

LUMPABILITY OF NETWORKS VIA A DYNAMICAL GENERALIZATION OF COSPECTRAL VERTICES

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By
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Lumpability of Networks via a Dynamical Generalization of Cospectral
Vertices

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We certify that we have read this thesis and that in our opinion it is fully adequate,
in scope and in quality, as a thesis for the degree of Master of Science.

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ABSTRACT

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A new vertex relation in networks corresponding to dynamical symmetry and inducing lumpability is defined with respect to dynamics modeled by the adjacency or the Laplacian matrix. Several constructions and operations that preserve these constructions are given, both for this vertex relation, called coprobable, as well as for its subclass, cospectral vertices. Further results are obtained for cospectral vertices, including a construction of “almost” strongly cospectral vertices and an investigation of dynamically symmetric subgraphs induced by cospectral vertices.

Keywords: Coprobable Vertices, Cospectral Vertices, Lumpability, Strongly Cospectral Vertices.

ÖZET

EŞSPEKTRAL DÜĞÜMLERİN DİNAMİK BİR GENELLEMEŞİ VASİTASIYLA KÜMELEŞTİRİLEBİLİRLİK

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Düğümler arası yeni bir simetri türü tanımlanmıştır. Graf üstünde komşuluk matrisi ya da Laplas matrisi vasıtasıyla tanımlanan bir dinamik altındaki bir simetriye tekabül eden bu simetri türü, aynı zamanda bu dinamiğin kümeleştirilebilmesine aracı olmaktadır. Hem eşolasılıksal olarak isimlendirilen bu simetri türü için, hem de onun bir altkümesini oluşturan eşspektral düğümler için birtakım yapımlar ve bu yapımları koruyan bazı işlemler verilmiştir. Buna ek olarak, güçlü eşspektral düğüm yapımına dair ve eşspektral düğümler aracılığıyla dinamik olarak simetrik olan altgraflara dair bazı sonuçlar da ilave edilmiştir.

Anahtar sözcükler: Eşolasılıksal Düğümler, Eşspektral Düğümler, Kümeleştirilebilirlik, Güçlü Eşspektral Düğümler.

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Chapter 1

Introduction

In many real and theoretical contexts, one can think of dynamical systems over networks where the parameters of the dynamical system are induced by the values of functions over the vertices of the network. Such systems, modeled through the use of $N \times N$ matrices associated with the network such as the adjacency matrix or the Laplacian matrix; can model systems as diverse as populations, power grids, transportation infrastructure, or communication networks of any kind.

Although dynamical systems over networks can in general be thought of as ordinary dynamical systems, the associated discrete topological structure of the graph/network is often of central importance for the dynamics and could provide us with significant information about it. In this thesis, keeping this in mind, we define and obtain vertices that are dynamically symmetric in networks, with respect to either the adjacency matrix or the Laplacian matrix. This dynamical symmetry between vertices facilitates the well known phenomena of lumpability, a method of dimension reduction in dynamical systems. Furthermore, we establish a wide range of different constructions and operations that preserve these constructions to obtain these dynamically symmetric vertex pairs, called “coprobable vertices” as well as their stronger versions, cospectral vertices. The latter is a well known vertex relationship with algebraic origins, which has primarily been of focus in the graph theory literature.

Beyond constructions of coprobable and cospectral vertex pairs given in Section 4.1, in Section 4.2 we digress into the special case of strongly cospectral vertices, finding out that our construction of cospectral vertices is “almost” strongly cospectral. Further expanding on the properties and uses of cospectral vertices, in Section 4.3.1, we expand on the literature to obtain dynamically symmetric subgraphs or components that could be interchanged with one another without interfering with the dynamics over the rest of the graph.

The constructions and operations that we provide work in arbitrarily large and complex graphs and therefore enable the construction of a diverse class of graphs containing coprobable or cospectral vertices. In particular, this diverse class of graphs enable us to explain numerous existing cases of cospectral vertices from the literature, many of which are provided as examples.

Chapter 2

Literature Survey

Contemporary interest in network science has, in recent decades, facilitated a growing body of research aimed at developing a theoretical understanding of networks. Early efforts focused on statistical and generative models designed to explain observed features such as degree distributions, the small-world property, centrality, and hierarchical structure [1, 2, 3, 4]. More recently, attention has also focused on analyzing substructures and components of networks. Despite significant theoretical and empirical work on network motifs and community structures, a comprehensive and unified theoretical framework for understanding network structure remains elusive.

One promising approach for understanding network structure involves identifying generalized notions of symmetry that extend beyond classical graph automorphisms. Recent work in various fields have shown that vertices of a network/graph indeed have different symmetries of interest besides the classical symmetries induced by graph automorphisms. Among these, a recently popular one is latently symmetric vertices [5]. These symmetries arise in the context of isospectral reductions, which reduce the dimensionality of a network while preserving the spectrum of its adjacency matrix [6, 7]. These latently symmetric vertices are defined to be those that are symmetric in an isospectral reduction of the network but not necessarily under traditional automorphisms. It has been suggested that through

this generalization one can better understand network structure. Indeed, these latent symmetries can be organized hierarchically using a parameter known as the measure of latency, offering a novel lens through which to interpret network architecture [5].

Another notable form of vertex symmetry is the concept of cospectral vertices—vertices whose removal gives graphs with identical adjacency spectra [8]. Relatedly, the recently popular strongly cospectral vertices can also be considered a type of symmetry relation between vertices, albeit a much stricter one [8]. It was also mentioned in [8] that whether two vertices are cospectral is equivalent to whether there exists an orthogonal involution matrix commuting with the adjacency matrix mapping these vertices to one another. It therefore follows that cospectrality corresponds to a form of dynamical symmetry governed by the graph’s adjacency matrix. It is also interesting here that the relationship between cospectrality and latent symmetries has been explored in [9], where it was demonstrated that all cospectral vertices are, in fact, latently symmetric. It was further shown that for undirected graphs, the converse also holds, that is, all latently symmetric vertices are cospectral.

In a different development, a new form of structural symmetry was proposed in [10]. This approach constructs an infinite tree rooted at each vertex by tracing all possible paths terminating at that vertex. Vertices are then defined as symmetric if the corresponding trees are isomorphic. In the same study it was shown in particular that these symmetries arise in the context of gene regulation networks and indeed do have a function within the biological system; thereby showing their relevance for real networks.

There has also been growing interest in identifying generalized vertex symmetries in networks from the perspective of network dynamics. Various studies have explored either specific dynamical models or more general frameworks to define dynamically symmetric vertices. For example, in [11], symmetry is defined in the context of the Kuramoto-Sakaguchi model: two vertices are considered symmetric if they exhibit no phase difference in the steady state. In a broader approach, [12] defines dynamical symmetry as any symmetry of the dynamical system defined

on the network. This general formulation is then applied to large-scale graphs and graphons, allowing for the analysis of symmetry in the continuum limit.

Beyond the theoretical interest in such generalized symmetries justified by the need to understand the structure of networks, such symmetries have also been shown to be relevant for a wide range of practical applications. Most notably, cospectral vertices and their rare cousins, strongly cospectral vertices, are known to be directly related to the problem of perfect state transfer in continuous quantum walks [8]. On the other hand, latently symmetric vertices have been shown to share the same eigenvector centrality, a key indicator of a vertex’s importance within a network [5]. Furthermore, latent symmetries not only has implications for network analysis but also arises in developments in physics: they have been linked to the emergence of flat bands in physical systems and have enabled the construction of lattices lacking any apparent symmetries [13, 14].

The problem of dynamical symmetries in networks is closely related to the issues of controllability and observability, since dynamical symmetries can render symmetric components indistinguishable, thereby limiting the full controllability or observability of the system [15].

Interest in the controllability and observability of complex networks has grown significantly in recent years. A foundational contribution was made in [16], where the authors introduced a method based on the maximum matching algorithm to determine the minimum number of driver nodes required for structural controllability. This same framework was subsequently applied to analyze observability in networks [17]. Beyond structural controllability, the problem of exact controllability has also been investigated. In particular, it has been shown that for linear systems, the minimum number of driver nodes required for controllability depends on the eigenvalue degeneracies of the system matrix governing the network dynamics [18].

In the network science and control literature, works on controllability often focus on theoretical necessities to control or observe a system and therefore, do not directly take dynamical symmetries into account. As an exception to this,

[19] investigates the effect of graph symmetries on controllability by numerically analyzing motifs with three vertices under a nonlinear dynamics. Another exception, although not directly related with symmetries, is [20], in which it is shown that the existence of equitable partitions in graph can break controllability in nontrivial ways.

It is also worth mentioning that there have also been some theoretical work towards constructive methods to obtain controllable and observable networks. In [21] for example, the controllability of cartesian product networks has been investigated.

In the graph theory literature, a graph is said to be controllable if the set of vectors $\{\mathbf{1}, A\mathbf{1}, \dots, A^{n-1}\mathbf{1}\}$ is linearly independent where $\mathbf{1}$ is the all-ones vector, A is the adjacency matrix of the graph and n is the number of nodes in the graph. With this definition in mind, there have also been interest towards the controllability of graphs from the perspective of graph theory [22, 23, 24, 25]. However, from the perspective of network science, such works remain very specific due to their specialized definition of controllability.

Regardless of the character and interest of these diverse range of studies, they all focus on controllability as an objective and do not explicitly investigate when controllability might break down for arbitrary networks. Such a perspective is obviously intimately related to the existence of dynamical symmetries in networks and could perhaps be more fruitful towards understanding network structure. From a practical standpoint, it also provides a clearer framework for identifying which networked systems are controllable and which are inherently resistant to control. It is well known [15] that this breakdown of controllability and observability is inextricably linked with the concept of lumpability—a property describing whether the system’s phase space can be reduced while retaining a meaningful relation to the original dynamics. Accordingly, the study of generalized network symmetries is not only conceptually aligned with, but also directly relevant to, the analysis of lumpability in dynamical systems on networks.

Various work has been done on the lumpability of network systems. In the

Markov chain literature, the lumpability of Markov chains over networks has been investigated. For instance, in [26] graph automorphisms were used to lump a Markov chain over networks modeling epidemic spread. Extending this idea in [27], the lumpability investigation, albeit only approximately, has been expanded from graph automorphisms to local symmetries defined as isomorphisms between k -neighborhoods of vertices.

The lumpability of networks has also been referred indirectly, most notably in [28] which talks about symmetries and patterns of synchrony in networks. Related to these, it in particular mentions quotient networks, which are in practice, dynamics preserving network reductions, and points out some important observations about them, such as the emergence of self-coupling and multiple edges in the reduced models. Dynamics on quotient networks has also been considered in [29] where the relation between the structure of the symmetry group of a network and the synchronizability of clusters of nodes was investigated. Finally, the relationship between the reduction of dynamical systems on networks and the structure of these networks was investigated in [30] using a category theoretic perspective.

Most work regarding lumpability in networks are either too specific, especially among the Markov chain literature as well as among works that use graph automorphisms; or too general, providing general frameworks towards reducing the dimension of the dynamics but falling short of practicability. These limitations stem, in large part, from the inherent complexity and diversity of network structures, especially when considered in their most general form. It is also important to note that many large-scale networks, whether real or synthetic, exhibit pronounced non-random features such as community structures and hubs. As previously discussed [5, 10], such structural regularities often give rise to generalized symmetries that are not captured by traditional graph-theoretic notions. This suggests that complex networks may harbor rich forms of dynamical symmetry beyond standard graph symmetries, and may therefore support substantial lumpability. Taken together, these observations indicate that the lumpability of dynamical systems on networks is deeply connected to network structure and more line of research from this perspective could be done.

In this thesis, building on the insights discussed above, we propose an approach to lumpability in networks with linear dynamics which also complements our understanding of the effect of network topology on the dynamics. To characterize and construct lumpable networks under linear dynamics, we adopt equal eigenvector centrality as a criterion for defining equivalence between vertices. It must be mentioned here that this connection between eigenvector centrality and lumpability has been noted in previous work. For instance, [31] investigates the relationship between centrality measures, including eigenvector centrality, and lumpability of dynamical systems on networks. Specifically, it was shown that vertices that are backward differential equivalent are also equivalent under exact role assignment, and thus share the same eigenvector centrality. It has also been noted that latently symmetric vertices also have equal eigenvector centrality, though this is not an if and only if statement [5].

Chapter 3

Background

3.1 Notation

A graph G is a pair (V, E) such that V is a set of finite size called the vertex set of G and $E \subseteq V \times V$ is called the edge set of G . In general, we denote the pair (V, E) by $G(V, E)$ or just G . When speaking about the vertex and edge sets of a graph, we denote them by $V(G)$ and $E(G)$ to indicate which graph's set of vertices and edges we are talking about. If the graph is clear from the context, we might omit G and just talk about V and E . Throughout the thesis, the capital letter N denotes the number of vertices of G , $|V|$. The letter v in all its forms, such as v' , v_i or v_i^1 , always denotes a vertex of a graph, i.e. an element of the vertex set of the appropriate graph. Generally, we will index the vertices of a graph G with subscripts like v_i . When there is an edge from a vertex v_i to a vertex v_j , i.e. $(v_i, v_j) \in E$, we will indicate this by the notation $v_i \sim v_j$. Lastly, we say that a graph $G'(V', E')$ is a subgraph of $G(V, E)$ if $V' \subseteq V$ and $E' \subseteq E$.

Definition 3.1.1. (Undirected Graph) A graph G is said to be undirected if its edge set E satisfies the property that $(v_i, v_j) \in E$ if and only if $(v_j, v_i) \in E$.

Definition 3.1.2. (Loop) An edge $(v_i, v_j) \in E$ of a graph G is said to be a loop if $v_i = v_j$.

Definition 3.1.3. (Path/Walk) Let G be a graph. A finite sequence of vertices $v_{i_1}, v_{i_2}, \dots, v_{i_n} \in V$ of G is called a path from v_{i_1} to v_{i_n} or just a path if we have $(v_{i_j}, v_{i_{j+1}}) \in E$ for all $j = 1, \dots, n - 1$. We also occasionally refer to a path as a walk.

The length of a path/walk $v_{i_1}, v_{i_2}, \dots, v_{i_n}$ is equal to $n - 1$. Note that the vertices of a path $v_{i_1}, v_{i_2}, \dots, v_{i_n}$ need not in general be distinct.

Definition 3.1.4. (Closed Path/Walk) We say that a path/walk from v_i to v_j is closed if $v_i = v_j$.

Definition 3.1.5. (Strongly Connected Graph, Connected Graph) A graph G is said to be strongly connected if for every $v_i, v_j \in V$, there exists a path from v_i to v_j . For an undirected graph, this property is called connected instead of strongly connected.

Rather than a normal graph, one can define a weighted graph, which is defined exactly the same as a normal graph but with an extra map $W : E \rightarrow \mathbb{R}$ called the weight map. In weighted graphs, for every edge $e \in E$, $W(e)$ denotes the weight associated with that edge. A graph is said to be unweighted if it is not weighted. Throughout this thesis, all graphs will be assumed to be undirected, unweighted, without any loops and connected; although our results and approach can in principle be extended to graphs that has neither of the aforementioned properties.

Given a graph $G(V, E)$, we will also consider the vector space $\mathbb{R}^N$ where $N = |V|$, called the state space induced by G . If the vertices of G are denoted as $v_1, v_2, \dots, v_N \in V$, then for all $i \in \{1, \dots, N\}$ we can associate the vertex v_i with the i -th standard basis vector $[0, \dots, 1, \dots, 0]^T$ of $\mathbb{R}^N$ where the non-zero entry is in the i -th index. With this association in mind, we will denote the elements of V as $v_i \in V$ and the associated standard basis vectors as their bold counterparts $\mathbf{v}_i \in \mathbb{R}^N$, although we will generally refer to both of them as vertices of G . Hence, from now on we will be assuming $\mathbf{v}_i = [0, \dots, 1, \dots, 0]^T$ where the non-zero entry is in the i -th index. For an arbitrary vector of $\mathbb{R}^N$, we will use the bold letters $\mathbf{x}, \mathbf{y} \in \mathbb{R}^N$. Since the i -th standard basis vector is denoted by $\mathbf{v}_i$, we will refer

to the i -th component of an arbitrary vector $\mathbf{x} \in \mathbb{R}^N$ as $(\mathbf{x})_{v_i}$. Similarly, for an $N \times N$ matrix A , we will denote the (i, j) -th entry as $(A)_{v_i, v_j}$ or A_{v_i, v_j} . In situations where we have to represent a vertex of a graph with a label other than an index, such as $v, v', \hat{v} \in V$, we will denote the standard basis vectors associated with these vertices as $\mathbf{v}, \mathbf{v}', \hat{\mathbf{v}}$ and so on. We will also denote the vector components corresponding to these vertices as $(\mathbf{x})_v, (\mathbf{x})_{v'}, (\mathbf{x})_{\hat{v}}$ and so on.

With this notation we can now define the adjacency matrix of a graph G , denoted by A , as an $N \times N$ matrix with entries defined by:

$$A_{v_i, v_j} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$$

We will also make use of the Laplacian matrix, denoted by L and defined as follows:

$$L_{v_i, v_j} = \begin{cases} -1 & \text{if } (v_i, v_j) \in E \\ d_{v_i} & \text{if } v_i = v_j \\ 0 & \text{otherwise} \end{cases}$$

where d_{v_i} is the degree of the vertex v_i , i.e. the number of vertices $v_k \neq v_i$ of G for which $(v_i, v_k) \in E$. By the above definitions, it is clear that the adjacency and Laplacian matrices of an undirected graph are symmetric matrices. Lastly, it is well known that for the adjacency matrix A of a graph G , the entry $(A^k)_{v_i, v_j}$ gives us the number of paths of length k from v_i to v_j in G .

Unless otherwise mentioned, we will always denote by the capital letters A and L the adjacency matrix and the Laplacian matrix of a graph. When there are multiple graphs labeled in some different way such as $\tilde{G}$, G' or G_i , their corresponding adjacency and Laplacian matrices will be labeled accordingly $\tilde{A}$, A' , A_i and so on.

3.2 Linear Algebra

In this section we provide the necessary background material from linear algebra, focusing on subspaces generated by linear maps.

Suppose we are given a vector space $\mathbb{R}^N$ and a linear map $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ on the vector space. Given a vector $\mathbf{x} \in \mathbb{R}^N$, we define the subspace generated by $\mathbf{x}$ under the action of A by $\langle \mathbf{x} \rangle_A = \text{span}\{\mathbf{x}, A\mathbf{x}, \dots, A^{N-1}\mathbf{x}\} = \text{span}\{\mathbf{x}, A\mathbf{x}, \dots, A^{N-1}\mathbf{x}, \dots\}$, the last equality being by the Cayley-Hamilton Theorem. We denote the subspace orthogonal to $\langle \mathbf{x} \rangle_A$ by $\langle \mathbf{x} \rangle_A^\perp$.

Given an $N \times N$ matrix A , we can consider it as a linear map $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ on $\mathbb{R}^N$ through direct matrix multiplication. In this way, we will consider matrices as linear maps on $\mathbb{R}^N$. Conversely, we also know from linear algebra that given a linear map $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$, we can consider it as a matrix by choosing a basis for $\mathbb{R}^N$ and we will always be using the most obvious choice, the standard basis in $\mathbb{R}^N$. In giving our results, we will implicitly be keeping these in mind.

Now we had mentioned that given a graph G , we always have a corresponding vector space $\mathbb{R}^N$ where $N = |V|$, by associating the standard unit basis vectors $\mathbf{v}_i = [0, \dots, 1, \dots, 0]^T$ with vertices $v_i \in V$. Furthermore, we also naturally have two matrices A and L , respectively the adjacency and the Laplacian matrix, acting on this vector space through direct matrix multiplication. With these in mind, for every graph G and every vertex $v_i \in V$, we directly have associated subspaces $\langle \mathbf{v}_i \rangle_A$ and $\langle \mathbf{v}_i \rangle_L$ of $\mathbb{R}^N$.

Definition 3.2.1. (Spectrum of a linear map) Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map. We call the set of eigenvalues of A , denoted Λ_A , the spectrum of A .

We will generally denote an eigenvector corresponding to an eigenvalue λ of a linear map A as $\mathbf{w}_\lambda$. We will occasionally call this eigenvector a λ -eigenvector. In a similar fashion, we will call the eigenspace associated with an eigenvalue λ simply as the λ -eigenspace of A . We will denote by $E_\lambda : \mathbb{R}^N \rightarrow \mathbb{R}^N$ the orthogonal projection map onto the λ -eigenspace of A . In cases where it is not clear to which

linear map's λ -eigenspace E_λ is projecting onto, we will denote it by E_λ^A .

Now, because we are working with undirected graphs, all matrices used in this thesis will be symmetric. It is known from linear algebra that finite dimensional symmetric matrices are diagonalizable by an orthonormal set of eigenvectors. Because of this, for all matrices A used in this thesis; we will be able to talk about the spectral decomposition of A ,

$$A = \sum_{\lambda \in \Lambda_A} \lambda E_\lambda.$$

Since A is a symmetric matrix, it is clear from this decomposition that E_λ are symmetric matrices as well. In a similar way, for all vectors $\mathbf{x} \in \mathbb{R}^N$ we will be able to talk about the spectral decomposition of $\mathbf{x}$ with respect to (the dynamics) A , that is;

$$\mathbf{x} = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda$$

where $c_\lambda \in \mathbb{R}$, $\mathbf{w}_\lambda$ is a unit eigenvector with eigenvalue λ and $c_\lambda \mathbf{w}_\lambda = E_\lambda \mathbf{x}$. In cases where λ is a simple eigenvalue of A , we have $E_\lambda = \mathbf{w}_\lambda \mathbf{w}_\lambda^T$ and $c_\lambda = \mathbf{w}_\lambda^T \mathbf{x}$.

We can now state the following lemma:

Lemma 3.2.2. *Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map whose matrix form is symmetric and let $\mathbf{x} \in \mathbb{R}^N$ be a vector. Let $\mathbf{x} = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda$ be the spectral decomposition of $\mathbf{x}$ with respect to A . Then, we have that*

$$\langle \mathbf{x} \rangle_A = \text{span}\{\mathbf{w}_\lambda \in \mathbb{R}^N | c_\lambda \neq 0, \lambda \in \Lambda_A\}$$

that is, the subspace generated by $\mathbf{x}$ under the action of A is spanned by the eigenvectors $\mathbf{w}_\lambda$ in the spectral decomposition of $\mathbf{x}$.

Proof. Because A is symmetric, all eigenvalues of A are real. Now, since there are only finitely many eigenvalues λ of A , there exists an eigenvalue λ_{max} of maximum modulus $|\lambda_{max}|$ in $\{\lambda \in \Lambda_A | c_\lambda \neq 0\}$. Then, if $-\lambda_{max} \notin \{\lambda \in \Lambda_A | c_\lambda \neq 0\}$ we have $\lim_{k \rightarrow \infty} \frac{A^k \mathbf{x}}{\lambda_{max}^k} = c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}}$. Since subspaces of vector spaces are closed, this implies $\mathbf{w}_{\lambda_{max}} \in \langle \mathbf{x} \rangle_A$.

If $-\lambda_{max} \in \{\lambda \in \Lambda_A | c_\lambda \neq 0\}$, then we have, $\lim_{k \rightarrow \infty} \frac{A^{2k} \mathbf{x}}{\lambda_{max}^{2k}} = c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}} + c_{-\lambda_{max}} \mathbf{w}_{-\lambda_{max}}$ and $\lim_{k \rightarrow \infty} \frac{A^{2k+1} \mathbf{x}}{\lambda_{max}^{2k+1}} = c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}} - c_{-\lambda_{max}} \mathbf{w}_{-\lambda_{max}}$. Since subspaces of vector spaces are closed, this implies that $c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}} \pm c_{-\lambda_{max}} \mathbf{w}_{-\lambda_{max}} \in \langle \mathbf{x} \rangle_A$, which clearly implies $\mathbf{w}_{\lambda_{max}}, \mathbf{w}_{-\lambda_{max}} \in \langle \mathbf{x} \rangle_A$.

Now, consider the set $S_1 := \{\lambda \in \Lambda_A | c_\lambda \neq 0\} \setminus \{\lambda_{max}, -\lambda_{max}\}$. This set again is a set of finite size and so must contain an eigenvalue λ_1 of maximum modulus $|\lambda_1|$. If $-\lambda_1 \notin S_1$, then we have

$$\lim_{k \rightarrow \infty} \frac{A^k \mathbf{x} - \lambda_{max}^k c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}} - (-\lambda_{max})^k c_{-\lambda_{max}} \mathbf{w}_{-\lambda_{max}}}{\lambda_1^k} = c_{\lambda_1} \mathbf{w}_{\lambda_1}$$

or

$$\lim_{k \rightarrow \infty} \frac{A^k \mathbf{x} - \lambda_{max}^k c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}}}{\lambda_1^k} = c_{\lambda_1} \mathbf{w}_{\lambda_1}$$

depending on whether $-\lambda_{max} \in \{\lambda \in \Lambda_A | c_\lambda \neq 0\}$ or not. Since $\mathbf{w}_{\lambda_{max}}, \mathbf{w}_{-\lambda_{max}} \in \langle \mathbf{x} \rangle_A$ or $\mathbf{w}_{\lambda_{max}} \in \langle \mathbf{x} \rangle_A$ depending on whether $-\lambda_{max} \in \{\lambda \in \Lambda_A | c_\lambda \neq 0\}$ or not and since subspaces of vector spaces are closed, this implies $\mathbf{w}_{\lambda_1} \in \langle \mathbf{x} \rangle_A$.

If $-\lambda_1 \in S_1$, then we have $\lim_{k \rightarrow \infty} \frac{A^{2k} \mathbf{x} - \lambda_{max}^{2k} c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}}}{\lambda_1^{2k}} = c_{\lambda_1} \mathbf{w}_{\lambda_1} + c_{-\lambda_1} \mathbf{w}_{-\lambda_1}$ and $\lim_{k \rightarrow \infty} \frac{A^{2k+1} \mathbf{x} - \lambda_{max}^{2k+1} c_{\lambda_{max}} \mathbf{w}_{\lambda_{max}}}{\lambda_1^{2k+1}} = c_{\lambda_1} \mathbf{w}_{\lambda_1} - c_{-\lambda_1} \mathbf{w}_{-\lambda_1}$ in the case where $-\lambda_{max} \notin \{\lambda \in \Lambda_A | c_\lambda \neq 0\}$. Hence, we have $c_{\lambda_1} \mathbf{w}_{\lambda_1} \pm c_{-\lambda_1} \mathbf{w}_{-\lambda_1} \in \langle \mathbf{x} \rangle_A$, which implies $\mathbf{w}_{\lambda_1}, \mathbf{w}_{-\lambda_1} \in \langle \mathbf{x} \rangle_A$. A similar argument works if $-\lambda_{max} \in \{\lambda \in \Lambda_A | c_\lambda \neq 0\}$.

By repeating this process for $S_2 := \{\lambda \in \Lambda_A | c_\lambda \neq 0\} \setminus \{\lambda_{max}, -\lambda_{max}, \lambda_1, -\lambda_1\}$, S_3 and so on, it clearly follows that

$$\text{span}\{\mathbf{w}_\lambda \in \mathbb{R}^N | c_\lambda \neq 0, \lambda \in \Lambda_A\} \subseteq \langle \mathbf{x} \rangle_A.$$

But any vector $\mathbf{y} \in \langle \mathbf{x} \rangle_A$ is of the form $\mathbf{y} = \sum_{k=0}^{N-1} A^k \mathbf{x}$ and so necessarily is in $\text{span}\{\mathbf{w}_\lambda \in \mathbb{R}^N | c_\lambda \neq 0, \lambda \in \Lambda_A\}$. Hence we have

$$\langle \mathbf{x} \rangle_A \subseteq \text{span}\{\mathbf{w}_\lambda \in \mathbb{R}^N | c_\lambda \neq 0, \lambda \in \Lambda_A\}$$

and so

$$\langle \mathbf{x} \rangle_A = \text{span}\{\mathbf{w}_\lambda \in \mathbb{R}^N | c_\lambda \neq 0, \lambda \in \Lambda_A\}$$

as desired. $\square$

The following corollaries will be relevant for lumpability.

Corollary 3.2.3. *Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map whose matrix form is symmetric and let $\mathbf{x} \in \mathbb{R}^N$ be a vector. Let $\mathbf{x} = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda$ be the spectral decomposition of $\mathbf{x}$ with respect to A . Then $\dim \langle \mathbf{x} \rangle_A^\perp = N - \dim \langle \mathbf{x} \rangle_A$ counts the number of linearly independent unit eigenvectors $\mathbf{w}_\lambda$ of A satisfying $\mathbf{w}_\lambda^T \mathbf{x} = 0$.*

Proof. Note that there can be at most $\dim \langle \mathbf{x} \rangle_A^\perp$ linearly independent unit eigenvectors $\mathbf{w}_\lambda$ of A satisfying $\mathbf{w}_\lambda^T \mathbf{x} = 0$, since all such eigenvectors satisfy $\mathbf{w}_\lambda \in \langle \mathbf{x} \rangle_A^\perp$ by definition. By Lemma 3.2.2 we have $\langle \mathbf{x} \rangle_A = \text{span}\{\mathbf{w}_\lambda \in \mathbb{R}^N | c_\lambda \neq 0, \lambda \in \Lambda_A\}$ and so the space $\langle \mathbf{x} \rangle_A$ is spanned by a subset of eigenvectors of A . Since A is symmetric, its eigenspaces are orthogonal to one another. This implies that the space $\langle \mathbf{x} \rangle_A^\perp$ is also spanned by a subset of eigenvectors of A , from which the claim follows. $\square$

Corollary 3.2.4. *Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map whose matrix form is symmetric and let $\mathbf{x} \in \mathbb{R}^N$ be a vector. Then, there exists an eigenbasis $\{\mathbf{w}_\lambda^i\}_{i=1,\dots,N}$ of A which satisfies either $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A$ or $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A^\perp$ for all $i = 1, 2, \dots, N$.*

Proof. We will show that for all eigenspaces of A , a basis $\{\mathbf{w}_\lambda^i\}_{i=1,\dots,k}$ can be chosen such that either $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A$ or $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A^\perp$ for all $i = 1, 2, \dots, k$.

Suppose λ is simple and its eigenvector $\mathbf{w}_\lambda^1 \notin \langle \mathbf{x} \rangle_A$. Since A is symmetric and since λ is a simple eigenvalue, $\mathbf{w}_\lambda^1$ is orthogonal to all other eigenvectors of A . In particular, since $\langle \mathbf{x} \rangle_A$ is spanned by a subset of eigenvectors of A by Lemma 3.2.2, $\mathbf{w}_\lambda^1 \notin \langle \mathbf{x} \rangle_A$ implies that $\mathbf{w}_\lambda^1 \perp \langle \mathbf{x} \rangle_A$, or equivalently, $\mathbf{w}_\lambda^1 \in \langle \mathbf{x} \rangle_A^\perp$.

