

Chapter 2

Dynamical Networks and Isospectral Graph Reductions

This is a fundamental chapter of the book. It deals with networks, which are here considered as graphs, and is built on the theory developed in the previous chapter, on matrices.

Although, the dynamical networks described in Chap. 3 are richer objects than their weighted adjacency matrices, the latter still carry the most important information about a dynamical network. Indeed, from a theoretical point of view, a network's weighted adjacency matrix describes a linearization of the network's dynamics, which in applications is often the only network information available. In fact, it is not uncommon to have only the unweighted adjacency matrix of a network.

In this chapter, we introduce the notion of an isospectral graph reduction, which is based on the essential idea of the branch structure of a graph (network). A graph's collection of branches, which are related to the more familiar concepts of paths and cycles, form the foundation of the isospectral transformations considered in this book, both in this chapter and later in applications of this theory.

The isospectral graph reductions that we study in this chapter allow us to reduce the size of a graph (number of vertices) while maintaining the graph's spectrum, up to a known set. Besides these reductions, we also introduce and analyze a number of other graph transformations that affect the graph's spectrum in a specific way. These include the operations of branch expansions, reweightings, and mergings.

These graph transformations can be used to simplify the structure of a graph (network) while preserving the graph's (network's) spectrum, up to a known set, as well as its collection of edge weights. For example, it is possible to reduce a network in which all edges have weight 1 to a smaller network with the same property. That is, these isospectral transformations do not somehow shift the complexity of the original network to the edge weights of the reduced network.

We begin this chapter by introducing the fundamental operation of isospectral graph reduction. After analyzing its properties, we show that a sequence of isospectral reductions of the same graph results in the same reduced network,

regardless of the order in which the vertices were removed, i.e., the result depends only on the final collection of vertices.

It is worthwhile mentioning that the procedure of isospectral graph reduction can be applied not only to the vertices of graphs (elements of networks) but also to the graph's edges. To do this, one need only consider the line (dual) graph, in which all edges of the initial graph are vertices, and apply the same procedure to it. Because all the results and operations are the same, we will deal only with removal of vertices.

We also introduce a new equivalence relation on the collection of graphs (networks) that we consider. Namely, two graphs (networks) are said to be *spectrally equivalent* if they can be isospectrally reduced to one and the same graph (network). The basic idea here is that two graphs may look very different but be spectrally equivalent, suggesting that the corresponding networks have similar dynamics.

Although each of these results is rigorously proved, we have attempted to make the exposition as visual and accessible as possible. With this goal in mind, the definitions and results of this chapter are illustrated by numerous examples and figures.

2.1 Dynamical Networks as Graphs

To begin, we note that to each dynamical network there is an associated weighted directed graph G , which we call the network's *graph of interactions*. As the name suggests, this graph describes the various interactions among the network's elements. In network theory, the unweighted version of this graph is often called the network's *topology*. Here, we do not use this term, since it might be confused with the unrelated branch of mathematics called topology.

The graph $G = (V, E, \omega)$ is composed of a *vertex set* V , a set of directed *edges* E , and a function ω that gives a weight to each edge in E . The *vertex set* V represents the elements of the network, and the *edge set* E , the interactions among these elements. Because it is assumed that the graph G corresponds to a network, we consider only *finite graphs*, or those graphs in which V and E are finite and nonempty.

For $V = \{v_1, \dots, v_n\}$, we let e_{ij} denote the edge from vertex v_i to v_j . The edge e_{ij} is an element of E if the i th network element interacts with (or directly influences) the j th network element. The function ω gives the edge weights of G , where $\omega(e_{ij})$, or the edge weight of e_{ij} , corresponds to the strength of the interaction between the i th and j th elements of a network. We adopt the standard convention that each edge of G has a nonzero weight. More formally, $\omega(e_{ij}) = 0$ if and only if $e_{ij} \notin E$, or the i th element of the network does not directly influence the j th network element.

Suppose the graph $G = (V, E, \omega)$ has the vertex set $V = \{v_1, \dots, v_n\}$. We define the $n \times n$ matrix $M(G)$ by

$$M(G)_{ij} = \omega(e_{ij}).$$

The matrix $M(G)$ is called the *weighted adjacency matrix* of G . If G is the graph of interactions of a dynamical network, we say that the eigenvalues of the matrix $M(G)$ make up the spectrum of this dynamical network. In later chapters, we will connect the spectrum of a network with its dynamics. For now, we simply assume that to each dynamical network there is an associated graph G with adjacency matrix $M(G)$.

To compute the spectrum of a network, we need to know the weights of its graph of interactions $G = (V, E, \omega)$. At this point, we have yet to formally define the *weight set* $\omega(E) = \{\omega(e) : e \in E\}$ that will be considered here. In practice, one often chooses $\omega(E)$ to be some subset of the real numbers. For example, if we consider the graph G to be an unweighted graph, then $M(G)$ is the matrix with 0–1 entries given by

$$M(G)_{ij} = \begin{cases} 1 & \text{if } e_{ij} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

However, the set of weights we will use is not a subset of the real or even complex numbers but the set of rational functions $\mathbb{W}$, defined in Chap. 1. The class of graphs we consider is defined as follows.

Definition 2.1. Let $\mathbb{G}$ be the collection of weighted directed graphs given by

$$\mathbb{G} = \{G = (V, E, \omega) : \omega : E \rightarrow \mathbb{W}\}.$$

The *spectrum*, or set of eigenvalues, of a graph $G \in \mathbb{G}$ is the set $\sigma(G) = \sigma(M(G))$. The *inverse spectrum* of G is the set $\sigma^{-1}(G) = \sigma^{-1}(M(G))$.

Equivalently, one could define $\mathbb{G}$ as the set of all graphs $G = (V, E, \omega)$ for which $M(G) \in \mathbb{W}^{n \times n}$ for some $n \in \mathbb{N}$. In either case, Definition 1.1 gives the spectrum and inverse spectrum of the graph $G \in \mathbb{G}$.

To stress the generality of considering the set $\mathbb{G}$, we note that graphs that are either undirected or have parallel edges can be considered graphs in $\mathbb{G}$. In particular, an undirected graph can be made into a directed graph by orienting each of its edges in both directions. If a graph G has multiple edges between two vertices, a single edge can be put in their place whose weight is the sum of the weights of the edges that it is replacing.

Example 2.1. Consider the graphs G and H shown in Fig. 2.1. The weighted adjacency matrices $M(G) \in \mathbb{W}^{4 \times 4}$ and $M(H) \in \mathbb{C}^{6 \times 6}$ are given in (1.4) and (1.5), respectively. Hence,

$$\sigma(G) = \sigma(H) = \{-2, -2, -1 \pm i, -1 \pm \sqrt{3}\}.$$

That is, G and H have the same spectrum, although H has more vertices than G .

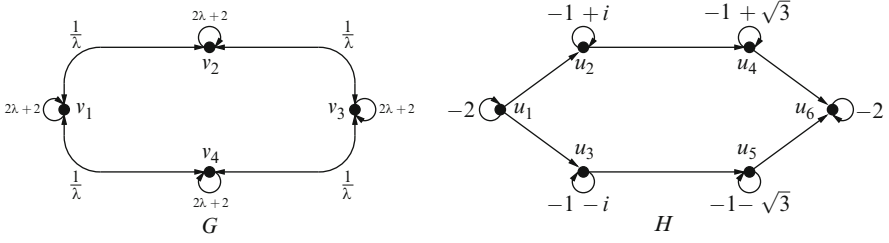


Fig. 2.1 The graph $G \in \mathbb{W}^{4 \times 4}$ (left) given in Example 2.1 and $H \in \mathbb{C}^{6 \times 6}$, where $\sigma(G) = \sigma(H)$

Again, our main question is whether a graph can be reduced to a smaller graph in such a way that its spectrum is preserved. Equivalently, we ask whether there is a way to reduce a graph H to a graph G such that $M(H)$ and $M(G)$ have the same eigenvalues.

The answer from Chap. 1 is that this is indeed possible. The goal, then, of this chapter is to describe what isospectral graph reductions means in terms of the original graph (network) and second how to use this understanding to develop other isospectral transformations of a graph (network).

One point we hope to make is that there are a number of useful isospectral transformations that can be developed using the theory of isospectral graph reductions as an initial starting point. In this chapter, we introduce a handful of such transformations that will be useful later for different purposes. The major point is that one can develop the most relevant transformation for a given problem with respect to both analytic simplicity and effectiveness as a computational tool.

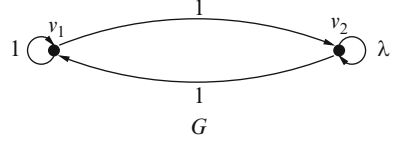
2.2 Isospectral Graph Reductions

Because of the structural complexity and considerable size of many networks, the corresponding graph of interactions $G = (V, E, \omega)$ may have an extremely large vertex set V as well as a large and irregular set of edges. To reduce this complexity while maintaining the network's spectral properties, we introduce the concept of isospectral graph reductions, which is related to isospectral matrix reduction, studied in the previous chapter.

The spectrum of a graph is intimately related to its structure. Specifically, knowing the graph's path and cycle structure along with its weights gives us enough information to compute the graph's spectrum. Simply put, a path is a sequence of distinct vertices that can be traversed by moving along edges of the graph. A cycle is a path that begins and ends at the same vertex.

More formally, a *path* P in the graph $G = (V, E, \omega)$ is an ordered sequence of distinct vertices $P = v_1, \dots, v_m \in V$ such that $e_{i,i+1} \in E$ for $1 \leq i \leq m-1$. We call the vertices $v_2, \dots, v_{m-1}$ of P the *interior vertices* of P . If the vertices v_1

Fig. 2.2 The graph $G \in \mathbb{W}^{4 \times 4}$ with adjacency matrix $M(G)$ considered in Example 1.5



and v_m are the same, then P is a *cycle*. If it is the case that a cycle contains a single vertex, then we call this cycle a *loop*. In addition, since v_i is a loop of G if and only if $e_{ii} \in E$, we may refer to the edge e_{ii} as a loop.

The main idea behind the isospectral reduction of a graph $G = (V, E, \omega)$ is that we reduce G to a smaller graph on some subset $S \subset V$. Equating a graph G with its adjacency matrix $M(G)$, we note that formally, an isospectral reduction of G could be defined as the graph with the “reduced” adjacency matrix $\mathcal{R}(M(G); S)$. Indeed, this will be the case. However, to investigate how the structure of a graph is affected by an isospectral reduction, we deliberately limit the type of vertex sets over which we can reduce a graph. Such sets, called structural sets, are defined as follows.

Definition 2.2. Let $G = (V, E, \omega) \in \mathbb{G}$. A nonempty vertex set $S \subset V$ is a *structural set* of G if

- (i) each cycle of G that is not a loop contains a vertex in S ; and
- (ii) $\omega(e_{ii}) \neq \lambda$ for each $v_i \in \bar{S} = V - S$.

For $G = (V, E, \omega)$, suppose S is a subset of the vertex set V . Then the graph $G|_S$ is called the *subgraph of G induced over the vertex set S* and is given by

$$G|_S = (S, \mathcal{E}, \mu) \text{ where } \mathcal{E} = \{e_{ij} \in E : v_i, v_j \in S\} \text{ and } \mu = \omega|_{\mathcal{E}}.$$

If S is a structural set of G , part (i) of Definition 2.2 says that the subgraph $G|_{\bar{S}}$ has no cycles except possibly for loops. Part (ii) of Definition 2.2 is the formal assumption that the loops of the vertices in $\bar{S}$, i.e., the complement of S , do not have weight equal to $\lambda \in \mathbb{W}$. That is, these loops are not weighted by the rational function $\lambda/1 \in \mathbb{W}$.

Consider the graph $G \in \mathbb{G}$ with adjacency matrix

$$M(G) = \begin{bmatrix} 1 & 1 \\ 1 & \lambda \end{bmatrix},$$

as in Example (1.5). The graph G is shown in Fig. 2.2. Notice that $\omega(e_{22}) = \lambda$. Hence, the set $S = \{v_2\}$ is not a structural set of G .

