcup K_2^c \vee K_{14}$
01000111111111111111	$K_2 \sqcup K_3^c \vee K_{13}$
0100001111111111111	$K_2 \sqcup K_4^c \vee K_{12}$
0110001111111111111	$K_3 \sqcup K_3^c \vee K_{12}$
0100000111111111111	$K_2 \sqcup K_5^c \lor K_{11}$
0110000111111111111	$K_3 \sqcup K_4^c \lor K_{11}$
010000001111111111	$K_2 \sqcup K_6^c \lor K_{10}$
011000001111111111	$K_3 \sqcup K_5^c \vee K_{10}$
011100001111111111	$K_4 \sqcup K_4^c \vee K_{10}$
Co	ontinued on next page

Graph
$K_2^c \lor K_2 \sqcup K_4^c \lor K_{10}$
$K_2 \sqcup K_7^c \lor K_9$
$K_3 \sqcup K_6^c \vee K_9$
$K_4 \sqcup K_5^c \lor K_9$
$K_2^c \vee K_2 \sqcup K_5^c \vee K_9$

Appendix B

THRESHOLD GRAPHS THAT ARE WHD

<i>n</i> = 3	
Binary Sequence	Graph
011	K_3
Number of Graphs: 1	

n = 4

Binary Sequence	Graph
0111	K_4
0011	$K_2^c \vee K_2$
Number of G	Graphs: 2

n	=	5	
n	=	0	

Binary Sequence	Graph
01111	K_5
00111	$K_2^c \vee K_3$
Number of O	Graphs: 2

<i>n</i> = 6	
Binary Sequence	Graph
011111	K_6
001111	$K_2^c \vee K_4$
000111	$K_3^c \vee K_3$
Continued on	next page

Binary sequence Graph	Binary Sequence Graph
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Number	of	Graphs:	3
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n = 7

Binary Sequence	Graph
0111111	K_7
0011111	$K_2^c \vee K_5$
0001111	$K_3^c \vee K_4$
Number of G	Fraphs: 3

n = 8

Binary S	equence	Graph
01111111		K_8
00111111		$K_2^c \vee K_6$
00011111		$K_3^c \lor K_5$
00001111		$K_4^c \vee K_4$
01001111		$K_2 \sqcup K_2^c \vee K_4$
	Number	of Graphs: 5

<i>n</i> = 9

Binary Sequence	Graph
011111111	K_9
001111111	$K_2^c \vee K_7$
000011111	$K_4^c \vee K_5$
010011111	$K_2 \sqcup K_2^c \vee K_5$

Number of Graphs: 4

n	=	10
10	_	10

Binary Sequence	Graph	
0111111111	K_{10}	
0011111111	$K_2^c \vee K_8$	
0000111111	$K_4^c \lor K_6$	
0000011111	$K_5^c \lor K_5$	
0100111111	$K_2 \sqcup K_2^c \vee K_6$	
0100011111	$K_2 \sqcup K_3^c \vee K_5$	
Number of Graphs: 6		

<i>n</i> = 11

Binary Sequence	Graph	
01111111111	K_{11}	
00111111111	$K_2^c \lor K_9$	
00000111111	$K_5^c \vee K_6$	
01000111111	$K_2 \sqcup K_3^c \vee K_6$	
Number of Graphs: 4		

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Binary Sequence	Graph	
011111111111	K_{12}	
001111111111	$K_2^c \vee K_{10}$	
000111111111	$K_3^c \lor K_9$	
000001111111	$K_5^c \lor K_7$	
000000111111	$K_6^c \lor K_6$	
010001111111	$K_2 \sqcup K_3^c \lor K_7$	
010000111111	$K_2 \sqcup K_4^c \lor K_6$	
011000111111	$K_3 \sqcup K_3^c \vee K_6$	
Number of Graphs: 8		

um	\mathbf{per}	of	Grap	hs: 8	8	
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<i>n</i> =	13
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Binary Sequence	Graph	
0111111111111	K_{13}	
0011111111111	$K_2^c \vee K_{11}$	
0001111111111	$K_3^c \vee K_{10}$	
0000001111111	$K_6^c \vee K_7$	
0100001111111	$K_2 \sqcup K_4^c \vee K_7$	
0110001111111	$K_3 \sqcup K_3^c \vee K_7$	
Number of Graphs: 6		