Now let $\mathbf{x} = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda$ be the spectral decomposition of $\mathbf{x}$ with respect to A . If λ is an eigenvalue of order k ; either $c_\lambda = 0$, in which case $\mathbf{w}_\lambda \perp \langle \mathbf{x} \rangle_A$ for all λ -eigenvectors by Lemma 3.2.2 and by the fact that A is orthogonally diagonalizable; or $c_\lambda \neq 0$, in which case an eigenbasis $\{\mathbf{w}_\lambda^i\}_{i=1,\dots,k}$ for the eigenspace of λ can be chosen such that $\mathbf{w}_\lambda^1 \in \langle \mathbf{x} \rangle_A$ for a single eigenvector defined by $\mathbf{w}_\lambda^1 = \frac{E_\lambda \mathbf{x}}{c_\lambda}$ and $\mathbf{w}_\lambda^i \perp \langle \mathbf{x} \rangle_A$ for $i = 2, \dots, k$.

By appropriately relabeling the eigenvectors for all eigenspaces, the claim follows. $\square$

Corollary 3.2.5. *Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map whose matrix form is symmetric and let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^N$ be vectors such that $\langle \mathbf{x} \rangle_A \perp \langle \mathbf{y} \rangle_A$. Then, there exists an eigenbasis $\{\mathbf{w}_\lambda^i\}_{i=1, \dots, N}$ of A which satisfies either $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A$, $\mathbf{w}_\lambda^i \in \langle \mathbf{y} \rangle_A$ or $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A^\perp \cap \langle \mathbf{y} \rangle_A^\perp = (\langle \mathbf{x} \rangle_A \oplus \langle \mathbf{y} \rangle_A)^\perp$ for all $i = 1, 2, \dots, N$.*

Proof. Apply Corollary 3.2.4 twice, first to the vector $\mathbf{x} \in \mathbb{R}^N$ with linear map A acting on the space $\mathbb{R}^N$ and then to the vector $\mathbf{y} \in \langle \mathbf{x} \rangle_A^\perp$ with the map $A|_{\langle \mathbf{x} \rangle_A^\perp}$ acting on the space $\langle \mathbf{x} \rangle_A^\perp$. $\square$

Lastly, we have another lemma which will be of use.

Lemma 3.2.6. *Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map whose matrix form is symmetric and let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^N$. Then, the following are equivalent*

1. $\mathbf{x} \in \langle \mathbf{y} \rangle_A^\perp$
2. $\mathbf{y} \in \langle \mathbf{x} \rangle_A^\perp$
3. $\langle \mathbf{y} \rangle_A \perp \langle \mathbf{x} \rangle_A$

Proof. We have $\mathbf{x} \in \langle \mathbf{y} \rangle_A^\perp$ if and only if $\mathbf{x}^T(A^k \mathbf{y}) = 0$ for all $k \in \mathbb{N}$. Since A is symmetric, this is equivalent to $\mathbf{x}^T(A^k \mathbf{y}) = (\mathbf{x}^T(A^k)^T) \mathbf{y} = (A^k \mathbf{x})^T \mathbf{y} = 0$ for all $k \in \mathbb{N}$. This is equivalent to $\mathbf{y} \in \langle \mathbf{x} \rangle_A^\perp$. The equivalence of these two with 3 follows from $\mathbf{x}^T(A^k)^T A^j \mathbf{y} = \mathbf{x}^T A^{k+j} \mathbf{y}$. $\square$

3.3 Controllability, Observability and Lumpability

In this section we will introduce the required background for controllability, observability and our eventual goal, lumpability. The introduced concepts are for

general dynamical systems with linear dynamics, but as a particular case, they apply to linear dynamical systems over a graph.

Consider a discrete linear time-invariant dynamical system of the form:

$$\begin{aligned}\mathbf{x}(t+1) &= A\mathbf{x}(t) + B\mathbf{u}(t) \\ \mathbf{y}(t+1) &= C\mathbf{x}(t)\end{aligned}\tag{3.1}$$

where $\mathbf{x}(t) \in \mathbb{R}^N$ is the state vector, $\mathbf{u}(t) \in \mathbb{R}^k$ is the input vector, and $\mathbf{y}(t) \in \mathbb{R}^m$ is the output vector at time t , and $A \in \mathbb{R}^{N \times N}$, $B \in \mathbb{R}^{N \times k}$ and $C \in \mathbb{R}^{m \times N}$ are matrices. In a general dynamical system, the matrix A need not represent the adjacency matrix of a graph. As was said before, we will only use the adjacency matrix and Laplacian matrix of a graph to induce a dynamical system over a graph.

Definition 3.3.1 (Controllability). The dynamical system 3.1 is said to be controllable if for any initial state $\mathbf{x}(0) \in \mathbb{R}^N$ and any final state $\mathbf{x}_f \in \mathbb{R}^N$, there exists a finite sequence of inputs $\mathbf{u}(0), \mathbf{u}(1), \dots, \mathbf{u}(T-1) \in \mathbb{R}^k$ such that the state $\mathbf{x}(T) = \mathbf{x}_f$.

Example 3.3.2. Consider the graph G in Figure 3.1 and consider the state space $\mathbb{R}^N$ induced by the graph G where $N = |G|$. Consider a dynamical system on this space, for example that induced by the action of the adjacency matrix $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ or the Laplacian matrix $L : \mathbb{R}^N \rightarrow \mathbb{R}^N$ by direct matrix multiplication. Consider now an input from the vertex labeled v_i , that is, the input matrix B in the dynamical system 3.1 is an $N \times 1$ matrix with only the i -th entry $(B)_{v_i} = 1$ non-zero. With this input, this dynamical system is not controllable because no matter how the inputs are given, we will always have that $(\mathbf{x}(t))_{v_1} = (\mathbf{x}(t))_{v_2}$ implies $(\mathbf{x}(t+1))_{v_1} = (\mathbf{x}(t+1))_{v_2}$ for any $t \in \mathbb{N}$, due to the symmetry between vertices v_1 and v_2 .

Definition 3.3.3 (Observability). The dynamical system 3.1 is said to be observable if for any initial state $\mathbf{x}(0) \in \mathbb{R}^N$, the state $\mathbf{x}(0)$ can be uniquely determined from the output sequence $\mathbf{y}(0), \mathbf{y}(1), \dots, \mathbf{y}(T-1) \in \mathbb{R}^m$, for some finite number $T \in \mathbb{N}$.

Example 3.3.4. Similar to controllability, the graph in Figure 3.2 with the outputs taken from vertex v_i , and the dynamical system induced by the adjacency

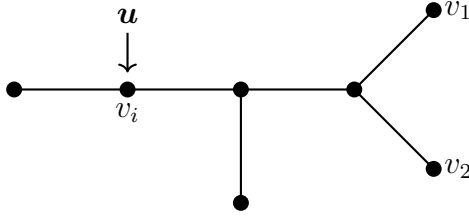


Figure 3.1: The graph with the associated dynamical system induced by its adjacency or the Laplacian matrix, is not controllable with the inputs $\mathbf{u}(t)$ given from the vertex v_i .

or the Laplacian matrix of the graph, is not observable. Similar to the case in Figure 3.1, this stems from the symmetry between vertices v_1 and v_2 . Indeed, the two initial conditions $\mathbf{x}_1(0) = \mathbf{v}_1$ and $\mathbf{x}_2(0) = \mathbf{v}_2$ are indistinguishable from observations made at vertex v_i .

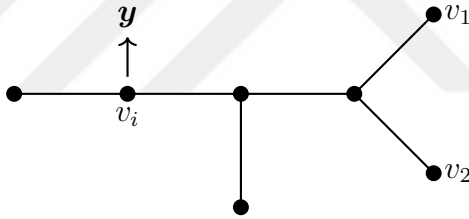


Figure 3.2: The graph with the associated dynamical system induced by its adjacency or the Laplacian matrix, is not observable with the outputs $\mathbf{y}(t)$ taken from the vertex v_i .

Definition 3.3.5 (Lumpability). The dynamical system 3.1 is said to be lumpable if there exists a surjective linear map $M : \mathbb{R}^N \rightarrow \mathbb{R}^r$ with $r < N$ such that the following diagram commutes:

$$\begin{array}{ccc} \mathbb{R}^N & \xrightarrow{A} & \mathbb{R}^N \\ \downarrow M & & \downarrow M \\ \mathbb{R}^r & \xrightarrow{\hat{A}} & \mathbb{R}^r \end{array}$$

where $\hat{A} \in \mathbb{R}^{r \times r}$ is the system matrix of the lumped system. Note that lumpability is a condition that solely pertains to the matrix A representing the system dynamics and is independent from the input matrix B and the output matrix C . We therefore talk about lumpability with respect to a pair (X, A) where $X = \mathbb{R}^N$

is the state space and $A : X \rightarrow X$ is a linear map and we say that the pair (X, A) is lumpable if the associated dynamical system 3.1 is lumpable.

The following well known theorem, due to Kalman [32], is central for controllability and observability in linear systems.

Theorem 3.3.6 (Kalman Rank Condition [32]). *The system 3.1 is controllable if and only if the controllability matrix $\mathcal{C} = [B, AB, \dots, A^{N-1}B]$ has full row rank. Similarly, the system is observable if and only if the observability matrix $\mathcal{O} = [C; CA; \dots; CA^{N-1}]$ has full column rank.*

The following two theorems are similarly central to the problem of lumpability in linear systems [15]. Although the theorem extends to Banach spaces with slight modifications, we present it with finite dimensional vector spaces over $\mathbb{R}$ as this version is enough for our purposes.

Theorem 3.3.7. [15] *Let $X = \mathbb{R}^N$ and $Y = \mathbb{R}^r$ be finite dimensional vector spaces. Let $A : X \rightarrow X$ and $M : X \rightarrow Y$ be linear maps. Assume that M is surjective. Then the following are equivalent:*

1. *There exists a linear map $\hat{A} : Y \rightarrow Y$ such that $MA = \hat{A}M$.*
2. *$\ker(M)$ is invariant under A . Equivalently, $\ker(M) \subseteq \ker(MA)$.*
3. *The dynamical system 3.1 is lumpable by the map M .*

The following theorem [15] is essential for our purposes.

Theorem 3.3.8. [15] *If the system 3.1 is not observable, then it is lumpable by a linear map $M : \mathbb{R}^N \rightarrow \mathbb{R}^r$ with $r = \text{rank}(\mathcal{O})$ where $\mathcal{O}$ is the observability matrix.*

Proof. Consider the matrix $\mathcal{O} = [C; CA; \dots; CA^{N-1}]$. Since the system is not observable, $\mathcal{O}$ has rank $r < N$ by assumption. Consider the matrix M defined by taking r independent rows of $\mathcal{O}$. Now, $\mathcal{O}$ is an $Nm \times N$ matrix. Hence, clearly M is an $r \times N$ matrix with rank r . Therefore, it defines a surjective map from $\mathbb{R}^N$ to

$\mathbb{R}^r$. Now, consider the matrix $\mathcal{O}A = [CA; CA^2; \dots; CA^N]$. Since by the Cayley-Hamilton theorem, $A^N = \sum_{i=0}^{N-1} c_i A^i$, the rows of $\mathcal{O}A$ are linear combinations of the rows of $\mathcal{O}$ and thus of the rows of M . Since the rows of MA are a subset of the rows of $\mathcal{O}A$, this implies that the rows of MA are linear combinations of the rows of M . In other words, there exists a matrix $\hat{A}$ such that $MA = \hat{A}M$ and the claim follows by Theorem 3.3.7. $\square$

3.4 Lumpability and Graphs

We will now briefly consider how controllability, observability and lumpability translate to dynamical systems over graphs.

Remark 3.4.1 (SISO version of Theorem 3.3.6). In the single input case where B is an $N \times 1$ vector, the controllability matrix which has the form $\mathcal{C} = [B, AB, \dots, A^{N-1}B]$ becomes an $N \times N$ matrix and so the condition that it has full row rank is equivalent to just being full rank. This last condition is equivalent to the condition $\text{span}\{B, AB, \dots, A^{N-1}B\} = \langle B \rangle_A = \mathbb{R}^N$. Similarly, in the single output case we have that C is a $1 \times N$ vector and the observability matrix $\mathcal{O}$ has full rank if and only if $\text{span}\{C^T, A^T C^T, \dots, (A^T)^{N-1} C^T\} = \langle C^T \rangle_{A^T} = \mathbb{R}^N$.

Now in this thesis, our system 3.1 represents the dynamics of a graph $G(V, E)$, that is, the state space is $\mathbb{R}^N = \mathbb{R}^{|V|}$ and the dynamics is represented by the adjacency A or the Laplacian matrix L of G . Since we are working with undirected graphs, A and L are both symmetric matrices. Consequently, we have $\langle C^T \rangle_{A^T} = \langle C^T \rangle_A$. Hence, for dynamics on undirected graphs with single input and single output, the only relevant subspaces for both controllability and observability are $\langle \mathbf{x} \rangle_A$, where $\mathbf{x} \in \mathbb{R}^N$ is a vector.

In network systems, we often have access to only a subset of the vertices to/from which we can send/receive inputs. In cases where we have access to only one vertex $v_i \in V(G)$, the input and output matrices B and C have the form $[0, \dots, 1, \dots, 0]^T$ and $[0, \dots, 1, \dots, 0]$ respectively, with the nonzero entry in the i -th index. Hence in such cases, the controllability/observability of the dynamical

system over G is determined, depending on the dynamics, by the subspace $\langle \mathbf{v}_i \rangle_A$ or $\langle \mathbf{v}_i \rangle_L$ where $\mathbf{v}_i = [0, \dots, 1, \dots, 0]^T \in \mathbb{R}^N$. Lastly, it might also be useful to mention here that the subspace $\langle \mathbf{v}_i \rangle_A$ is also equal to the order- n Krylov subspace $\mathcal{K}_n(A, \mathbf{v}_i) := \text{span}\{\mathbf{v}_i, A\mathbf{v}_i, \dots, A^{n-1}\mathbf{v}_i\}$.

Now, in light of the above remark, we provide a corollary of Theorem 3.3.8 that we will be making use of.

Corollary 3.4.2 (of Theorem 3.3.8). *Let $G(V, E)$ be a graph, let A be its adjacency matrix and let $\mathbf{y} \in \mathbb{R}^N$ be a vector in the state space induced by G . Suppose that we have $\langle \mathbf{y} \rangle_A \neq \mathbb{R}^N$. Then, the dynamical system defined by*

$$\mathbf{x}(t+1) = A\mathbf{x}(t)$$

is lumpable by a linear map $M : \mathbb{R}^N \rightarrow \langle \mathbf{y} \rangle_A$ defined as identity on $\langle \mathbf{y} \rangle_A \subseteq \mathbb{R}^N$ and zero on $\langle \mathbf{y} \rangle_A^\perp$.

Proof. By Lemma 3.2.2, $\langle \mathbf{y} \rangle_A$ is spanned by a subset of eigenvectors of A . Since A is undirected, by Corollary 3.2.4 an eigenbasis of A can be chosen such that all eigenvectors in the eigenbasis are either in $\langle \mathbf{y} \rangle_A^\perp$ or $\langle \mathbf{y} \rangle_A$. This implies, by the fact that $\dim \langle \mathbf{y} \rangle_A + \dim \langle \mathbf{y} \rangle_A^\perp = N$, that $\langle \mathbf{y} \rangle_A^\perp$ is spanned by a subset of eigenvectors of A . Hence, $\langle \mathbf{y} \rangle_A^\perp$ is A -invariant. Since $\langle \mathbf{y} \rangle_A^\perp = \ker M$, the claim follows by Theorem 3.3.7. $\square$

The analogue of this corollary for lumpability under Laplacian matrix induced dynamics is obtained by replacing A with L .

Remark 3.4.3. Note that for linear dynamics induced by symmetric maps lumpability is a trivial condition, related to the A -invariant subspaces, i.e. eigenspaces of A . However as we will provide below, what will be of interest in this thesis are graph-theoretic methods to obtain easily lumpable graphs under adjacency/Laplacian induced dynamics.

3.5 The Perron-Frobenius Theorem

There are many facts pertaining to the Perron-Frobenius theorem. We will state only some of these here. Specifically, we are only interested in the Perron-Frobenius theorem for non-negative matrices. We will start with some definitions.

Definition 3.5.1. Let A be an $N \times N$ matrix over $\mathbb{R}$. Let $G(V, E)$ be the graph defined by $V = \{v_1, \dots, v_N\}$ and $E = \{(v_i, v_j); A_{i,j} \neq 0\} \subseteq V \times V$. Then the graph G is called the graph associated with the matrix A . Note that this graph is in general a directed graph.

Definition 3.5.2 (Irreducible matrix). Let A be an $N \times N$ matrix over $\mathbb{R}$. A is said to be irreducible if the graph G associated with the matrix A is strongly connected (connected, if G is undirected).

Definition 3.5.3 (Spectral Radius). Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map. The spectral radius of A , denoted $\rho(A)$ is defined to be

$$\rho(A) = \sup\{|\lambda|; \lambda \in \Lambda_A\}$$

Definition 3.5.4 (Period of A). Let A be an $N \times N$ non-negative matrix. For each index i , consider the numbers $m \in \mathbb{N}$ for which $(A^m)_{i,i} > 0$. The period of index i in A is defined to be the greatest common divisor of all natural numbers m such that $(A^m)_{i,i} > 0$. For irreducible matrices, the period of each index in A is the same and is called the period of A [33].

Note that when A is the adjacency matrix of a graph, the period of A is the greatest common divisor of the lengths of all closed paths. Therefore, for most graphs of concern to us, the period of the adjacency matrix A can be assumed to be 1. As an example, the adjacency matrix A of any undirected graph which has a triangle has period 1 since it has closed paths of length 2 and 3.

Theorem 3.5.5 (The Perron-Frobenius Theorem for Non-Negative Irreducible Matrices [33]). *Let A be an $N \times N$ non-negative irreducible matrix with spectral radius $\rho(A) = \lambda_p$. Then the following hold:*

1. $\lambda_p > 0$ is an eigenvalue of the matrix A . It is called the Perron–Frobenius eigenvalue.
2. A has both a left and a right unit eigenvector, respectively $\mathbf{w}_p$ and $\mathbf{y}_p$, with eigenvalue λ_p and whose components are all positive. Moreover the only eigenvectors whose components are all positive are those associated with the eigenvalue λ_p .
3. The Perron–Frobenius eigenvalue λ_p is simple. Both right and left eigenspaces associated with λ_p are one-dimensional.
4. The matrix A has exactly h complex eigenvalues with absolute value λ_p where h is the period of A . Each of them is a simple root of the characteristic polynomial and is the product of λ_p with an h -th root of unity.

Since all graphs that we are working with are undirected and connected, their adjacency matrices satisfy Theorem 3.5.5. Furthermore, because we are working with symmetric matrices A , the left and right Perron-Frobenius eigenvectors are equal, hence we will denote them both by $\mathbf{w}_p$ and refer them simply as the Perron-Frobenius eigenvector. Now we have a simple lemma which we are going to make use of later in our results.

Lemma 3.5.6. *Let $A : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a linear map whose matrix form is symmetric and let $\mathbf{x} \in \mathbb{R}^N$. Suppose that there exists an index i such that for every $\mathbf{y} \in \langle \mathbf{x} \rangle_A$, we have $(\mathbf{y})_i = 0$. Then, the Perron-Frobenius eigenvector of A satisfies $\mathbf{w}_p \in \langle \mathbf{x} \rangle_A^\perp$.*

Proof. Since all indices of the Perron-Frobenius eigenvector is positive, $\mathbf{w}_p \in \langle \mathbf{x} \rangle_A$ gives the contradiction $(\mathbf{w}_p)_i = 0$. Hence $\mathbf{w}_p \notin \langle \mathbf{x} \rangle_A$. Now, by Corollary 3.2.4 there exists an eigenbasis $\{\mathbf{w}_\lambda^i\}_{i=1,\dots,N}$ of A which satisfies either $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A$ or $\mathbf{w}_\lambda^i \in \langle \mathbf{x} \rangle_A^\perp$ for all $i = 1, 2, \dots, N$. Since λ_p is a simple eigenvalue, a scalar multiple of the Perron-Frobenius eigenvector $\mathbf{w}_p$ has to be in this eigenbasis. Hence, we have $c\mathbf{w}_p \in \{\mathbf{w}_\lambda^i\}_{i=1,\dots,N}$ where $c \in \mathbb{R}$ is a non-zero scalar. Since $\mathbf{w}_p \notin \langle \mathbf{x} \rangle_A$, we also have $c\mathbf{w}_p \notin \langle \mathbf{x} \rangle_A$. By Corollary 3.2.4, this implies $c\mathbf{w}_p \in \langle \mathbf{x} \rangle_A^\perp$ or equivalently, $\mathbf{w}_p \in \langle \mathbf{x} \rangle_A^\perp$. $\square$

Corollary 3.5.7. *Let G be a graph with adjacency matrix A and let $v_i, v_j, v_k \in V(G)$ be vertices of G . Then, the following are equivalent:*

1. $\mathbf{v}_i - \mathbf{v}_j \in \langle \mathbf{v}_k \rangle_A^\perp$
2. $\mathbf{v}_k \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A^\perp$
3. For every vector $\mathbf{y} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, we have $(\mathbf{y})_{v_k} = 0$

Furthermore, if the vertices v_i, v_j and v_k satisfy these equivalent conditions, then the v_i and v_j entries of the Perron-Frobenius eigenvector $\mathbf{w}_p$ of A are equal, that is, $(\mathbf{w}_p)_{v_i} = (\mathbf{w}_p)_{v_j}$.

Proof. By Lemma 3.2.6 conditions 1 and 2 are equivalent. For the equivalence of these two with 3, note that $(\mathbf{y})_{v_k} = 0$ if and only if $\mathbf{y}^T \mathbf{v}_k = 0$, or $\mathbf{y} \perp \mathbf{v}_k$. Hence; for every $\mathbf{y} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, we have $(\mathbf{y})_{v_k} = 0$ if and only if for every $\mathbf{y} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, we have $\mathbf{y} \perp \mathbf{v}_k$. The last condition is equivalent to 2 by definition.

Now, suppose the equivalent conditions hold. Then by Lemma 3.5.6, $\mathbf{w}_p \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A^\perp$. In particular, this means $\mathbf{w}_p \perp \mathbf{v}_i - \mathbf{v}_j$ or $\mathbf{w}_p^T (\mathbf{v}_i - \mathbf{v}_j) = 0$. In other words, $(\mathbf{w}_p)_{v_i} = \mathbf{w}_p^T \mathbf{v}_i = \mathbf{w}_p^T \mathbf{v}_j = (\mathbf{w}_p)_{v_j}$. $\square$

3.6 Cospectral vertices

In this section we introduce the notion of cospectral vertices and their characterization. The eventual characterization that we want to reach is Theorem 3.6.3.

We start by some notation. Let $G(V, E)$ be a graph and let $v_i \in V$ be a vertex of G . We denote by $G \setminus v_i$ the graph with vertex set $V \setminus \{v_i\}$ and edge set $E \setminus v_i := \{(v_j, v_k) \in E \mid v_j, v_k \neq v_i\}$. To follow the notation among the literature, for the purposes of this section we will denote by $\phi(G, t)$ the characteristic polynomial $\det(tI - A)$ of the adjacency matrix A of G and by $\phi(G)$ the set of eigenvalues of

A. The following is the original definition of cospectral vertices, first mentioned in [34].

Definition 3.6.1 (Cospectral). Let G be a graph and let $v_i, v_j \in V(G)$ be two distinct vertices of G . Then, v_i and v_j are cospectral in G if the spectrums of the adjacency matrices of graphs $G \setminus v_i$ and $G \setminus v_j$ are equal; or in other words, if $\phi(G \setminus v_i) = \phi(G \setminus v_j)$.

Example 3.6.2. In Figure 3.3, two graph with cospectral vertices are shown. In the top graph, two cospectral vertex pairs are shown. As can be immediately seen, the blue pair is cospectral as a consequence of being symmetric, whereas the red pair is not symmetric but still cospectral. A similar non-symmetric cospectral vertex pair can be seen in the bottom graph as well.

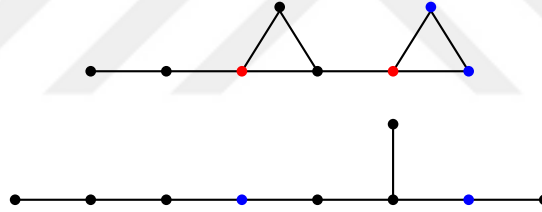


Figure 3.3: Two graphs containing cospectral vertices are shown with the cospectral pairs colored in the same color. No other cospectral pairs exist in these graphs.

Recall that for any undirected graph $G(V, E)$ the adjacency matrix A is a symmetric matrix and has the spectral decomposition

$$A = \sum_{\lambda \in \phi(G)} \lambda E_\lambda$$

where E_λ are the orthogonal projection maps onto the λ -eigenspaces of A as was mentioned before. We now state the main theorem of this section.

Theorem 3.6.3. [8] *Let G be a graph and let $v_i, v_j \in V(G)$ be two distinct vertices. Then, the following are equivalent:*

1. v_i and v_j are cospectral, i.e. $\phi(G \setminus v_i) = \phi(G \setminus v_j)$.

2. $(A^k)_{(v_i, v_i)} = (A^k)_{(v_j, v_j)}$ for all $k \in \mathbb{N}$.
3. $(E_\lambda)_{(v_i, v_i)} = (E_\lambda)_{(v_j, v_j)}$ for all $\lambda \in \phi(G)$.
4. The subspaces $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ and $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ are orthogonal.

It is clear that 4 implies that if two vertices v_i, v_j are cospectral, then the subspaces satisfy $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A, \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A \neq \mathbb{R}^N$. Recalling Corollary 3.4.2 we see that cospectral vertices v_i, v_j induce lumpability onto the subspaces $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ and $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$.

Before proving Theorem 3.6.3, we will need one final definition and a lemma.

Definition 3.6.4. [35] Let G be a graph and let A be its adjacency matrix. Then, the matrix valued formal power series

$$W(G, t) = \sum_{k=0}^{\infty} A^k t^k = (I - tA)^{-1}$$

is called the Walk generating function of G . The name is justified by observing that $W_{v_i, v_j}(G, t) := (W(G, t))_{v_i, v_j} = \sum_{k=0}^{\infty} (A^k)_{v_i, v_j} t^k$ is a generating function for the number of walks from vertex v_i to v_j in G . Clearly, the formal power series converges for $t \in (-\frac{1}{\lambda_p}, \frac{1}{\lambda_p})$ where λ_p is the Perron-Frobenius eigenvalue of A .

Lemma 3.6.5. [35] Let $G(V, E)$ be a graph and let $A = \sum_{\lambda \in \phi(G)} \lambda E_\lambda$ be its adjacency matrix. Then we have the following:

1. $W(G, t) = \sum_{\lambda \in \phi(G)} \frac{E_\lambda}{1-t\lambda}$. As such, we have $W_{v_i, v_j}(G, t) = \sum_{\lambda \in \phi(G)} \frac{(E_\lambda)_{v_i, v_j}}{1-t\lambda}$ where $v_i, v_j \in V$.
2. If $v_i \in V$ is a vertex of G , $\frac{\phi(G \setminus v_i, t)}{\phi(G, t)} = t^{-1} W_{v_i, v_i}(G, t^{-1}) = \sum_{\lambda \in \phi(G)} \frac{(E_\lambda)_{v_i, v_i}}{t-\lambda}$.

Proof. For 1, we have

$$\begin{aligned} W(G, t) &= (I - tA)^{-1} = (I - t \sum_{\lambda \in \phi(G)} \lambda E_\lambda)^{-1} = (\sum_{\lambda \in \phi(G)} E_\lambda - t \sum_{\lambda \in \phi(G)} \lambda E_\lambda)^{-1} = \\ &= (\sum_{\lambda \in \phi(G)} (1 - t\lambda) E_\lambda)^{-1} = \sum_{\lambda \in \phi(G)} \frac{E_\lambda}{1 - t\lambda}. \end{aligned}$$

where the last equality is by direct matrix multiplication. To prove 2, consider the adjugate matrix of an $N \times N$ matrix M defined by

$$\text{adj}(M) := \det(M)M^{-1}$$

or equivalently,

$$\text{adj}(M)_{i,j} = (-1)^{i+j} \det(M[j, i])$$

where $M[j, i]$ is the matrix obtained by removing the j -th row and i -th column of M . With this definition in mind, we have

$$W(G, t) = (I - tA)^{-1} = \frac{\text{adj}(I - tA)}{\det(I - tA)}$$

and so

$$W_{v_i, v_i}(G, t) = \frac{\text{adj}(I - tA)_{v_i, v_i}}{\det(I - tA)} = \frac{\det((I - tA)[v_i, v_i])}{\det(I - tA)} = \frac{\det(I - tA_{G \setminus v_i})}{\det(I - tA)}$$

where $A_{G \setminus v_i}$ is the adjacency matrix of the graph $G \setminus v_i$. The claim follows by noting

$$\frac{\phi(G \setminus v_i, t)}{\phi(G, t)} = \frac{\det(tI - A_{G \setminus v_i})}{\det(tI - A)} = \frac{t^{-1} \det(I - t^{-1}A_{G \setminus v_i})}{\det(I - t^{-1}A)} = t^{-1} W_{v_i, v_i}(G, t^{-1})$$

where the second equality is obtained by noting that $\det(cA) = c^N \det(A)$ for an $N \times N$ matrix A . $\square$

Now we conclude with the proof of Theorem 3.6.3

Proof of Theorem 3.6.3. By the spectral decomposition $A = \sum_{\lambda \in \phi(G)} \lambda E_\lambda$, clearly 2 and 3 are equivalent. By the second claim of Lemma 3.6.5, 1 is equivalent to 3. For 4, note that $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ and $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ are orthogonal if and only if

$$(A^k(\mathbf{v}_i + \mathbf{v}_j))^T (A^\ell(\mathbf{v}_i - \mathbf{v}_j)) = 0 \quad \forall k, \ell \in \mathbb{N}$$

This is equivalent to $(\mathbf{v}_i + \mathbf{v}_j)^T A^{k+\ell}(\mathbf{v}_i - \mathbf{v}_j) = 0$ for all $k, \ell \in \mathbb{N}$, or equivalently, just $(\mathbf{v}_i + \mathbf{v}_j)^T A^k(\mathbf{v}_i - \mathbf{v}_j) = 0$ for all $k \in \mathbb{N}$. Using $A = \sum_{\lambda \in \phi(G)} \lambda E_\lambda$ this is equivalent to $(\mathbf{v}_i + \mathbf{v}_j)^T E_\lambda(\mathbf{v}_i - \mathbf{v}_j) = 0$ for all $\lambda \in \phi(G)$. Expanding this out,

we get $\mathbf{v}_i^T E_\lambda \mathbf{v}_i - \mathbf{v}_j^T E_\lambda \mathbf{v}_j + \mathbf{v}_j^T E_\lambda \mathbf{v}_i - \mathbf{v}_i^T E_\lambda \mathbf{v}_j = (E_\lambda)_{v_i, v_i} - (E_\lambda)_{v_j, v_j} + (E_\lambda)_{v_j, v_i} - (E_\lambda)_{v_i, v_j} = 0$. Since E_λ is symmetric, this reduces to

$$(E_\lambda)_{v_i, v_i} - (E_\lambda)_{v_j, v_j} = 0 \text{ for all } \lambda \in \phi(G).$$

This is equivalent to 3. □

Corollary 3.6.6 (of Theorem 3.6.3). *Let $G(V, E)$ be a graph and let $v_i, v_j \in V$ be two vertices of G . Then, v_i and v_j are cospectral if and only if there exists an orthogonal eigenbasis $\{\mathbf{w}_\lambda^k\}_{k=1, \dots, N}$ with respect to the adjacency matrix A of G such that all eigenvectors $\mathbf{w}_\lambda^k$ satisfy $(\mathbf{w}_\lambda^k)_{v_i} = \pm(\mathbf{w}_\lambda^k)_{v_j}$.*

Proof. Suppose that $\{\mathbf{w}_\lambda^k\}_{k=1, \dots, N}$ is an orthogonal eigenbasis of A such that all eigenvectors $\mathbf{w}_\lambda^k$ in the basis satisfy $(\mathbf{w}_\lambda^k)_{v_i} = \pm(\mathbf{w}_\lambda^k)_{v_j}$. Now, consider the spectral decomposition $\mathbf{v}_i + \mathbf{v}_j = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}'_\lambda$ where $\mathbf{w}'_\lambda$ are unit eigenvectors with eigenvalue λ and $c_\lambda \mathbf{w}'_\lambda = E_\lambda(\mathbf{v}_i + \mathbf{v}_j)$. By Lemma 3.2.2, $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ is spanned by eigenvectors $\mathbf{w}'_\lambda$ such that $c_\lambda \neq 0$ in the spectral decomposition of $\mathbf{v}_i + \mathbf{v}_j$, represented by the set $\{\mathbf{w}'_\lambda \in \mathbb{R}^N \mid c_\lambda \neq 0, \mathbf{v}_i + \mathbf{v}_j = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}'_\lambda\}$.