For $G \in \mathbb{G}$, we let $st(G)$ denote the set of all structural sets of the graph G . The idea behind the notion of a structural set $S \in st(G)$ is the following. Every random walk along edges of G that begins at a vertex in S eventually finds its way to another vertex of S , if we ignore loops. Therefore, a structural set allows us essentially to partition a random walk on G into finite paths and cycles that begin and end with vertices of S . We give these paths and cycles the following name.

Definition 2.3. Suppose $G = (V, E, \omega)$ with the structural set $S = \{v_1, \dots, v_m\}$. Let $\mathcal{B}_{ij}(G; S)$ be the set of paths from v_i to v_j , or cycles if $i = j$, with no interior vertices in S . We call a path or cycle $\beta \in \mathcal{B}_{ij}(G; S)$ a *branch* of G with respect to S . We let

$$\mathcal{B}_S(G) = \bigcup_{1 \leq i, j \leq m} \mathcal{B}_{ij}(G; S)$$

denote the *branch set* of all branches of G with respect to S .

If $\beta = v_1, \dots, v_m$ is a branch of G with respect to S and $m > 2$, we define

$$\mathcal{P}_\omega(\beta) = \omega(e_{12}) \prod_{i=2}^{m-1} \frac{\omega(e_{i,i+1})}{\lambda - \omega(e_{ii})}. \quad (2.1)$$

For $m = 1, 2$, we let $\mathcal{P}_\omega(\beta) = \omega(e_{1m})$. We call $\mathcal{P}_\omega(\beta)$ the *branch product* of β .

Notice that assumption (ii) in Definition 2.2 implies that the branch product of every $\beta \in \mathcal{B}_S(G)$ is always defined and is a rational function in $\mathbb{W}$. In fact, the reason we require that part (ii) of Definition 2.2 hold is to ensure that the branch product of each branch in $\mathcal{B}_S(G)$ exists.

To *isospectrally reduce* a graph over the set $S \in st(G)$, we replace each branch $\mathcal{B}_{ij}(G; S)$ with a single edge $e_{ij} \in \mathcal{E}$. The following definition specifies the weights of these edges.

Definition 2.4. Let $G = (V, E, \omega)$ with structural set $S = \{v_1, \dots, v_m\}$. Define the edge weights

$$\mu(e_{ij}) = \begin{cases} \sum_{\beta \in \mathcal{B}_{ij}(G; S)} \mathcal{P}_\omega(\beta) & \text{if } \mathcal{B}_{ij}(G; S) \neq \emptyset, \\ 0 & \text{otherwise,} \end{cases} \quad \text{for } 1 \leq i, j \leq m. \quad (2.2)$$

The graph $\mathcal{R}_S(G) = (S, \mathcal{E}, \mu)$ in which $e_{ij} \in \mathcal{E}$ if $\mu(e_{ij}) \neq 0$ is the *isospectral reduction* of G over S .

Observe that $\mu(e_{ij})$ in Definition 2.4 is the weight of the edge e_{ij} in $\mathcal{R}_S(G)$. Moreover, since $\mathbb{W}$ is closed under both addition and multiplication, it follows that the edge weights $\mu(e_{ij})$ of $\mathcal{R}_S(G)$ are also in the set $\mathbb{W}$. Hence the isospectral reduction $\mathcal{R}_S(G)$ is again a graph in $\mathbb{G}$.

Example 2.2. Consider the graph $G = (V, E, \omega)$ given in Fig. 2.3 (left), where G is an unweighted graph, i.e., each edge of G is given unit weight. Note that the vertex set $S = \{v_1, v_3\} \subset V$ is a structural set of G , since

- (i) the three nonloop cycles of G , namely v_1, v_2, v_3, v_4, v_1 ; v_1, v_5, v_1 ; and v_3, v_6, v_3 , each contains a vertex in S ; and

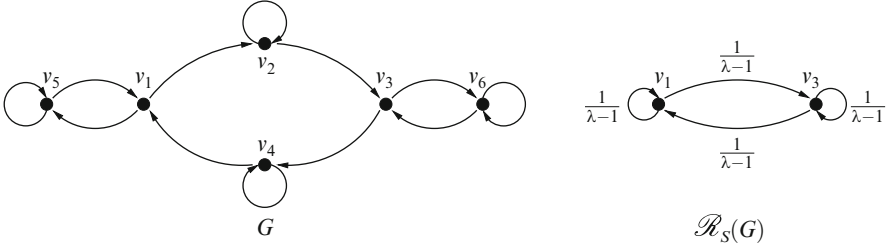


Fig. 2.3 Reduction of G over $S = \{v_1, v_3\}$ from Example 2.2, where each edge in G has unit weight

- (ii) the loop weights of vertices in $\tilde{S} = \{v_2, v_4, v_5, v_6\}$ are $\omega(e_{22}) = 1$, $\omega(e_{44}) = 1$, $\omega(e_{55}) = 1$, and $\omega(e_{66}) = 1$ respectively.

Hence, $\omega(e_{ii}) = 1 \in \mathbb{W}$ is not equal to the rational function $\lambda/1 \in \mathbb{W}$ for each $v_i \in \tilde{S}$.

In contrast, the vertex set $T = \{v_1, v_2, v_5\}$ is not a structural set of G , since the (nonloop) cycle v_3, v_6, v_3 does not contain a vertex of T . Phrased another way, the random walk $v_2, v_3, v_6, v_3, v_6, \dots$ cannot be partitioned into finite paths and cycles that begin and end with vertices in T .

Returning to the structural set S , we see that the branches in $\mathcal{B}_S(G)$ are respectively given by $\mathcal{B}_{11}(G; S) = \{v_1, v_5, v_1\}$, $\mathcal{B}_{13}(G; S) = \{v_1, v_2, v_3\}$, $\mathcal{B}_{31}(G; S) = \{v_3, v_4, v_1\}$, and $\mathcal{B}_{33}(G; S) = \{v_3, v_6, v_3\}$. Using (2.1), we conclude that the branch product of each branch is given by

$$\mathcal{P}_\omega(v_1, v_5, v_1) = \mathcal{P}_\omega(v_1, v_2, v_3) = \mathcal{P}_\omega(v_3, v_4, v_1) = \mathcal{P}_\omega(v_3, v_6, v_3) = \frac{1}{\lambda - 1}.$$

Equation (2.2) then gives each edge of $\mathcal{R}_S(G) = (S, \mathcal{E}, \mu)$ the weight

$$\mu(e_{11}) = \mu(e_{13}) = \mu(e_{31}) = \mu(e_{33}) = \frac{1}{\lambda - 1}.$$

Since each edge weight is nonzero, the edge set $\mathcal{E}$ of $\mathcal{R}_S(G)$ is $\mathcal{E} = \{e_{11}, e_{13}, e_{31}, e_{33}\}$. In particular, an edge of $\mathcal{E}$ need not be an edge of E . The graph $\mathcal{R}_S(G)$ is shown in Fig. 2.3 (right).

To relate an isospectral graph reduction to an isospectral matrix reduction, we need a way of connecting a structural set with a submatrix. For the graph $G = (V, E, \omega)$, suppose that $S, T \subset V$ are nonempty. By a slight abuse of notation, let $M(G)_{ST}$ denote the submatrix of the graph's weighted adjacency matrix with rows indexed by the vertices in S and columns indexed by the vertices in T . This allows us to state the following fundamental relation between isospectral graph and matrix reductions.

Theorem 2.1. *Let S be a structural set of the graph $G \in \mathbb{G}$. Then*

$$M(\mathcal{R}_S(G)) = \mathcal{R}(M(G); S).$$

Before proving Theorem 2.1, we note the following. A matrix $P \in \mathbb{C}^{n \times n}$ is a *permutation matrix* if each row and column of P has exactly one entry that is 1 with all other entries equal to 0. We will use the fact that every permutation matrix is invertible. Moreover, for $G = (V, E, \omega) \in \mathbb{G}$, the matrix $PM(G)P^{-1}$ is the adjacency matrix of G in which the vertices V have been relabeled by the permutation P .

Proof. Let $G = (V, E, \omega)$, where $V = \{v_1, \dots, v_n\}$. Without loss in generality, suppose $S = \{v_1, \dots, v_m\}$ is a structural set of the graph G . Since the subgraph $G|_{\bar{S}}$ has no cycles except loops, the vertices of $G|_{\bar{S}}$ can be relabeled such that the matrix $M(G|_{\bar{S}})$ is upper triangular. By assumption (ii) of Definition 2.2, the diagonal entries $M(G|_{\bar{S}})_{ii}$ are not equal to λ , implying

$$(M(G|_{\bar{S}}) - \lambda I)_{ii} \neq 0 \text{ for all } m < i \leq n.$$

Hence, $M(G)_{\bar{S}\bar{S}} - \lambda I$ is an upper triangular matrix with nonzero diagonal and is therefore invertible.

Letting $M = M(G)$, the upper triangular matrix $M_{\bar{S}\bar{S}} - \lambda I$ can be written as

$$M_{\bar{S}\bar{S}} - \lambda I = D(I + N),$$

where $D = \text{diag}[M_{m+1, m+1} - \lambda \dots M_{nn} - \lambda]$ and $N \in \mathbb{W}^{(n-m) \times (n-m)}$ is the nilpotent matrix given by

$$N_{ij} = \begin{cases} \frac{M_{i+m, j+m} - \lambda}{M_{i+m, i+m} - \lambda} & \text{for } i < j, \\ 0 & \text{otherwise.} \end{cases} \quad (2.3)$$

The inverse of $M_{\bar{S}\bar{S}} - \lambda I$ is then

$$(I + N)^{-1} D^{-1} = (I + N - N^2 - \dots + (-1)^{n-m-1} N^{n-m-1}) D^{-1}, \quad (2.4)$$

where $D^{-1} = \text{diag}[\frac{1}{M_{m+1, m+1} - \lambda} \dots \frac{1}{M_{nn} - \lambda}]$.

For $1 \leq \ell \leq n - m - 1$, the matrix N^ℓ is given by

$$N_{ij}^\ell = \begin{cases} \sum \prod_{k=1}^\ell N_{i_{k-1}, i_k} & \text{for } i < j, \\ 0 & \text{otherwise,} \end{cases}$$

where the sum is taken over all strictly increasing $(\ell + 1)$ -tuples $i = i_0 < \dots < i_\ell = j$ starting at i and ending at j . Hence for $1 \leq i, j \leq m$, we have

$$\begin{aligned}
M_{ij} + (M_{S\bar{S}}(M_{\bar{S}\bar{S}} - \lambda I)^{-1}M_{\bar{S}S})_{ij} \\
&= M_{ij} + (M_{S\bar{S}}(I + N - N^2 - \dots + (-1)^{n-m-1}N^{n-m-1})D^{-1}M_{\bar{S}S})_{ij} \\
&= M_{ij} + \sum_{p=m+1}^n \sum_{q=m+1}^n M_{pi} \left(\sum_{\ell=0}^{n-m-1} (-1)^\ell N^\ell D^{-1} \right)_{pq} M_{qj}.
\end{aligned}$$

Observe that the entries of the matrix $(-1)^\ell N^\ell D^{-1}$ are

$$(-1)^\ell (N^\ell D^{-1})_{ij} = \begin{cases} \left(\sum \prod_{k=1}^{\ell} \frac{M_{i_{k-1}+m, i_k+m}}{\lambda - M_{i_{k-1}+m, i_{k-1}+m}} \right) \left(\frac{1}{\lambda - M_{j+m, j+m}} \right) & \text{for } i < j, \\ 0 & \text{otherwise,} \end{cases}$$

where as before, the sum is taken over all increasing $(\ell + 1)$ -tuples $i = i_0 < \dots < i_\ell = j$ starting at i and ending at j . Therefore,

$$M_{ij} + (M_{S\bar{S}}(M_{\bar{S}\bar{S}} - \lambda I)^{-1}M_{\bar{S}S})_{ij} = M_{ij} + \sum \left(\sum_{\ell=0}^{n-m-1} \frac{M_{ip}}{\lambda - M_{pp}} \prod_{k=1}^{\ell} \frac{M_{i_{k-1}, i_k}}{\lambda - M_{i_k, i_k}} M_{qj} \right),$$

where the sum is taken over all increasing $(\ell + 1)$ -tuples $p = i_0 < i_1 < \dots < i_\ell = q$ for $m < p, q \leq n$.