Binary Sequence	Graph	
011111111111111	K_{14}	
001111111111111	$K_2^c \vee K_{12}$	
00011111111111	$K_3^c \vee K_{11}$	
00000011111111	$K_6^c \vee K_8$	
00000001111111	$K_7^c \lor K_7$	
01000011111111	$K_2 \sqcup K_4^c \lor K_8$	
01000001111111	$K_2 \sqcup K_5^c \vee K_7$	
01100011111111	$K_3 \sqcup K_3^c \vee K_8$	
01100001111111	$K_3 \sqcup K_4^c \vee K_7$	
Number of Graphs: 9		

<i>n</i> = 15	
Binary Sequence	Graph
0111111111111111	K_{15}
0011111111111111	$K_2^c \vee K_{13}$
0001111111111111	$K_3^c \vee K_{12}$
000000011111111	$K_7^c \lor K_8$
010000011111111	$K_2 \sqcup K_5^c \vee K_8$
Continue	ed on next page

Binary Sequence	Graph
011000011111111	$K_3 \sqcup K_4^c \vee K_8$
Number of Graphs: 6	

		10	
n	_	In	
10	_	TO	

Binary Sequence	Graph
011111111111111111	K_{16}
00111111111111111	$K_2^c \lor K_{14}$
00011111111111111	$K_3^c \vee K_{13}$
00001111111111111	$K_4^c \vee K_{12}$
0000000111111111	$K_7^c \lor K_9$
0000000011111111	$K_8^c \vee K_8$
01001111111111111	$K_2 \sqcup K_2^c \lor K_{12}$
0100000111111111	$K_2 \sqcup K_5^c \lor K_9$
0100000011111111	$K_2 \sqcup K_6^c \lor K_8$
0110000111111111	$K_3 \sqcup K_4^c \lor K_9$
0110000011111111	$K_3 \sqcup K_5^c \lor K_8$
0111000011111111	$K_4 \sqcup K_4^c \lor K_8$
0011000011111111	$K_2^c \vee K_2 \sqcup K_4^c \vee K_8$

Number of Graphs: 13

<i>n</i> = 17	
Binary Sequence	Graph
0111111111111111111	K_{17}
0011111111111111111	$K_2^c \vee K_{15}$
0001111111111111111	$K_3^c \vee K_{14}$
000011111111111111	$K_4^c \vee K_{13}$
00000000111111111	$K_8^c \lor K_9$
010011111111111111	$K_2 \sqcup K_2^c \vee K_{13}$
01000000111111111	$K_2 \sqcup K_6^c \lor K_9$

Continued on next page

Binary Sequence	Graph
01100000111111111	$K_3 \sqcup K_5^c \lor K_9$
01110000111111111	$K_4 \sqcup K_4^c \lor K_9$
00110000111111111	$K_2^c \lor K_2 \sqcup K_4^c \lor K_9$

Number of	Graphs:	10
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n	=	18
		-

Binary Sequence	Graph
0111111111111111111111	K_{18}
001111111111111111111	$K_2^c \vee K_{16}$
000111111111111111111	$K_3^c \vee K_{15}$
00001111111111111111	$K_4^c \vee K_{14}$
000000001111111111	$K_8^c \vee K_{10}$
000000000111111111	$K_9^c \lor K_9$
01001111111111111111	$K_2 \sqcup K_2^c \lor K_{14}$
010000001111111111	$K_2 \sqcup K_6^c \lor K_{10}$
010000000111111111	$K_2 \sqcup K_7^c \lor K_9$
011000001111111111	$K_3 \sqcup K_5^c \lor K_{10}$
0111000011111111111	$K_4 \sqcup K_4^c \lor K_{10}$
011100000111111111	$K_4 \sqcup K_5^c \lor K_9$
001100001111111111	$K_2^c \vee K_2 \sqcup K_4^c \vee K_{10}$
001100000111111111	$K_2^c \lor K_2 \sqcup K_5^c \lor K_9$
Nur	nber of Graphs: 14