Suppose for the sake of contradiction that there exists a unit eigenvector $\mathbf{w}'_{\lambda_1} \in \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ for some eigenvalue $\lambda_1 \in \Lambda_A$ that doesn't satisfy $(\mathbf{w}'_{\lambda_1})_{v_i} = \pm(\mathbf{w}'_{\lambda_1})_{v_j}$. Then, since $\{\mathbf{w}_\lambda^k\}_{k=1, \dots, N}$ is an eigenbasis, there exists (appropriately scaled) eigenvectors $\mathbf{w}_{\lambda_1}^{k_1}, \mathbf{w}_{\lambda_2}^{k_2}, \dots, \mathbf{w}_{\lambda_\ell}^{k_\ell} \in \{\mathbf{w}_\lambda^k\}_{k=1, \dots, N}$ such that $\mathbf{w}'_{\lambda_1} = \mathbf{w}_{\lambda_1}^{k_1} + \mathbf{w}_{\lambda_2}^{k_2} + \dots + \mathbf{w}_{\lambda_\ell}^{k_\ell}$. Clearly, it follows that $\lambda_1 = \lambda_2 = \dots = \lambda_\ell$. Since the eigenvectors $\mathbf{w}_\lambda^k$ of the eigenbasis $\{\mathbf{w}_\lambda^k\}_{k=1, \dots, N}$ satisfy $(\mathbf{w}_\lambda^k)_{v_i} = \pm(\mathbf{w}_\lambda^k)_{v_j}$, we can assume $\mathbf{w}'_{\lambda_1} = \mathbf{w}_{\lambda_1}^+ + \mathbf{w}_{\lambda_1}^-$ where $\mathbf{w}_{\lambda_1}^+$ and $\mathbf{w}_{\lambda_1}^-$ are orthogonal λ_1 -eigenvectors satisfying $(\mathbf{w}_{\lambda_1}^+)_{v_i} = (\mathbf{w}_{\lambda_1}^+)_{v_j}$ and $(\mathbf{w}_{\lambda_1}^-)_{v_i} = -(\mathbf{w}_{\lambda_1}^-)_{v_j}$, respectively. Note that $\mathbf{w}_{\lambda_1}^+$ and $\mathbf{w}_{\lambda_1}^-$ have magnitude strictly smaller than 1 because $\mathbf{w}'_{\lambda_1} = \mathbf{w}_{\lambda_1}^+ + \mathbf{w}_{\lambda_1}^-$ and $\mathbf{w}'_{\lambda_1}$ is a unit vector.

Because $c_\lambda \mathbf{w}'_\lambda = E_\lambda(\mathbf{v}_i + \mathbf{v}_j)$ and E_λ is the orthogonal projection onto the λ -eigenspace; $\mathbf{w}'_{\lambda_1}$, by definition should be the unit λ_1 -eigenvector that has the largest dot product with the vector $\mathbf{v}_i + \mathbf{v}_j$. But since

$$\begin{aligned} (\mathbf{w}'_{\lambda_1})^T(\mathbf{v}_i + \mathbf{v}_j) &= (\mathbf{w}_{\lambda_1}^+ + \mathbf{w}_{\lambda_1}^-)^T(\mathbf{v}_i + \mathbf{v}_j) = (\mathbf{w}_{\lambda_1}^+)^T(\mathbf{v}_i + \mathbf{v}_j) + (\mathbf{w}_{\lambda_1}^-)^T(\mathbf{v}_i + \mathbf{v}_j) = \\ &= (\mathbf{w}_{\lambda_1}^+)^T(\mathbf{v}_i + \mathbf{v}_j) + ((\mathbf{w}_{\lambda_1}^-)_{v_i} + (\mathbf{w}_{\lambda_1}^-)_{v_j}) = (\mathbf{w}_{\lambda_1}^+)^T(\mathbf{v}_i + \mathbf{v}_j) > 0 \end{aligned}$$

and since $\mathbf{w}_{\lambda_1}^+$ has magnitude strictly smaller than 1, an appropriately scaled up unit $\mathbf{w}_{\lambda_1}^+$ has higher dot product with $\mathbf{v}_i + \mathbf{v}_j$; which is a contradiction. Therefore, all eigenvectors $\mathbf{w}'_\lambda \in \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ must satisfy $(\mathbf{w}'_\lambda)_{v_i} = \pm(\mathbf{w}'_\lambda)_{v_j}$. In fact, they satisfy $(\mathbf{w}'_\lambda)_{v_i} = (\mathbf{w}'_\lambda)_{v_j}$, because $(\mathbf{w}'_\lambda)_{v_i} = -(\mathbf{w}'_\lambda)_{v_j}$ implies $(\mathbf{w}'_\lambda)^T(\mathbf{v}_i + \mathbf{v}_j) = 0$ and consequently $\mathbf{w}'_\lambda \perp \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$; which is a contradiction. Since $(\mathbf{w}'_\lambda)_{v_i} = (\mathbf{w}'_\lambda)_{v_j}$ implies $\mathbf{w}'_\lambda \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ and since $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ is spanned by these eigenvectors $\mathbf{w}'_\lambda$, we thus have $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$; which implies the cospectrality of v_i and v_j by Theorem 3.6.3.

For the other direction; note that by Corollary 3.2.4, there exists an eigenbasis $\{\mathbf{w}_\lambda^k\}_{k=1,\dots,N}$ of A such that the basis eigenvectors $\mathbf{w}_\lambda^k$ satisfy $\mathbf{w}_\lambda^k \in \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ or $\mathbf{w}_\lambda^k \perp \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$. If v_i and v_j are cospectral, we have that $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. Hence the basis eigenvectors $\mathbf{w}_\lambda^k$ are orthogonal to either $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ or $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ depending on whether $\mathbf{w}_\lambda^k \in \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ or $\mathbf{w}_\lambda^k \perp \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$. Hence, they satisfy either $(\mathbf{w}_\lambda^k)_{v_i} = (\mathbf{w}_\lambda^k)_{v_j}$ or $(\mathbf{w}_\lambda^k)_{v_i} = -(\mathbf{w}_\lambda^k)_{v_j}$, respectively. $\square$

Chapter 4

Results

Having equipped ourselves with the necessary background material, we now present our results. We will begin with the definition of cospectral vertices that we will use in this thesis. Although cospectral vertices are defined under the adjacency matrix dynamics, using the equivalent definition provided in Corollary 3.6.6, we extend this definition for our purposes to Laplacian dynamics as well.

Definition 4.0.1 (A -cospectral and L -cospectral). Let $G(V, E)$ be a graph and let $v_i, v_j \in V$ be two vertices of G . Consider the adjacency (Laplacian) matrix A (L) of G . If there exists an eigenbasis $\{\mathbf{w}_\lambda\}_{\lambda \in \Lambda_A}$ ($\{\mathbf{w}_\lambda\}_{\lambda \in \Lambda_L}$) of A (L) such that the eigenvectors $\mathbf{w}_\lambda$ of the basis satisfy $(\mathbf{w}_\lambda)_{v_i} = \pm(\mathbf{w}_\lambda)_{v_j}$ for all $\lambda \in \Lambda_A$ (Λ_L), then we say that v_i and v_j are A -cospectral (L -cospectral) in G or just cospectral in G if the dynamics is clear from the context.

Note that the “ A ” in the term A -cospectral is to indicate that the cospectrality is with respect to the dynamics induced by the adjacency matrix and not to indicate which graph we are talking about. Hence, for the adjacency matrices of graphs $\tilde{G}, \hat{G}$ etc. that are denoted as $\tilde{A}, \hat{A}$ and so on; we still say that two vertices v_i and v_j are A -cospectral in $\tilde{G}$ or $\hat{G}$ rather than $\tilde{A}$ -cospectral or $\hat{A}$ -cospectral. The same statement also holds for L -cospectrality as well as coprobability defined below.

Remark 4.0.2. As a side note, we should mention that there is a concept of

Laplace cospectral or L -cospectral graphs in the literature, defined by having equal Laplacian spectrum. Our definition of Laplace cospectral vertices is not a direct generalization of A -cospectral vertices in this sense; since with our definition of L -cospectral vertices, the graphs that are left after one of the vertices is taken out do not necessarily have equal Laplacian spectrums. We are using a different definition based on the dynamics induced by the Laplacian matrix. Although the two definitions coincide for the adjacency matrix as was explained in Section 3.6, they are different for the Laplacian matrix. The reason for this is that for the Laplacian matrix, adding/deleting edges between vertices v_i and v_j not only changes the matrix in the L_{v_i, v_j} and L_{v_j, v_i} entries but also changes it in the L_{v_i, v_i} and L_{v_j, v_j} entries. Consequently Lemma 3.6.5 does not apply.

Following its adjacency analogue, we provide an equivalent characterization for the L -cospectral vertices.

Lemma 4.0.3. *Let $G(V, E)$ be a graph and let $v_i, v_j \in V$ be two vertices of G . The following are equivalent:*

1. v_i and v_j are L -cospectral vertices.
2. $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_L \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L$

Proof. Same as Corollary 3.6.6 □

We now make a generalization of cospectral vertices.

Definition 4.0.4 (A -coprobable). Let $G(V, E)$ be a graph with adjacency matrix A , and let $v_i, v_j \in V$ be two vertices of G . Consider the Perron-Frobenius eigenvector $\mathbf{w}_p$ of A . If $(\mathbf{w}_p)_{v_i} = (\mathbf{w}_p)_{v_j}$, then we say that v_i and v_j are A -coprobable or just coprobable in G .

Remark 4.0.5. Setting $\mathbf{x} = \mathbf{v}_i - \mathbf{v}_j$ in Corollary 3.2.3 we see that if v_i and v_j are coprobable in G , then $\dim \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A \neq N$ and thus by Corollary 3.4.2, coprobable vertices also induce lumpability onto the subspace $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. In fact for this to be true, we need not use the Perron-Frobenius eigenvector at all. It is sufficient for any eigenvector $\mathbf{w}_\lambda$ of A to satisfy $(\mathbf{w}_\lambda)_{v_i} = (\mathbf{w}_\lambda)_{v_j}$.

We now provide the analogous definition for Laplacian dynamics. However, although the Laplacian matrix also indirectly satisfies the Perron-Frobenius Theorem, the Perron-Frobenius eigenvector $\mathbf{w}_p$ for L is the all-ones vector $[1, 1, \dots, 1]$. Therefore, if we follow the definition of A -coprobable vertices, then all vertices would be L -coprobable. We are therefore forced to make the generalization described in Remark 4.0.5 and use arbitrary eigenvectors for the Laplacian case. The actual wording of the definition is slightly different.

Definition 4.0.6 (L -coprobable). Let $G(V, E)$ be a graph and let $v_i, v_j \in V$ be two vertices of G . Consider the subspaces $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_L$ and $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L$ with respect to the Laplacian matrix L of G . Since the vector $[1, 1, \dots, 1]$ is always an eigenvector of L , we have $\dim(\langle \mathbf{v}_i + \mathbf{v}_j \rangle_L) \leq N$ and $\dim(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L) \leq N - 1$ where $N = |V|$. If $\dim(\langle \mathbf{v}_i + \mathbf{v}_j \rangle_L) < N$ or $\dim(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L) < N - 1$, then we say that v_i and v_j are L -coprobable or just coprobable in G .

Remark 4.0.7. This definition has a major drawback in cases where there are eigenspaces of L that have dimensions greater than 1; in such cases, all pairs of vertices trivially satisfy the definition. By including a lot of unwanted cases into the definition, we have in a sense, a “noisy” definition. However, although this is a significant formal problem, it does not cloud our understanding. Indeed as we will see, our results derive from structural symmetries and are impervious to eigenvalue manipulations. Consequently, the eigenvalues of the Laplacian can be changed by modifying the graph, while the L -coprobability in our results is preserved as long as the structural considerations that induce it are preserved. In this way, the trivial cases can be distinguished from actual structural dynamical symmetries. As a last note, it might be the case that a modification of the definition, excluding trivial cases while retaining others, is possible; perhaps by considering a special eigenvalue as in A -coprobable or using special graphs with or without certain structures.

Lemma 4.0.8. *Let $G(V, E)$ be a graph and let $v_i, v_j \in V$. Suppose v_i and v_j are A -cospectral (L -cospectral) vertices in G . Then v_i and v_j are A -coprobable (L -coprobable) in G .*

Proof. For L -cospectral, the claim is trivial. Now, suppose v_i and v_j be A -cospectral. Then we have that $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ as subspaces. Since these subspaces are orthogonal, the Perron-Frobenius eigenvector $\mathbf{w}_p$ is orthogonal to at least one of them, by Corollary 3.2.4. It cannot be orthogonal to $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ since if so, then $(\mathbf{w}_p)_{v_i} = -(\mathbf{w}_p)_{v_j}$ contradicts the positivity of $\mathbf{w}_p$. Hence, it must be orthogonal to $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, which implies $(\mathbf{w}_p)_{v_i} = (\mathbf{w}_p)_{v_j}$. $\square$

With this lemma we see that all cospectral vertices are in fact coprobable. Noting that all symmetric vertices; i.e. vertices that can be mapped to one another via a graph automorphism, are also A (L)-cospectral we also have that all symmetric vertices are A (L)-coprobable.

In the rest of the chapter, we will provide constructions and operations to obtain coprobable and in some cases cospectral vertices. We will be concerned with the adjacency and Laplacian matrices as linear maps. In theorems and lemmas, we will indicate which graph dynamics the theorem/lemma works with and whether it applies to cospectral vertices in particular or coprobable vertices in general via titles such as (A -cospectral), (L -coprobable) or (A -cospectral and L -coprobable) etc.

4.1 Constructions of Coprobable Vertices

We start with constructive methods to obtain coprobable vertices.

Theorem 4.1.1 (A -coprobable). *Let G and H be two graphs with vertices labeled as $v_1, v_2, \dots, v_N \in V(G)$ and $v'_1, v'_2, \dots, v'_r \in V(H)$ where $N = |V(G)|$ and $r = |V(H)|$. Construct a graph $\tilde{G}$ as follows: Select any two vertices v_i and v_j of G . Take two copies of G , labeled $G^1(V^1, E^1)$ and $G^2(V^2, E^2)$. Label the vertices $v_1, v_2, \dots, v_N$ in these as $v_1^1, v_2^1, \dots, v_N^1$ and $v_1^2, v_2^2, \dots, v_N^2$, respectively. Now, take any vertex $v'_\alpha \in V(H)$ and connect both v_i^1 and v_j^2 with this vertex.*

Then, we have that v_j^1 and v_i^2 are A -coprobable in $\tilde{G}$, and the spectrum of $\tilde{A}$ contains that of A . Moreover, there exists an eigenbasis $\{\tilde{\mathbf{w}}_\lambda^k\}_{k=1, \dots, 2N+r}$ of $\tilde{A}$ such

that for any eigenvector $\tilde{\mathbf{w}}_\lambda^k$ which has a nonzero v'_α -th entry, that is, $(\tilde{\mathbf{w}}_\lambda^k)_{v'_\alpha} \neq 0$, we have

$$(\tilde{\mathbf{w}}_\lambda^k)_{v_j^1} = (\tilde{\mathbf{w}}_\lambda^k)_{v_i^2}.$$

In particular, this is true for the Perron-Frobenius eigenvector.

Remark 4.1.2. The new graph $\tilde{G}$ of Theorem 4.1.1 has $2N+r$ vertices with vertex set $V(\tilde{G}) = V(G^1) \cup V(G^2) \cup V(H)$. For simplicity, one can think of the vectors $\mathbf{x} \in \mathbb{R}^{2N+r}$ associated with the graph $\tilde{G}$ as being indexed by vertices of G^1 , G^2 and H ; in this order. Hence; $(\mathbf{x})_{v_m^1}$, $(\mathbf{x})_{v_m^2}$ and $(\mathbf{x})_{v'_m}$ can be thought of as the m -th, $(N+m)$ -th and $(2N+m)$ -th component of $\mathbf{x}$, respectively. The $2N+r \times 2N+r$ adjacency matrix $\tilde{A}$ of $\tilde{G}$ can then be represented as follows:

$$\tilde{A} = \begin{bmatrix} A & \mathbf{0} & \mathbf{v}_i \mathbf{v}'_\alpha{}^T \\ \mathbf{0} & A & \mathbf{v}_j \mathbf{v}'_\alpha{}^T \\ \mathbf{v}'_\alpha \mathbf{v}_i^T & \mathbf{v}'_\alpha \mathbf{v}_j^T & A_H \end{bmatrix}$$

where A and A_H are the adjacency matrices of the graphs G and H respectively, and the four blocks with the outer products of vectors each contain a single non-zero value in the (v_i^1, v'_α) , (v'_α, v_i^1) , (v_j^2, v'_α) and (v'_α, v_j^2) entries, corresponding to the edges between v_i^1 , v_j^2 and v'_α .

Proof. Firstly, we show that for all $v'_\beta \in V(H) \subseteq V(\tilde{G})$, we have $\langle \mathbf{v}_i^2 - \mathbf{v}_j^1 \rangle_{\tilde{A}} \perp \mathbf{v}'_\beta$. We claim, by induction on $k \in \mathbb{N}$, that we have for all $v'_\beta \in V(H)$ and $v_m \in V(G)$;

1. $(\tilde{A}^k(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_m^1} = -(A^k(\mathbf{v}_j))_{v_m}$ and $(\tilde{A}^k(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_m^2} = (A^k(\mathbf{v}_i))_{v_m}$
2. $(\tilde{A}^k(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\alpha} = 0$
3. $(\tilde{A}^k(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\beta} = 0$

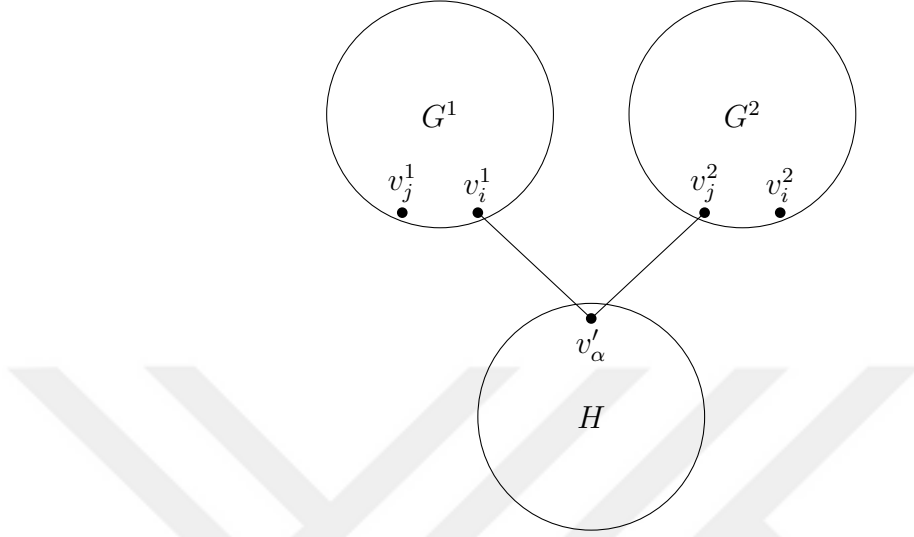


Figure 4.1: Figure illustrating the construction of $\tilde{G}$ explained in the Theorem 4.1.1. Here, the subgraphs G^1, G^2 and H are shown as spheres to illustrate that they are arbitrary graphs.

where A is the adjacency matrix of G and $\tilde{A}$ is the adjacency matrix of the whole graph $\tilde{G}$. It is obvious that 3 proves $\langle \mathbf{v}_i^2 - \mathbf{v}_j^1 \rangle_{\tilde{A}} \perp \mathbf{v}'_\beta$ for all $v'_\beta \in V(H) \subseteq V(\tilde{G})$, since $(\tilde{A}^k(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\beta} = (\tilde{A}^k(\mathbf{v}_i^2 - \mathbf{v}_j^1))^T \mathbf{v}'_\beta$.

Base case $k = 0$: Trivial.

Inductive Step: Now, assume that the claims hold for $k = n - 1$. We will prove the claims for $k = n$.

1. For any $v_m^1 \in V(G^1)$, if $v_m^1 \neq v_i^1$ we have

$$(\tilde{A}^n(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_m^1} = \sum_{v_m \sim v_\ell} (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_\ell^1} = - \sum_{v_m \sim v_\ell} (A^{n-1}(\mathbf{v}_j))_{v_\ell} = -(A^n(\mathbf{v}_j))_{v_m}$$

using **induction hypothesis (1)**. Now, if $v_m^1 = v_i^1$, we have

$$\begin{aligned} (\tilde{A}^n(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_i^1} &= \sum_{v_i \sim v_\ell} (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_\ell^1} + (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\alpha} = \\ &= - \sum_{v_i \sim v_\ell} (A^{n-1}(\mathbf{v}_j))_{v_\ell} = -(A^n(\mathbf{v}_j))_{v_i} \end{aligned}$$

where we used **induction hypothesis (2)** in the second equality. Similarly, we get

$$(\tilde{A}^n(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_m^2} = (A^n(\mathbf{v}_i))_{v_m} \quad \forall v_m \in V(G).$$

2.

$$(\tilde{A}^n(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\alpha} = \sum_{\substack{v'_\beta \sim v'_\alpha \\ v'_\beta \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\beta} + (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_i^1} + (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v_j^2}$$

Using **induction hypothesis (1) and (3)** and that A is symmetric we get,

$$\begin{aligned} &= 0 - (A^{n-1}(\mathbf{v}_j))_{v_i} + (A^{n-1}(\mathbf{v}_i))_{v_j} \\ &= -(A^{n-1})_{v_j, v_i} + (A^{n-1})_{v_i, v_j} = 0. \end{aligned}$$

3. For any $v'_\beta \in V(H)$, $v'_\beta \neq v'_\alpha$:

$$(\tilde{A}^n(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\beta} = \sum_{\substack{v'_\gamma \sim v'_\beta \\ v'_\gamma \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^2 - \mathbf{v}_j^1))_{v'_\gamma} = 0$$

by **induction hypothesis (3)**.

Thus, we have shown $\langle \mathbf{v}_i^2 - \mathbf{v}_j^1 \rangle_{\tilde{A}} \perp \mathbf{v}'_\beta$ for all $v'_\beta \in V(H) \subseteq V(\tilde{G})$. Now, we will show that the spectrum of $\tilde{A}$ contains that of A . Let $\lambda \in \Lambda_A$ and let $\mathbf{w}_\lambda$ be a λ -eigenvector (an eigenvector of A). We will construct an eigenvector of $\tilde{A}$ with eigenvalue λ . There are two cases. For the first case, suppose one of $(\mathbf{w}_\lambda)_{v_i}, (\mathbf{w}_\lambda)_{v_j} = 0$, say $(\mathbf{w}_\lambda)_{v_i} = 0$ without losing generality. Then construct an eigenvector $\tilde{\mathbf{w}}_\lambda$ of $\tilde{A}$ for all $v \in V(\tilde{G})$ by

$$(\tilde{\mathbf{w}}_\lambda)_v = \begin{cases} (\mathbf{w}_\lambda)_{v_m} & \text{if } v = v_m^1 \\ 0 & \text{otherwise} \end{cases}$$

That $\tilde{\mathbf{w}}_\lambda$ is an eigenvector of $\tilde{A}$ is obvious. For the second case, define the λ -eigenvector $\tilde{\mathbf{w}}_\lambda$ of $\tilde{A}$ for all $v \in V(\tilde{G})$ as follows:

$$(\tilde{\mathbf{w}}_\lambda)_v = \begin{cases} (\mathbf{w}_\lambda)_{v_m} & \text{if } v = v_m^1 \\ -\frac{(\mathbf{w}_\lambda)_{v_i}}{(\mathbf{w}_\lambda)_{v_j}} (\mathbf{w}_\lambda)_{v_m} & \text{if } v = v_m^2 \\ 0 & \text{otherwise} \end{cases}$$

It can be checked by matrix algebra that $\tilde{\mathbf{w}}_\lambda$ is an eigenvector of $\tilde{A}$ with eigenvalue λ .

For the last claim of the theorem, note that since $\mathbf{v}'_\alpha \perp \langle \mathbf{v}_i^2 - \mathbf{v}_j^1 \rangle_{\tilde{A}}$, we get $\langle \mathbf{v}'_\alpha \rangle_{\tilde{A}} \perp \langle \mathbf{v}_i^2 - \mathbf{v}_j^1 \rangle_{\tilde{A}}$ by Lemma 3.2.6. Now, by Corollary 3.2.4 eigenvectors $\tilde{\mathbf{w}}_\lambda$ of $\tilde{A}$ can be chosen such that either $\tilde{\mathbf{w}}_\lambda \perp \langle \mathbf{v}'_\alpha \rangle_{\tilde{A}}$ or $\tilde{\mathbf{w}}_\lambda \in \langle \mathbf{v}'_\alpha \rangle_{\tilde{A}}$. This implies that if $(\tilde{\mathbf{w}}_\lambda)_{v'_\alpha} \neq 0$ then $\tilde{\mathbf{w}}_\lambda \in \langle \mathbf{v}'_\alpha \rangle_{\tilde{A}}$ and so $\tilde{\mathbf{w}}_\lambda \perp \langle \mathbf{v}_i^2 - \mathbf{v}_j^1 \rangle_{\tilde{A}}$. Thus we have $(\tilde{\mathbf{w}}_\lambda)_{v_i^2} = (\tilde{\mathbf{w}}_\lambda)_{v_j^1}$. In fact, the claim holds for any $v'_\beta \in V(H)$ in place of v'_α in this last part of the theorem. Finally, since we have $(\tilde{\mathbf{w}}_p)_{v'_\alpha} \neq 0$ where $\tilde{\mathbf{w}}_p$ is the Perron-Frobenius eigenvector of $\tilde{A}$, the coprobability of v_i^2 and v_j^1 follows. $\square$

Example 4.1.3. A common simple example for Theorem 4.1.1 is given in Figure 4.2. The graph G in this example is the path graph on 4 vertices shown with red. Here, the vertices v_1^2 and v_2^1 are coprobable. In addition, a relabeling of vertices shows that the vertices v_4^2 and v_3^1 are also coprobable. In networks with a power law degree distribution, this structure can be seen.

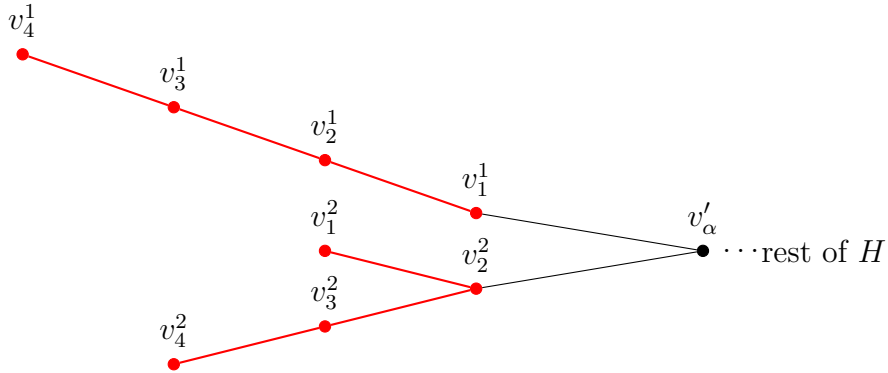


Figure 4.2: A simple example to the construction in Theorem 4.1.1. Here the red subgraphs are G^1 and G^2 .

Remark 4.1.4. From the proof of Theorem 4.1.1, it is obvious that one can connect the G 's in more nontrivial ways. One such way is to connect the G 's to more than one vertex in H . A schematic example of this can be seen in Figure 4.3 below. Here the vertices v_i^1 and v_j^2 are connected to v'_{α_1} and v'_{α_2} in H . Again, vertices v_i^2 and v_j^1 are coprobable in the entire graph.

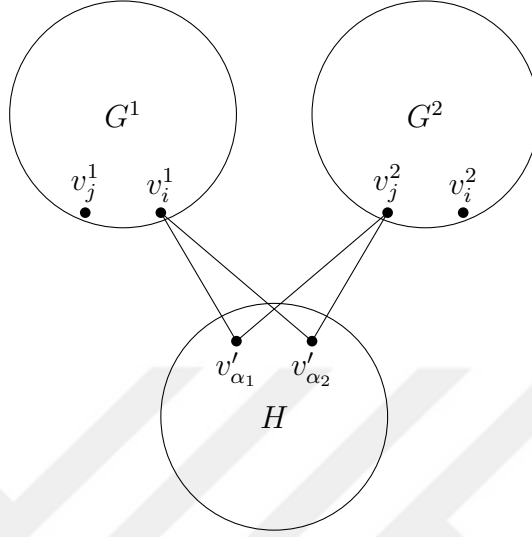


Figure 4.3: The proof of Theorem 4.1.1 can easily be replicated to show that v_j^1 and v_i^2 are coprobable in these cases as well.

We have a slightly different analogue of this construction for Laplacian dynamics.

Theorem 4.1.5 (*L*-coprobable). *Let G be a graph. Construct a graph $\tilde{G}$ as follows: Select any two vertices v_i and v_j of G . Take two copies of G , labeled $G^1(V^1, E^1)$ and $G^2(V^2, E^2)$. Label $v_1, v_2, \dots, v_n$ in these as $v_1^1, v_2^1, \dots, v_N^1$ and $v_1^2, v_2^2, \dots, v_N^2$, respectively. Now, connect v_i^1 and v_j^2 to obtain the larger graph $\tilde{G}$.*

Then, v_j^1 and v_i^2 are L -coprobable in $\tilde{G}$, and the spectrum of $\tilde{L}$ contains that of L .

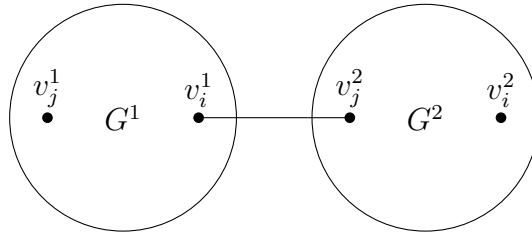


Figure 4.4: Figure illustrating the construction of $\tilde{G}$ for the Laplacian case. That the subgraphs G^1 and G^2 must be connected to each other and not to a separate graph H makes this version slightly different than its adjacency analogue.