Under the assumption that $M(G)_{\bar{S}\bar{S}} - \lambda I$ is upper triangular, the graph G has the following property: if $\beta = v_i, v_{i_2}, \dots, v_{i_{\ell-1}}, v_j \in \mathcal{B}_S(G)$, then $i_2 < \dots < i_{\ell-1}$, where $i, j \leq m$ and $i_2, \dots, i_{\ell-1} > m$.

Thus, the branch product of β can be written as

$$\mathcal{P}_\omega(\beta) = \frac{M_{i, i_2}}{\lambda - M_{i_2, i_2}} \prod_{k=1}^{\ell} \frac{M_{i_{k-1}, i_k}}{\lambda - M_{i_k, i_k}} M_{i_{\ell-1}, j}.$$

Summing over all branches of $\mathcal{B}_S(G)$ from v_i to v_j , we arrive at

$$M(\mathcal{R}_S(G))_{ij} = M_{ij} + \sum \left(\sum_{\ell=0}^{n-m-1} \frac{M_{ip}}{\lambda - M_{pp}} \prod_{k=1}^{\ell} \frac{M_{i_{k-1}, i_k}}{\lambda - M_{i_k, i_k}} M_{qj} \right).$$

Therefore, the weighted adjacency matrix of $\mathcal{R}_S(G)$ is

$$M(\mathcal{R}_S(G)) = M(G)_{SS} - M(G)_{S\bar{S}}(M(G)_{\bar{S}\bar{S}} - \lambda I)^{-1}M(G)_{\bar{S}S} = \mathcal{R}(M(G), S),$$

which completes the proof. $\square$

The reason we consider both graph and matrix reductions is that both points of view have their advantages. For one, graphs allow one to analyze network structure visually, while matrices allow for easy storage and manipulation of this network

information. More to the point, equation (2.2) indicate how the spectrum of a graph is preserved in terms of the graph's branch structure. This observation will allow us, in Sects. 2.5 and 2.6 of this chapter, to develop other types of isospectral transformations. These transformations will be based on manipulating a graph's path and cycle structure in ways that modify the graph's spectrum in a predictable way.

For now, we note that if S is a structural set of the graph $G \in \mathbb{G}$, then the isospectral reduction $\mathcal{R}_S(G)$ is also a graph in $\mathbb{G}$. Hence, both G and $\mathcal{R}_S(G)$ have well-defined spectra. The relation between $\sigma(G)$ and $\sigma(\mathcal{R}_S(G))$ is given in the following corollary of Theorems 1.1 and 2.1.

Corollary 2.1. *Let S be a structural set of the graph $G \in \mathbb{G}$. Then*

$$\begin{aligned}\sigma(\mathcal{R}_S(G)) &= (\sigma(G) \cup \sigma^{-1}(G|_{\bar{S}})) - (\sigma(G|_{\bar{S}}) \cup \sigma^{-1}(G)); \text{ and} \\ \sigma^{-1}(\mathcal{R}_S(G)) &= (\sigma(G|_{\bar{S}}) \cup \sigma^{-1}(G)) - (\sigma(G) \cup \sigma^{-1}(G|_{\bar{S}})).\end{aligned}$$

Suppose that $G = (V, E, \omega)$ has the structural set S . Because the graph $G|_{\bar{S}}$ has a particular form, it is possible to compute both $\sigma(G|_{\bar{S}})$ and $\sigma^{-1}(G|_{\bar{S}})$ quickly. That is, since $M(G|_{\bar{S}}) - \lambda I$ is similar to an upper triangular matrix via some permutation, it follows that

$$\det(M(G|_{\bar{S}}) - \lambda I) = \prod_{v_i \in \bar{S}} (\omega(e_{ii}) - \lambda). \quad (2.5)$$

Since the product $\prod_{v_i \in \bar{S}} (\omega(e_{ii}) - \lambda) = p(\lambda)/q(\lambda)$ for some $p(\lambda)/q(\lambda) \in \mathbb{W}$ then

$$\sigma(G|_S) = \{\lambda \in \mathbb{C} : p(\lambda) = 0\} \text{ and } \sigma^{-1}(G|_S) = \{\lambda \in \mathbb{C} : q(\lambda) = 0\}. \quad (2.6)$$

For complex-valued matrices, Corollary 2.1 together with (2.5) and (2.6) implies the following corollary.

Corollary 2.2. *Let S be a structural set of the graph $G \in \mathbb{G}$. If $M(G) \in \mathbb{C}^{n \times n}$, then*

- (i) $\sigma^{-1}(G) = \emptyset$ and $\sigma^{-1}(G|_{\bar{S}}) = \emptyset$;
- (ii) $\sigma(G|_{\bar{S}}) = \{\omega(e_{ii}) : v_i \in \bar{S}\}$;
- (iii) $\sigma(\mathcal{R}_S(G)) = \sigma(G) - \sigma(G|_{\bar{S}})$; and
- (iv) $\sigma^{-1}(\mathcal{R}_S(G)) = \sigma(G|_{\bar{S}}) - \sigma(G)$.

In many applications, the graphs (matrices) that are used have real or positive weights (entries). If $G = (V, E, \omega)$ has complex-valued weights and $S \in st(G)$, then part (iii) of Corollary 2.2 states that the spectra of $\mathcal{R}_S(G)$ and G differ at most by the spectrum of $G|_{\bar{S}}$. Moreover, part (ii) of Corollary 2.2 states that the spectrum $\sigma(G|_{\bar{S}})$ consists of the weights of the loops e_{ii} for $v_i \in \bar{S}$ and is therefore easily identified.

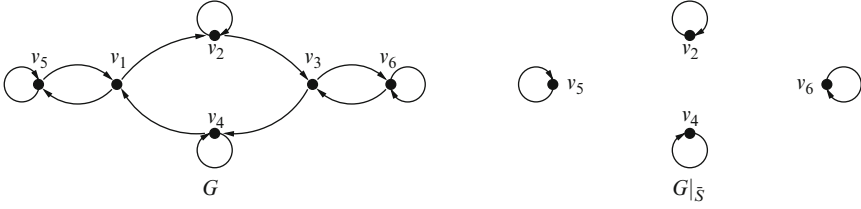


Fig. 2.4 The restriction of the graph G in Example 2.5 to $\bar{S} = \{v_2, v_4, v_5, v_6\}$, where each edge in each of G and $G|_{\bar{S}}$ has unit weight

Similar to Theorem 1.1 for matrices, Corollary 2.1 describes exactly which eigenvalues we may gain from an isospectral reduction and which we may lose. In this way, an isospectral reduction of a graph preserves the spectral information of the original graph. This will be important, for instance, in Sect. 2.6, where we consider isospectral reductions that do not affect the nonzero eigenvalues of a graph.

Example 2.3. Let G be the graph considered in Example 2.2. As previously shown, the vertex set $S = \{v_1, v_3\}$ is a structural set of G . Moreover, $M(G) \in \mathbb{C}^{6 \times 6}$. Hence, Corollary 2.2 allows us to compute the eigenvalues of the reduced graph $\mathcal{R}_S(G)$ quickly once the eigenvalues of G are known.

As one can compute, the eigenvalues of the graph G are $\sigma(G) = \{2, -1, 1, 1, 1, 0\}$. The restricted graph $G|_{\bar{S}}$, shown in Fig. 2.4 (right), has loop weights $\omega(e_{22}) = 1$, $\omega(e_{44}) = 1$, $\omega(e_{55}) = 1$, and $\omega(e_{66}) = 1$. Corollary 2.2 then implies that $\sigma(G|_{\bar{S}}) = \{1, 1, 1, 1\}$. Additionally, since $\sigma(\mathcal{R}_S(G)) = \sigma(G) - \sigma(G|_{\bar{S}})$, the spectrum of the reduced graph is $\sigma(\mathcal{R}_S(G)) = \{2, -1, 0\}$.

Since the graph $\mathcal{R}_S(G)$ has two vertices, the matrix $M(\mathcal{R}_S(G))$ belongs to $\mathbb{W}_{\pi}^{2 \times 2}$. However, notice that

$$\det(M(\mathcal{R}_S(G)) - \lambda I) = \frac{\lambda^3 - \lambda^2 - 2\lambda}{\lambda - 1},$$

which is zero for $\lambda = 2, -1, 0$. Similar to Example 1.1, this is an explicit demonstration of the fact that an $n \times n$ matrix in $\mathbb{W}_{\pi}^{n \times n}$ may have more than n eigenvalues.

Therefore, the effect of reducing G over S is that we lose the eigenvalues $\{1, 1, 1, 1\}$. However, even if $\sigma(G)$ is unknown, we still know the following. The set of eigenvalues $\sigma(G|_{\bar{S}}) = \{1, 1, 1, 1\}$ is the most by which $\sigma(\mathcal{R}_S(G))$ and $\sigma(G)$ can differ.

We note that this example is equivalent to Example 1.3 in Chap. 1. The difference is that this example is taken from the point of view of a graph reduction. This is done to emphasize the differences and similarities between isospectral reductions of matrices and graphs.

We note that for every $G \in \mathbb{G}$, both $\sigma(G|_{\bar{S}})$ and $\sigma^{-1}(G|_{\bar{S}})$ are easily calculated via equation (2.5). Therefore, Corollary 2.1 offers a quick way of computing the eigenvalues of a reduced graph if the spectrum of the original unreduced graph is known.

Before moving on to the following section, on sequential graph reductions, we note that undirected graphs are often studied in the theory of networks. This is the case whenever the interaction between two network elements has the same effect on both of them, i.e., when the interaction between elements is *symmetric*.

Undirected graphs are particular types of directed graphs and as such can be reduced using Definition 2.4. For the moment, we consider the theory of isospectral graph reductions restricted to the class of undirected graphs.

Definition 2.5. A graph $G = (V, E, \omega)$ in $\mathbb{G}$ is an *undirected graph* if whenever the edge e_{ij} is in E , then $e_{ji} \in E$ and $\omega(e_{ij}) = \omega(e_{ji})$.

A consequence of Definition 2.5 is that a graph $G \in \mathbb{G}$ is undirected if and only if its adjacency matrix $M(G)$ is symmetric. Typically, an undirected graph is assumed to have no loops. The reason we allow undirected graphs to be graphs possibly with loops is that it allows us to state the following results more concisely.

Theorem 2.2. Suppose S is a structural set of the undirected graph $G \in \mathbb{G}$. Then the reduced graph $\mathcal{R}_S(G)$ is an undirected graph.

Proof. If $G \in \mathbb{G}$ is undirected, then its adjacency matrix $M = M(G)$ is symmetric. For $S \in st(G)$, we have

$$(M_{S\bar{S}}(M - \lambda I)_{\bar{S}\bar{S}}^{-1}M_{\bar{S}S})^T = M_{\bar{S}S}^T((M - \lambda I)_{\bar{S}\bar{S}}^{-1})^T M_{SS}^T = M_{S\bar{S}}(M - \lambda I)_{\bar{S}\bar{S}}^{-1}M_{\bar{S}S},$$

where the second inequality follows from the fact that $M_{\bar{S}S}^T = M_{S\bar{S}}$, $M_{SS}^T = M_{SS}$, and the fact that the inverse of the symmetric matrix $(M - \lambda I)_{\bar{S}\bar{S}}$ is also symmetric. Hence, the matrix $M_{S\bar{S}}(M - \lambda I)_{\bar{S}\bar{S}}^{-1}M_{\bar{S}S}$ is symmetric.

It then follows that the reduced matrix

$$\mathcal{R}(M; S) = (M - \lambda I)_{SS} - M_{S\bar{S}}(M - \lambda I)_{\bar{S}\bar{S}}^{-1}M_{\bar{S}S}$$

is symmetric, implying that $\mathcal{R}_S(G)$ is an undirected graph. $\square$

Example 2.4. Let G be the undirected graph shown in Fig. 2.5 (left). The edges found in this figure are undirected, but each can be thought of as being two directed edges oriented in opposite directions with equal (unit) weights.

As one can check, the set $S = \{v_1, v_3, v_4, v_6\}$ is a structural set of G . Theorem 2.2 then implies that the reduced graph $\mathcal{R}_S(G)$ is undirected, which can be seen in Fig. 2.5 (right).

Given a graph $G = (V, E, \omega)$, recall that two vertices $v_i, v_j \in V$ are *adjacent* if $e_{ij} \in E$. Since two adjacent vertices form a cycle in an undirected graph, this

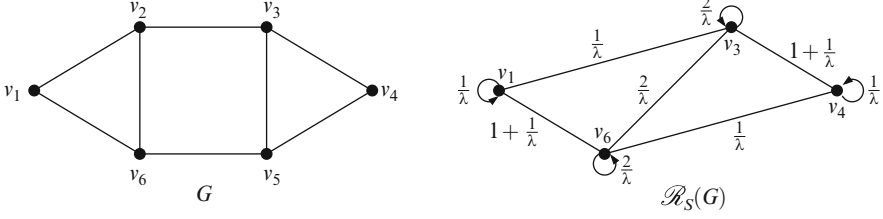


Fig. 2.5 The undirected graph G with unit edge weights and its reduction $\mathcal{R}_S(G)$, where the structural set S is given by $S = \{v_1, v_3, v_4, v_6\}$

naturally restricts which sets can be its structural sets. In fact, this observation allows us to characterize which sets can and cannot be structural sets of an undirected graph.

Theorem 2.3. *Let $G = (V, E, \omega)$ be an undirected graph. Then $S \in st(G)$ if and only if no two vertices $v_i, v_j \in \bar{S}$ are adjacent and $\omega(e_{kk}) \neq \lambda$ for all $v_k \in \bar{S}$.*

Proof. For $S \in st(G)$, suppose $v_i, v_j \in \bar{S}$, where $i \neq j$. Then v_i and v_j are not adjacent, since otherwise, v_i, v_j would form a cycle. Moreover, $\omega(e_{kk}) \neq \lambda$ for all $v_k \in \bar{S}$ by Definition 2.2.

Conversely, suppose that no two vertices $v_i, v_j \in \bar{S}$ are adjacent. Assuming that $v_1, \dots, v_m$ for $m \geq 2$ is a cycle of G , then if it is the case that $v_1 \in \bar{S}$, it follows that $v_2 \in S$, since v_1 and v_2 are adjacent. Otherwise, if $v_1 \in S$, then in either case, the cycle $v_1, \dots, v_m$ will contain a vertex of S . Additionally, if $\omega(e_{kk}) \neq \lambda$ for all $v_k \in \bar{S}$, then it follows that S is a structural set of G . $\square$

Based on Theorem 2.3, the set $S = \{v_1, v_3, v_4, v_6\}$ of the graph G in Fig. 2.5 (left) is a structural set, since G has no loops and v_2, v_5 are not adjacent.

2.3 Sequential Graph Reductions

Observe that if $G \in \mathbb{G}$, then every reduction $\mathcal{R}_S(G)$ is again a graph in $\mathbb{G}$. Since $\mathcal{R}_S(G)$ may have a structural set T , it may be possible to consider a sequence of reductions on the graph $G \in \mathbb{G}$. However, to do so formally requires that we first extend our notation to sequences of isospectral graph reductions.

For $G = (V, E, \omega)$, suppose $S_m \subset S_{m-1} \subset \dots \subset S_1 \subset V$ such that $S_1 \in st(G)$, $\mathcal{R}_1(G) = \mathcal{R}_{S_1}(G)$, and

$$S_{i+1} \in st(\mathcal{R}_i(G)) \text{ where } \mathcal{R}_{S_{i+1}}(\mathcal{R}_i(G)) = \mathcal{R}_{i+1}(G), \quad 1 \leq i \leq m-1.$$

If this is the case, we say that $S_1, \dots, S_m$ induce a sequence of reductions on G with final vertex set S_m . By way of notation, we write $\mathcal{R}_m(G) = \mathcal{R}(G; S_1, \dots, S_m)$,

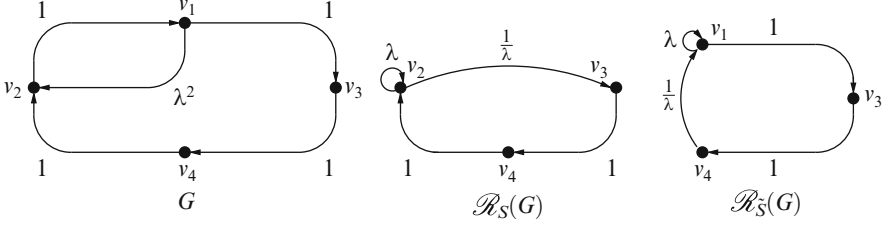


Fig. 2.6 The graph G and its reductions considered in Example 2.5

where $\mathcal{R}(G; S_1, \dots, S_m)$ denotes the graph G reduced over the vertex set S_1 , then over S_2 , and so on until G is reduced over the final vertex set S_m .

Because an isospectral graph reduction is a special type of matrix reduction, Theorem 2.1 has the following corollary.

Corollary 2.3. *If $S_1, \dots, S_m$ induces a sequence of reductions on $G \in \mathbb{G}$, then*

$$M(\mathcal{R}(G; S_1, \dots, S_m)) = \mathcal{R}(M(G); S_m).$$

If $S \notin st(G)$, it is natural to ask whether there exists a sequence of vertex sets $S \subset S_{m-1} \subset \dots \subset S_1 \subset V$ that induce a sequence of reductions on G , and if such a sequence exists, whether it is the only such sequence.

To address these questions we consider the following example.

Example 2.5. Consider the graph $G = (V, E, \omega) \in \mathbb{G}$ shown in Fig. 2.6 (left) with adjacency matrix

$$M(G) = \begin{bmatrix} 0 & \lambda^2 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

Here, our goal is to remove the vertices v_1 and v_2 from G . However, since the set $\{v_3, v_4\}$ is not in $st(G)$ our only option is to remove these vertices sequentially, one at a time.

Removing v_1 then v_2 amounts to finding the isospectral reduction $\mathcal{R}(G; S, T)$, where $S = \{v_2, v_3, v_4\}$ and $T = \{v_3, v_4\}$. Since the set $S = \{v_2, v_3, v_4\}$ is a structural set of G , it is possible to find the reduction $\mathcal{R}(G; S)$, which is shown in Fig. 2.6 (center). However, $\mathcal{R}(G; S)$ cannot be reduced over the vertex set T , since the weight of v_2 in this graph is equal to λ .

Suppose we attempt to reverse the order in which we reduce G by first removing v_2 , and then v_1 . To do so, we let $\tilde{S} = \{v_1, v_3, v_4\}$, where we attempt to compute the reduction $\mathcal{R}(G; \tilde{S}, T)$. However, the reduction $\mathcal{R}(G; \tilde{S})$ shown in Fig. 2.6 (right) has the same problem as before. Namely, the vertex set T is not a structural set of

$\mathcal{R}(G; \tilde{S})$. Since we cannot remove v_1 and v_2 together or sequentially from G , we are forced to conclude that it is not possible to reduce G isospectrally to a graph with vertex set T .

To determine when it is possible to reduce a graph $G = (V, E, \omega)$ and when it is not, we note the following. If the weight $\omega(e_{ii})$ is not equal to λ for some $v_i \in V$, then the vertex set $S = V - \{v_i\}$ is a structural set of G . This follows from the fact that $\tilde{S} = \{v_i\}$. Hence, the graph $G|_{\tilde{S}}$ is the graph restricted to the single vertex v_i , and every cycle of $G|_{\tilde{S}}$ is a loop. Therefore, $G \in \mathbb{G}$ can be reduced over the structural set $S = V - \{v_i\}$ if it is known that $\omega(e_{ii}) \neq \lambda$.

Another way to state this is to say that it is possible to remove the vertex v_i from G via an isospectral graph reduction if $\omega(e_{ii}) \neq \lambda$ even when nothing is known about the graph structure of G .

This has the following important implication. Suppose it is known that no loop of G and no loop of any sequential reduction of G has weight λ . If this is the case, then it is possible to remove any sequence of single vertices from G via some sequence of isospectral reductions. Consequently, the graph G can be reduced to a graph on any subset of its vertex set by sequentially removing any “unwanted” vertices.

In general, though, there is no way to know beforehand whether a set of vertices can be removed from a graph without actually going through the process of trying to remove those vertices. However, as with matrices, there is a way to overcome this problem.

Definition 2.6. Let $\mathbb{G}_\pi$ be the set of graphs given by

$$\mathbb{G}_\pi = \{G \in \mathbb{G} : M(G) \in \mathbb{W}_\pi^{n \times n} \text{ for some } n \in \mathbb{N}\}.$$

Lemma 2.1. *If $G \in \mathbb{G}_\pi$ and $S \in st(G)$, then $\mathcal{R}_S(G) \in \mathbb{G}_\pi$. In particular, no loop of G and no loop of any reduction of G can have weight λ .*

Proof. Suppose $G = (V, E, \omega) \in \mathbb{G}_\pi$ has the structural set S . Hence, $M(G) \in \mathbb{W}_\pi^{n \times n}$ for some $n \in \mathbb{N}$. Using Theorems 2.1 and 1.2, it follows that

$$M(\mathcal{R}_S(G)) = \mathcal{R}(M(G); S) \in \mathbb{W}_\pi^{|S| \times |S|},$$

implying $\mathcal{R}_S(G) \in \mathbb{G}_\pi$. Since each edge weight of G and $\mathcal{R}_S(G)$ belongs to $\mathbb{W}_\pi$, it follows that no edge of these graphs can have the weight $\lambda/1 \notin \mathbb{W}_\pi$. This completes the proof. $\square$

A direct consequence of Lemma 2.1 is that if $G \in \mathbb{G}_\pi$, then G can be (sequentially) reduced to a graph on any subset of its vertex set. This result is stated in the following theorem.

Theorem 2.4 (Existence of Sequential Graph Reductions). *Suppose $G = (V, E, \omega)$ is in $\mathbb{G}_\pi$. If $S \subset V$ is nonempty, then there are vertex sets $S \subset S_{m-1} \subset \dots \subset S_1 \subset V$ such that $S_1, \dots, S_{m-1}, S$ induces a sequence of reductions on G .*

Proof. Let $G = (V, E, \omega)$ be in $\mathbb{G}_\pi$. If $S \subset V$ is nonempty, then suppose, without loss of generality, that $S = \{v_1, \dots, v_{n-m}\}$, where $|V| = n$. Letting $S_i = \{v_1, \dots, v_{n-i}\}$, we see that for each $1 \leq i < n - m$, the claim is that vertex set S_i is in $st(\mathcal{R}_{S_{i+1}}(G))$.

Since S_i and S_{i+1} differ by a single vertex v_{i+1} , it follows that S_i is a structural set of $\mathcal{R}_{S_{i+1}}(G)$, as long as the weight of the loop $e_{i+1,i+1}$ in $\mathcal{R}_{S_{i+1}}(G)$ is not equal to $\lambda \in \mathbb{W}$. Under the assumption that $G \in \mathbb{G}_\pi$, repeated use of Lemma 2.1 implies that this is not the case for each $1 \leq i < n - m$, verifying the claim. Therefore, the sets $S_1, \dots, S_{m-1}, S$ induce a sequence of reductions on G . $\square$

It is therefore possible to reduce a graph $G \in \mathbb{G}_\pi$ to a graph on any (nonempty) subset of its vertex set via some sequence of isospectral reductions. Observe that Theorem 2.4 does not apply to the graph in Example 2.5, since that graph does not have all weights in the set $\mathbb{W}_\pi$.

Theorem 2.4 can be thought of as an existence result for sequences of isospectral graph reductions. That is, assuming that S is a vertex subset of $G \in \mathbb{G}_\pi$, there is always a sequence of reductions on G with final vertex S . Sequences of reductions also have the following uniqueness property.