Remark 4.1.6. The new graph $\tilde{G}$ of Theorem 4.1.5 has $2N$ vertices with vertex set $V(\tilde{G}) = V(G^1) \cup V(G^2)$. For simplicity, one can think of the vectors $\mathbf{x} \in \mathbb{R}^{2N}$

associated with the graph $\tilde{G}$ as being indexed by vertices of G^1 and G^2 , in this order. Hence; $(\mathbf{x})_{v_m^1}$ and $(\mathbf{x})_{v_m^2}$ can be thought of as the m -th and $(N + m)$ -th component of $\mathbf{x}$, respectively. The $2N \times 2N$ Laplacian matrix $\tilde{L}$ of $\tilde{G}$ can then be represented as follows:

$$\tilde{L} = \begin{bmatrix} L & \mathbf{0} \\ \mathbf{0} & L \end{bmatrix} + \begin{bmatrix} \mathbf{v}_i \mathbf{v}_i^T & -\mathbf{v}_i \mathbf{v}_j^T \\ -\mathbf{v}_j \mathbf{v}_i^T & \mathbf{v}_j \mathbf{v}_j^T \end{bmatrix}$$

where L is the Laplacian matrix of the graph G and the four blocks in the second term with the outer products of vectors, contain a single non-zero value in the $(v_i^1, v_i^1), (v_i^1, v_j^2), (v_j^2, v_i^1)$ and (v_j^2, v_j^2) entries, corresponding to the edge between v_i^1 and v_j^2 .

Proof. Firstly, we will show by induction on $k \in \mathbb{N}$ that we have $\forall v_m \in V(G)$,

$$\begin{aligned} (\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1))_{v_m^1} &= (L^k(\mathbf{v}_j))_{v_m} \\ (\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1))_{v_m^2} &= (L^k(\mathbf{v}_i))_{v_m}. \end{aligned}$$

Base case $k = 0$: Trivial.

Inductive step: Assume that the claim holds for $k = n - 1$. We will prove the claim for $k = n$. For any $v_m^1 \in V(G^1)$, such that $v_m^1 \neq v_i^1$, we have

$$\begin{aligned} (\tilde{L}^n(\mathbf{v}_i^2 + \mathbf{v}_j^1))_{v_m^1} &= d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_m^1} - \sum_{v_m \sim v_\ell} \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_\ell^1} = \\ &= d_{v_m} (L^{n-1}(\mathbf{v}_j))_{v_m} - \sum_{v_m \sim v_\ell} (L^{n-1}(\mathbf{v}_j))_{v_\ell} = (L^n(\mathbf{v}_j))_{v_m} \end{aligned}$$

where we used the **induction hypothesis** in the second equality. Here, d_{v_m} is the degree of vertex v_m in the graph G . If $v_m^1 = v_i^1$, we have

$$(\tilde{L}^n(\mathbf{v}_i^2 + \mathbf{v}_j^1))_{v_i^1} = (d_{v_i} + 1) \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_i^1} - \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_j^2}$$

$$\begin{aligned}
& - \sum_{v_i \sim v_\ell} \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_\ell^1} \\
& = d_{v_i} \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_i^1} - \sum_{v_i \sim v_\ell} \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_\ell^1} \\
& \quad + \left[\left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_i^1} - \left(\tilde{L}^{n-1}(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_j^2} \right] \\
& = d_{v_i} (L^{n-1}(\mathbf{v}_j))_{v_i} - \sum_{v_m \sim v_\ell} (L^{n-1}(\mathbf{v}_j))_{v_\ell} + (L^{n-1}(\mathbf{v}_j))_{v_i} - (L^{n-1}(\mathbf{v}_i))_{v_j} \\
& = (L^n(\mathbf{v}_j))_{v_i} + 0 = (L^n(\mathbf{v}_j))_{v_i}
\end{aligned}$$

where we again used the **induction hypothesis** and the fact that $\tilde{G}$ is undirected in the third and fourth equalities, respectively. Similarly, we obtain

$$(\tilde{L}^n(\mathbf{v}_i^2 + \mathbf{v}_j^1))_{v_m^2} = (L^n(\mathbf{v}_i))_{v_m}$$

for all $v_m \in V(G)$, and so we conclude the induction. Now, we have shown that $\forall k \in \mathbb{N}$ and $\forall v_m \in V(G)$,

$$\left(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_m^1} = (L^k(\mathbf{v}_j))_{v_m} \quad \text{and} \quad \left(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_m^2} = (L^k(\mathbf{v}_i))_{v_m}.$$

In particular, $\forall k \in \mathbb{N}$ we have,

$$\left(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_i^1} = (L^k(\mathbf{v}_j))_{v_i} \quad \text{and} \quad \left(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_j^2} = (L^k(\mathbf{v}_i))_{v_j}.$$

Since $(L^k(\mathbf{v}_j))_{v_i} = (L^k(\mathbf{v}_i))_{v_j}$, this implies $\forall k \in \mathbb{N}$, $\left(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_i^1} = \left(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1) \right)_{v_j^2}$ or equivalently,

$$(\tilde{L}^k(\mathbf{v}_i^2 + \mathbf{v}_j^1))^T(\mathbf{v}_i^1 - \mathbf{v}_j^2) = 0$$

Hence $\mathbf{v}_i^1 - \mathbf{v}_j^2 \perp \langle \mathbf{v}_i^2 + \mathbf{v}_j^1 \rangle_{\tilde{L}}$ and so we have

$$\dim(\langle \mathbf{v}_i^2 + \mathbf{v}_j^1 \rangle_{\tilde{L}}) < \tilde{N},$$

where $\tilde{N} = |V(\tilde{G})|$, proving that v_i^2 and v_j^1 are L -coprobable in $\tilde{G}$.

Now as to the second claim of the theorem, let $\lambda \in \Lambda_L$. We will show that λ is also an eigenvalue of $\tilde{L}$. We will do so by explicitly constructing an eigenvector of $\tilde{L}$. Let $\mathbf{w}_\lambda$ be an eigenvector of L with eigenvalue λ . Suppose it satisfies

$(\mathbf{w}_\lambda)_{v_i}, (\mathbf{w}_\lambda)_{v_j} \neq 0$. Then, construct an eigenvector $\tilde{\mathbf{w}}_\lambda$ of $\tilde{L}$ by defining it on all $v \in V(\tilde{G})$ as

$$(\tilde{\mathbf{w}}_\lambda)_v = \begin{cases} (\mathbf{w}_\lambda)_{v_m} & \text{if } v = v_m^1 \\ \frac{(\mathbf{w}_\lambda)_{v_i}(\mathbf{w}_\lambda)_{v_m}}{(\mathbf{w}_\lambda)_{v_j}} & \text{if } v = v_m^2 \end{cases}$$

It can be checked that $\tilde{\mathbf{w}}_\lambda$ is an eigenvector of $\tilde{L}$ with eigenvalue λ . Consider now the case where we have one of $(\mathbf{w}_\lambda)_{v_i} = 0$ or $(\mathbf{w}_\lambda)_{v_j} = 0$, assume without loss of generality that $(\mathbf{w}_\lambda)_{v_i} = 0$. Construct $\tilde{\mathbf{w}}_\lambda$ on all $v \in V(\tilde{G})$ as

$$(\tilde{\mathbf{w}}_\lambda)_v = \begin{cases} (\mathbf{w}_\lambda)_{v_m} & \text{if } v = v_m^1 \\ 0 & \text{if } v = v_m^2 \end{cases}$$

It is clear that $\tilde{\mathbf{w}}_\lambda$ is an eigenvector of $\tilde{L}$ with eigenvalue λ . $\square$

We have another construction involving identical subgraphs and this time the obtained vertices are not only coprobable, but also cospectral.

Theorem 4.1.7 (*A-cospectral*). *Let G be a graph whose vertices are labeled as $v_1, v_2, \dots, v_N \in V(G)$ where $N = |V(G)|$. Select a vertex $v_i \in V(G)$. Let the group of graph automorphisms of G fixing v_i be denoted as $\text{Aut}(G, v_i)$ and the orbits of vertices under this action as $[v_j]_{v_i} \subseteq V(G)$, i.e. $[v_j]_{v_i}$ is the set of vertices of G that are in the same orbit as v_j under the action of $\text{Aut}(G, v_i)$. Let H be another graph with vertices labeled as $v'_1, v'_2, \dots, v'_r \in V(H)$, where $r = |V(H)|$. Construct the graph $\tilde{G}$ as follows. Similar to Theorem 4.1.1, take a copy of H and two copies of G , denoted as $G^1(V^1, E^1)$ and $G^2(V^2, E^2)$. Denote the vertices of G^1 and G^2 as v_j^1, v_k^2 , etc. Now, add an arbitrary amount of edges between H and G^1, G^2 as follows:*

For every added edge connecting a vertex $v_j^1 \in V(G^1)$ and a vertex $v'_\alpha \in V(H)$, add exactly one edge between v'_α and a vertex $v_m^2 \in V(G^2)$ such that $v_m \in [v_j]_{v_i}$; that is, v_j and v_m should be in the same orbit in G under the action of $\text{Aut}(G, v_i)$. In other words, all vertices $v'_\alpha \in V(H)$ should have the same number of neighbours in corresponding orbits of the subgraphs G^1 and G^2 of $\tilde{G}$. A schematic representation of this construction is shown in Figure 4.5.

Then, v_i^1 and v_i^2 are A -cospectral in $\tilde{G}$.

Remark 4.1.8. The new graph $\tilde{G}$ of Theorem 4.1.7 has $2N+r$ vertices with vertex set $V(\tilde{G}) = V(G^1) \cup V(G^2) \cup V(H)$. For simplicity, one can think of the vectors $\mathbf{x} \in \mathbb{R}^{2N+r}$ associated with the graph $\tilde{G}$ as being indexed by vertices of G^1, G^2 and H ; in this order. Hence; $(\mathbf{x})_{v_m^1}, (\mathbf{x})_{v_m^2}$ and $(\mathbf{x})_{v'_m}$ can be thought of as the m -th, $(N+m)$ -th and $(2N+m)$ -th component of $\mathbf{x}$, respectively. The $2N+r \times 2N+r$ adjacency matrix $\tilde{A}$ of $\tilde{G}$ can then be represented as follows:

$$\tilde{A} = \begin{bmatrix} A & \mathbf{0} & \\ \mathbf{0} & A & \\ & & A_H \end{bmatrix}$$

where A and A_H are the adjacency matrices of the graphs G and H respectively, and the four empty blocks contain non-zero entries representing the edges between vertices of H and G^1, G^2 ; whose construction was outlined in the theorem.

Proof. We claim that $\forall k \in \mathbb{N}$,

1. $(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v'_\alpha} = 0$ for all $v'_\alpha \in V(H)$
2. $(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = -(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^2}$ for all $v_m \in V(G)$
3. $(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = (\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^1}$ for any $v_m, v_\ell \in V(G)$ such that $v_\ell \in [v_m]_{v_i}$.

Clearly, claims (2) and (3) together also imply

$$(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^2} = (\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^2}, \quad \text{for any } v_m, v_\ell \in V(G) \text{ such that } v_\ell \in [v_m]_{v_i}.$$

We prove by induction on k .

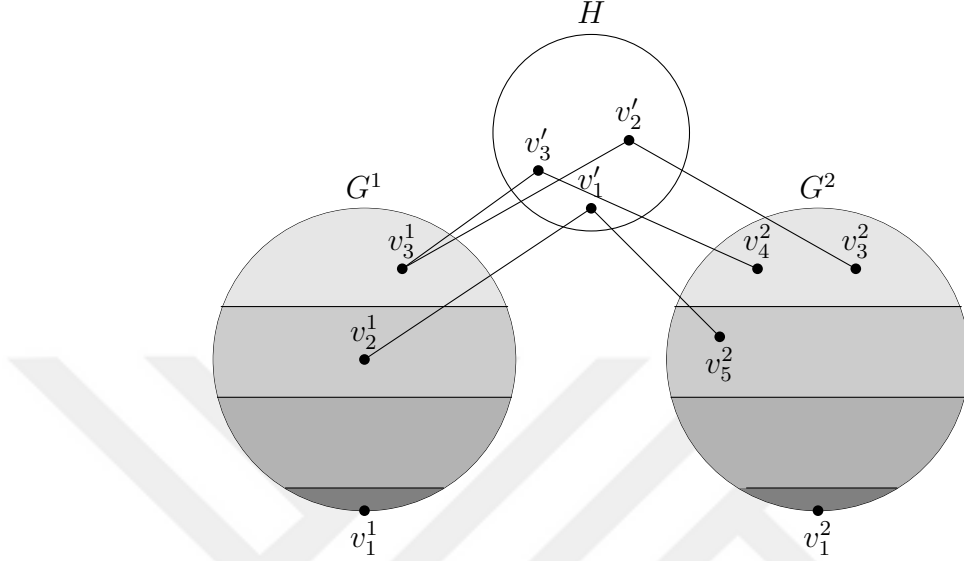


Figure 4.5: Construction of $\tilde{G}$ explained in Theorem 4.1.7 illustrated. Here, the graphs G^1 and G^2 are divided into orbits under the action of $\text{Aut}(G, v_1)$. These orbits are shown by shades of grey in which the darkest grey contains only v_1 . The vertices v_2, v_5 and v_3, v_4 are in the same orbit. As can be seen in the Figure, for every edge from a vertex in G^1 to a vertex $v'_\alpha \in V(H)$, there is a corresponding edge from a vertex of G^2 of the same orbit. Here, the vertices v_1^1 and v_1^2 are A -cospectral in the graph $\tilde{G}$.

Base Case $k = 0$: Trivial.

Inductive Step: Suppose case $k = n - 1$. We will prove case $k = n$. For any $v'_\alpha \in V(H)$ we have

$$\begin{aligned} & (\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v'_\alpha} = \\ &= \sum_{\substack{v'_\beta \sim v'_\alpha \\ v'_\beta \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v'_\beta} + \sum_{\substack{v_m^1 \sim v'_\alpha \\ v_m \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} + \sum_{\substack{v_\ell^2 \sim v'_\alpha \\ v_\ell \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^2}. \end{aligned}$$

Using **induction hypothesis (1)**, we know that $(\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v'_\beta} = 0$ for all $v'_\beta \in V(H)$. So we have $\sum_{\substack{v'_\beta \sim v'_\alpha \\ v'_\beta \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v'_\beta} = 0$. By the construction in the theorem and using **induction hypothesis (2) and (3)** respectively in the second and third equalities below, we also have

$$\sum_{\substack{v_m^1 \sim v'_\alpha \\ v_m \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} + \sum_{\substack{v_\ell^2 \sim v'_\alpha \\ v_\ell \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^2} =$$

$$\begin{aligned}
&= \sum_{\substack{v_m^1 \sim v_\alpha' \\ v_m \in V(G)}} [(\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} + (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_{\ell_m}^2}] = \\
&= \sum_{\substack{v_m^1 \sim v_\alpha' \\ v_m \in V(G)}} [(\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} - (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_{\ell_m}^1}] = 0
\end{aligned}$$

where $v_{\ell_m} \in [v_m]_{v_i}$ by construction. This proves claim (1) for $k = n$. Now to prove claim (2), we have for any $v_m^1 \in V(G^1)$,

$$(\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = \sum_{v_\ell \sim v_m} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^1} + \sum_{\substack{v_\alpha' \sim v_m^1 \\ v_\alpha' \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\alpha'}.$$

Using **induction hypothesis (1)**, the second term is 0 and so we have

$$(\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = \sum_{v_\ell \sim v_m} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^1}.$$

Now by **induction hypothesis (2)** and then (1), we have

$$\begin{aligned}
&\sum_{v_\ell \sim v_m} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^1} = - \sum_{v_\ell \sim v_m} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^2} \\
&= - \sum_{v_\ell \sim v_m} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^2} - \sum_{\substack{v_\alpha' \sim v_m^2 \\ v_\alpha' \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\alpha'} \\
&= -(\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^2}
\end{aligned}$$

proving claim (2). Finally to prove claim (3), let $v_m, v_\ell \in V(G)$ be two vertices such that $v_\ell \in [v_m]_{v_i}$. Since $v_\ell \in [v_m]_{v_i}$, there must exist a graph automorphism $\gamma \in \text{Aut}(G, v_i)$ such that $\gamma(v_\ell) = v_m$. Now, we have

$$(\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = \sum_{\substack{v_j \sim v_m \\ v_j \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_j^1} + \sum_{\substack{v_\alpha' \sim v_m^1 \\ v_\alpha' \in V(H)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\alpha'}.$$

Using **induction hypothesis (1)**, the second term is 0, so we obtain

$$= \sum_{\substack{v_j \sim v_m \\ v_j \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_j^1} = \sum_{\substack{v_s \sim v_\ell \\ v_s \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_s^1}$$

where the last equality follows from **induction hypothesis (3)** and the fact that neighbors of v_m and v_ℓ are in the same automorphism orbit in G via γ . Since

$(\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = \sum_{\substack{v_j \sim v_m \\ v_j \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_j^1}$ holds for any vertex $v_m \in V(G)$, it now follows that

$$(\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = \sum_{\substack{v_j \sim v_m \\ v_j \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_j^1} = \sum_{\substack{v_s \sim v_\ell \\ v_s \in V(G)}} (\tilde{A}^{n-1}(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_s^1} = (\tilde{A}^n(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_\ell^1}$$

proving claim (3) and finishing the induction. Now, we have proved (2), which says that

$$(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^1} = -(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_m^2}, \quad \forall v_m \in V(G) \text{ and } k \in \mathbb{N}.$$

In particular, this implies for all $k \in \mathbb{N}$,

$$(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_i^1} + (\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))_{v_i^2} = 0.$$

This is equivalent to $(\tilde{A}^k(\mathbf{v}_i^1 - \mathbf{v}_i^2))^T(\mathbf{v}_i^1 + \mathbf{v}_i^2) = 0$. Thus, we conclude that $\mathbf{v}_i^1 + \mathbf{v}_i^2 \perp \langle \mathbf{v}_i^1 - \mathbf{v}_i^2 \rangle_{\tilde{A}}$ or equivalently,

$$\langle \mathbf{v}_i^1 + \mathbf{v}_i^2 \rangle_{\tilde{A}} \perp \langle \mathbf{v}_i^1 - \mathbf{v}_i^2 \rangle_{\tilde{A}}.$$

Hence by Theorem 3.6.3 v_i^1 and v_i^2 are A -cospectral in $\tilde{G}$. □

Example 4.1.9. We provide a simple example to the construction explained in Theorem 4.1.7. In Figure 4.6, the subgraphs G^1 and G^2 are highlighted with red vertices and edges and the black vertices can be regarded as H . The cospectral vertices v_1^1 and v_1^2 are indicated with blue. As one can see, the red vertices v_2 , v_3 and v_4 are all in the same orbit under graph automorphisms of the graph G fixing v_1 . Hence, we can see that the edges connecting vertices in H and the two G 's satisfy the theorem's requirements and so the vertices v_1^1 and v_1^2 are A -cospectral in this graph.

Example 4.1.10. Another example of cospectral vertices, taken from the literature [9], is explained by the construction in Theorem 4.1.7, as can be observed in Figure 4.7.

One can modify this construction in various ways as long as one does not break the inherent dynamical symmetry. One such useful way is given below.

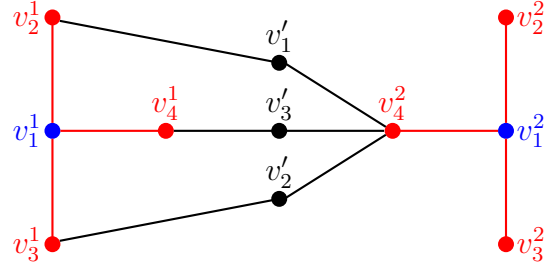


Figure 4.6: It is clear from the figure that the red subgraphs together with the blue A -cospectral vertices, are isomorphic to one another and that their connections to the middle vertices satisfy Theorem 4.1.7.

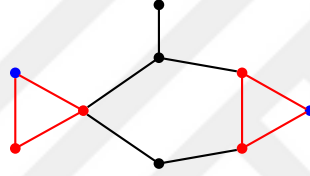


Figure 4.7: The red subgraphs correspond to G^1 and G^2 in the construction of Theorem 4.1.7, and the blue vertices correspond to the A -cospectral vertices.

Lemma 4.1.11. *Let $\tilde{G}$ be a graph constructed as outlined in Theorem 4.1.7, with subgraphs G^1 , G^2 , H and cospectral vertices $v_i^1 \in V(G^1)$ and $v_i^2 \in V(G^2)$ as explained. Now, consider an orbit $[v_j]_{v_i}$ of vertices under the action of $\text{Aut}(G, v_i)$ on G . In the graph $\tilde{G}$, there are two copies of G ; G^1 and G^2 . Hence, these orbits also have two copies, denoted*

$$[v_j^1]_{v_i} \subseteq V(G^1), \quad [v_j^2]_{v_i} \subseteq V(G^2).$$

Consider the graph $\hat{G}$ obtained by modifying $\tilde{G}$ by connecting vertices in $[v_j^1]_{v_i}$ with vertices in $[v_j^2]_{v_i}$ in a bijective manner, that is; $\forall v_m^1 \in [v_j^1]_{v_i}$, connect v_m^1 to exactly one vertex in $[v_j^2]_{v_i}$ such that $\forall v_k^2 \in [v_j^2]_{v_i}$, v_k^2 is also connected to exactly one vertex in $[v_j^1]_{v_i}$. Then, v_i^1 and v_i^2 are still A -cospectral in $\hat{G}$.

Proof. In the proof of Theorem 4.1.7 we laid three separate claims and proved them together inductively. It is easy to see that all three claims are unaffected by the operation of connecting orbits. Thus, the proof of Theorem 4.1.7 applies and hence, v_i^1 and v_i^2 are A -cospectral in $\hat{G}$. $\square$

Remark 4.1.12. It is useful to note that one can apply Lemma 4.1.11 in different ways to create different graphs. We provide an example to this in Figure 4.8 below.

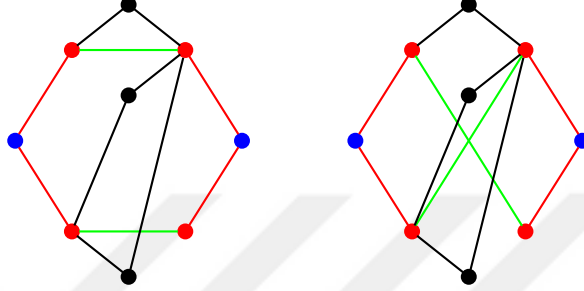


Figure 4.8: Lemma 4.1.11 applied to a graph constructed via Theorem 4.1.7, in two different ways. Here, the red subgraphs correspond to G^1 and G^2 in Theorem 4.1.7 with the blue vertices corresponding to the A -cospectral vertices. The green edges are those that are added in applying Lemma 4.1.11 in two different ways. It is easy to see that the two graphs are not isomorphic: in the right graph the two vertices with degrees 4 and 5 are connected, in the left one they are not.

Example 4.1.13. Using Theorem 4.1.7 and Lemma 4.1.11 we can illuminate many examples of cospectral vertices and latent symmetries in the literature. Three such examples are provided below in Figure 4.9 with the subgraphs that correspond to G^1 and G^2 indicated in red and the A -cospectral vertices indicated by blue.

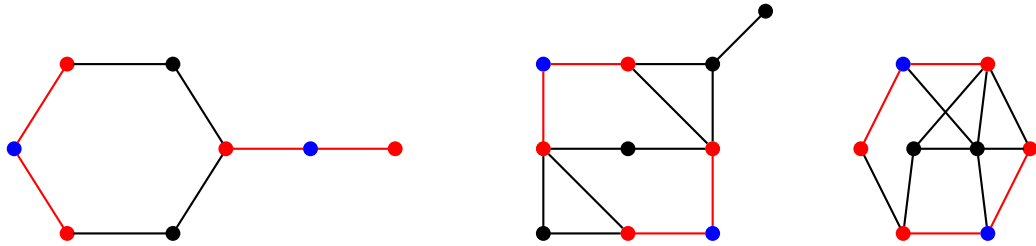


Figure 4.9: All three of these graphs are from [7]. In all three of them, the indicated blue vertex pairs are not symmetric but A -cospectral and therefore, latently symmetric. Through the indicated subgraphs, it is easy to see that the left one can be obtained by applying Theorem 4.1.7 and the other two can be obtained by applying Lemma 4.1.11 after Theorem 4.1.7.

There is also a slightly different Laplacian version of Theorem 4.1.7 where

instead of vertices of G^1 and G^2 connecting to vertices of H , they connect to each other, respecting the orbit structure.

Theorem 4.1.14 (*L*-cospectral). *Let G be a graph and select a vertex $v_i \in V(G)$. Divide the vertices of G into orbits under the action of $\text{Aut}(G, v_i)$, the group of graph automorphisms that fix v_i . Denote the orbits of vertices under this action as $[v_j]_{v_i} \subseteq V(G)$. Now, take two copies of G and label them $G^1(V^1, E^1)$ and $G^2(V^2, E^2)$. Denote the vertices of G^1 and G^2 as v_j^1, v_k^2 , etc. Finally, in order to construct the graph $\tilde{G}$, add any number of edges between G^1 and G^2 satisfying the following:*

*Every edge connecting a vertex $v_j^1 \in V(G^1)$ and a vertex $v_m^2 \in V(G^2)$ should be between vertices of the same orbit; that is if $(v_j^1, v_m^2) \in E(\tilde{G})$, then we must have $v_m \in [v_j]_{v_i}$. Then v_i^1 and v_i^2 are *L*-cospectral in $\tilde{G}$.*

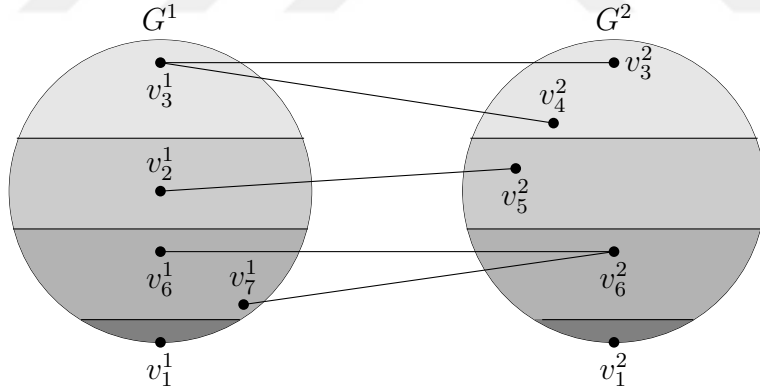


Figure 4.10: Construction of Theorem 4.1.14 illustrated. Here, the graphs G^1 and G^2 are divided into orbits under the action of $\text{Aut}(G, v_1)$. These orbits are shown by shades of grey in which the darkest grey contains only v_1 . The vertices v_6, v_7 ; v_2, v_5 and v_3, v_4 are in the same orbit. As can be seen in the Figure, every edge between vertices of G^1 and G^2 are between vertices of the same orbit. Hence, the vertices v_1^1 and v_1^2 are *L*-cospectral in the graph $\tilde{G}$.

Proof. We will claim $\forall k \in \mathbb{N}$;

$$1. \left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} = \left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^2}, \forall v_m \in V(G),$$

$$2. \left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} = \left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^1}, \forall v_m, v_j \in V(G) \text{ such that } v_j \in [v_m]_{v_i}.$$

Clearly, (1) and (2) together imply $\left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^2} = \left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^2}$ as well. We will prove by induction.

Base Case $k = 0$: Trivial.

Inductive Step: To prove claim (1), we have for any $v_m \in V(G)$,

$$\begin{aligned} \left(\tilde{L}^n(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} &= d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} - \sum_{v_j \sim v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^1} \\ &\quad + \sum_{\substack{v_\ell \in V(G) \\ v_\ell^2 \sim v_m^1}} \left[\left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} - \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_\ell^2} \right] \\ &= d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^2} - \sum_{v_j \sim v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^2} \end{aligned}$$

by **induction hypothesis (1) and (2)** along with the by construction fact that if $v_\ell^2 \sim v_m^1$ then $v_\ell \in [v_m]_{v_i}$. In the same way we obtain,

$$\begin{aligned} &= d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^2} - \sum_{v_j \sim v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^2} \\ &\quad + \sum_{\substack{v_\ell \in V(G) \\ v_\ell^1 \sim v_m^2}} \left[\left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^2} - \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_\ell^1} \right] = \left(\tilde{L}^n(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^2} \end{aligned}$$

proving claim (1). Now to prove claim (2), consider two vertices $v_m, v_j \in V(G)$ such that $v_j \in [v_m]_{v_i}$. We have

$$\begin{aligned} \left(\tilde{L}^n(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} &= d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} - \sum_{v_\ell \sim v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_\ell^1} \\ &\quad + \sum_{\substack{v_r \in V(G) \\ v_r^2 \sim v_m^1}} \left[\left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} - \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_r^2} \right] \\ &= d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} - \sum_{v_\ell \sim v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_\ell^1} \end{aligned}$$

where similar to claim (1), we used **induction hypotheses (1) and (2)** along with the fact that if $v_r^2 \sim v_m^1$ then $v_r \in [v_m]_{v_i}$. Now, since v_j and v_m are in the same automorphism orbit, their neighbors are also in the same automorphism orbits. Hence, we have by **induction hypothesis (2)**

$$\begin{aligned}
& d_{v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_m^1} - \sum_{v_\ell \sim v_m} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_\ell^1} = \\
& = d_{v_j} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^1} - \sum_{v_s \sim v_j} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_s^1} \\
& = d_{v_j} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^1} - \sum_{v_s \sim v_j} \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_s^1} \\
& + \sum_{\substack{v_r \in V(G) \\ v_r^2 \sim v_j^1}} \left[\left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^1} - \left(\tilde{L}^{n-1}(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_r^2} \right] = \left(\tilde{L}^n(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_j^1}
\end{aligned}$$

where we implicitly used the fact that $d_{v_m} = d_{v_j}$ in the first equality and **induction hypothesis (1) and (2)** along with the fact that if $v_r^2 \sim v_j^1$ then $v_r \in [v_j]_{v_i}$ in the second equality, similar to before. Hence, we have proved claim (2) and so the induction is finished. Now, we have shown in particular that $\forall k \in \mathbb{N}$, we have $\left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_i^1} = \left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)_{v_i^2}$. Equivalently, we have $\forall k \in \mathbb{N}$,

$$\left(\tilde{L}^k(\mathbf{v}_i^1 + \mathbf{v}_i^2) \right)^T (\mathbf{v}_i^1 - \mathbf{v}_i^2) = 0$$

Hence, $\langle \mathbf{v}_i^1 + \mathbf{v}_i^2 \rangle_{\tilde{L}} \perp \langle \mathbf{v}_i^1 - \mathbf{v}_i^2 \rangle_{\tilde{L}}$ and so v_i^1 and v_i^2 are L -cospectral in $\tilde{G}$ by Lemma 4.0.3. $\square$

There is another example of some kind of nontrivial symmetries giving rise to coprobable vertices, this time, only for the Laplacian.