Theorem 2.5 (Uniqueness of Sequential Graph Reductions). *Suppose the graph $G = (V, E, \omega)$ is in $\mathbb{G}_\pi$. If $S \subset V$ is nonempty, where both $S_1, \dots, S_{m-1}, S$ and $T_1, \dots, T_{n-1}, S$ induce a sequence of reductions on G , then*

$$\mathcal{R}(G; S_1, \dots, S_{m-1}, S) = \mathcal{R}(G; T_1, \dots, T_{n-1}, S).$$

Proof. Suppose $G = (V, E, \omega) \in \mathbb{G}_\pi$. If both $S_1, \dots, S_{m-1}, S$ and $T_1, \dots, T_{n-1}, S$ induce a sequence of reductions on G , then

$$M(\mathcal{R}(G; S_1, \dots, S_{m-1}, S)) = \mathcal{R}(M(G); S) = M(\mathcal{R}(G; T_1, \dots, T_{n-1}, S)),$$

using Corollary 2.3. Since these isospectral graph reductions have the same adjacency matrix, they are the same graph. $\square$

Suppose the graph $G = (V, E, \omega)$ is a graph in $\mathbb{G}_\pi$ and that $S \subset V$ is nonempty. By combining the existence and uniqueness results of Theorems 2.4 and 2.5, it follows that there is exactly one graph that results from sequentially reducing G by any sequence of reductions with final vertex set S . This fact allows us to introduce the following definition.

Definition 2.7. Let $G = (V, E, \omega)$ be a graph in $\mathbb{G}_\pi$. If $S \subseteq V$ is nonempty, define

$$\mathcal{R}_S[G] = \mathcal{R}(G; S_1, \dots, S_{m-1}, S),$$

where $S_1, \dots, S_{m-1}, S$ is any sequence that induces a sequence of reductions on G with final vertex set S .

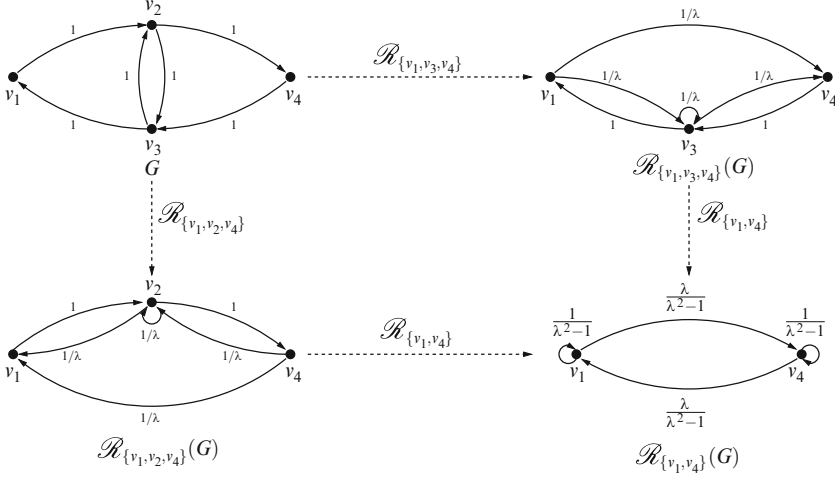


Fig. 2.7 Distinct sequences of isospectral reductions with the same final vertex set and outcome

The graph $\mathcal{R}_S[G]$ is well defined as a result of Theorems 2.4 and 2.5. The notation $\mathcal{R}_S[G]$ given in Definition 2.7 is intended to emphasize the fact that S need not be a structural set of G .

Similar to Remark 1.1, we note that if the adjacency matrix $M(G)$ is in $\mathbb{C}^{n \times n}$, then $G \in \mathbb{G}_\pi$. Therefore, every graph with complex weights can be uniquely reduced over every nonempty subset of its vertex set.

Example 2.6. Let $G = (V, E, \omega)$ be the graph shown in Fig. 2.7. Our goal is to reduce G over the vertex set $\{v_1, v_4\} \subset V$. Note that since $G \in \mathbb{G}_\pi$, Theorem 2.4 guarantees that there is at least one sequence of reductions that reduces G to the graph $\mathcal{R}_{\{v_1, v_4\}}[G]$.

In fact, there are exactly two. This follows from the fact that $\{v_1, v_4\} \notin st(G)$. Hence, G cannot be reduced over $\{v_1, v_4\}$ with a single reduction. However, every (nontrivial) reduction of G removes at least one vertex from G . Therefore, the two possible ways of reducing G over the vertex set $\{v_1, v_4\}$ are

$$\mathcal{R}_{\{v_1, v_4\}}[G] = \mathcal{R}(G; \{v_1, v_2, v_4\}, \{v_1, v_4\}) \text{ and} \quad (2.7)$$

$$\mathcal{R}_{\{v_1, v_4\}}[G] = \mathcal{R}(G; \{v_1, v_3, v_4\}, \{v_1, v_4\}). \quad (2.8)$$

Both of the reductions given in (2.7) and (2.8) are shown in Fig. 2.7. The dashed arrows labeled $\mathcal{R}_T$ in this figure represent the reduction of a graph over some structural set $T \subset V$. This notation is meant to emphasize that this diagram commutes. That is,

$$\mathcal{R}_{\{v_1, v_4\}}(\mathcal{R}_{\{v_1, v_2, v_4\}}(G)) = \mathcal{R}_{\{v_1, v_4\}}(\mathcal{R}_{\{v_1, v_3, v_4\}}(G)),$$

as guaranteed by Theorem 2.5.

Using Definition 2.7, we state the following general result for isospectral graph reductions, which follows from Theorems 1.1, 2.4, and 2.5.

Theorem 2.6. *If $G = (V, E, \omega) \in \mathbb{G}_\pi$ and $S \subset V$ is nonempty, then*

$$\begin{aligned}\sigma(\mathcal{R}_S[G]) &= (\sigma(G) \cup \sigma^{-1}(G|_{\bar{S}})) - (\sigma(G|_{\bar{S}}) \cup \sigma^{-1}(G)); \text{ and} \\ \sigma^{-1}(\mathcal{R}_S[G]) &= (\sigma(G|_{\bar{S}}) \cup \sigma^{-1}(G)) - (\sigma(G) \cup \sigma^{-1}(G|_{\bar{S}})).\end{aligned}$$

Theorem 2.6 can be thought of as a generalization of Corollary 2.1 from structural sets to any nonempty vertex subset of a graph. However, Theorem 2.6 holds only for graphs in $\mathbb{G}_\pi$, whereas Corollary 2.1 holds for every graph $G \in \mathbb{G}$.

In the following section, the results established here will be used to give rules for devising equivalence relations on the set of graphs $\mathbb{G}_\pi$.

2.4 Equivalence Relations

Theorems 2.4 and 2.5 from the previous section assert that a graph $G \in \mathbb{G}_\pi$ has a unique reduction to any (nonempty) subset of its vertex set via some sequence of isospectral reductions. In this section, this fact will allow us to define equivalence relations on the collection of graphs in $\mathbb{G}_\pi$. To define these equivalence relations, we need first to introduce the notion of isomorphic graphs.

Two weighted digraphs $G_1 = (V_1, E_1, \omega_1)$ and $G_2 = (V_2, E_2, \omega_2)$ are *isomorphic* if there is a bijection $b : V_1 \rightarrow V_2$ such that there is an edge e_{ij} in G_1 from v_i to v_j if and only if there is an edge $\tilde{e}_{ij}$ between $b(v_i)$ and $b(v_j)$ in G_2 with $\omega_2(\tilde{e}_{ij}) = \omega_1(e_{ij})$. If the map b exists, it is called an *isomorphism*, and we write $G_1 \simeq G_2$.

An isomorphism is essentially a relabeling of the vertices of a graph. Therefore, if two graphs are isomorphic, then their spectra are identical. The equivalent notion for matrices is that $A(\lambda) \in \mathbb{W}^{n \times n}$ is similar to $B(\lambda) \in \mathbb{W}^{n \times n}$ by some perturbation matrix P , i.e., $A(\lambda) = PB(\lambda)P^{-1}$. This notion of being isomorphic, together with the uniqueness and existence of sequential graph reductions, allows us to define the following equivalence relations on the graphs $\mathbb{G}_\pi$.

Theorem 2.7 (Spectral Equivalence). *Suppose that for each graph $G = (V, E, \omega)$ in $\mathbb{G}_\pi$, τ is a rule that selects a unique nonempty subset $\tau(G) \subset V$. Then τ induces an equivalence relation $\sim$ on the set $\mathbb{G}_\pi$, where $G \sim H$ if $\mathcal{R}_{\tau(G)}[G] \simeq \mathcal{R}_{\tau(H)}[H]$.*

Proof. If $G \in \mathbb{G}_\pi$ the set $\tau(G) \subseteq V$ is unique and nonempty, then the graph $\mathcal{R}_{\tau(G)}[G]$ is uniquely determined by the rule τ . Hence, τ induces a unique reduction on $G \in \mathbb{G}_\pi$.

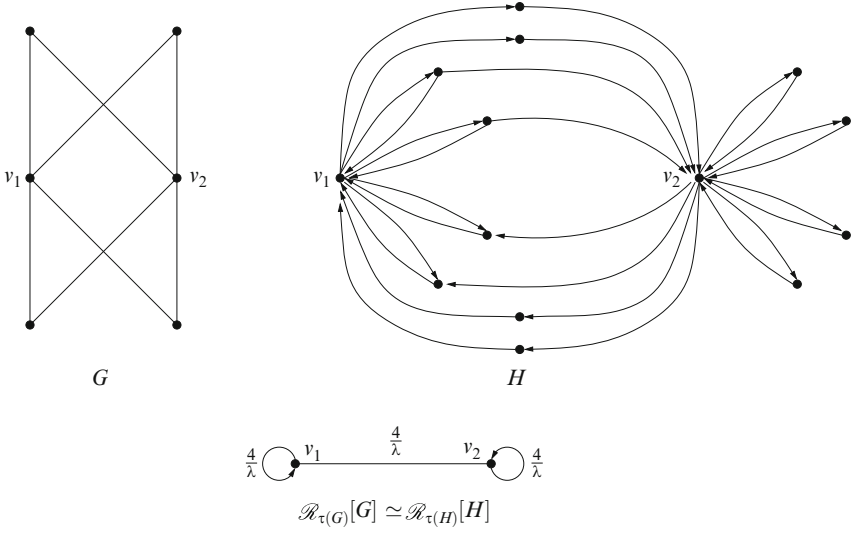


Fig. 2.8 The unweighted undirected graph G is equivalent to the unweighted directed graph H under the relation induced by the rule τ given in Example 2.7. Here, $\tau(G) = \tau(H) = \{v_1, v_2\}$

The claim, then, is that the relation $G \sim H$ if $\mathcal{R}_{\tau(G)}[G] \cong \mathcal{R}_{\tau(H)}[H]$ is an equivalence relation on $\mathbb{G}_\pi$. This follows from the fact that the relation of being isomorphic is reflexive, symmetric, and transitive, which completes the proof. $\square$

Two graphs may look very different but be spectrally equivalent, suggesting that the corresponding networks have similar dynamics. The major idea in this section is that by choosing an appropriate rule τ , one can discover this similarity.

Example 2.7. Suppose $G = (V, E, \omega)$. For $v \in V$, let $d_{\text{in}}(v)$ be the *in-degree* of v , which is the number of incoming edges incident to v , excluding loops. In an undirected graph, the in-degree of a vertex v is then the same as the number of nonloop edges incident to v .

If $\Delta(G) = \max_{v \in V} d_{\text{in}}(G)$ indicates the *maximum in-degree* of G , let τ be the rule

$$\tau(G) := \{v \in V : d_{\text{in}}(v) > \Delta(G)/2\}.$$

Observe that for each graph $G \in \mathbb{G}_\pi$, the set $\tau(G)$ both exists and is unique. Thus, the relation of having an isomorphic reduction with respect to this rule induces an equivalence relation on $\mathbb{G}_\pi$.