Theorem 4.1.15 (L -coprobable). *Let G be a graph, and let v_i, v_j and v_k, v_ℓ be two pairs of vertices in the same automorphism orbits, that is, v_i and v_j are in the same orbit and v_k and v_ℓ are in the same orbit. Since these vertex pairs are L -cospectral vertex pairs in G , we have that*

$$\langle \mathbf{v}_i + \mathbf{v}_j \rangle_L \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L \quad \text{and} \quad \langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \perp \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L.$$

Let $n = \dim(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp \cap \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp)$. Since the constant vector $[1, 1, \dots, 1]$ is an eigenvector of L that is orthogonal to both subspaces, $n > 0$. Now, consider the graph $\widehat{G}$ obtained from G by adding/deleting an edge between v_k and v_ℓ . Then, we have that:

1. $\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} = \langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L$ and $\langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}} = \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L$
2. If λ is an eigenvalue of L with eigenvector $\mathbf{w}_\lambda \perp \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L$, then it is also an eigenvalue of $\widehat{L}$ with the same eigenvector.
3. $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\widehat{L}} \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp \cap \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp$ and so $\dim(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\widehat{L}}) \leq |G| - n = N - n$.

In particular, (3) shows that depending on k , v_i and v_j are L -coprobable in $\widehat{G}$ as well.

Proof. Firstly, we prove (2). Let λ be an eigenvalue of L with eigenvector $\mathbf{w}_\lambda \perp \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L$. This implies that $(\mathbf{w}_\lambda)_{v_k} = (\mathbf{w}_\lambda)_{v_\ell}$. Because the Laplacian only involves differences between vertices, for these eigenvectors satisfying $(\mathbf{w}_\lambda)_{v_k} = (\mathbf{w}_\lambda)_{v_\ell}$, deleting or adding an edge between v_k and v_ℓ does not change it being an eigenvector of the Laplacian. The eigenvector $\mathbf{w}_\lambda$ is also an eigenvector of $\widehat{L}$ with the same eigenvalue λ . This proves (2).

Now for (1), let $\mathbf{v}_k + \mathbf{v}_\ell = \sum_{\lambda \in \Lambda_L} c_\lambda \mathbf{w}_\lambda$ be the spectral decomposition of $\mathbf{v}_k + \mathbf{v}_\ell$ with respect to L where $\mathbf{w}_\lambda$ is a unit eigenvector with eigenvalue λ and $c_\lambda \mathbf{w}_\lambda = E_\lambda(\mathbf{v}_k + \mathbf{v}_\ell)$. By Lemma 3.2.2, all eigenvectors $\mathbf{w}_\lambda$ in the spectral decomposition such that $c_\lambda \neq 0$, satisfy $\mathbf{w}_\lambda \in \langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L$ and so $\mathbf{w}_\lambda \perp \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L$ by the L -cospectrality of v_k and v_ℓ . Hence by (2), all such $\mathbf{w}_\lambda$ are eigenvectors of $\widehat{L}$ with eigenvalues λ . Since all eigenvectors with nonzero coefficients in the spectral decomposition of $\mathbf{v}_k + \mathbf{v}_\ell$ with respect to L continue to remain eigenvectors with respect to $\widehat{L}$, we have that $\mathbf{v}_k + \mathbf{v}_\ell = \sum_{\lambda \in \Lambda_L} c_\lambda \mathbf{w}_\lambda$ is also the spectral decomposition of $\mathbf{v}_k + \mathbf{v}_\ell$ with respect to $\widehat{L}$. By Lemma 3.2.2, this implies that

$$\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} = \langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L.$$

Now, consider the space $(\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L)^\perp$. By Corollary 3.2.5, there exists eigenvectors $\{\mathbf{w}_\lambda^i\}_{i \in I}$ that form a basis for this space. For $i \in I$ the eigenvector $\mathbf{w}_\lambda^i$ satisfies $\mathbf{w}_\lambda^i \perp \langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L$, and so claim (2) implies that $\mathbf{w}_\lambda^i$ is still an eigenvector of $\widehat{L}$. Since $\mathbf{w}_\lambda^i$ satisfies $(\mathbf{w}_\lambda^i)_{v_3} = (\mathbf{w}_\lambda^i)_{v_4} = 0$ for all $i \in I$, this implies by the undirectedness of $\widehat{G}$,

$$\mathbf{w}_\lambda^i \perp \langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}}.$$

Thus, we have

$$(\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L)^\perp \subseteq (\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}})^\perp.$$

Because the operations of deleting/adding an edge are inverses of each other, we also have

$$(\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}})^\perp \subseteq (\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L)^\perp$$

and so

$$(\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L)^\perp = (\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} \oplus \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}})^\perp.$$

Now, in both G and $\widehat{G}$, v_k and v_ℓ are in the same automorphism orbit and consequently, are L -cospectral. Thus, we already have $\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_L \perp \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L$ and $\langle \mathbf{v}_k + \mathbf{v}_\ell \rangle_{\widehat{L}} \perp \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}}$ which, together with the equalities above, imply

$$\langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L = \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_{\widehat{L}},$$

proving claim (1).

Finally, we show claim (3). By Corollary 3.2.4, $\langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp$ is spanned by some eigenvectors $\{\mathbf{w}_\lambda^i\}_{i \in I'}$ of L . By claim (2), we know these eigenvectors are also eigenvectors of $\widehat{L}$ with the same eigenvalues. Now let $\mathbf{x} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp \cap \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp$. Since $\mathbf{x} \in \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp$, it can be written as a sum of eigenvectors $\{\mathbf{w}_\lambda^i\}_{i \in I'}$. We thus have $\mathbf{x} = \sum_{i \in I'} \alpha_i \mathbf{w}_\lambda^i$ where $\alpha_i \in \mathbb{R}$. Furthermore, since $\mathbf{x} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp$ it also satisfies $(\mathbf{x})_{v_i} = (\mathbf{x})_{v_j}$. Hence for any $m \in \mathbb{N}$, we have

$$\mathbf{x}^T \widehat{L}^m (\mathbf{v}_i - \mathbf{v}_j) = (\widehat{L}^m \mathbf{x})^T (\mathbf{v}_i - \mathbf{v}_j) = (L^m \mathbf{x})^T (\mathbf{v}_i - \mathbf{v}_j) = \mathbf{x}^T L^m (\mathbf{v}_i - \mathbf{v}_j) = 0$$

where the first and third equality follows by the undirectedness of $\widehat{G}$, the second by the fact that $\mathbf{x}$ is a linear combination of eigenvectors $\{\mathbf{w}_\lambda^i\}_{i \in I'}$ of L which

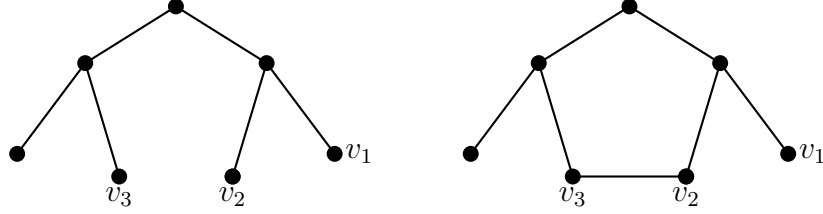


Figure 4.11: An example to Theorem 4.1.15 with symmetric vertices v_1, v_2 and v_3 ($v_\ell = v_j = v_2$) in the left graph and L -coprovable vertices v_1 and v_2 in the right graph.

are also eigenvectors of $\widehat{L}$ with the same eigenvalues, and the last equality follows from the fact that $\mathbf{x} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp$. Hence we have shown $\mathbf{x} \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\widehat{L}}$ for all $\mathbf{x} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp \cap \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp$. In other words,

$$\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\widehat{L}} \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_L^\perp \cap \langle \mathbf{v}_k - \mathbf{v}_\ell \rangle_L^\perp$$

as claimed in (3). Therefore we have, $\dim(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\widehat{L}}) \leq |G| - n = N - n$ as was claimed. $\square$

Example 4.1.16. With this construction, one can obtain L -coprovable vertices whose underlying symmetry is not very apparent. A simple example of how this might occur is given in Figure 4.11. As can be seen in the left graph, vertices v_1, v_2 and v_3 are all in the same automorphism orbit (here $v_\ell = v_j = v_2$ in the theorem). When we add an edge between v_2 and v_3 , this relationship breaks down. Now in the right graph, v_1 is no longer in the same automorphism orbit with v_2 . However, v_1 and v_2 remain L -coprovable vertices because of Theorem 4.1.15.

4.2 Constructing Strongly Cospectral Vertices

In this section we will digress into investigating whether the A -cospectral vertices constructed in Theorem 4.1.7 are strongly cospectral or not. We will find out that they are “almost” strongly cospectral and consequently can be “made” strongly cospectral, the meanings of these terms to be made clear later. We will start with the definition of strongly cospectral vertices.

Definition 4.2.1 (Strongly Cospectral vertices). Let $G(V, E)$ be a graph and let $A = \sum_{\lambda \in \Lambda_A} \lambda E_\lambda$ be its adjacency matrix where E_λ are the orthogonal projection onto the λ -eigenspaces of A . Let $v_i, v_j \in V$ be two vertices of G . Then the vertices v_i and v_j are called strongly cospectral if $\forall \lambda \in \Lambda_A$ we have $E_\lambda \mathbf{v}_i = \pm E_\lambda \mathbf{v}_j$.

To move on, we require some preparatory results. The first of these is the following lemma.

Lemma 4.2.2. *Let G be a graph and let $v_i \in V(G)$ be a vertex of G . Consider the orbits $[v_j]_{v_i}$ of G under the action of the group $\text{Aut}(G, v_i)$. Consider also the spectral decomposition of $\mathbf{v}_i$ with respect to the adjacency matrix A of G ;*

$$\mathbf{v}_i = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda.$$

For all $\lambda \in \Lambda_A$ such that $c_\lambda \neq 0$ and for all vertices v_ℓ, v_m in the same orbit, that is, for all $v_\ell, v_m \in V(G)$ satisfying $v_m \in [v_\ell]_{v_i}$; we have $(\mathbf{w}_\lambda)_{v_\ell} = (\mathbf{w}_\lambda)_{v_m}$.

Proof. Since v_ℓ and v_m are in the same orbit $[v_\ell]_{v_i}$, we have

$$(A^k \mathbf{v}_i)_{v_\ell} = (A^k \mathbf{v}_i)_{v_m}, \quad \forall k \in \mathbb{N}.$$

Now, we can write $(A^k \mathbf{v}_i)_{v_\ell}$ and $(A^k \mathbf{v}_i)_{v_m}$ as

$$(A^k \mathbf{v}_i)_{v_\ell} = \sum_{\lambda \in \Lambda_A} \lambda^k c_\lambda (\mathbf{w}_\lambda)_{v_\ell} \quad \text{and} \quad (A^k \mathbf{v}_i)_{v_m} = \sum_{\lambda \in \Lambda_A} \lambda^k c_\lambda (\mathbf{w}_\lambda)_{v_m}.$$

Therefore, the equality $(A^k \mathbf{v}_i)_{v_\ell} = (A^k \mathbf{v}_i)_{v_m}$, $\forall k \in \mathbb{N}$, is equivalent to

$$\sum_{\lambda \in \Lambda_A} \lambda^k c_\lambda (\mathbf{w}_\lambda)_{v_\ell} = \sum_{\lambda \in \Lambda_A} \lambda^k c_\lambda (\mathbf{w}_\lambda)_{v_m}, \quad \forall k \in \mathbb{N}$$

which implies that $\forall \lambda \in \Lambda_A$ such that $c_\lambda \neq 0$, we have

$$(\mathbf{w}_\lambda)_{v_\ell} = (\mathbf{w}_\lambda)_{v_m}.$$

□

Besides being useful later, the following theorem might be of interest in itself.

Theorem 4.2.3. *Let $\tilde{G}$ be a graph constructed as outlined in Theorem 4.1.7, with subgraphs G^1 , G^2 , H and A -cospectral vertices v_i^1 and v_i^2 . Consider the vertex v_i in the graph G . The vertex has a spectral decomposition with respect to the adjacency matrix A of G as follows:*

$$\mathbf{v}_i = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda.$$

If $c_\lambda \neq 0$, then we have that λ is also an eigenvalue of $\tilde{A}$. We call such eigenvalues, eigenvalues of $\tilde{A}$ induced by G and denote the set of such eigenvalues by $\Lambda_G^{\tilde{A}}$.

Proof. We know that the vertices of $\tilde{G}$ can be partitioned into the vertices of the subgraphs G^1 , G^2 and H . Let $\lambda \in \Lambda_A$ be an eigenvalue of A such that $c_\lambda \neq 0$ in the spectral decomposition of $\mathbf{v}_i$. Consider the vector $\tilde{\mathbf{w}}_\lambda$ associated with the eigenvector $\mathbf{w}_\lambda$ of A , defined $\forall v \in V(\tilde{G})$ as

$$(\tilde{\mathbf{w}}_\lambda)_v := \begin{cases} 0 & \text{if } v = v'_\alpha \in V(H) \\ (\mathbf{w}_\lambda)_{v_k} & \text{if } v = v_k^1 \in V(G^1) \\ -(\mathbf{w}_\lambda)_{v_k} & \text{if } v = v_k^2 \in V(G^2) \end{cases}$$

We will show that $\tilde{\mathbf{w}}_\lambda$ is an eigenvector of $\tilde{A}$. For vertices $v'_\alpha \in V(H)$ of $\tilde{G}$, we have:

$$\begin{aligned} (\tilde{A}\tilde{\mathbf{w}}_\lambda)_{v'_\alpha} &= \sum_{v_k^1 \sim v'_\alpha} (\tilde{\mathbf{w}}_\lambda)_{v_k^1} + \sum_{v_\ell^2 \sim v'_\alpha} (\tilde{\mathbf{w}}_\lambda)_{v_\ell^2} + \sum_{\substack{v'_\beta \sim v'_\alpha \\ v'_\beta \in V(H)}} (\tilde{\mathbf{w}}_\lambda)_{v'_\beta} = \\ &= \sum_{v_k^1 \sim v'_\alpha} (\tilde{\mathbf{w}}_\lambda)_{v_k^1} + \sum_{v_\ell^2 \sim v'_\alpha} (\tilde{\mathbf{w}}_\lambda)_{v_\ell^2} \end{aligned}$$

where the last equality follows from definition of $\tilde{\mathbf{w}}_\lambda$ on subgraph H . Now, by the construction of Theorem 4.1.7, vertices $v'_\alpha \in V(H)$ have equal number of edges connecting it to corresponding orbits. In other words, for every edge between $v'_\alpha \in V(H)$ and a vertex $v_k^1 \in V(G^1)$, there exists a corresponding edge between v'_α and a vertex $v_\ell^2 \in V(G^2)$ such that $v_\ell \in [v_k]_{v_i}$ and vice versa. This fact, together with the definition of $\tilde{\mathbf{w}}_\lambda$ on subgraphs G^1 , G^2 and Lemma 4.2.2 implies that we have

$$= \sum_{v_k^1 \sim v'_\alpha} (\tilde{\mathbf{w}}_\lambda)_{v_k^1} + \sum_{v_\ell^2 \sim v'_\alpha} (\tilde{\mathbf{w}}_\lambda)_{v_\ell^2} = 0 = \lambda(\tilde{\mathbf{w}}_\lambda)_{v'_\alpha}.$$

For vertices $v_k^1 \in V(G^1)$ we have:

$$(\tilde{A}\tilde{\mathbf{w}}_\lambda)_{v_k^1} = \sum_{v_\ell \sim v_k} (\tilde{\mathbf{w}}_\lambda)_{v_\ell^1} + \sum_{\substack{v'_\alpha \sim v_k^1 \\ v'_\alpha \in V(H)}} (\tilde{\mathbf{w}}_\lambda)_{v'_\alpha} = \sum_{v_\ell \sim v_k} (\mathbf{w}_\lambda)_{v_\ell} = \lambda(\mathbf{w}_\lambda)_{v_k} = \lambda(\tilde{\mathbf{w}}_\lambda)_{v_k^1}$$

where the second equality is by the definition of $\tilde{\mathbf{w}}_\lambda$, the third equality is because $\mathbf{w}_\lambda$ is an eigenvector of A with eigenvalue λ . A similar argument works for vertices of G^2 . Hence we have

$$\tilde{A}\tilde{\mathbf{w}}_\lambda = \lambda\tilde{\mathbf{w}}_\lambda$$

and so λ is an eigenvalue of $\tilde{A}$ as was claimed. $\square$

The eigenvectors $\tilde{\mathbf{w}}_\lambda$ constructed in Theorem 4.2.3 are called eigenvectors of $\tilde{A}$ induced by G . The next result establishes why eigenvectors of $\tilde{A}$ induced by G are relevant for us.

Lemma 4.2.4. *Let $\tilde{G}$ be a graph constructed as outlined in Theorem 4.1.7, with subgraphs G^1 , G^2 , H and cospectral vertices v_i^1 and v_i^2 . Consider the adjacency matrix $\tilde{A}$, its eigenvectors and the vector $\mathbf{v}_i^1 - \mathbf{v}_i^2$. The spectral decomposition*

$$\mathbf{v}_i^1 - \mathbf{v}_i^2 = \sum_{\lambda \in \Lambda_{\tilde{A}}} c_\lambda \mathbf{y}_\lambda$$

of $\mathbf{v}_i^1 - \mathbf{v}_i^2$ contains precisely those eigenvectors of $\tilde{A}$ that are induced by G ; that is if $c_\lambda \neq 0$ then λ is an eigenvalue of $\tilde{A}$ induced by G and the eigenvector $\mathbf{y}_\lambda$ equals the eigenvector $\tilde{\mathbf{w}}_\lambda$ of $\tilde{A}$ induced by G .

Proof. Let $\mathbf{v}_i = \sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda$ be the spectral decomposition of $\mathbf{v}_i$ with respect to A and let $\tilde{\mathbf{w}}_\lambda$ denote eigenvectors of $\tilde{A}$ induced by G . Consider the vector $\sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda$. We will show that $\mathbf{v}_i^1 - \mathbf{v}_i^2 = \sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda$.

Let $v'_\alpha \in V(H)$. Then $(\sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda)_{v'_\alpha} = \sum_{\lambda \in \Lambda_A} c_\lambda (\tilde{\mathbf{w}}_\lambda)_{v'_\alpha} = 0$ since $(\tilde{\mathbf{w}}_\lambda)_{v'_\alpha} = 0$ for all eigenvectors of $\tilde{A}$ induced by G .

Let $v_k^1 \in V(G^1)$. Then

$$\left(\sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda \right)_{v_k^1} = \sum_{\lambda \in \Lambda_A} c_\lambda (\tilde{\mathbf{w}}_\lambda)_{v_k^1} = \sum_{\lambda \in \Lambda_A} c_\lambda (\mathbf{w}_\lambda)_{v_k} =$$

$$= \left(\sum_{\lambda \in \Lambda_A} c_\lambda \mathbf{w}_\lambda \right)_{v_k} = (\mathbf{v}_i)_{v_k} = \delta_{ik}.$$

Similarly, we have

$$\left(\sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda \right)_{v_k^2} = -\delta_{ik}.$$

Hence, we have $\sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda = \mathbf{v}_i^1 - \mathbf{v}_i^2$. Now by Theorem 4.2.3, all $\lambda \in \Lambda_A$ and $\tilde{\mathbf{w}}_\lambda$ such that $c_\lambda \neq 0$ are eigenvalues and eigenvectors of $\tilde{A}$. Because the spectral decomposition of a vector is unique, this implies that $\sum_{\lambda \in \Lambda_A} c_\lambda \tilde{\mathbf{w}}_\lambda$ is the spectral decomposition of $\mathbf{v}_i^1 - \mathbf{v}_i^2$ with respect to $\tilde{A}$. $\square$

The next result shows that to ensure strong cospectrality for the cospectral vertices obtained by the construction in Theorem 4.1.7, we need only check eigenvalues of $\tilde{A}$ induced by G .

Theorem 4.2.5. *Let $\tilde{G}$ be a graph constructed as outlined in Theorem 4.1.7, with subgraphs G^1, G^2, H and cospectral vertices v_i^1 and v_i^2 . Then, the vertices v_i^1 and v_i^2 are strongly cospectral if eigenvalues of $\tilde{A}$ induced by G are simple in $\tilde{A}$.*

Proof. Consider the cospectral vertices v_i^1 and v_i^2 . Now, with respect to the dynamics $\tilde{A}$ of $\tilde{G}$, $\mathbf{v}_i^1$ and $\mathbf{v}_i^2$ have spectral decompositions:

$$\mathbf{v}_i^1 = \sum_{\lambda \in \Lambda_{\tilde{G}}^{\tilde{A}}} \alpha_\lambda^1 \tilde{\mathbf{w}}_\lambda + \sum_{\lambda \in X} \beta_\lambda^1 \mathbf{y}_\lambda \quad \text{and} \quad \mathbf{v}_i^2 = \sum_{\lambda \in \Lambda_{\tilde{G}}^{\tilde{A}}} \alpha_\lambda^2 \tilde{\mathbf{w}}_\lambda + \sum_{\lambda \in X} \beta_\lambda^2 \mathbf{y}_\lambda$$

where $\tilde{\mathbf{w}}_\lambda$ are the eigenvectors of $\tilde{A}$ induced by G defined in Theorem 4.2.3, $\mathbf{y}_\lambda$ denotes other eigenvectors of $\tilde{A}$ and

$$X := \left[\Lambda_{\tilde{A}} \setminus \Lambda_{\tilde{G}}^{\tilde{A}} \right] \cup \left\{ \lambda \in \Lambda_{\tilde{G}}^{\tilde{A}} \mid \lambda \text{ has order } > 1 \text{ in } \Lambda_{\tilde{A}} \right\}$$

denotes the set of eigenvalues of $\tilde{A}$ not induced by G , which includes potentially some of the eigenvalues of $\tilde{A}$ induced by G (if they have order > 1 in $\Lambda_{\tilde{A}}$). Now, the vector $\mathbf{v}_i^1 - \mathbf{v}_i^2$ also has a spectral decomposition, and by Lemma 4.2.4 it should contain only eigenvectors $\tilde{\mathbf{w}}_\lambda$ of $\tilde{A}$ induced by G , i.e. it has the form:

$$\mathbf{v}_i^1 - \mathbf{v}_i^2 = \sum_{\lambda \in \Lambda_{\tilde{G}}^{\tilde{A}}} (\alpha_\lambda^1 - \alpha_\lambda^2) \tilde{\mathbf{w}}_\lambda$$

This directly implies $\forall \lambda \in X$,

$$\beta_\lambda := \beta_\lambda^1 = \beta_\lambda^2 \quad \text{and} \quad \mathbf{y}_\lambda := \mathbf{y}_\lambda^1 = \mathbf{y}_\lambda^2.$$

The latter was not obvious as $\mathbf{y}_\lambda^1$ and $\mathbf{y}_\lambda^2$ could have been different eigenvectors of the same eigenvalue if the eigenspace of λ is more than one dimensional. Moreover, we also have:

$$\alpha_\lambda := \alpha_\lambda^1 = \tilde{\mathbf{w}}_\lambda^T \mathbf{v}_i^1 = -\tilde{\mathbf{w}}_\lambda^T \mathbf{v}_i^2 = -\alpha_\lambda^2$$

where the equalities follow from the definition of $\tilde{\mathbf{w}}_\lambda$, scaled to be a unit vector. Now let E_λ be the orthogonal projection map onto the λ -eigenspace of $\tilde{A}$. Then, we have the following:

$$\begin{aligned} E_\lambda \mathbf{v}_i^1 &= E_\lambda \mathbf{v}_i^2 = \beta_\lambda \mathbf{y}_\lambda & \text{if } \lambda \in X \text{ and } \lambda \notin \Lambda_G^{\tilde{A}} \\ E_\lambda \mathbf{v}_i^1 &= -E_\lambda \mathbf{v}_i^2 = \alpha_\lambda \tilde{\mathbf{w}}_\lambda & \text{if } \lambda \notin X \text{ and } \lambda \in \Lambda_G^{\tilde{A}} \end{aligned}$$

This implies that if $X \cap \Lambda_G^{\tilde{A}} = \emptyset$, i.e., if all eigenvalues in $\tilde{A}$ induced by G are simple in $\Lambda_{\tilde{A}}$, then $\mathbf{v}_i^1$ and $\mathbf{v}_i^2$ are strongly cospectral in $\tilde{G}$. $\square$

The reason that we cannot claim certain strongly cospectrality in Theorem 4.2.5 is that if there are eigenvalues λ of $\tilde{A}$ such that $\lambda \in X$ and $\lambda \in \Lambda_G^{\tilde{A}}$, then we have $E_\lambda \mathbf{v}_i^1 = \beta_\lambda \mathbf{y}_\lambda + \alpha_\lambda \tilde{\mathbf{w}}_\lambda$ and $E_\lambda \mathbf{v}_i^2 = \beta_\lambda \mathbf{y}_\lambda - \alpha_\lambda \tilde{\mathbf{w}}_\lambda$ and so these vectors become linearly independent from one another. However, as we explain in the remark below, such cases actually can be avoided.

Remark 4.2.6. There are three ways for eigenvalues in $\tilde{A}$ induced by G to have order > 1 in $\Lambda_{\tilde{A}}$. Firstly, there may be local substructures in the subgraph H that induces the same eigenvalue. For example, the substructure shown in Figure 4.12 induces the eigenvalue 0 to whatever graph it is connected to. This case actually does not present a problem for strong cospectrality, as eigenvectors $\mathbf{y}_\lambda$ induced by such eigenvalues are local in the subgraph H , in particular they satisfy $(\mathbf{y}_\lambda)_{v_i^1} = (\mathbf{y}_\lambda)_{v_i^2} = 0$ and consequently do not arise in the spectral decompositions of $\mathbf{v}_i^1$ and $\mathbf{v}_i^2$.

The second way for eigenvalues in $\tilde{A}$ induced by G to have order > 1 is for G to “induce” more than one λ -eigenvector in $\tilde{A}$. This can happen if the $\mathbf{w}_\lambda$

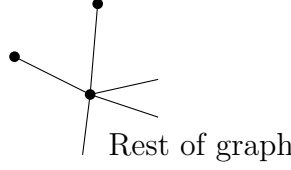


Figure 4.12: Two vertices attached to the same vertex induce a 0-eigenvalue for the adjacency matrix A with eigenvector $\mathbf{w}_0$ whose components are zero on all vertices of the graph except for those two.

eigenvector of A has the value 0 at those indices where G^1 and G^2 is connected to H . In other words, if for all $v_k^1 \in V(G^1)$ such that $v_k^1 \sim v'_\alpha$ for a vertex $v'_\alpha \in V(H)$, we have $(\mathbf{w}_\lambda)_{v_k} = 0$; then $\mathbf{w}_\lambda^1$ defined $\forall v \in V(\tilde{G})$ as

$$(\mathbf{w}_\lambda^1)_v := \begin{cases} (\mathbf{w}_\lambda)_{v_k} & \text{if } v = v_k^1 \in V(G^1) \\ 0 & \text{else} \end{cases}$$

is a λ -eigenvector of $\tilde{A}$, and one can similarly obtain another λ -eigenvector $\mathbf{w}_\lambda^2$ of $\tilde{A}$. Obviously we have $\tilde{\mathbf{w}}_\lambda = \mathbf{w}_\lambda^1 - \mathbf{w}_\lambda^2$ where $\tilde{\mathbf{w}}_\lambda$ is the λ -eigenvector of $\tilde{A}$ induced by G . In such a case v_i^1 and v_i^2 would not be strongly cospectral. However, this case can easily be remedied by adding new edges between vertices of G^1 , G^2 and vertices of H ; through vertices $v_k^1 \in V(G^1)$ and $v_\ell^2 \in V(G^2)$ satisfying $(\mathbf{w}_\lambda)_{v_k}, (\mathbf{w}_\lambda)_{v_\ell} \neq 0$; all the while respecting the construction of Theorem 4.1.7.

Lastly, there are the rest of the cases where the second λ -eigenvector exists “over” the whole graph, i.e. there is a λ -eigenvector $\mathbf{y}_\lambda$ of $\tilde{A}$ who satisfies neither of the two other cases’ conditions:

1. $(\mathbf{y}_\lambda)_{v_k^1} = (\mathbf{y}_\lambda)_{v_k^2} = 0, \quad \forall v_k \in V(G)$
2. $(\mathbf{y}_\lambda)_{v'_\alpha} = 0, \quad \forall v'_\alpha \in V(H)$

Similar to the second case, this case also prevents strong cospectrality in general but is easy to remedy. Because $(\mathbf{y}_\lambda)_{v'_\alpha} \neq 0$ for some $v'_\alpha \in V(H)$, we can attach a new vertex $\hat{v}$ to v'_α to modify the graph $\tilde{G}$. This operation preserves cospectrality as it preserves the construction in Theorem 4.1.7. Furthermore it slightly changes the eigenvalues of those eigenvectors which satisfy $(\mathbf{y}_\lambda)_{v'_\alpha} \neq 0$. Hence, in the

modified graph, λ should have lower order. A formal proof for this argument is given by Lemma 4.2.7. With this remark, Theorem 4.2.5 in practice almost ensures the strong cospectrality of v_i^1 and v_i^2 in $\tilde{G}$. Finally we should mention that heuristically, cases 2 and 3 above are difficult to obtain or even construct. It is therefore highly unlikely that they should arise frequently in constructions.

Lemma 4.2.7. *Let $\tilde{G}$ be a graph. Suppose that λ is an eigenvalue of $\tilde{A}$ of order $\ell > 1$. Let $\mathbf{y}_\lambda$ be a λ -eigenvector of $\tilde{A}$. We have $(\mathbf{y}_\lambda)_{v_m} \neq 0$ for some $v_m \in V(\tilde{G})$. Now, modify $\tilde{G}$ by attaching a single vertex $\hat{v}$ to v_m and denote the modified graph by $\hat{G}$. Then, the order of λ in $\hat{A}$ equals $\ell - 1$.*

Proof. We can suppose that the vertices of the graph $\hat{G}$ are indexed in the same order as those of $\tilde{G}$ with the exception that the extra vertex $\hat{v}$ is the final $N + 1$ -th vertex where $N = |V(\tilde{G})|$. Hence the adjacency matrix of $\hat{G}$ can be assumed to have the form

$$\hat{A} = \begin{bmatrix} & & & & 0 \\ & & & & \vdots \\ & & \tilde{A} & & 1 \\ & & & & \vdots \\ 0 & \dots & 1 & \dots & 0 \end{bmatrix}$$

where the non-zero entries in the final row and column are in the $(\hat{v}, v_m)$ and $(v_m, \hat{v})$ entries.

We will follow the proof of Theorem 9.5.1 of [36] with slight modifications. Let $\lambda_i(\tilde{A})$ and $\lambda_i(\hat{A})$ denote the i -th eigenvalue of $\tilde{A}$ and $\hat{A}$ respectively, counting multiplicity and with the first eigenvalue being the largest. Now suppose that the λ -eigenvalues of $\tilde{A}$ are from $i = j$ to $i = j + \ell - 1$. Since $\tilde{A}$ is obtained from $\hat{A}$ by deleting a vertex (i.e., a row and a column corresponding to $\hat{v}$), Theorem 9.5.1 of [36] applies and so the eigenvalues of $\tilde{A}$ interlace those of $\hat{A}$, i.e.

$$\lambda_i(\hat{A}) \geq \lambda_i(\tilde{A}) \geq \lambda_{i+1}(\hat{A}) \quad \text{for } i = 1, \dots, N; \quad \text{where } N = |V(\tilde{G})|.$$

Now, let $\mathbf{w}_1, \dots, \mathbf{w}_N$ be an orthonormal set of eigenvectors of $\tilde{A}$ with eigenvalues $\lambda_1(\tilde{A}), \lambda_2(\tilde{A}), \dots, \lambda_N(\tilde{A})$ such that $\mathbf{w}_j = \mathbf{y}_\lambda$ and let $\mathbf{u}_1, \dots, \mathbf{u}_{N+1}$ be an orthonormal set of eigenvectors of $\hat{A}$ with eigenvalues $\lambda_1(\hat{A}), \lambda_2(\hat{A}), \dots, \lambda_{N+1}(\hat{A})$. Let W_i

and U_i denote the subspaces spanned by $\mathbf{w}_1, \dots, \mathbf{w}_i$ and $\mathbf{u}_1, \dots, \mathbf{u}_i$ respectively. Finally, let

$$R = \begin{bmatrix} I_{N \times N} \\ 0_{1 \times N} \end{bmatrix}$$

be the matrix that deletes from $\hat{A}$ the row and column corresponding to the vertex $\hat{v}$ via

$$R^T \hat{A} R = \tilde{A}$$

Now, for any $i = 1, \dots, N$ we have that W_i is i -dimensional and $R^T U_{i-1}$ is at most $(i-1)$ -dimensional. Therefore taking $i = j$, there exists a vector $\mathbf{y} \in W_j \cap (R^T U_{j-1})^\perp$. This vector satisfies

$$\mathbf{y}^T R^T \mathbf{u}_k = 0 \quad \text{for } k = 1, \dots, j-1$$

and so $R\mathbf{y} \in U_{j-1}^\perp$. By Rayleigh's inequalities this yields

$$\lambda_j(\hat{A}) \geq \frac{(R\mathbf{y})^T \hat{A} (R\mathbf{y})}{(R\mathbf{y})^T R\mathbf{y}} = \frac{\mathbf{y}^T \tilde{A} \mathbf{y}}{\mathbf{y}^T \mathbf{y}} \geq \lambda_j(\tilde{A}) = \lambda$$

with equality if and only if $\mathbf{y}$ and $R\mathbf{y}$ are λ -eigenvectors of $\tilde{A}$ and $\hat{A}$ respectively. Now if $\mathbf{y}$ and $R\mathbf{y}$ are λ -eigenvectors, then necessarily $\mathbf{y} = \mathbf{y}_\lambda$ because there is only one linearly independent λ -eigenvector in W_j . But this means $R\mathbf{y}_\lambda$ is a λ -eigenvector of $\hat{A}$. However we have

$$(\hat{A} R\mathbf{y}_\lambda)_{\hat{v}} = (R\mathbf{y}_\lambda)_{v_m} \neq 0 \quad \text{and} \quad (R\mathbf{y}_\lambda)_{\hat{v}} = 0$$

where the equality on the left follows from the fact that $\hat{v}$ has only one neighbour, v_m , and that $(\mathbf{y}_\lambda)_{v_m} \neq 0$ by assumption and the equality on the right follows from the definition of R . Thus

$$0 \neq (\hat{A} R\mathbf{y}_\lambda)_{\hat{v}} = \lambda (R\mathbf{y}_\lambda)_{\hat{v}} = \lambda \cdot 0 = 0$$

which is a contradiction. So the Rayleigh inequalities that we obtained are strict and therefore we must have $\lambda_j(\hat{A}) > \lambda_j(\tilde{A})$. Using the same argument on $-\hat{A}$ and $-\tilde{A}$ we get

$$-\lambda_{j+\ell}(\hat{A}) = \lambda_{N+2-j-\ell}(-\hat{A}) > \lambda_{N+2-j-\ell}(-\tilde{A}) = -\lambda_{j+\ell-1}(\tilde{A}).$$

and so

$$\lambda_{j+\ell-1}(\tilde{A}) > \lambda_{j+\ell}(\hat{A}).$$

Since

$$\lambda_j(\tilde{A}) = \lambda_{j+1}(\tilde{A}) = \cdots = \lambda_{j+\ell-1}(\tilde{A})$$

the interlacing implies that only the eigenvalues $\lambda_{j+1}(\hat{A}), \dots, \lambda_{j+\ell-1}(\hat{A})$ of $\hat{A}$ are equal to λ . Thus λ is of order $\ell - 1$ in $\hat{A}$. $\square$

4.3 Operations on Coprobable Vertices

There are several operations that can be done on graphs to obtain new coprobable vertices from existing ones. We explain these operations as well as some of their corollaries here.

4.3.1 Vertex Addition/Deletion

Our results from Lemma 4.3.1 leading up to Corollary 4.3.7 follow work done in [37], but we generalize the results to coprobable vertices from the special case of cospectral vertices. We also prove for the cospectral case further results in Lemma 4.3.9 and Theorem 4.3.10.

Lemma 4.3.1 (Vertex Addition/Deletion, A -cospectral, A -coprobable). *Let G be a graph, and let v_i and v_j be A -coprobable (A -cospectral) vertices in G . Consider the subspace $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. If there exists a vertex v_m such that*

$$\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A,$$

that is, if for any vector $\mathbf{x} \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, we have $(\mathbf{x})_{v_m} = 0$; then v_i and v_j remain A -coprobable (A -cospectral) in the graph $G \setminus v_m$. Conversely, suppose there exist vertices $\{v_\ell\}_{\ell \in I}$ of G such that

$$\sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A.$$

Then, in the graph $G + v$ where the extra vertex v is connected to the vertices $\{v_\ell\}_{\ell \in I}$, the vertices v_i and v_j remain A -coprobable (A -cospectral).

Proof. Suppose that there exists a vertex $v_m \in V(G)$, such that $\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. Now, since the vertex set $V(G \setminus v_m)$ of the subgraph $G \setminus v_m$ is a subset of the vertex set $V(G)$ of G , we can consider the associated spaces $\mathbb{R}^{N_{G \setminus v_m}}$ and $\mathbb{R}^N$ where $N_{G \setminus v_m} = |V(G \setminus v_m)| = N - 1$, as subspaces $\mathbb{R}^{N_{G \setminus v_m}} \leq \mathbb{R}^N$ of one another. Hence, we can talk about vectors $\mathbf{v}_i \in \mathbb{R}^{N_{G \setminus v_m}}$ and $\mathbf{v}_i \in \mathbb{R}^N$ associated with vertices $v_m \in V(G \setminus v_m) \cap V(G)$ as the same vector. With this in mind, we will show inductively for all $k \in \mathbb{N}$:

$$(A_{G \setminus v_m})^k(\mathbf{v}_i - \mathbf{v}_j) = \text{Ann}_{v_m}(A^k(\mathbf{v}_i - \mathbf{v}_j))$$

where $A_{G \setminus v_m}$ denote the adjacency matrix of $G \setminus v_m$ and $\text{Ann}_{v_m} : \mathbb{R}^N \rightarrow \mathbb{R}^{N_{G \setminus v_m}}$ is the annihilation map on vertex v_m , defined as:

$$[(\mathbf{x})_{v_1}, \dots, (\mathbf{x})_{v_{m-1}}, (\mathbf{x})_{v_m}, (\mathbf{x})_{v_{m+1}}, \dots, (\mathbf{x})_{v_N}] \mapsto [(\mathbf{x})_{v_1}, \dots, (\mathbf{x})_{v_{m-1}}, (\mathbf{x})_{v_{m+1}}, \dots, (\mathbf{x})_{v_N}].$$

Base Case $k = 0$: Trivial.

Inductive Step: Now, assume that the induction hypothesis holds for $k = n - 1$. We will show now that it holds for $k = n$. By the **induction hypothesis** we have, $(A_{G \setminus v_m})^{n-1}(\mathbf{v}_i - \mathbf{v}_j) = \text{Ann}_{v_m}(A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))$. We thus obtain,

$$\begin{aligned} (A_{G \setminus v_m})^n(\mathbf{v}_i - \mathbf{v}_j) &= A_{G \setminus v_m}(\text{Ann}_{v_m}(A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))) = \\ &= \text{Ann}_{v_m}(A^n(\mathbf{v}_i - \mathbf{v}_j) - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} \mathbf{v}_m - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_m} \mathbf{v}_\ell). \end{aligned}$$

Since $\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, we have $(A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_m} = (A^n(\mathbf{v}_i - \mathbf{v}_j))_{v_m} = 0$. This, together with $\sum_{v_\ell \sim v_m} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} = (A^n(\mathbf{v}_i - \mathbf{v}_j))_{v_m}$ implies that

$$\begin{aligned} (A_{G \setminus v_m})^n(\mathbf{v}_i - \mathbf{v}_j) &= \\ &= \text{Ann}_{v_m}(A^n(\mathbf{v}_i - \mathbf{v}_j) - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} \mathbf{v}_m - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_m} \mathbf{v}_\ell) \\ &= \text{Ann}_{v_m}(A^n(\mathbf{v}_i - \mathbf{v}_j)), \end{aligned}$$

proving the induction step. It is now easily seen that

$$\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}} = \text{Ann}_{v_m}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A).$$

To conclude that v_i and v_j are A -coprobable in $G \setminus v_m$, note that by Lemma 3.2.2, $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ is spanned by a subset of eigenvectors $\{\mathbf{w}_\lambda\}_{\lambda \in I}$ of A , all of which have different eigenvalues. Clearly, since $\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ we have to have $(\mathbf{w}_\lambda)_{v_m} = 0$ for all $\lambda \in I$. Hence, we have $\forall \lambda \in I$,

$$\begin{aligned} A_{G \setminus v_m} \text{Ann}_{v_m}(\mathbf{w}_\lambda) &= \text{Ann}_{v_m}(A\mathbf{w}_\lambda - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (\mathbf{w}_\lambda)_{v_\ell} \mathbf{v}_m - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (\mathbf{w}_\lambda)_{v_m} \mathbf{v}_\ell) = \\ &= \text{Ann}_{v_m}(A\mathbf{w}_\lambda - (A\mathbf{w}_\lambda)_{v_m} \mathbf{v}_m - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v_m}} (\mathbf{w}_\lambda)_{v_m} \mathbf{v}_\ell) = \text{Ann}_{v_m}(A\mathbf{w}_\lambda) \end{aligned}$$

where the last equality follows from the fact that $\mathbf{w}_\lambda$ is an eigenvector and that $(\mathbf{w}_\lambda)_{v_m} = 0$. Hence, we have that

$$A_{G \setminus v_m} \text{Ann}_{v_m}(\mathbf{w}_\lambda) = \text{Ann}_{v_m}(A\mathbf{w}_\lambda) = \text{Ann}_{v_m}(\lambda \mathbf{w}_\lambda) = \lambda \text{Ann}_{v_m}(\mathbf{w}_\lambda)$$

and so $\text{Ann}_{v_m}(\mathbf{w}_\lambda)$ is also an eigenvector of $A_{G \setminus v_m}$ with eigenvalue λ , for all eigenvectors $\mathbf{w}_\lambda \in \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. Hence using,

$$\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}} = \text{Ann}_{v_m}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A)$$

we see that $\{\text{Ann}_{v_m}(\mathbf{w}_\lambda)\}_{\lambda \in I}$ are eigenvectors that are spanning the subspace $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}}$. Furthermore, all eigenvectors $\{\mathbf{w}_\lambda\}_{\lambda \in I}$ contain both positive and negative entries because, by the A -coprobability of v_i and v_j in G , they are orthogonal to the Perron-Frobenius eigenvector of A . In particular, this implies that the eigenvectors $\{\text{Ann}_{v_m}(\mathbf{w}_\lambda)\}_{\lambda \in I}$ of $A_{G \setminus v_m}$ also contain both positive and negative entries and hence, are orthogonal to the Perron-Frobenius eigenvector of $A_{G \setminus v_m}$. Thus, the Perron-Frobenius eigenvector of $A_{G \setminus v_m}$ is orthogonal to $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}}$ and so we conclude that v_i and v_j are A -coprobable in $G \setminus v_m$ as well.

Now, if v_i and v_j were A -cospectral, then we would have $\mathbf{v}_i + \mathbf{v}_j \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. By $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}} = \text{Ann}_{v_m}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A)$, this implies $\mathbf{v}_i + \mathbf{v}_j \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}}$ and consequently,

$$\langle \mathbf{v}_i + \mathbf{v}_j \rangle_{A_{G \setminus v_m}} \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}}$$

as well. Therefore, we would see that v_i and v_j are A -cospectral in $G \setminus v_m$ also.

For the converse side, suppose that v_i and v_j are A -coprobable in G and suppose that there exist vertices $\{v_\ell\}_{\ell \in I}$ such that

$$\sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A.$$

Consider the graph $G + v$ with an extra vertex v connected to vertices $\{v_\ell\}_{\ell \in I}$. We will again show by induction that for all $k \in \mathbb{N}$:

1. $A^k(\mathbf{v}_i - \mathbf{v}_j) = \text{Ann}_v(A_{G+v}^k(\mathbf{v}_i - \mathbf{v}_j))$
2. $(A_{G+v}^k(\mathbf{v}_i - \mathbf{v}_j))_v = 0$

where A_{G+v} denotes the adjacency matrix of $G + v$.

Base Case $k = 0$: Trivial.

Inductive Step: Assume the case $k = n - 1$. We will prove case $k = n$. For (2), we have

$$(A_{G+v}^n(\mathbf{v}_i - \mathbf{v}_j))_v = \sum_{v_\ell \sim v} (A_{G+v}^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell}.$$

Since $v_\ell \sim v$ if and only if $\ell \in I$ by construction and using **induction hypothesis (1)**, this summation becomes:

$$\begin{aligned} \sum_{v_\ell \sim v} (A_{G+v}^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} &= \sum_{\ell \in I} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} = \\ &= \sum_{\ell \in I} (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))^T \mathbf{v}_\ell = (A^{n-1}(\mathbf{v}_i - \mathbf{v}_j))^T \sum_{\ell \in I} \mathbf{v}_\ell = 0 \end{aligned}$$

where the last equality is by $\sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$. For (1), using **induction hypothesis (1)** we have

$$\begin{aligned} A^n(\mathbf{v}_i - \mathbf{v}_j) &= A(\text{Ann}_v(A_{G+v}^{n-1}(\mathbf{v}_i - \mathbf{v}_j))) = \\ &= \text{Ann}_v(A_{G+v}^n(\mathbf{v}_i - \mathbf{v}_j)) - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v}} (A_{G+v}^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} \mathbf{v} - \sum_{\substack{v_\ell \in V(G) \\ v_\ell \sim v}} (A_{G+v}^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_v \mathbf{v}_\ell \end{aligned}$$

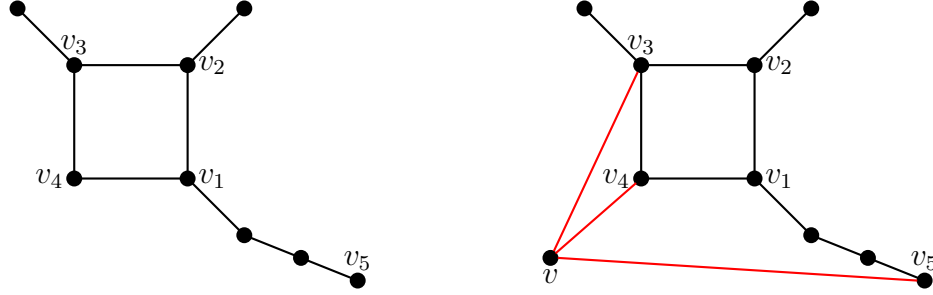


Figure 4.13: An example to Lemma 4.3.1. Here the vertices v_1 and v_2 are A -cospectral and the added vertex v preserves this cospectrality.

By **induction hypothesis (2)**, the last term is zero. The second term is zero since we have just shown

$$\sum_{v_\ell \sim v} (A_{G+v}^{n-1}(\mathbf{v}_i - \mathbf{v}_j))_{v_\ell} = (A_{G+v}^n(\mathbf{v}_i - \mathbf{v}_j))_v = 0$$

so we conclude $A^n(\mathbf{v}_i - \mathbf{v}_j) = \text{Ann}_v(A_{G+v}^n(\mathbf{v}_i - \mathbf{v}_j))$, finishing the induction. Now clearly,

$$A^k(\mathbf{v}_i - \mathbf{v}_j) = \text{Ann}_v(A_{G+v}^k(\mathbf{v}_i - \mathbf{v}_j)), \quad \forall k \in \mathbb{N}$$

implies $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A = \text{Ann}_v(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G+v}})$. To conclude that v_i and v_j are A -coprobable, note again by Lemma 3.2.2 that $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ is spanned by a subset of eigenvectors $\{\mathbf{w}_\lambda\}_{\lambda \in I}$ of A , all of which have different eigenvalues. Clearly, since $\sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ we have to have $(\mathbf{w}_\lambda)^T \sum_{\ell \in I} \mathbf{v}_\ell = 0$ for all $\lambda \in I$. Thus, defining the vector $\hat{\mathbf{w}}_\lambda$, $\forall \lambda \in I$ for all $v' \in V(G+v)$ by

$$(\hat{\mathbf{w}}_\lambda)_{v'} = \begin{cases} (\mathbf{w}_\lambda)_{v_s} & \text{if } v' = v_s \in V(G) \\ 0 & \text{if } v' = v \end{cases}$$

we see that $\hat{\mathbf{w}}_\lambda$ is an eigenvector of A_{G+v} with eigenvalue λ . The rest of the proof is identical to that of vertex deletion. $\square$

Example 4.3.2. An example for Lemma 4.3.1 is seen in Figure 4.13. In the left graph, vertices v_1 and v_2 are A -cospectral. Since the subspace $\langle \mathbf{v}_1 - \mathbf{v}_2 \rangle_A$ is orthogonal to the vector $\mathbf{v}_3 + \mathbf{v}_4 + \mathbf{v}_5$ in this graph, we can construct the graph on the right where the extra edges are indicated in red. By the lemma, v_1 and v_2 are A -cospectral in the right graph too.

Definition 4.3.3. (0-nodes) Let G be a graph. Vertices $v_m \in V(G)$ satisfying $\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ are called 0-nodes of G with respect to the pair (v_i, v_j) or just 0-nodes of G . We denote the set of all 0-nodes by $V^0(v_i, v_j)$ or just V^0 .

Remark 4.3.4. It is clear that a vertex v_m being a 0-node with respect to (v_i, v_j) is preserved by addition/deletion of other vertices. This is because, by the proof of Lemma 4.3.1,

$$\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{G \setminus v_\ell} = \text{Ann}_{v_\ell}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_G) \quad \text{and} \quad \langle \mathbf{v}_i - \mathbf{v}_j \rangle_G = \text{Ann}_{v_\ell}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{G+v})$$

for deleted vertex $v_\ell \in V(G)$ and added vertex v . Hence, we still have

$$\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{G \setminus v_\ell} \quad \text{or} \quad \mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{G+v}$$

in the graphs $G \setminus v_\ell$ and $G + v$.

By the below lemma, we have that a vertex v added by the operation in Lemma 4.3.1 is also a 0-node of $G + v$ with respect to (v_i, v_j) .

Lemma 4.3.5. *Let G be a graph, let v_i, v_j be A -coprable vertices and let v be a vertex added to G by the vertex addition operation of Lemma 4.3.1. Then v is a 0-node of $G + v$ with respect to (v_i, v_j) .*

Proof. Since v is connected to vertices $\{v_\ell\}_{\ell \in I}$ such that

$$\sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$$

and since by the proof of Lemma 4.3.1 we have

$$\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A = \text{Ann}_v(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G+v}}),$$

we also have that

$$\sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G+v}}$$

or equivalently,

$$\sum_{\ell \in I} \mathbf{v}_\ell \perp A_{G+v}^k(\mathbf{v}_i - \mathbf{v}_j), \quad \forall k \in \mathbb{N}$$

Using this, we have $\forall k \in \mathbb{N}$,

$$\left(\sum_{\ell \in I} \mathbf{v}_\ell \right)^T A_{G+v}^k (\mathbf{v}_i - \mathbf{v}_j) = (A_{G+v} \mathbf{v})^T (A_{G+v}^k (\mathbf{v}_i - \mathbf{v}_j)) = \mathbf{v}^T A_{G+v}^{k+1} (\mathbf{v}_i - \mathbf{v}_j) = 0.$$

where the first equality is by the definition of vertex addition and the second is by undirectedness. Thus $\mathbf{v}^T A_{G+v}^k (\mathbf{v}_i - \mathbf{v}_j) = 0$ for $k = 1, \dots, N+1$. Since $\mathbf{v}^T (\mathbf{v}_i - \mathbf{v}_j) = 0$ is obvious, we have

$$\mathbf{v} \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G+v}}$$

as was claimed. $\square$

The following lemma is more or less clear.

Lemma 4.3.6. *Let G be a graph, let v_i and v_j be A -coprable (A -cospectral) vertices and let $V^0(v_i, v_j)$ be the set of 0-nodes of G with respect to (v_i, v_j) . Now let $G+v$ be the graph constructed by adding a vertex v to G by connecting it to a subset of 0-nodes $S \subseteq V^0(v_i, v_j)$. Then v_i and v_j are A -coprable (A -cospectral) in $G+v$ and v is a 0-node with respect to (v_i, v_j) .*

Proof. By Lemma 4.3.1 and Lemma 4.3.5 we need only show that

$$\sum_{v_\ell \in S} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$$

But $\forall v_\ell \in V^0(v_i, v_j)$, we have

$$\mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A.$$

The claim follows directly by noting $S \subseteq V^0(v_i, v_j)$. $\square$

Corollary 4.3.7. *Let G be a graph, let v_i and v_j be A -coprable (A -cospectral) vertices and let H be another graph. Let $\tilde{G}$ be a graph constructed by attaching H to the 0-nodes of G with respect to (v_i, v_j) in an arbitrary way; that is, by connecting a subset $S \subseteq V(H)$ of vertices of H to a subset $R \subseteq V^0$ of 0-nodes of G through a subset of $S \times R$. Then, v_i and v_j are A -coprable (A -cospectral) in $\tilde{G}$ and all of $V(H) \subseteq V(\tilde{G})$ are 0-nodes of $\tilde{G}$.*

Proof. Follows directly from Lemma 4.3.6 and Remark 4.3.4. $\square$

When v_i and v_j are A -cospectral, a further operation which will be relevant below, preserves the 0-nodes.

Lemma 4.3.8. *Let $G(V, E)$ be a graph and let v_i and v_j be A -cospectral vertices in G . Let $v_m \in V^0$ be a 0-node of G with respect to (v_i, v_j) that does not have an edge with neither v_i nor v_j . Now, let $\tilde{G}(V, E)$ be the graph defined by $V(\tilde{G}) = V(G)$ and $E(\tilde{G}) = E(G) \cup \{(v_m, v_i), (v_i, v_m), (v_j, v_m), (v_m, v_j)\}$, i.e. with the same vertex set and with the same edge set, except from extra edges between v_m and v_i, v_j . Then, v_i and v_j are A -cospectral in $\tilde{G}$ and v_m is a 0-node in $\tilde{G}$.*

Proof. Let $\{v_\ell\}_{\ell \in I}$ be the set of vertices in G that v_m is connected to. Since v_m is a 0-node in G , we can take it out without affecting the cospectrality of v_i and v_j by Lemma 4.3.1. Furthermore, by the proof of the lemma we have $\text{Ann}_{v_m}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A) = \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}}$. Now, since we have $A\mathbf{v}_m = \sum_{\ell \in I} \mathbf{v}_\ell \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ and $\mathbf{v}_i + \mathbf{v}_j \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ by the definition of v_m and the cospectrality of v_i and v_j ; we can claim that

$$\sum_{\ell \in I \cup \{i, j\}} \mathbf{v}_\ell = \left(\sum_{\ell \in I} \mathbf{v}_\ell \right) + \mathbf{v}_i + \mathbf{v}_j \perp \text{Ann}_{v_m}(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_A) = \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{A_{G \setminus v_m}}$$

Hence, again by Lemma 4.3.1 we can add v_m back to the graph $G \setminus v_m$, this time through the set $\{v_\ell\}_{\ell \in I} \cup \{v_i, v_j\}$. The claim follows from Lemma 4.3.1 and 4.3.5. $\square$

We have an important theorem regarding 0-nodes and the vertex deletion operation of Lemma 4.3.1 when the vertices are A -cospectral. The proof of the lemma comprises the essential part of the proof of Theorem 4.3.10.

Lemma 4.3.9 (A -cospectral). *Let G be a graph and let v_i and v_j be A -cospectral vertices. Suppose that $v_m \in V^0$ is a 0-node of G with respect to (v_i, v_j) . Now, let $G_i := G \setminus v_i$ and $G_j := G \setminus v_j$. Since v_i and v_j are A -cospectral, we have that the spectrum of A_i and A_j , counting multiplicity, are the same; call it Λ . Hence, for an eigenvalue λ of A_i and A_j of order r , λ has r copies in Λ . Now, for any*

$\lambda \in \Lambda$, consider the unit eigenvectors corresponding to λ with respect to both A_i and A_j . Denote these eigenvectors by $\mathbf{w}_\lambda^i$ and $\mathbf{w}_\lambda^j$ respectively. Then, there exists orthonormal eigenbases $\{\mathbf{w}_\lambda^i\}_{\lambda \in \Lambda}$ and $\{\mathbf{w}_\lambda^j\}_{\lambda \in \Lambda}$ for A_i and A_j such that $\forall \lambda \in \Lambda$, we have

$$(\mathbf{w}_\lambda^i)_{v_j} = (\mathbf{w}_\lambda^j)_{v_i} \quad \text{and} \quad (\mathbf{w}_\lambda^i)_{v_m} = (\mathbf{w}_\lambda^j)_{v_m}$$

Proof. Since the vertex v_m is a 0-node, it satisfies $\mathbf{v}_m \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$ and hence the relation

$$(A^k)_{v_i, v_m} = (A^k)_{v_j, v_m} \quad \forall k \in \mathbb{N}.$$

Furthermore, since v_i and v_j are A -cospectral, we also have

$$(A^k)_{v_i, v_i} = (A^k)_{v_j, v_j} \quad \forall k \in \mathbb{N}$$

by Theorem 3.6.3. Now, we will firstly show

$$((A_j)^k)_{v_i, v_i} = ((A_i)^k)_{v_j, v_j}, \quad \forall k \in \mathbb{N}.$$

Let $W_{v_a, v_b}(k)$ denote the number of paths from v_a to v_b of length k in the graph G . Let $W_{v_a, v_b; v_c}(k)$ denote the number of paths from v_a to v_b of length k not passing through v_c in between. (This means $W_{v_a, v_b; v_b}(k)$ is meaningful and describes the number of paths passing through v_b only at the end and not in between.) Similarly, define $W_{v_a, v_b; v_c, v_d}(k)$ to be the number of paths from v_a to v_b of length k not passing through v_c or v_d in between and so on. With this notation, the claim $((A_j)^k)_{v_i, v_i} = ((A_i)^k)_{v_j, v_j}$, $\forall k \in \mathbb{N}$ becomes

$$W_{v_i, v_i; v_j}(k) = W_{v_j, v_j; v_i}(k), \quad \forall k \in \mathbb{N}$$

The proof of the claim will be by strong induction.

Base case $k = 1$: Trivial, since $W_{v_i, v_i; v_j}(1) = W_{v_j, v_j; v_i}(1) = 0$.

Inductive Step: We assume cases $k = 1, 2, \dots, n-1$; we now prove the case $k = n$. We can rewrite $W_{v_i, v_i}(n)$ as follows:

$$W_{v_i, v_i}(n) = W_{v_i, v_i; v_j}(n) + \sum_{\substack{k_1 + k_2 + k_3 = n \\ k_1 \geq 0, k_2, k_3 \geq 1}} W_{v_i, v_i; v_j}(k_1) W_{v_i, v_j; v_i, v_j}(k_2) W_{v_j, v_i}(k_3)$$

where the first term $W_{v_i, v_i; v_j}(n)$ is the number of paths from v_i to v_i not passing through v_j , and the second term describes the number of paths from v_i to v_i passing through v_j . This second term can be explained as follows:

Any path from v_i to v_i passing through v_j can pass through v_i and v_j arbitrarily many times. However, all such paths can be uniquely divided into three parts:

1. A path from v_i to v_i not passing through v_j .
2. A path from v_i to v_j not passing through v_i or v_j in between.
3. A path from v_j to v_i .

This division can be constructed as follows. Consider a path γ from v_i to v_i passing through v_j . The path might pass through v_j multiple times, but there must be a unique first instance it passes through v_j . Since the path started at v_i , there also has to exist a unique last instance that the path passes through v_i , before passing through the first v_j . These two instances divide the path into three unique parts shown in Figure 4.14. By construction, the first part is a path from v_i to v_i not passing through v_j since it comprises the path before the first instance of passing through v_j . The second part is a path from v_i to v_j not passing through v_i or v_j in between since the first instance of passing through v_j is at the end of this path and the last instance of passing through v_i before the first v_j , is at the beginning of this path. Finally, the third part is a path from v_j to v_i without any constraint.

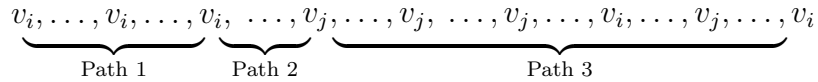


Figure 4.14: A hypothetical path with all stops at v_i and v_j shown. The division of the path into three unique parts can easily be seen.