Here, the rule τ selects all those vertices that have an in-degree greater than $\Delta(G)/2$. In Fig. 2.8, the graphs G and H have the vertex set $\tau(G) = \tau(H) = \{v_1, v_2\}$. Moreover, as shown in the figure, the graph $\mathcal{R}_{\tau(G)}[G]$ is isomorphic to $\mathcal{R}_{\tau(H)}[H]$, implying $G \sim H$ under the relation $\sim$ induced by the rule τ . What

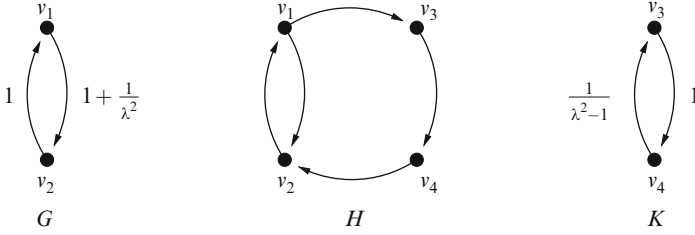


Fig. 2.9 We have $G = \mathcal{R}_S[H]$ and $\mathcal{R}_T[H] = K$ for $S = \{v_1, v_2\}$ and $T = \{v_3, v_4\}$, but the graphs G and K do not have isomorphic reductions

is interesting here is that although these graphs do not appear to have a similar structure, they are the same when reduced with respect to the rule τ .

We note that not every rule that one could propose will select a unique vertex set of a graph. The simplest example is the rule that randomly selects a single vertex of a graph. This selection is, of course, nonunique. The reason it does not lead to an equivalence relation is that without a unique vertex set, the relation cannot be reflexive.

Importantly, choosing a rule that selects a unique vertex set of each graph allows one to study the graphs in $\mathbb{G}_\pi$ modulo some particular graph feature. In Example 2.7, this graph feature, or vertex set, is the set of vertices that have in-degree less than or equal to $\Delta(G)/2$ for every graph G .

From a practical point of view, this allows those studying a particular class of networks a way of comparing the *reduced topology* of these networks. Of course, the particular reduction rule τ should be designed by the particular biologist, chemist, physicist, etc., to have some significance with respect to the networks under consideration.

Before continuing to the next section, we note that the relation of simply having isomorphic reductions is not transitive. That is, if both $\mathcal{R}_S[G] \simeq \mathcal{R}_T[H]$ and $\mathcal{R}_U[H] \simeq \mathcal{R}_V[K]$, it is not necessarily the case that there are sets X and Y , subsets of the vertex sets of G and K respectively, such that $\mathcal{R}_X[G] \simeq \mathcal{R}_Y[K]$.

As an example, in Fig. 2.9, we have both $\mathcal{R}_S[G] \simeq \mathcal{R}_S[H]$ and $\mathcal{R}_T[H] \simeq \mathcal{R}_T[K]$, where $S = \{v_1, v_2\}$ and $T = \{v_3, v_4\}$. However, one can quickly check that for no subsets $X \subseteq S$ and $Y \subseteq T$ do we have $\mathcal{R}_X[G] \simeq \mathcal{R}_Y[K]$. That is, the relation of having isomorphic reductions is not an equivalence relation on $\mathbb{G}$, since it is not transitive. Overcoming this intransitivity requires some rule τ that selects a unique set of vertices from each graph in $\mathbb{G}$ (as in Theorem 2.7).

2.5 Weight-Preserving Isospectral Transformations

Suppose $G = (V, E, \omega)$ is a graph in $\mathbb{G}$. Recall that the *weight set* of G , or the collection of edge weights of G , is the set

$$\omega(E) = \{\omega(e_{ij}) : e \in E\}.$$

The isospectral graph reductions introduced in Sect. 2.2 modify not only the graph structure but also the weight set of a graph. That is, if $\mathcal{R}_S(G) = (S, \mathcal{E}, \mu)$ is a reduction of $G = (V, E, \omega)$, then typically, $\omega(E) \neq \mu(\mathcal{E})$.

This may lead one to assume that the procedure of reducing a graph simply shifts the complexity of the graph's structure to its set of edge weights. While the edge weights can become more complicated in the case of isospectral reductions, this is not the case for the transformations we will consider in this section.

In this section, we introduce graph transformations that modify the structure of a graph but preserve the weights of the graph's edges. As before, this procedure preserves the spectrum of the graph up to a known set of eigenvalues. The idea behind an isospectral graph transformation that preserves a graph's edge weights is based on the following. If two graphs $G, H \in \mathbb{G}$ have the same branch structure (including weights), then they should have similar spectra.

To make this precise, suppose $G = (V, E, \omega)$ and $S \in st(G)$. For the branch $\beta = v_1, \dots, v_m \in \mathcal{B}_S(G)$, we define $\Omega_G(\beta)$ to be the ordered sequence of weights

$$\Omega_G(\beta) = \omega(e_{12}), \dots, \omega(e_{i-1,i}), \omega(e_{ii}), \omega(e_{i,i+1}), \dots, \omega(e_{m-1,m})$$

for $m > 1$, and $\omega(e_{ii})$ if $m = 1$.

Let $G, H \in \mathbb{G}$ and suppose $S = \{v_1, \dots, v_m\}$ is a structural set of both G and H . We say that the branch set $\mathcal{B}_{ij}(G; S)$ is *isomorphic* to $\mathcal{B}_{ij}(H; S)$ if there is a bijection

$$b : \mathcal{B}_{ij}(G; S) \rightarrow \mathcal{B}_{ij}(H; S)$$

such that $\Omega_G(\beta) = \Omega_H(b(\beta))$ for each $\beta \in \mathcal{B}_{ij}(G; S)$.

If such a map exists, we write $\mathcal{B}_{ij}(G; S) \simeq \mathcal{B}_{ij}(H; S)$. If

$$\mathcal{B}_{ij}(G; S) \simeq \mathcal{B}_{ij}(H; S) \text{ for all } 1 \leq i, j \leq m,$$

we say that $\mathcal{B}_S(G)$ is *isomorphic* to $\mathcal{B}_S(H)$ and write $\mathcal{B}_S(G) \simeq \mathcal{B}_S(H)$.

Definition 2.8. For $G, H \in \mathbb{G}$, suppose S is a structural set of both G and H . If

- (i) $\mathcal{B}_S(G) \simeq \mathcal{B}_S(H)$, and
- (ii) each vertex of G and H belong to a branch of $\mathcal{B}_S(G)$ and $\mathcal{B}_S(H)$ respectively,

we call H is a *weight-preserving isospectral transformation (wpit)* of G over S .

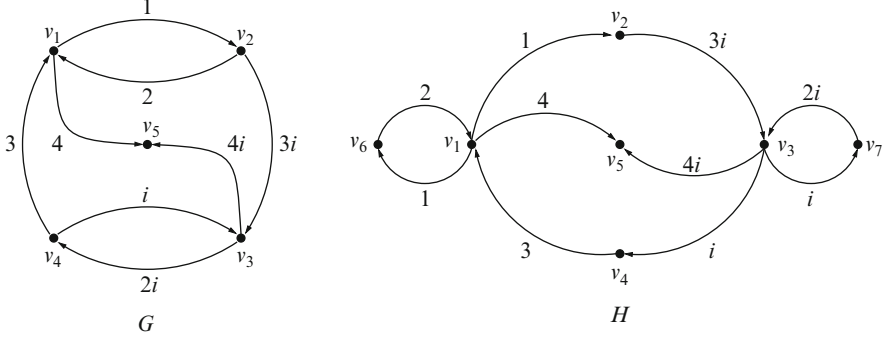


Fig. 2.10 The graph H is a weight-preserving isospectral transformation of the graph G with respect to the structural set $S = \{v_1, v_3, v_5\}$

Notice that if $\mathcal{B}_S(G) \simeq \mathcal{B}_S(H)$ and each vertex of G and H belongs to some branch, then G and H have the same weight set. This justifies the term “weight-preserving” given in Definition 2.8.

More formally, suppose $H = (\mathcal{V}, \mathcal{E}, \mu)$ is a *wpit* of $G = (V, E, \omega)$. By assumption, then, each vertex of G and H belongs to a branch of $\mathcal{B}_S(G)$ and $\mathcal{B}_S(H)$ respectively. Suppose that $e_{ij} \in E$. If $i = j$, then since the vertex v_i belongs to some branch $\beta \in \mathcal{B}_S(G)$, $\omega(e_{ij})$ belongs to the weight sequence $\Omega_G(\beta)$. If $i \neq j$, then there are branches $v_1, \dots, v_i, \dots, v_s$ and $u_1, \dots, u_j, \dots, u_t$ in $\mathcal{B}_S(G)$ containing v_i and $v_j = u_j$ respectively. Hence, $\beta = v_1, \dots, v_i, v_j, \dots, u_t \in \mathcal{B}_S(G)$. Therefore, $\omega(e_{ij})$ belongs to the weight sequence $\Omega_G(\beta)$.

Thus, each edge weight of G belongs to a weight sequence of some $\beta \in \mathcal{B}_S(G)$. By similar reasoning, each edge weight of H belongs to a weight sequence of some $\beta \in \mathcal{B}_S(H)$. Since $\mathcal{B}_S(G) \simeq \mathcal{B}_S(H)$, then $\omega(e_{ij})$ is an edge weight of G if and only if $\omega(e_{ij})$ is an edge weight of H . Therefore, G and H have the same set of edge weights.

Example 2.8. Suppose $G = (V, E, \omega)$ and $H = (\mathcal{V}, \mathcal{E}, \mu)$ are the graphs shown in Fig. 2.10. We note that the vertex set $S = \{v_1, v_3, v_5\}$ is a structural set of both G and H . Moreover,

$$\begin{aligned}
 \mathcal{B}_{11}(G; S) &= \{v_1, v_2, v_1\}, & \mathcal{B}_{11}(H; S) &= \{v_1, v_6, v_1\}; \\
 \mathcal{B}_{13}(G; S) &= \{v_1, v_2, v_3\}, & \mathcal{B}_{13}(H; S) &= \{v_1, v_2, v_3\}; \\
 \mathcal{B}_{15}(G; S) &= \{v_1, v_5\}, & \mathcal{B}_{15}(H; S) &= \{v_1, v_5\}; \\
 \mathcal{B}_{31}(G; S) &= \{v_3, v_4, v_1\}, & \mathcal{B}_{31}(H; S) &= \{v_3, v_4, v_1\}; \\
 \mathcal{B}_{33}(G; S) &= \{v_3, v_4, v_3\}, & \mathcal{B}_{33}(H; S) &= \{v_3, v_7, v_3\}; \\
 \mathcal{B}_{35}(G; S) &= \{v_3, v_5\}, & \mathcal{B}_{35}(H; S) &= \{v_3, v_5\}; \\
 \mathcal{B}_{51}(G; S) &= \emptyset, & \mathcal{B}_{51}(H; S) &= \emptyset;
 \end{aligned}$$

$$\begin{aligned}\mathcal{B}_{53}(G; S) &= \emptyset, & \mathcal{B}_{53}(H; S) &= \emptyset; \\ \mathcal{B}_{55}(G; S) &= \emptyset, & \mathcal{B}_{55}(H; S) &= \emptyset.\end{aligned}$$

Hence, there is a bijection $b : \mathcal{B}_{ij}(G; S) \rightarrow \mathcal{B}_{ij}(H; S)$ for all $i, j \in \{1, 3, 5\}$.

To determine whether the branch sets $\mathcal{B}_S(G)$ and $\mathcal{B}_S(H)$ are isomorphic, we need to check whether each branch $\beta \in \mathcal{B}_S(G)$ and the corresponding branch $b(\beta) \in \mathcal{B}_S(H)$ have the same sequence of weights. Observe that the branch $\beta = v_1, v_2, v_1$ in $\mathcal{B}_{11}(G; S)$ has the weight sequence $\Omega_G(\beta) = 1, 0, 2$. Similarly, note that the branch $b(\beta) = v_1, v_6, v_1$ in $\mathcal{B}_{11}(H; S)$ has the weight sequence $\Omega_H(b(\beta)) = 1, 0, 2$. Hence, $\mathcal{B}_{11}(G; S) \simeq \mathcal{B}_{11}(H; S)$. Continuing in this manner, one can check that each $\mathcal{B}_{ij}(G; S)$ is isomorphic to $\mathcal{B}_{ij}(H; S)$ for $i, j \in \{1, 3, 5\}$, so that $\mathcal{B}_S(G) \simeq \mathcal{B}_S(H)$. Since every vertex of G and H belongs to a branch of $\mathcal{B}_S(G)$ or $\mathcal{B}_S(H)$ respectively, H is a *wpit* of G over S .