Now, rewriting $W_{v_j, v_j}(n)$ similarly to $W_{v_i, v_i}(n)$, we obtain:

$$W_{v_i, v_i}(n) = W_{v_i, v_i; v_j}(n) + \sum_{\substack{k_1 + k_2 + k_3 = n \\ k_1 \geq 0, k_2, k_3 \geq 1}} W_{v_i, v_i; v_j}(k_1) W_{v_i, v_j; v_i, v_j}(k_2) W_{v_j, v_i}(k_3).$$

$$W_{v_j, v_j}(n) = W_{v_j, v_j; v_i}(n) + \sum_{\substack{k_1 + k_2 + k_3 = n \\ k_1 \geq 0, k_2, k_3 \geq 1}} W_{v_j, v_j; v_i}(k_1) W_{v_j v_i; v_j v_i}(k_2) W_{v_i, v_j}(k_3).$$

Now, we have $W_{v_i, v_i}(n) = W_{v_j, v_j}(n)$ by A -cospectrality. In the second term, we have

$$W_{v_i, v_i; v_j}(k_1) = W_{v_j, v_j; v_i}(k_1), \quad \forall k_1 \in \{0, 1, \dots, n-1\}$$

by strong induction ($k_1 < n$ since $k_2, k_3 \geq 1$). We also have

$$W_{v_i, v_j; v_i, v_j}(k_2) = W_{v_j, v_i; v_j, v_i}(k_2)$$

since by undirectedness, there is a bijective correspondence between paths from v_i to v_j not passing through v_i and v_j in between, and paths from v_j to v_i not passing through v_i and v_j in between. Finally, we also have

$$W_{v_j, v_i}(k_3) = W_{v_i, v_j}(k_3)$$

again, by undirectedness. Hence, the second terms are also equal, and so we have

$$W_{v_i, v_i; v_j}(n) = W_{v_j, v_j; v_i}(n)$$

which completes the induction. Now, in a similar way we will show

$$((A_i)^k)_{v_j, v_m} = ((A_j)^k)_{v_i, v_m}, \quad \forall k \in \mathbb{N}$$

With the previous notation, this is equivalent to $W_{v_j, v_m; v_i}(k) = W_{v_i, v_m; v_j}(k)$ for all $k \in \mathbb{N}$. Like before, we can rewrite $W_{v_i, v_m}(k)$ and $W_{v_j, v_m}(k)$ as:

$$W_{v_i, v_m}(k) = W_{v_i, v_m; v_j}(k) + \sum_{\substack{k_1 + k_2 + k_3 = k \\ k_1 \geq 0, k_2, k_3 \geq 1}} W_{v_i, v_i; v_j}(k_1) W_{v_i, v_j; v_i, v_j}(k_2) W_{v_j, v_m}(k_3)$$

and similarly,

$$W_{v_j, v_m}(k) = W_{v_j, v_m; v_i}(k) + \sum_{\substack{k_1 + k_2 + k_3 = k \\ k_1 \geq 0, k_2, k_3 \geq 1}} W_{v_j, v_j; v_i}(k_1) W_{v_j, v_i; v_j, v_i}(k_2) W_{v_i, v_m}(k_3)$$

Now, we have for all appropriate $k, k_1, k_2 \in \mathbb{N}$:

$$W_{v_i, v_m}(k) = W_{v_j, v_m}(k) \quad (\text{by } v_m \text{ being a 0-node, } (A^k)_{v_i, v_m} = (A^k)_{v_j, v_m})$$

$$W_{v_i, v_i; v_j}(k_1) = W_{v_j, v_j; v_i}(k_1) \quad (\text{Proved above})$$

$$W_{v_i, v_j; v_i, v_j}(k_2) = W_{v_j, v_i; v_i, v_j}(k_2) \quad (\text{Undirectedness})$$

Hence, we obtain $W_{v_i, v_m; v_j}(k) = W_{v_j, v_m; v_i}(k)$, $\forall k \in \mathbb{N}$. Lastly, we will show

$$((A_i)^k)_{v_m, v_\ell} = ((A_j)^k)_{v_m, v_\ell} \quad \forall k \in \mathbb{N}$$

where $v_\ell \in V^0$ is a 0-node of G , possibly the same as v_m . With the previous notation, this is equivalent to $W_{v_m, v_\ell; v_i}(k) = W_{v_m, v_\ell; v_j}(k)$ for all $k \in \mathbb{N}$. We now rewrite $W_{v_m, v_\ell}(k)$ in two different ways as:

$$\begin{aligned} W_{v_m, v_\ell}(k) &= W_{v_m, v_\ell; v_j}(k) + \sum_{\substack{k_1+k_2=k \\ k_1, k_2 \geq 1}} W_{v_m, v_j; v_j}(k_1) W_{v_j, v_\ell}(k_2) \\ W_{v_m, v_\ell}(k) &= W_{v_m, v_\ell; v_i}(k) + \sum_{\substack{k_1+k_2=k \\ k_1, k_2 \geq 1}} W_{v_m, v_i; v_i}(k_1) W_{v_i, v_\ell}(k_2) \end{aligned}$$

where the second terms are constructed by the fact that paths from v_m to v_ℓ passing through v_j can be uniquely factorized into a path from v_m to v_j not passing through v_j and a path from v_j to v_ℓ without any constraint. Now, we will again apply a strong induction on k in order to show $W_{v_m, v_\ell; v_i}(k) = W_{v_m, v_\ell; v_j}(k)$ for all $k \in \mathbb{N}$. Since the left sides of the equations $W_{v_m, v_\ell}(k)$ are already equal, we need only show $W_{v_j, v_\ell}(k_2) = W_{v_i, v_\ell}(k_2)$ and $W_{v_m, v_j; v_j}(k_1) = W_{v_m, v_i; v_i}(k_1)$. Since v_ℓ is a 0-node, we have $W_{v_j, v_\ell}(k_2) = W_{v_i, v_\ell}(k_2) \quad \forall k_2 \in \mathbb{N}$. For $W_{v_m, v_j; v_j}(k_1) = W_{v_m, v_i; v_i}(k_1)$, let $r = k_1 < k$. We will prove the claim $W_{v_m, v_i; v_i}(r) = W_{v_m, v_j; v_j}(r)$ by applying another strong induction on r , nested within the strong induction on k ; which we are able to do because we have $r < k$. We have

$$W_{v_m, v_j}(r) = W_{v_m, v_j; v_j}(r) + \sum_{\substack{r_1+r_2+r_3=r \\ r_1 \geq 0, r_2, r_3 \geq 1}} W_{v_m, v_m; v_j}(r_1) W_{v_m, v_j; v_j}(r_2) W_{v_j, v_j}(r_3)$$

and

$$W_{v_m, v_i}(r) = W_{v_m, v_i; v_i}(r) + \sum_{\substack{r_1+r_2+r_3=r \\ r_1 \geq 0, r_2, r_3 \geq 1}} W_{v_m, v_m; v_i}(r_1) W_{v_m, v_i; v_i}(r_2) W_{v_i, v_i}(r_3)$$

the same way as explained in Figure 4.14. Since v_i and v_j are A -cospectral and since v_m is a 0-node, we have $W_{v_m, v_j}(r) = W_{v_m, v_i}(r)$ and $W_{v_j, v_j}(r_3) = W_{v_i, v_i}(r_3)$. We have $W_{v_m, v_i; v_i}(r_2) = W_{v_m, v_j; v_j}(r_2)$ by strong induction on r since $r_2 < r$. Lastly

since we have $r_1 < r < k$, by the strong induction on k we have $W_{v_m, v_m; v_i}(r_1) = W_{v_m, v_m; v_j}(r_1)$ where $v_\ell = v_m$.

Hence, we conclude $W_{v_m, v_i; v_i}(r) = W_{v_m, v_j; v_j}(r) \quad \forall r < k$ by the strong induction on r and using this, we have $W_{v_m, v_\ell; v_i}(k) = W_{v_m, v_\ell; v_j}(k)$, $\forall k \in \mathbb{N}$ by the strong induction on k .

We have now shown, for all $k \in \mathbb{N}$ and 0-nodes $v_m, v_\ell \in V^0$:

$$W_{v_i, v_m; v_j}(k) = W_{v_j, v_m; v_i}(k)$$

$$W_{v_i, v_i; v_j}(k) = W_{v_j, v_j; v_i}(k)$$

$$W_{v_m, v_\ell; v_j}(k) = W_{v_m, v_\ell; v_i}(k)$$

which are equivalent to

$$((A_j)^k)_{v_i, v_m} = ((A_i)^k)_{v_j, v_m},$$

$$((A_j)^k)_{v_i, v_i} = ((A_i)^k)_{v_j, v_j},$$

$$((A_j)^k)_{v_m, v_\ell} = ((A_i)^k)_{v_m, v_\ell}.$$

These are equivalent to

$$(E_\lambda^{A_j})_{v_i, v_m} = (E_\lambda^{A_i})_{v_j, v_m}$$

$$(E_\lambda^{A_j})_{v_i, v_i} = (E_\lambda^{A_i})_{v_j, v_j},$$

$$(E_\lambda^{A_j})_{v_m, v_\ell} = (E_\lambda^{A_i})_{v_m, v_\ell}.$$

$\forall \lambda \in \Lambda$, where $E_\lambda^{A_i}$ and $E_\lambda^{A_j}$ denote the orthogonal projection onto the λ -eigenspace of A_i and A_j , respectively. Now to finally prove the lemma, we consider the eigenvalues and eigenspaces. Let $\lambda \in \Lambda$ be an eigenvalue with order $r > 1$. Let $\mathbf{w}_1^i, \mathbf{w}_2^i, \dots, \mathbf{w}_r^i$ and $\mathbf{w}_1^j, \mathbf{w}_2^j, \dots, \mathbf{w}_r^j$ be λ -eigenvectors of respectively A_i and A_j , forming an orthonormal basis of the λ -eigenspace. Here the λ subscript is not shown for notational clarity. We will show the existence of the said eigenbasis only for the eigenspace of λ , the rest of the claim follows since the orthonormal eigenbases of all eigenspaces together make up an orthonormal eigenbasis of the whole space. The claim of the lemma is now equivalent to showing that these

eigenvectors can be chosen such that $(\mathbf{w}_k^i)_{v_m} = (\mathbf{w}_k^j)_{v_m}$ and $(\mathbf{w}_k^j)_{v_i} = (\mathbf{w}_k^i)_{v_j}$. Now, since $\{\mathbf{w}_k^i\}_{k=1,\dots,r}$ and $\{\mathbf{w}_k^j\}_{k=1,\dots,r}$ form orthonormal bases, we have

$$E_\lambda^{A_i} = \mathbf{w}_1^i(\mathbf{w}_1^i)^T + \dots + \mathbf{w}_r^i(\mathbf{w}_r^i)^T$$

$$E_\lambda^{A_j} = \mathbf{w}_1^j(\mathbf{w}_1^j)^T + \dots + \mathbf{w}_r^j(\mathbf{w}_r^j)^T$$

Hence, $(E_\lambda^{A_j})_{v_m, v_m} = (E_\lambda^{A_i})_{v_m, v_m}$ implies that

$$(\mathbf{w}_1^j)_{v_m}^2 + (\mathbf{w}_2^j)_{v_m}^2 + \dots + (\mathbf{w}_r^j)_{v_m}^2 = (\mathbf{w}_1^i)_{v_m}^2 + (\mathbf{w}_2^i)_{v_m}^2 + \dots + (\mathbf{w}_r^i)_{v_m}^2$$

If for all $\mathbf{w}_k^i$, we have $(\mathbf{w}_k^i)_{v_m} = 0$ then clearly we have $(\mathbf{w}_k^j)_{v_m} = (\mathbf{w}_k^i)_{v_m} = 0$ for all $\mathbf{w}_k^j$. If for any one of $\mathbf{w}_k^i$ we have $(\mathbf{w}_k^i)_{v_m} \neq 0$, we can rechoose the orthonormal eigenvectors (so that they remain orthonormal) by taking a linear combination such that they satisfy

$$(\mathbf{w}_1^i)_{v_m} \neq 0, (\mathbf{w}_k^i)_{v_m} = 0, \quad \forall k \in \{2, \dots, r\}.$$

Similarly we can choose

$$(\mathbf{w}_1^j)_{v_m} \neq 0, (\mathbf{w}_k^j)_{v_m} = 0, \quad \forall k \in \{2, \dots, r\}.$$

Thus, with this choice we trivially have $(\mathbf{w}_k^i)_{v_m} = (\mathbf{w}_k^j)_{v_m}$, $\forall k \in \{2, \dots, r\}$. We also have that

$$(\mathbf{w}_1^i)_{v_m}^2 + (\mathbf{w}_2^i)_{v_m}^2 + \dots + (\mathbf{w}_r^i)_{v_m}^2 = (\mathbf{w}_1^j)_{v_m}^2 + (\mathbf{w}_2^j)_{v_m}^2 + \dots + (\mathbf{w}_r^j)_{v_m}^2$$

implies $(\mathbf{w}_1^i)_{v_m}^2 = (\mathbf{w}_1^j)_{v_m}^2$. By a suitable choice of $\mathbf{w}_1^i$ and $\mathbf{w}_1^j$, we would have $(\mathbf{w}_1^i)_{v_m} = (\mathbf{w}_1^j)_{v_m}$. In the case where all $\mathbf{w}_k^i, \mathbf{w}_k^j$, satisfy $(\mathbf{w}_k^i)_{v_m} = (\mathbf{w}_k^j)_{v_m} = 0$; this argument applied to

$$(E_\lambda^{A_j})_{v_i, v_i} = (E_\lambda^{A_i})_{v_j, v_j} =$$

$$= (\mathbf{w}_1^j)_{v_i}^2 + (\mathbf{w}_2^j)_{v_i}^2 + \dots + (\mathbf{w}_r^j)_{v_i}^2 = (\mathbf{w}_1^i)_{v_j}^2 + (\mathbf{w}_2^i)_{v_j}^2 + \dots + (\mathbf{w}_r^i)_{v_j}^2$$

proves the result $(\mathbf{w}_k^j)_{v_i} = (\mathbf{w}_k^i)_{v_j}$, $\forall k \in \{1, \dots, r\}$ and finishes the lemma.

Now, continuing the case where for at least one of $\mathbf{w}_k^i$ we have $(\mathbf{w}_k^i)_{v_m} \neq 0$; we use $(E_\lambda^{A_j})_{v_i, v_m} = (E_\lambda^{A_i})_{v_j, v_m}$. This equality implies in the same way as before,

$$(\mathbf{w}_1^j)_{v_i}(\mathbf{w}_1^j)_{v_m} + \dots + (\mathbf{w}_r^j)_{v_i}(\mathbf{w}_r^j)_{v_m} = (\mathbf{w}_1^i)_{v_j}(\mathbf{w}_1^i)_{v_m} + \dots + (\mathbf{w}_r^i)_{v_j}(\mathbf{w}_r^i)_{v_m}$$

Since $(\mathbf{w}_k^i)_{v_m} = (\mathbf{w}_k^j)_{v_m} = 0$, $\forall k \in \{2, \dots, r\}$ by our choice, we thus have $(\mathbf{w}_1^j)_{v_i}(\mathbf{w}_1^j)_{v_m} = (\mathbf{w}_1^i)_{v_j}(\mathbf{w}_1^i)_{v_m}$. Noting that we have $(\mathbf{w}_1^i)_{v_m} = (\mathbf{w}_1^j)_{v_m} \neq 0$ by choice also, we obtain $(\mathbf{w}_1^j)_{v_i} = (\mathbf{w}_1^i)_{v_j}$.

Now, if $r = 1$ or if we have $(\mathbf{w}_k^j)_{v_i} = (\mathbf{w}_k^i)_{v_j} = 0$, $\forall k \in \{2, \dots, r\}$, we are done. If not, then consider $(E_\lambda^{A_j})_{v_i, v_i} = (E_\lambda^{A_i})_{v_j, v_j}$. Similar to before, this implies

$$(\mathbf{w}_1^j)_{v_i}^2 + (\mathbf{w}_2^j)_{v_i}^2 + \dots + (\mathbf{w}_r^j)_{v_i}^2 = (\mathbf{w}_1^i)_{v_j}^2 + (\mathbf{w}_2^i)_{v_j}^2 + \dots + (\mathbf{w}_r^i)_{v_j}^2.$$

By $(\mathbf{w}_1^j)_{v_i} = (\mathbf{w}_1^i)_{v_j}$, this implies that there must exist both $k, \ell \in \{2, \dots, r\}$ such that $(\mathbf{w}_k^j)_{v_i}, (\mathbf{w}_\ell^i)_{v_j} \neq 0$. Then, we can rechoose the orthonormal eigenvectors $\{\mathbf{w}_k^i\}_{k=2, \dots, r}$ and $\{\mathbf{w}_k^j\}_{k=2, \dots, r}$ by taking a linear combination such that

$$(\mathbf{w}_k^j)_{v_i} = (\mathbf{w}_k^i)_{v_j} = 0, \quad \forall k \in \{3, \dots, r\}$$

and $(\mathbf{w}_2^j)_{v_i}, (\mathbf{w}_2^i)_{v_j} \neq 0$. This choice does not interfere with our previous construction satisfying $(\mathbf{w}_k^i)_{v_m} = (\mathbf{w}_k^j)_{v_m}$ for all $k \in \{1, \dots, r\}$, since we had

$$(\mathbf{w}_k^i)_{v_m} = (\mathbf{w}_k^j)_{v_m} = 0, \quad \forall k \in \{2, \dots, r\}.$$

With this choice, we have that

$$(\mathbf{w}_1^j)_{v_i}^2 + (\mathbf{w}_2^j)_{v_i}^2 + \dots + (\mathbf{w}_r^j)_{v_i}^2 = (\mathbf{w}_1^i)_{v_j}^2 + (\mathbf{w}_2^i)_{v_j}^2 + \dots + (\mathbf{w}_r^i)_{v_j}^2,$$

together with $(\mathbf{w}_1^j)_{v_i} = (\mathbf{w}_1^i)_{v_j}$, implies that

$$(\mathbf{w}_2^j)_{v_i}^2 = (\mathbf{w}_2^i)_{v_j}^2$$

and hence $(\mathbf{w}_2^j)_{v_i} = (\mathbf{w}_2^i)_{v_j}$ by a suitable choice of direction and concluding the proof. $\square$

With this lemma and the previous parts, the following theorem follows.

Theorem 4.3.10. *Let G be a graph with vertices $v_1, v_2, \dots, v_N \in V(G)$ and let v_i and v_j be A -cospectral vertices in G . Let H be another graph with vertices $v'_1, v'_2, \dots, v'_r \in V(H)$. Let $\tilde{G}$ be a graph constructed by attaching H to the 0-nodes of G with respect to (v_i, v_j) in an arbitrary way as explained in Corollary 4.3.7 and possibly further modified by adding edges pairwise between vertices $v'_\alpha \in V(H)$ and*

v_i, v_j as explained in Lemma 4.3.8. Finally select two vertices $v, \hat{v} \in V(H) \cup V^0$ where V^0 are the 0-nodes of G with respect to (v_i, v_j) . Now, let

$$\tilde{G}_i = \tilde{G} \setminus v_i, \quad \tilde{G}_j = \tilde{G} \setminus v_j.$$

Then, the adjacency matrices $\tilde{A}_i$ and $\tilde{A}_j$ of $\tilde{G}_i$ and $\tilde{G}_j$ share the same spectrum, counting multiplicity; we call it Λ . Hence, for an eigenvalue λ of A_i and A_j of order r , λ has r copies in Λ . Furthermore, there exists orthonormal eigenbases $\{\mathbf{w}_\lambda^i\}_{\lambda \in \Lambda}$ and $\{\mathbf{w}_\lambda^j\}_{\lambda \in \Lambda}$ of $\tilde{A}_i$ and $\tilde{A}_j$, for which eigenvectors $\mathbf{w}_\lambda^i$ and $\mathbf{w}_\lambda^j$ corresponding to the same eigenvalue λ satisfy

$$(\mathbf{w}_\lambda^i)_{v_j} = (\mathbf{w}_\lambda^j)_{v_i}, \quad (\mathbf{w}_\lambda^i)_v = (\mathbf{w}_\lambda^j)_v, \quad (\mathbf{w}_\lambda^i)_{\hat{v}} = (\mathbf{w}_\lambda^j)_{\hat{v}}$$

Proof. By Corollary 4.3.7 and Lemma 4.3.8 we have

$$V(H) \cup V^0 \subseteq \tilde{V}^0(v_i, v_j) \quad (\text{In fact, this is an equality by exclusion})$$

where $\tilde{V}^0(v_i, v_j)$ denotes the set of 0-nodes of $\tilde{G}$ with respect to (v_i, v_j) . Now, let $\lambda \in \Lambda$ be an eigenvalue of $\tilde{A}_i$ and $\tilde{A}_j$ of order r . We will show the existence of the said eigenbasis only for the eigenspace of λ , the rest of the claim follows since the orthonormal eigenbases of all eigenspaces together make up an orthonormal eigenbasis of the whole space. Clearly, if $r = 1$ the claim follows immediately from Lemma 4.3.9. If not, by Lemma 4.3.9 there exists orthonormal eigenbases $\{\mathbf{w}_k^i\}_{k=1, \dots, r}$ and $\{\mathbf{w}_k^j\}_{k=1, \dots, r}$ for the λ -eigenspaces of $\tilde{A}_i$ and $\tilde{A}_j$ such that $(\mathbf{w}_k^i)_v = (\mathbf{w}_k^j)_v$ and $(\mathbf{w}_k^i)_{v_j} = (\mathbf{w}_k^j)_{v_i}$ for all $k \in \{1, \dots, r\}$. By the proof of Lemma 4.3.9, we have constructed these eigenvectors so that they satisfy

$$(\mathbf{w}_1^i)_{v_j} = (\mathbf{w}_1^j)_{v_i} \neq 0, \quad (\mathbf{w}_2^i)_{v_j} = (\mathbf{w}_2^j)_{v_i} \neq 0, \quad (\mathbf{w}_k^i)_{v_j} = (\mathbf{w}_k^j)_{v_i} = 0, \quad \forall k \in \{3, \dots, r\}$$

$$(\mathbf{w}_1^i)_v = (\mathbf{w}_1^j)_v \neq 0, \quad (\mathbf{w}_k^i)_v = (\mathbf{w}_k^j)_v = 0, \quad \forall k \in \{2, \dots, r\}.$$

We had also shown that

$$(E_\lambda^{\tilde{A}_j})_{\tilde{v}_m, \tilde{v}_\ell} = (E_\lambda^{\tilde{A}_i})_{\tilde{v}_m, \tilde{v}_\ell}$$

for all 0-nodes $\tilde{v}_m, \tilde{v}_\ell \in \tilde{V}^0(v_i, v_j)$ where $E_\lambda^{\tilde{A}_i}$ and $E_\lambda^{\tilde{A}_j}$ are the orthogonal projections onto the λ -eigenspaces of $\tilde{A}_i$ and $\tilde{A}_j$, respectively. We have additionally put

tildes on the vertices and adjacency matrices for notational consistency. Now, we consider specifically the 0-nodes $v, \hat{v} \in \tilde{V}^0(v_i, v_j)$, and so we have

$$(E_{\lambda}^{\tilde{A}_j})_{v, \hat{v}} = (E_{\lambda}^{\tilde{A}_i})_{v, \hat{v}}.$$

Since $\{\mathbf{w}_k^i\}_{k=1, \dots, r}$ and $\{\mathbf{w}_k^j\}_{k=1, \dots, r}$ form orthonormal bases for the λ -eigenspaces, we have

$$\begin{aligned} E_{\lambda}^{\tilde{A}_i} &= \mathbf{w}_1^i(\mathbf{w}_1^i)^T + \dots + \mathbf{w}_r^i(\mathbf{w}_r^i)^T \\ E_{\lambda}^{\tilde{A}_j} &= \mathbf{w}_1^j(\mathbf{w}_1^j)^T + \dots + \mathbf{w}_r^j(\mathbf{w}_r^j)^T. \end{aligned}$$

Therefore, the relation $(E_{\lambda}^{\tilde{A}_j})_{v, \hat{v}} = (E_{\lambda}^{\tilde{A}_i})_{v, \hat{v}}$ implies

$$(\mathbf{w}_1^j)_v(\mathbf{w}_1^j)_{\hat{v}} + \dots + (\mathbf{w}_r^j)_v(\mathbf{w}_r^j)_{\hat{v}} = (\mathbf{w}_1^i)_v(\mathbf{w}_1^i)_{\hat{v}} + \dots + (\mathbf{w}_r^i)_v(\mathbf{w}_r^i)_{\hat{v}}.$$

Since we have $(\mathbf{w}_k^i)_v = (\mathbf{w}_k^j)_v = 0$, $\forall k \in \{2, \dots, r\}$ and $(\mathbf{w}_1^i)_v = (\mathbf{w}_1^j)_v \neq 0$, this implies $(\mathbf{w}_1^i)_{\hat{v}} = (\mathbf{w}_1^j)_{\hat{v}}$. From the proof of Lemma 4.3.9 we also had

$$(E_{\lambda}^{\tilde{A}_j})_{v_i, \hat{v}} = (E_{\lambda}^{\tilde{A}_i})_{v_j, \hat{v}}.$$

In the same way as before, this implies

$$(\mathbf{w}_1^j)_{v_i}(\mathbf{w}_1^j)_{\hat{v}} + \dots + (\mathbf{w}_r^j)_{v_i}(\mathbf{w}_r^j)_{\hat{v}} = (\mathbf{w}_1^i)_{v_j}(\mathbf{w}_1^i)_{\hat{v}} + \dots + (\mathbf{w}_r^i)_{v_j}(\mathbf{w}_r^i)_{\hat{v}}.$$

Since we have $(\mathbf{w}_k^i)_{v_i} = (\mathbf{w}_k^j)_{v_j} = 0$, $\forall k \in \{3, \dots, r\}$ this simplifies to

$$(\mathbf{w}_1^j)_{v_i}(\mathbf{w}_1^j)_{\hat{v}} + (\mathbf{w}_2^j)_{v_i}(\mathbf{w}_2^j)_{\hat{v}} = (\mathbf{w}_1^i)_{v_j}(\mathbf{w}_1^i)_{\hat{v}} + (\mathbf{w}_2^i)_{v_j}(\mathbf{w}_2^i)_{\hat{v}}.$$

Since we also have $(\mathbf{w}_1^i)_{v_j} = (\mathbf{w}_1^j)_{v_i} \neq 0$, $(\mathbf{w}_2^i)_{v_j} = (\mathbf{w}_2^j)_{v_i} \neq 0$ and $(\mathbf{w}_1^i)_{\hat{v}} = (\mathbf{w}_1^j)_{\hat{v}}$; this equality implies $(\mathbf{w}_2^i)_{\hat{v}} = (\mathbf{w}_2^j)_{\hat{v}}$. Now, if $r = 2$ or if we have $(\mathbf{w}_k^i)_{\hat{v}} = (\mathbf{w}_k^j)_{\hat{v}} = 0$, $\forall k \in \{3, \dots, r\}$ we are done. If not, then there must exist $m, \ell \in \{3, \dots, r\}$ such that $(\mathbf{w}_m^i)_{\hat{v}} \neq 0$ and $(\mathbf{w}_\ell^j)_{\hat{v}} \neq 0$. Then we can rechoose the orthonormal eigenvectors $\{\mathbf{w}_k^i\}_{k=3, \dots, r}$ and $\{\mathbf{w}_k^j\}_{k=3, \dots, r}$ by taking a linear combination of them so that we have $(\mathbf{w}_k^i)_{\hat{v}} = (\mathbf{w}_k^j)_{\hat{v}} = 0$, $\forall k \in \{4, \dots, r\}$ and $(\mathbf{w}_3^i)_{\hat{v}} \neq 0$, $(\mathbf{w}_3^j)_{\hat{v}} \neq 0$. Since we had $(\mathbf{w}_k^i)_{v_j} = (\mathbf{w}_k^j)_{v_i} = 0$ and $(\mathbf{w}_k^i)_v = (\mathbf{w}_k^j)_v = 0$ for all $k \in \{3, \dots, r\}$, after rechoosing $\{\mathbf{w}_k^i\}_{k=3, \dots, r}$ and $\{\mathbf{w}_k^j\}_{k=3, \dots, r}$ we still have $(\mathbf{w}_k^i)_{v_j} = (\mathbf{w}_k^j)_{v_i} = 0$ and $(\mathbf{w}_k^i)_v = (\mathbf{w}_k^j)_v = 0$ for all $k \in \{3, \dots, r\}$. Finally, to show $(\mathbf{w}_3^i)_{\hat{v}} = (\mathbf{w}_3^j)_{\hat{v}}$, note that again, by Lemma 4.3.9 we have

$$(E_{\lambda}^{\tilde{A}_j})_{\hat{v}, \hat{v}} = (E_{\lambda}^{\tilde{A}_i})_{\hat{v}, \hat{v}}$$

which implies

$$(\mathbf{w}_1^j)_{\hat{v}}^2 + (\mathbf{w}_2^j)_{\hat{v}}^2 + \cdots + (\mathbf{w}_r^j)_{\hat{v}}^2 = (\mathbf{w}_1^i)_{\hat{v}}^2 + (\mathbf{w}_2^i)_{\hat{v}}^2 + \cdots + (\mathbf{w}_r^i)_{\hat{v}}^2.$$

Since we have $(\mathbf{w}_1^i)_{\hat{v}} = (\mathbf{w}_1^j)_{\hat{v}}$, $(\mathbf{w}_2^i)_{\hat{v}} = (\mathbf{w}_2^j)_{\hat{v}}$ and $(\mathbf{w}_k^i)_{\hat{v}} = (\mathbf{w}_k^j)_{\hat{v}} = 0$, $\forall k \in \{4, \dots, r\}$; this equality implies, by a suitable choice of direction, $(\mathbf{w}_3^i)_{\hat{v}} = (\mathbf{w}_3^j)_{\hat{v}}$. This proves the claim. $\square$

It more or less clear that the proofs of Lemma 4.3.9 and Theorem 4.3.10 can be similarly continued in order to extend Theorem 4.3.10 from two vertices $v, \hat{v} \in V(H) \cup V^0$ to an arbitrary subset of $S \subseteq V(H) \cup V^0$. The true meaning of this becomes apparent with the following corollary.

Corollary 4.3.11. *Let G be a graph with vertices $v_1, v_2, \dots, v_N \in V(G)$ and let v_i and v_j be A -cospectral vertices in G . Let H be another graph with vertices $v'_1, v'_2, \dots, v'_r \in V(H)$. Let $\tilde{G}$ be a graph constructed by attaching H to the 0-nodes of G with respect to (v_i, v_j) in an arbitrary way as explained in Corollary 4.3.7 and possibly further modified by adding edges pairwise between vertices $v'_\alpha \in V(H)$ and v_i, v_j as explained in Lemma 4.3.8. Now, let*

$$\tilde{G}_i = \tilde{G} \setminus v_i, \quad \tilde{G}_j = \tilde{G} \setminus v_j.$$

Let $N = |V(\tilde{G}_i)| = |V(\tilde{G}_j)|$ and let $\mathbf{x} \in \mathbb{R}^N$ be a vector, whose only non-zero components are those associated with vertices $V(H) \cup V^0$ where V^0 are the 0-nodes of G with respect to (v_i, v_j) . In other words the vector $\mathbf{x}$ is such that if $(\mathbf{x})_v \neq 0$ for some $v \in V(\tilde{G})$, then we have $v \in V(H) \cup V^0$.

Then, we have $((\tilde{A}_i)^k \mathbf{x})_{\hat{v}} = ((\tilde{A}_j)^k \mathbf{x})_{\hat{v}}$ for all $\hat{v} \in V(H) \cup V^0$.