Observe that the set S is not the only structural set that is common to both G and H . Another structural set of both graphs is the set $T = \{v_1, v_3\}$. For this set, one can again show that $\mathcal{B}_T(G) \simeq \mathcal{B}_T(H)$. However, since the vertex v_5 does not belong to any branch in either $\mathcal{B}_T(G)$ or $\mathcal{B}_T(H)$, it follows that the graph H is not a *wpit* of G over T .

The reason we do not consider H to be a *wpit* of G with respect to the set T is that some edge weights of these graphs are unaccounted for by the branch sets $\mathcal{B}_T(G)$ and $\mathcal{B}_T(H)$. For instance, if $\omega(e_{15}) = \pi/2$, rather than $\omega(e_{15}) = 4$, as shown in Fig. 2.10, then $\omega(E) \neq \mu(\mathcal{E})$, although the branch sets $\mathcal{B}_T(G)$ and $\mathcal{B}_T(H)$ would still be isomorphic. That is, part (ii) of Definition 2.8 is a necessary condition for ensuring that a *wpit* of a graph has the same weights as the original untransformed graph.

Suppose that two graphs $G, H \in \mathbb{G}$ both have the structural set S . If it is the case that $\mathcal{B}_S(G) \simeq \mathcal{B}_S(H)$, then $\mathcal{R}_S(G) = \mathcal{R}_S(H)$. This leads to the following result, which is a corollary of Theorem 2.1.

Corollary 2.4. *If the graph $G \in \mathbb{G}$ is a weight-preserving isospectral transformation of H over S , then*

$$\sigma(\mathcal{R}_S(G)) = G_* - G^* = H_* - H^* \quad \text{and} \quad \sigma^{-1}(\mathcal{R}_S(G)) = G^* - G_* = H^* - H_*,$$

where $G_* = \sigma(G) \cup \sigma^{-1}(G|_{\bar{S}})$, $G^* = \sigma(G|_{\bar{S}}) \cup \sigma^{-1}(G)$, $H_* = \sigma(H) \cup \sigma^{-1}(H|_{\bar{S}})$, and $H^* = \sigma(H|_{\bar{S}}) \cup \sigma^{-1}(H)$.

Example 2.9. As a demonstration of Corollary 2.4, consider the graphs G and H in Fig. 2.10, which are *wpits* of each other over the set $S = \{v_1, v_3, v_5\}$. Since $M(G)$ and $M(H)$ have complex-valued entries, each of $\sigma^{-1}(G)$, $\sigma^{-1}(G|_{\bar{S}})$, $\sigma^{-1}(H)$, and $\sigma^{-1}(H|_{\bar{S}})$ is the empty set. Hence, Corollary 2.4 implies that

$$\sigma(\mathcal{R}_S(G)) = \sigma(G) - \sigma(G|_{\bar{S}}) = \sigma(H) - \sigma(H|_{\bar{S}}).$$

Indeed, as one can compute, $\sigma(G) = \{\pm(-5)^{\frac{1}{4}}, \pm(-5)^{\frac{1}{4}}i, 0\}$, $\sigma(G|_{\bar{S}}) = \{0, 0\}$, $\sigma(H) = \{\pm(-5)^{\frac{1}{4}}, \pm(-5)^{\frac{1}{4}}i, 0, 0, 0\}$, and $\sigma(H|_{\bar{S}}) = \{0, 0, 0, 0\}$, verifying this fact. Additionally, this implies that

$$\sigma^{-1}(\mathcal{B}_S(G)) = \sigma(G|_{\bar{S}}) - \sigma(G) = \sigma(H|_{\bar{S}}) - \sigma(H),$$

demonstrating the second half of Corollary 2.4.

2.5.1 Branch Expansions

Typically, a graph $G \in \mathbb{G}$ will have many weight-preserving isospectral transformations over some $S \in st(G)$. Because G and each of these transformations have the same branch structure, there is some largest isospectral transformation of G . This is the transformation H in which the branches $\mathcal{B}_S(H)$ overlap the least. We call such a *wpit* the *isospectral expansion* of G .

More precisely, suppose $\alpha = v_1, \dots, v_m$ and $\beta = u_1, \dots, u_n$ are branches in $\mathcal{B}_S(G)$. Then these branches are said to be *independent* if

$$\{v_2, \dots, v_{m-1}\} \cap \{u_2, \dots, u_{n-1}\} = \emptyset.$$

That is, α and β are independent if they share no interior vertices.

Definition 2.9. Let $G, H \in \mathbb{G}$ and $S \in st(G), st(H)$. Suppose

- (i) H is a weight-preserving isospectral transformation of G over S , and
- (ii) the branches of $\mathcal{B}_S(H)$ are independent.

Then we call H an *isospectral expansion* of G with respect to S .

Isospectral expansions are particular types of weight-preserving isospectral transformations and moreover, are unique up to a labeling of vertices. That is, every two isospectral expansions of G with respect to S are isomorphic. By slight abuse of terminology, we let $\mathcal{X}_S(G)$ be any representative from the set of isospectral expansions and call $\mathcal{X}_S(G)$ the *isospectral expansion* of G with respect to S .

Since an isospectral expansion transforms a graph in a very specific way, it is possible to relate the spectrum of a graph with its expansion. This relation is given in the following theorem.

Theorem 2.8. Let $G = (V, E, \omega)$ with structural set S . Then

$$\det(M(\mathcal{X}_S(G)) - \lambda I) = \det(M(G) - \lambda I) \prod_{v_i \in V-S} (\omega(e_{ii}) - \lambda)^{n_i-1},$$

where n_i is the number of branches in $\mathcal{B}_S(G)$ containing v_i .

Proof. Let $\mathcal{X}_S(G) = (\mathcal{V}, \mathcal{E}, \mu)$ be an isospectral expansion of the graph $G = (V, E, \omega)$. Suppose $\beta = v_1, \dots, v_\ell \in \mathcal{B}_S(\mathcal{X}_S(G))$. Since $\mathcal{B}_S(G) \simeq \mathcal{B}_S(\mathcal{X}_S(G))$, there is a bijection

$$b : \mathcal{B}_S(G) \rightarrow \mathcal{B}_S(\mathcal{X}_S(G))$$

such that $\Omega_{\mathcal{X}_S(G)}(\beta) = \Omega_G(b^{-1}(\beta))$.

If $\beta(i) = v \notin S$, define

$$\tilde{b}(v_i) = (b^{-1}(\beta))(i) \text{ for } 1 < i < \ell.$$

Since $|\beta| = |b^{-1}(\beta)|$, then $\tilde{b}$ maps interior vertices of β to interior vertices of $b^{-1}(\beta)$. Since each vertex of $\mathcal{V} - S$ and $V - S$ belong to some branch of $\mathcal{B}_S(\mathcal{X}_S(G))$ and $\mathcal{B}_S(G)$ respectively, it follows that $\tilde{b} : \mathcal{V} - S \rightarrow V - S$ is onto.

Let

$$\mathcal{V}_i = \{v \in \mathcal{V} - S : \tilde{b}(v) = v_i \in V\}.$$

Note that $|\mathcal{V}_i| = n_i$ is then the number of branches in $\mathcal{B}_S(G)$ containing v_i . Moreover, $\mathcal{V} - S$ is the disjoint union

$$\mathcal{V} - S = \bigcup_{v_i \in V - S} \mathcal{V}_i.$$

Since $b : \mathcal{B}_S(G) \rightarrow \mathcal{B}_S(\mathcal{X}_S(G))$ preserves weight sequences, we have $\mu(e_{jj}) = \omega(e_{ii})$ for each $v_j \in \mathcal{V}_i$. Hence,

$$\prod_{v_j \in \mathcal{V} - S} (\mu(e_{jj}) - \lambda) = \prod_{v_i \in V - S} \left(\prod_{v_j \in \mathcal{V}_i} (\mu(e_{jj}) - \lambda) \right) = \prod_{v_i \in V - S} (\omega(e_{ii}) - \lambda)^{n_i}. \quad (2.9)$$

If $S = \{v_1, \dots, v_m\}$, then by assumption,

$$\mathcal{B}_{ij}(G; S) \simeq \mathcal{B}_{ij}(\mathcal{X}_S(G); S) \text{ for } 1 \leq i, j \leq m.$$

Equation (2.2) then implies that the edges e_{ij} in both $\mathcal{R}_S(G)$ and $\mathcal{R}_S(\mathcal{X}_S(G))$ have the same weight. Therefore, $\mathcal{R}_S(G) = \mathcal{R}_S(\mathcal{X}_S(G))$. Since

$$\det(M(\mathcal{R}_S(G)) - \lambda I) = \det(M(\mathcal{R}_S(\mathcal{X}_S(G))) - \lambda I),$$

equation (1.11), used in the context of the adjacency matrices of G and $\mathcal{X}_S(G)$, implies

$$\frac{\det(M(G) - \lambda I)}{\det(M(G|_{\bar{S}}) - \lambda I)} = \frac{\det(M(\mathcal{X}_S(G)) - \lambda I)}{\det(M(\mathcal{X}_S(G)|_{\bar{S}}) - \lambda I)}.$$

Equation (2.5) then implies that

$$\det(M(\mathcal{X}_S(G)) - \lambda I) = \det(M(G) - \lambda I) \frac{\prod_{v_j \in \mathcal{V}-S} (\mu(e_{jj}) - \lambda)}{\prod_{v_i \in V-S} (\omega(e_{ii}) - \lambda)}.$$

From (2.9) we then have that

$$\det(M(\mathcal{X}_S(G)) - \lambda I) = \det(M(G) - \lambda I) \prod_{v_i \in V-S} (\omega(e_{ii}) - \lambda)^{n_i-1},$$

completing the proof. $\square$

Example 2.10. Consider the graphs $G = (V, E, \omega)$ and $H = (\mathcal{V}, \mathcal{E}, \mu)$ in Fig. 2.10. As demonstrated in Example 2.8, if $S = \{v_1, v_3, v_5\}$, then the graph H is a *wpit* of G . Moreover, it can be seen from Fig. 2.10 that the six branches of $\mathcal{B}_S(H)$ share no interior vertices. That is, the branches of $\mathcal{B}_S(H)$ are pairwise independent.

Therefore, the graph H is an isospectral expansion of G with respect to S or $H = \mathcal{X}_S(G)$. Importantly, note that the edge weights of G and its expansion H are identical, i.e., as sets, $\omega(E) = \mu(\mathcal{E}) = \{1, 2, 3, 4, i, 2i, 3i, 4i\}$.

Moreover, since $V - S = \{v_2, v_4\}$, observe that the vertex v_2 of G is an interior vertex of the branches v_1, v_2, v_1 ; $v_1, v_2, v_3 \in \mathcal{B}_S(G)$. Similarly, the vertex v_4 of G is an interior vertex of the branches v_3, v_4, v_3 ; $v_3, v_4, v_1 \in \mathcal{B}_S(G)$. Since $\omega(e_{22}) = 0$ and $\omega(e_{44}) = 0$, Theorem 2.8 implies that $\sigma(\mathcal{X}_S(G)) = \sigma(G) \cup \{0, 0\}$.

The principal idea behind an isospectral expansion is the following. If $G \in \mathcal{G}$ and $S \in st(G)$, then the set of branches $\mathcal{B}_S(G)$ is uniquely defined. However, there are typically many other graphs H with the same branch structure as G , i.e., $S \in st(H)$, such that $\mathcal{B}_S(H) \simeq \mathcal{B}_S(G)$.

An isospectral expansion of G over S is then a graph $H = \mathcal{X}_S(G)$ with identical branch structure but with the following restriction. The branches of $\mathcal{B}_S(H)$ are pairwise independent, and every vertex of H belongs to a branch in $\mathcal{B}_S(H)$. That is, every vertex of $\bar{S}$ in H is part of exactly one branch in $\mathcal{B}_S(H)$.