Proof. Let $v, \hat{v} \in V(H) \cup V^0$ two vertices. By Theorem 4.3.10 we get orthonormal eigenbases $\{\mathbf{w}_\lambda^i\}_{\lambda \in \Lambda}$ and $\{\mathbf{w}_\lambda^j\}_{\lambda \in \Lambda}$ of $\tilde{A}_i$ and $\tilde{A}_j$ where the set Λ contains the eigenvalues of $\tilde{A}_i$ and $\tilde{A}_j$, counting multiplicity. Furthermore, by Theorem 4.3.10 eigenvectors $\mathbf{w}_\lambda^i$ and $\mathbf{w}_\lambda^j$ corresponding to the same eigenvalue λ satisfy

$$(\mathbf{w}_\lambda^i)_v = (\mathbf{w}_\lambda^j)_v, \quad (\mathbf{w}_\lambda^i)_{\hat{v}} = (\mathbf{w}_\lambda^j)_{\hat{v}}.$$

Since $\{\mathbf{w}_\lambda^i\}_{\lambda \in \Lambda}$ and $\{\mathbf{w}_\lambda^j\}_{\lambda \in \Lambda}$ are orthonormal eigenbases, we can decompose the vector $\mathbf{v}$ with respect to these bases as

$$\begin{aligned}\mathbf{v} &= \sum_{\lambda \in \Lambda} (\mathbf{w}_\lambda^i)^T \mathbf{v} \mathbf{w}_\lambda^i = \sum_{\lambda \in \Lambda} (\mathbf{w}_\lambda^i)_v \mathbf{w}_\lambda^i \\ \mathbf{v} &= \sum_{\lambda \in \Lambda} (\mathbf{w}_\lambda^j)^T \mathbf{v} \mathbf{w}_\lambda^j = \sum_{\lambda \in \Lambda} (\mathbf{w}_\lambda^j)_v \mathbf{w}_\lambda^j\end{aligned}$$

By $(\mathbf{w}_\lambda^i)_v = (\mathbf{w}_\lambda^j)_v$ and $(\mathbf{w}_\lambda^i)_{\hat{v}} = (\mathbf{w}_\lambda^j)_{\hat{v}}$, we have

$$((\tilde{A}_i)^k \mathbf{v})_{\hat{v}} = ((\tilde{A}_j)^k \mathbf{v})_{\hat{v}}$$

for all $k \in \mathbb{N}$. The claim follows by noting that this is true for any vertex $v \in V(H) \cup V^0$ and that the vector $\mathbf{x}$ is a linear combination of vectors $\mathbf{v}$ associated with these vertices. $\square$

Remark 4.3.12 (Discussion for Theorem 4.3.10). One way to interpret Corollary 4.3.11 is to think of the graphs $\tilde{G}_i$ and $\tilde{G}_j$ not as subgraphs of the same parent graph $\tilde{G}$ but instead as graphs with certain local structure changed. Since $\tilde{G}_i$ and $\tilde{G}_j$ share the vertices $V(H)$ and all its substructure (edges connecting them), we can think of $\tilde{G}_i$ and $\tilde{G}_j$ as the same graph H with the graph $G \setminus v_i$ or $G \setminus v_j$ attached in the same way to it. An example to this is given and explained below in Figure 4.15. In essence, the theorem and its corollary implies that certain substructures in graphs can be interchanged with each other without making a disturbance on the dynamics over the rest of the graph. This means that if we have inputs (or an initial condition) over a subset of vertices of $V(H) \cup V^0$, and if we are observing the dynamics again over a subset of $V(H) \cup V^0$; then we cannot decide whether the graph we are observing is $\tilde{G}_i$ or $\tilde{G}_j$; the dynamics would be identical. The meaning of these becomes clearer in large graphs such as the one in Figure 4.15.

Lastly, from this perspective, the use of Lemma 4.3.8 to add edge pairs between vertices $v'_\alpha \in V(H)$ and v_i, v_j implies that when interchanging the subgraph $G \setminus v_j$ with $G \setminus v_i$, we can interchange connections from v_i to $v'_\alpha \in V(H)$ with connections from v_j to v'_α . A representation for this is shown in Figure 4.16.

Example 4.3.13. The graph seen in the top left in Figure 4.15 is taken from [7]. The corresponding vertices in the two red subgraphs are latently symmetric (or

cospectral) as is mentioned in [7], as are those in the blue subgraphs. The reason for this becomes clear with Theorem 4.3.10; the blue and the red subgraphs are subgraphs of the same graph, obtained by deleting a cospectral vertex as can be seen in the top right. In the mother graph, the cospectral vertices are highlighted in red and the 0-nodes in blue. Below it are the two cospectral graphs with the same highlights. Notice that the right one is the red subgraph and the left one the blue subgraph; both connected to the large graph via their 0-nodes. By Corollary 4.3.11, without changing the dynamics of the graph over the other vertices, we can interchange the blue subgraph into the red subgraphs to obtain the symmetric graph shown in the bottom. Consequently, the dynamics of the unchanged vertices in the top left and the bottom graphs are the same. As cospectrality is a dynamical symmetry and since there is a dynamical symmetry induced by graph theoretic symmetry in the bottom graph; this explains why the non-symmetric vertices in the original graph are cospectral.

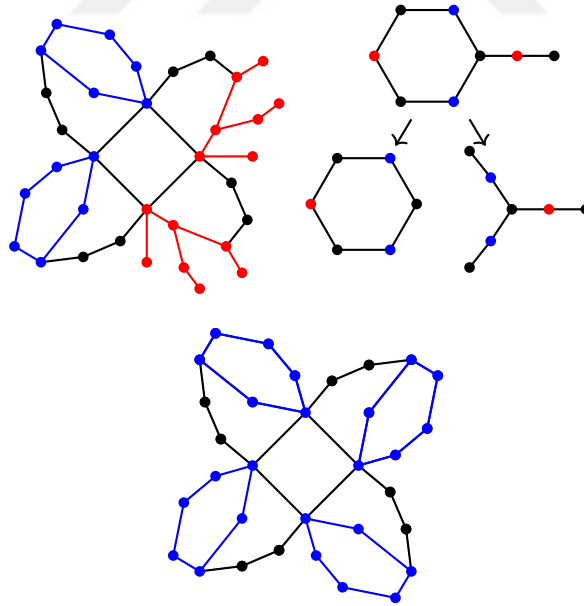


Figure 4.15: By Theorem 4.3.10 and Corollary 4.3.11, the top left and bottom graphs have exactly the same dynamics over the vertices that they share. Since the bottom graph is a highly symmetric graph, the dynamical system associated with it also contains dynamically symmetric vertices. Since these dynamical symmetries are preserved in the top left graph, the symmetric vertices in the bottom graph; although not symmetric anymore, remain A -cospectral in the top left graph.

We should note here that strictly speaking, Theorem 4.3.10 and Corollary 4.3.11 can only be applied once in order to change one of the subgraphs illustrated in Figure 4.15 and explained in Example 4.3.13. Be that as it may; locally speaking, there is no dynamical difference between the graphs $\tilde{G}_i$ and $\tilde{G}_j$ of Theorem 4.3.10 and Corollary 4.3.11. Consequently, Theorem 4.3.10 and Corollary 4.3.11 can in practice repeatedly be applied in order to change many subgraphs of a graph, such as the example given in Figure 4.15. A more rigorous version of this argument can be given by repeating the proofs of Lemma 4.3.9, Theorem 4.3.10 and Corollary 4.3.11 for each switched subgraph.

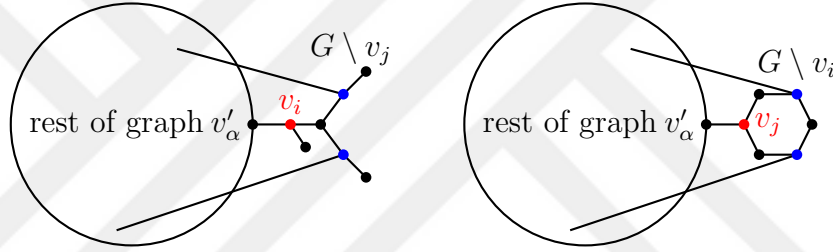


Figure 4.16: Schematic representation of the possibility to interchange connections from one cospectral vertex to the other. Here we used the cospectral graphs obtained through cospectral vertices that were used in Figure 4.15. The end of Remark 4.3.12 explains how we can switch subgraphs $G \setminus v_j$ and $G \setminus v_i$ by replacing connections from v_i to v'_α with connections from v_j to v'_α . Thus, by Corollary 4.3.11 the two graphs above have the same dynamics over the rest of the graph.

4.3.2 Other Operations

In this final section, we provide a few more operations.

Lemma 4.3.14 (*A-cospectral, L-cospectral and L-coprovable*). *Let G be a graph and let $v_i, v_j \in V(G)$ be $A(L)$ -cospectral vertices. Consider the graph $\hat{G}$ constructed from G by adding or deleting an edge between v_i and v_j . Then, v_i and v_j are $A(L)$ -cospectral in $\hat{G}$ as well. Furthermore, for any two vertices v_i and v_j , we have*

$$\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L = \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\hat{L}}.$$

In particular, if v_i and v_j are just L -coprovable in G and

$$\dim(\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L) < N - 1,$$

then v_i and v_j are L -coprable in $\widehat{G}$ as well.

Proof. Let $v_i, v_j \in V(G)$ be A -cospectral vertices. By Theorem 3.6.3 two vertices $v_i, v_j \in V(G)$ are A -cospectral if and only if $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A \perp \langle \mathbf{v}_i - \mathbf{v}_j \rangle_A$, or in other words,

$$\mathbf{v}_i - \mathbf{v}_j \perp \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$$

Thus, in order to prove that v_i and v_j are A -cospectral in $\widehat{G}$, we need to show that,

$$\mathbf{v}_i - \mathbf{v}_j \perp \langle \mathbf{v}_i + \mathbf{v}_j \rangle_{\widehat{A}}$$

Now, deleting or adding an edge between v_i and v_j only changes the edge set and not the underlying vertex set. Hence, we can regard the vectors $\mathbf{v}_m$ associated with vertices $v_m \in V(G)$ and $v_m \in V(\widehat{G})$ to be in the same vector space $\mathbb{R}^N$ with different operators A and $\widehat{A}$ acting on them. With this in mind, we claim the following: $\forall k \in \mathbb{N}$,

$$\text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^k(\mathbf{v}_i + \mathbf{v}_j)\} = \text{span}\{\mathbf{v}_i + \mathbf{v}_j, \widehat{A}(\mathbf{v}_i + \mathbf{v}_j), \dots, \widehat{A}^k(\mathbf{v}_i + \mathbf{v}_j)\}.$$

It is obvious that this proves $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_{\widehat{A}} = \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ and hence $\mathbf{v}_i - \mathbf{v}_j \perp \langle \mathbf{v}_i + \mathbf{v}_j \rangle_{\widehat{A}}$; showing that v_i and v_j are A -cospectral in $\widehat{G}$. We prove the claim by induction.

Base case $k = 0$: Trivial.

Inductive case: Suppose case $k = n - 1$. We will show case $k = n$. We have that

$$\text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^{n-1}(\mathbf{v}_i + \mathbf{v}_j)\} = \text{span}\{\mathbf{v}_i + \mathbf{v}_j, \widehat{A}(\mathbf{v}_i + \mathbf{v}_j), \dots, \widehat{A}^{n-1}(\mathbf{v}_i + \mathbf{v}_j)\}$$

Then, there must exist $\mathbf{x} \in \text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^{n-1}(\mathbf{v}_i + \mathbf{v}_j)\}$ such that

$$\mathbf{x} = \widehat{A}^{n-1}(\mathbf{v}_i + \mathbf{v}_j) = \sum_{\ell=0}^{n-1} \alpha_{\ell} A^{\ell}(\mathbf{v}_i + \mathbf{v}_j)$$

for some scalars α_{ℓ} . Now, we have

$$\widehat{A}^n(\mathbf{v}_i + \mathbf{v}_j) = \widehat{A}\mathbf{x} = A\mathbf{x} \pm ((\mathbf{x})_{v_i} \mathbf{v}_j + (\mathbf{x})_{v_j} \mathbf{v}_i)$$

where the $\pm$ sign depends on whether we added or removed an edge. Since $\mathbf{x} \in \text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^{n-1}(\mathbf{v}_i + \mathbf{v}_j)\} \subseteq \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$, we have that $\mathbf{x} \perp \mathbf{v}_i - \mathbf{v}_j$ and hence $(\mathbf{x})_{v_i} = (\mathbf{x})_{v_j}$. Therefore, we have $(\mathbf{x})_{v_i} \mathbf{v}_j + (\mathbf{x})_{v_j} \mathbf{v}_i = (\mathbf{x})_{v_i} (\mathbf{v}_i + \mathbf{v}_j)$. Since $A\mathbf{x}, \mathbf{v}_i + \mathbf{v}_j \in \text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^n(\mathbf{v}_i + \mathbf{v}_j)\}$, this implies that $\widehat{A}^n(\mathbf{v}_i + \mathbf{v}_j) \in \text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^n(\mathbf{v}_i + \mathbf{v}_j)\}$, and so

$$\text{span}\{\mathbf{v}_i + \mathbf{v}_j, \widehat{A}(\mathbf{v}_i + \mathbf{v}_j), \dots, \widehat{A}^n(\mathbf{v}_i + \mathbf{v}_j)\} \subseteq \text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^n(\mathbf{v}_i + \mathbf{v}_j)\}$$

Since this is true for both addition and deletion operations and since these are inverses of each other, we get

$$\text{span}\{\mathbf{v}_i + \mathbf{v}_j, \widehat{A}(\mathbf{v}_i + \mathbf{v}_j), \dots, \widehat{A}^n(\mathbf{v}_i + \mathbf{v}_j)\} = \text{span}\{\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^n(\mathbf{v}_i + \mathbf{v}_j)\}$$

as required. If v_i and v_j were L -cospectral, the proof would be the same by replacing A with L ; with the only difference that instead of

$$\widehat{A}^n(\mathbf{v}_i + \mathbf{v}_j) = \widehat{A}\mathbf{x} = A\mathbf{x} \pm ((\mathbf{x})_{v_i} \mathbf{v}_j + (\mathbf{x})_{v_j} \mathbf{v}_i)$$

we have

$$\widehat{L}^n(\mathbf{v}_i + \mathbf{v}_j) = \widehat{L}\mathbf{x} = L\mathbf{x}.$$

Hence, we have proved the cospectral part of the lemma. Now, for the second part of the lemma, let $v_i, v_j \in V(G)$ be any two vertices in G , not necessarily L -coprobable. We claim that $\forall k \in \mathbb{N}$,

$$\text{span}\{\mathbf{v}_i - \mathbf{v}_j, L(\mathbf{v}_i - \mathbf{v}_j), \dots, L^k(\mathbf{v}_i - \mathbf{v}_j)\} = \text{span}\{\mathbf{v}_i - \mathbf{v}_j, \widehat{L}(\mathbf{v}_i - \mathbf{v}_j), \dots, \widehat{L}^k(\mathbf{v}_i - \mathbf{v}_j)\}.$$

We prove by induction.

Base case $k = 0$: Trivial.

Inductive case: Suppose case $k = n - 1$. We will show case $k = n$. We have that

$$\text{span}\{\mathbf{v}_i - \mathbf{v}_j, L(\mathbf{v}_i - \mathbf{v}_j), \dots, L^{n-1}(\mathbf{v}_i - \mathbf{v}_j)\} = \text{span}\{\mathbf{v}_i - \mathbf{v}_j, \widehat{L}(\mathbf{v}_i - \mathbf{v}_j), \dots, \widehat{L}^{n-1}(\mathbf{v}_i - \mathbf{v}_j)\}.$$

Then, there must exist

$$\mathbf{x} \in \text{span}\{\mathbf{v}_i - \mathbf{v}_j, L(\mathbf{v}_i - \mathbf{v}_j), \dots, L^{n-1}(\mathbf{v}_i - \mathbf{v}_j)\}$$

such that

$$\mathbf{x} = \widehat{L}^{n-1}(\mathbf{v}_i - \mathbf{v}_j) = \sum_{\ell=0}^{n-1} \alpha_\ell L^\ell(\mathbf{v}_i - \mathbf{v}_j).$$

for some scalars α_ℓ . Now, we have

$$\widehat{L}^n(\mathbf{v}_i - \mathbf{v}_j) = \widehat{L}\mathbf{x} = L\mathbf{x} \pm [(\mathbf{x})_{v_i} - (\mathbf{x})_{v_j}](\mathbf{v}_i - \mathbf{v}_j)$$

where the $\pm$ sign depends on whether we added or deleted an edge between v_i and v_j . Since $(\mathbf{x})_{v_i} - (\mathbf{x})_{v_j}$ is a scalar, and since $L\mathbf{x}, \mathbf{v}_i - \mathbf{v}_j \in \text{span}\{\mathbf{v}_i - \mathbf{v}_j, L(\mathbf{v}_i - \mathbf{v}_j), \dots, L^n(\mathbf{v}_i - \mathbf{v}_j)\}$, we have

$$\widehat{L}^n(\mathbf{v}_i - \mathbf{v}_j) \in \text{span}\{\mathbf{v}_i - \mathbf{v}_j, L(\mathbf{v}_i - \mathbf{v}_j), \dots, L^n(\mathbf{v}_i - \mathbf{v}_j)\}.$$

Since edge addition and deletion are inverses of each other, this implies in the same way as before

$$\text{span}\{\mathbf{v}_i - \mathbf{v}_j, L(\mathbf{v}_i - \mathbf{v}_j), \dots, L^{n-1}(\mathbf{v}_i - \mathbf{v}_j)\} = \text{span}\{\mathbf{v}_i - \mathbf{v}_j, \widehat{L}(\mathbf{v}_i - \mathbf{v}_j), \dots, \widehat{L}^{n-1}(\mathbf{v}_i - \mathbf{v}_j)\}.$$

Thus, we have $\langle \mathbf{v}_i - \mathbf{v}_j \rangle_L = \langle \mathbf{v}_i - \mathbf{v}_j \rangle_{\widehat{L}}$ and the rest of the claims follow immediately. $\square$

Finally, we have a simple lemma for cospectral vertices. The operation described here does not preserve either cospectrality or coprobability, but as we are interested in lumpability, it might be useful.

Lemma 4.3.15 (*A-cospectral and L-cospectral*). *Let G be a graph and let v_i and v_j be $A(L)$ -cospectral vertices. Assume that v_i and v_j do not have any common neighbors. Then, construct the graph $\widehat{G}$ by merging v_i and v_j into a single vertex v_{ij} with edges connecting it to both the neighbors of v_i and v_j . Then, we have*

$$\dim\langle \mathbf{v}_i + \mathbf{v}_j \rangle_{A(L)} = \dim\langle \mathbf{v}_{ij} \rangle_{\widehat{A}(\widehat{L})} < N = |V(G)|.$$

Thus, this also implies $\langle \mathbf{v}_{ij} \rangle_{\widehat{A}(\widehat{L})} \neq \mathbb{R}^{\widehat{N}}$ where $\widehat{N} = N - 1 = |V(\widehat{G})|$, so long as $\dim\langle \mathbf{v}_i + \mathbf{v}_j \rangle_{A(L)} \neq N - 1$.

Proof. For notational simplicity, we will do the proof for A -cospectrality. For L -cospectrality, the proof is very similar. Firstly we assume v_i and v_j are not

connected by an edge by Lemma 4.3.14. Now, $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ is spanned by the vectors

$$\mathbf{v}_i + \mathbf{v}_j, A(\mathbf{v}_i + \mathbf{v}_j), \dots, A^{N-1}(\mathbf{v}_i + \mathbf{v}_j)$$

and similarly $\langle \mathbf{v}_{ij} \rangle_{\hat{A}}$ is spanned by

$$\mathbf{v}_{ij}, \hat{A}(\mathbf{v}_{ij}), \dots, \hat{A}^{N-1}(\mathbf{v}_{ij})$$

where $\hat{A}$ is the adjacency matrix of $\hat{G}$. We will show that $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A \cong \langle \mathbf{v}_{ij} \rangle_{\hat{A}}$ as vector spaces. Now, we define a map $S_{v_i v_j} : \mathbb{R}^N \rightarrow \mathbb{R}^{\hat{N}}$ by

$$[(\mathbf{x})_{v_i}, (\mathbf{x})_{v_j}, \dots, (\mathbf{x})_{v_N}] \mapsto \left[\frac{(\mathbf{x})_{v_i} + (\mathbf{x})_{v_j}}{2}, (\mathbf{x})_{v_3}, \dots, (\mathbf{x})_{v_N} \right]$$

where the v_i -th and v_j -th components of the vector $\mathbf{x} \in \mathbb{R}^N$ and the v_{ij} -th component of the vector $S_{v_i v_j}(\mathbf{x})$ has been put in front for notational simplicity. Clearly, the map $S_{v_i v_j}$ is linear. Now, suppose we have a vector $\mathbf{x} \in \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$. Since v_i and v_j are A -cospectral, the vector $\mathbf{x}$ satisfies $(\mathbf{x})_{v_i} = (\mathbf{x})_{v_j} = \alpha$. Now, letting $\hat{A}[\mathbf{v}_{ij}, \mathbf{v}_{ij}]$ denote the matrix $\hat{A}$ whose v_{ij} -th row and column is deleted, we thus have

$$\begin{aligned} \hat{A}(S_{v_i v_j}(\mathbf{x})) &= \begin{bmatrix} 0 & \dots & 1 & \dots & 1 & \dots \\ \vdots & & & & & \\ 1 & & & & & \\ \vdots & & \hat{A}[\mathbf{v}_{ij}, \mathbf{v}_{ij}] & & & \\ 1 & & & & & \\ \vdots & & & & & \end{bmatrix} (S_{v_i v_j}(\mathbf{x})) = \\ &= \begin{bmatrix} 0 & \dots & 1 & \dots & 1 & \dots \\ \vdots & & & & & \\ 1 & & & & & \\ \vdots & & \hat{A}[\mathbf{v}_{ij}, \mathbf{v}_{ij}] & & & \\ 1 & & & & & \\ \vdots & & & & & \end{bmatrix} \begin{bmatrix} \alpha \\ (\mathbf{x})_{v_3} \\ \vdots \\ (\mathbf{x})_{v_N} \end{bmatrix} = \end{aligned}$$

$$\begin{aligned}
&= S_{v_i v_j} \left(\begin{bmatrix} 0 & 0 & \cdots & 1 & \cdots & 0 & \cdots \\ 0 & 0 & \cdots & 0 & \cdots & 1 & \cdots \\ \vdots & \vdots & & & & & \\ 1 & 0 & & & & & \\ \vdots & \vdots & & \widehat{A}[\mathbf{v}_{ij}, \mathbf{v}_{ij}] & & & \\ 0 & 1 & & & & & \\ \vdots & \vdots & & & & & \end{bmatrix} \begin{bmatrix} \alpha \\ \alpha \\ (\mathbf{x})_{v_3} \\ \vdots \\ (\mathbf{x})_{v_N} \end{bmatrix} \right) + \sum_{v_k \sim v_i \text{ or } v_k \sim v_j} \frac{(\mathbf{x})_{v_k} \mathbf{v}_{ij}}{2} = \\
&= S_{v_i v_j} (A\mathbf{x}) + \sum_{v_k \sim v_i \text{ or } v_k \sim v_j} \frac{(\mathbf{x})_{v_k} \mathbf{v}_{ij}}{2}
\end{aligned}$$

where the equalities follow from direct matrix multiplication. Note that in establishing the third equality, we implicitly used the assumptions that v_i and v_j do not have any common neighbours and that v_i and v_j are not connected by an edge. Hence $S_{v_i v_j} A(\mathbf{x}) = \widehat{A} S_{v_i v_j}(\mathbf{x}) - \alpha_{\mathbf{x}} \mathbf{v}_{ij}$ for $\mathbf{x} \in \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ where $\alpha_{\mathbf{x}} = \sum_{v_k \sim v_i \text{ or } v_k \sim v_j} \frac{(\mathbf{x})_{v_k}}{2}$ is a constant that depends on $\mathbf{x}$. In particular, this is true for $\mathbf{x} = A^k(\mathbf{v}_i + \mathbf{v}_j)$ for any $k \in \mathbb{N}$. Thus we obtain,

$$S_{v_i v_j} A(\mathbf{v}_i + \mathbf{v}_j) = \widehat{A} S_{v_i v_j}(\mathbf{v}_i + \mathbf{v}_j) - \alpha_{(\mathbf{v}_i + \mathbf{v}_j)} \mathbf{v}_{ij} = \widehat{A}(\mathbf{v}_{ij}) - \alpha_{(\mathbf{v}_i + \mathbf{v}_j)} \mathbf{v}_{ij}$$

and

$$\begin{aligned}
S_{v_i v_j} A^k(\mathbf{v}_i + \mathbf{v}_j) &= \widehat{A} S_{v_i v_j}(A^{k-1}(\mathbf{v}_i + \mathbf{v}_j)) - \alpha_{A^{k-1}(\mathbf{v}_i + \mathbf{v}_j)} \mathbf{v}_{ij} = \\
&= \widehat{A}^k S_{v_i v_j}(\mathbf{v}_i + \mathbf{v}_j) + p_{k-1}(\widehat{A}) \mathbf{v}_{ij} = \widehat{A}^k \mathbf{v}_{ij} + p_{k-1}(\widehat{A}) \mathbf{v}_{ij}
\end{aligned}$$

where $p_{k-1}(\widehat{A})$ is a degree $k-1$ polynomial in $\widehat{A}$. Thus, the restriction $S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}$ of $S_{v_i v_j}$ to $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ is a surjection onto $\langle \mathbf{v}_{ij} \rangle_{\widehat{A}}$. It is obvious that the map $S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}^{-1} : \langle \mathbf{v}_{ij} \rangle_{\widehat{A}} \rightarrow \langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ defined by $S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}^{-1}([\alpha, (\mathbf{x})_{v_3}, \dots, (\mathbf{x})_{v_N}]) = ([\alpha, \alpha, (\mathbf{x})_{v_3}, \dots, (\mathbf{x})_{v_N}])$ is the inverse of $S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}$ since we have

$$\begin{aligned}
&S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}^{-1} S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}([\alpha, \alpha, (\mathbf{x})_{v_3}, \dots, (\mathbf{x})_{v_N}]) = \\
&= S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}^{-1}([\alpha, (\mathbf{x})_{v_3}, \dots, (\mathbf{x})_{v_N}]) = [\alpha, \alpha, (\mathbf{x})_{v_3}, \dots, (\mathbf{x})_{v_N}].
\end{aligned}$$

Hence $S_{v_i v_j}|_{\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A}$ is an isomorphism between $\langle \mathbf{v}_i + \mathbf{v}_j \rangle_A$ and $\langle \mathbf{v}_{ij} \rangle_{\widehat{A}}$. This completes the proof. $\square$

Chapter 5

Conclusion and Future Work

With several constructions and operations that preserve the vertex relations of cospectrality and coprobability, the latter being defined in this thesis; we have developed a large tool set to obtain these vertices in a variety of ways. Moreover, all of our constructive methods work for arbitrary graphs; meaning that our methods enable us to obtain vertices with these relations in arbitrarily large and complex networks. Because of their constructive nature, this means that our results can be applied to network design; being useful potentially in designing networks with redundant nodes or containing inherent symmetries that cannot be easily deciphered from the outside.

Several directions for future work can clearly be discerned. Although both coprobable and cospectral vertices can be defined for directed graphs, all of our results have been on undirected ones. Investigating the directed versions of these vertex relations could prove to be both theoretically and practically relevant, especially considering that undirected graphs are a subset of directed ones. Further generalization could be made in other ways, such as by considering weighted graphs or nonlinear dynamics over networks; although in such cases how to define coprobable and cospectral vertices might not be as clear as it seems.

Considering A -coprobable vertices in general, we have defined them through

the equality of the indices of the Perron-Frobenius eigenvector. These indices of the Perron-Frobenius eigenvector are also known as eigenvector centrality and are a widely used characteristic of vertex centrality. The concept of equal eigenvector centrality can thus potentially be related to different phenomena over networks and could provide connections between different areas of research on network theory.

Another obvious direction of research is further investigation of L -coprable and L -cospectral vertices. Indeed, the Laplacian analogues of our results are generally weaker. Furthermore, it is obvious that the definition of L -coprobability can be improved, perhaps making it clearer to discern the reasons for L -coprobability as well. Lastly but also significantly, results like Theorem 4.3.10 have been proved only in the A -cospectral case. Such results most likely have Laplacian analogues.

More specific directions could also be pointed out. For example, constructions of A -cospectral vertices have a special importance attached to them as the recently popular strongly cospectral vertices are a subclass of them. We followed that direction in Section 4.2, culminating in Theorem 4.2.5, which establishes the possibility to construct strongly cospectral vertices in graphs with arbitrary structure. Although, as was explained in Remark 4.2.6, the theorem in practice establishes the strong cospectrality of the A -cospectral vertices constructed in 4.1.7; the procedures described in the remark could still prove to be too heuristic. Consequently, results that improve upon Theorem 4.2.5 or algorithmize the processes described in Remark 4.2.6 might be required.

On another point, Theorem 4.2.5 only works for A -cospectral vertices constructed via Theorem 4.1.7 and not for any operations that preserve the A -cospectrality; such as Lemma 4.1.11 or Lemma 4.3.14. If similar to the cospectral case, some of these operations are also proven to be strong cospectrality preserving, it would increase the constructive possibilities of strongly cospectral vertices.

About Theorem 4.3.10 and Corollary 4.3.11, we should note that they might in fact be a special case of a larger phenomenon, possibly related to cospectral graphs in general (that are not necessarily derived from cospectral vertices). Indeed, the

theorem does not in principle require A -cospectral vertices and 0-nodes. It only requires two graphs and pairs of associated vertices in those graphs such that, when one graph is connected to a larger graph through these vertices, it can be interchanged with its pair via interchanging the vertices of the former with their associated pairs in the latter. This is precisely what is done in Theorem 4.3.10, with the two graphs being those obtained via deleting one of the cospectral vertices and the associated vertex pairs in the two graphs being the 0-nodes with respect to these cospectral vertices. However in principle, these graphs and the associated vertices need not derive from any underlying cospectral vertex pair. It therefore could be possible to obtain some form of generalization or analogue of the theorem for other types of subgraph pairs that are interchangeable with one another. In any case, whether this is true or not, it is clear that further research can facilitate a better understanding of this phenomenon.

Here we also note a potentially useful heuristic method for checking whether two vertices are symmetric in a graph or not in polynomial time, using A -cospectral and L -cospectral vertices. We already know that all symmetric vertex pairs are both A -cospectral and L -cospectral. However, we have also heuristically observed that all vertex pairs that are both A -cospectral and L -cospectral are symmetric. Furthermore, this heuristic also appears to be able to circumvent a fundamental shortcoming of spectral methods to establish vertex symmetry. Indeed, although two subgraphs $G \setminus v_i$ and $G \setminus v_j$ might be isomorphic and consequently have the same Laplacian and adjacency spectrum, this does not necessarily imply the symmetry of v_i and v_j in G . However, it also does not imply the L -cospectrality of v_i and v_j since our definition of L -cospectrality does not derive from the Laplacian spectra of these subgraphs. L -cospectrality is thus able to distinguish such unsymmetric cases from actual symmetries, something which cannot be done by just looking at various matrices associated with the subgraphs $G \setminus v_i$ and $G \setminus v_j$.

Although this heuristic need not in general be true and counterexamples could exist, we have been unable to attain them through generated networks. However, even if counterexamples exist, such cases appear to us to be extremely rare. In any case, a proper theoretical and experimental analysis has to be done in order

to propose the applicability of such a method.

Finally, we should also emphasize that our constructions do not characterize cospectral or coprobable vertices. As is well known, there are many unintuitive cospectral vertices that have no obvious explanation for their property. Similar examples of unintuitive coprobable vertices that our results are unable to explain exists. As such, there is still work to be done in characterizing and obtaining coprobable and cospectral vertices. Relatedly, it might also be fruitful to conduct a proper analysis of coprobable and cospectral vertices over existing networks in order to better understand the underlying reasons for the existence of such vertices. Such a research could illuminate when or if they arise in real or constructed networks, their frequency in various types of networks and could investigate whether they have a function or not, should they exist. As a last note, although we aren't able to fully characterize these vertex relations in a satisfactory manner, together with recent research [5][8][9]; for pairs of vertices, we have a hierarchy of these relations that might be of relevance:

$$\text{Strongly Cospectral} \subset \text{Cospectral} \subset \text{Latently Symmetric} \subset \text{Coprobable}$$

The first [8] and third [5] inclusions are known to be strict and the second is an equality only in the case where the graph is undirected [9].

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