Hence, given a graph G and structural set S , we can algorithmically construct the expansion $\mathcal{X}_S(G)$ as follows. Start with the vertices S . If $\beta \in \mathcal{B}_{ij}(G; S)$, then both v_i and v_j are in S . Construct a path (or cycle if $i = j$) from v_i to v_j with the weight sequence $\Omega(\beta)$ using “new” interior vertices. By *new*, we mean vertices that do not already appear on the graph we are constructing. Repeat this for each $\beta \in \mathcal{B}_{ij}(G; S)$. The resulting graph is the isospectral expansion $\mathcal{X}_S(G)$.

Importantly, an isospectral expansion is not the only example of an isospectral graph transformation that preserves the weight set of a graph. Many other weight-preserving isospectral transformations are possible.

2.6 Isospectral Graph Transformations over Modified Weight Sets

The isospectral expansions in Sect. 2.5 are a type of graph transformation that separates the various branches of a graph. In this section, we consider the reversal of this process. Specifically, we introduce a method of transforming a graph in a way that merges branches. This type of isospectral transformation has the additional property that it keeps the graph's weight set in a fixed subset $\mathbb{U} \subset \mathbb{W}$. The particular subsets for which this will hold are semirings of $\mathbb{W}$.

The set $\mathbb{U}$ is a *semiring* of $\mathbb{W}$ if it has the following properties: Both 0 and 1 belong to $\mathbb{U}$, and for every $u_1, u_2 \in \mathbb{U}$, both the product $u_1 u_2$ and the sum $u_1 + u_2$ are in $\mathbb{U}$. However, the additive and multiplicative inverses of u_1 and u_2 need not be in $\mathbb{U}$. Examples of such semirings include $\mathbb{C}[\lambda]$, $\mathbb{R}$, and $\mathbb{Z}^+ = \{0, 1, 2, \dots\}$.

In order to merge the branches of a graph G , we will first need to choose a structural set $S \in st(G)$, so that these branches are defined. The particular structural sets that we will consider in this section are defined as follows.

Definition 2.10. For $G = (V, E, \omega)$, let $S \in st(G)$. The set S is a *complete structural set* of G if each cycle of G , including loops, contains a vertex in S .

The difference between a structural set and a complete structural set of a graph G is the following. If S is a complete structural set of G , then every cycle of G contains a vertex in S . If S is simply a structural set of G , then loops of G need not contain a vertex of S .

For $G \in \mathbb{G}$, let $st_0(G)$ denote the set of all complete structural sets of G . Additionally, let $\sigma_0(G)$ be the nonzero elements of $\sigma(G)$ including multiplicities, which we refer to as the *nonzero spectrum* of G . Moreover, we denote by $\rho(G)$ the *spectral radius* of G . That is,

$$\rho(G) = \max_{\ell \in \sigma(G)} |\ell|.$$

Analogously, if $M \in \mathbb{W}^{n \times n}$, we say that $S \subset N$ is a complete structural set of M if there is a permutation matrix $P \in \mathbb{C}^{|\bar{S}| \times |\bar{S}|}$ such that the matrix $PM_{\bar{S}\bar{S}}P^{-1}$ is upper triangular and each diagonal entry is zero. Let $st_0(M)$ be the set of all complete structural sets of M , $\sigma_0(M)$ the nonzero eigenvalues of M , and $\rho(M)$ the spectral radius of M .

Note that if S is a complete structural set of a graph G , then $G|_{\bar{S}}$ has no cycles. Hence, one can show that

$$\det(M(G|_{\bar{S}}) - \lambda I) = \lambda^{|\bar{S}|}.$$

The following is then a corollary of Theorems 2.1 and 2.8.

Corollary 2.5. Let $G = (V, E, \omega)$ and suppose $S \in st_0(G)$. Then $\sigma_0(\mathcal{R}_S(G)) = \sigma_0(G) = \sigma_0(\mathcal{X}_S(G))$ and $\rho(\mathcal{R}_S(G)) = \rho(G) = \rho(\mathcal{X}_S(G))$.

Proof. Suppose $G = (V, E, \omega)$ and $S \in st_0(G)$. Since no vertex in $\bar{S}$ can have a loop, it follows that $\omega(e_{ii}) = 0$ for each $v_i \in \bar{S}$. Equation (2.5) then implies that

$$\det(M(G|_{\bar{S}}) - \lambda I) = \prod_{v_i \in \bar{S}} \lambda.$$

Hence $\sigma^{-1}(G|_{\bar{S}}) = \emptyset$ and $\sigma(G|_{\bar{S}}) = \{0, \dots, 0\}$, in which 0 has multiplicity $|\bar{S}|$. The corollary then follows from Theorem 2.1. $\square$

To phrase Corollary 2.5 in terms of matrices, suppose $M \in \mathbb{W}^{n \times n}$ and $S \in st_0(M)$. Then $\sigma_0(\mathcal{R}_S(M)) = \sigma_0(M) = \sigma_0(\mathcal{X}_S(M))$ and $\rho(\mathcal{R}_S(M)) = \rho(M) = \rho(\mathcal{X}_S(M))$.

In what follows, we demonstrate how the branches $\mathcal{B}_S(G)$ of a graph can be merged if $S \in st_0(G)$. To simplify the discussion, we will say the $e_{j,j+1}$ is the j th edge *belonging* to the branch β for each $1 \leq j \leq m-1$. This allows us to state the following result.

Lemma 2.2. *Let $G = (V, E, \omega)$ and $S \in st_0(G)$. Then $\mathcal{X}_S(G) = (\mathcal{V}, \mathcal{E}, \mu)$ has the following properties:*

- (i) *If $e_{ij} \in \mathcal{E}$, then e_{ij} belongs to exactly one branch of $\mathcal{B}_S(\mathcal{X}_S(G))$.*
- (ii) *If $\beta = v_1, \dots, v_m$ is a branch in $\mathcal{B}_S(\mathcal{X}_S(G))$, then*

$$\Omega_{\mathcal{X}_S(G)}(\beta) = \mu(e_{12}), 0, \dots, \mu(e_{k,k-1}), 0, \mu(e_{k,k+1}), \dots, 0, \mu(e_{m-1,m}). \quad (2.10)$$

Proof. Since each vertex of $\mathcal{X}_S(G)$ belongs to at least one branch of $\mathcal{B}_S(\mathcal{X}_S(G))$, the same holds for every $e_{ij} \in \mathcal{E}$. On the other hand, suppose e_{ij} belongs to both β_1 and β_2 in $\mathcal{B}_S(\mathcal{X}_S(G))$. Then neither v_i nor v_j can be an interior vertex of β_1 or β_2 , since these branches, if distinct, are independent. Hence $\beta_1 = \beta_2 = v_i, v_j$ or e_{ij} belongs to at most one branch of $\mathcal{B}_S(\mathcal{X}_S(G))$. This verifies property (i).

Since S is a complete structural set of G , it follows that $\omega(e_{ii}) = 0$ for each $v_i \in V - S$. This implies that for every $\beta = v_1, \dots, v_m \in \mathcal{B}_S(G)$, the weight sequence $\Omega_G(\beta)$ has the form given in equation (2.10). Since $\mathcal{B}_S(G) \simeq \mathcal{B}_S(\mathcal{X}_S(G))$, property (ii) holds. $\square$

2.6.1 Branch Reweighting

Given an isospectral expansion $\mathcal{X}_S(G)$, our goal is to construct a new graph $\mathcal{Y}_S(G)$ by reweighting the branches of $\mathcal{X}_S(G)$. The idea behind this construction is to reweight the branches $\mathcal{B}_S(\mathcal{X}_S(G))$ in such a way that it preserves their branch products.

Suppose the expansion $\mathcal{X}_S(G)$ is equal to $(\mathcal{V}, \mathcal{E}, \mu)$, where $S \in st_0(G)$. Let the graph $\mathcal{Y}_S(G)$ be equal to $(\mathcal{V}, \mathcal{E}, \nu)$. That is, $\mathcal{Y}_S(G)$ has the same vertex and edge

set as $\mathcal{X}_S(G)$ but possibly different edge weights. This implies that S is a complete structural set of $\mathcal{Y}_S(G)$ and moreover, that the branch set $\mathcal{B}_S(\mathcal{Y}_S(G))$ is identical to $\mathcal{B}_S(\mathcal{X}_S(G))$.

For the branch $\beta = v_1, \dots, v_m \in \mathcal{B}_S(\mathcal{Y}_S(G))$, let β have the weight sequence

$$\Omega_{\mathcal{Y}_S(G)}(\beta) = \prod_{k=1}^{m-1} \mu(e_{k,k+1}), 0, \dots, 1, 0, 1, \dots, 0, 1 \quad (2.11)$$

if $m > 1$. If $m = 1$, let $\Omega_{\mathcal{Y}_S(G)}(\beta) = \mu(e_{11})$. Since $\mathcal{X}_S(G)$ and $\mathcal{Y}_S(G)$ have the same vertex and edge sets, Lemma 2.2 implies that each edge of $\mathcal{Y}_S(G)$ belongs to exactly one branch of $\mathcal{B}_S(\mathcal{Y}_S(G))$. Therefore, equation (2.11) completely specifies the edge weights of the graph $\mathcal{Y}_S(G)$.

Observe that the edge $e_{ij} \in \mathcal{E}$ in $\mathcal{Y}_S(G)$ has weight $v(e_{ij}) = 1$ unless e_{ij} is the first edge of a branch in $\mathcal{B}_S(\mathcal{Y}_S(G))$. If e_{ij} happens to be the first edge of the branch $\beta \in \mathcal{B}_S(\mathcal{Y}_S(G))$, then its weight is the product of the nonzero entries of $\Omega_{\mathcal{Y}_S(G)}(\beta)$.

In effect, the branch reweighting process simply transfers the entire weight of the branch to the branch's first edge, leaving all other edges with unit weight. Hence, the branch product remains constant, but the entire weight of the branch is concentrated on its first edge. (Figure 2.11 gives an example of this branch reweighting.)

2.6.2 Branch Merging

From $\mathcal{Y}_S(G)$, we construct the graph $\mathcal{Z}_S(G)$. The major idea behind this construction is that the branches $\mathcal{B}_S(\mathcal{Y}_S(G))$ of the graph $\mathcal{Y}_S(G)$ can be merged together in a way that maintains the weight set of the graph as well as its nonzero spectrum. To define the graph $\mathcal{Z}_S(G)$, we will need the following terminology.

For $G = (V, E, \omega)$, suppose $S = \{v_1, \dots, v_m\}$ is a structural set of G . Let

$$\mathcal{B}_j(G; S) = \bigcup_{1 \leq i \leq m} \mathcal{B}_{ij}(G; S).$$

That is, $\mathcal{B}_j(G; S)$ are the branches in $\mathcal{B}_S(G)$ terminating at the same vertex $v_j \in V$. For every $\beta = u_1, \dots, u_k$ in $\mathcal{B}_S(G)$, let $|\beta| = k$, i.e., the number of vertices in β . Moreover, let $\{\beta\}_{\text{int}}$ denote the set of interior vertices of β .

To construct the graph $\mathcal{Z}_S(G)$, we first suppose that the graph $\mathcal{Y}_S(G)$ is equal to $(\mathcal{V}, \mathcal{E}, v)$ and that $S = \{v_1, \dots, v_m\} \in st_0(G)$. For each $v_j \in S$, we select a branch $\beta^j \in \mathcal{B}_j(\mathcal{Y}_S(G))$ with the property that $|\beta^j| \geq |\beta|$ for all branches $\beta \in \mathcal{B}_S(\mathcal{Y}_S(G))$. That is, the branch β^j is the “longest” branch that terminates at v_j . If $\mathcal{B}_j(\mathcal{Y}_S(G)) = \emptyset$, we set $\beta^j = \emptyset$.

Define $B = \mathcal{B}_S(\mathcal{Y}_S(G)) - \{\beta^1, \dots, \beta^m\}$, and let

$$\mathcal{U} = \bigcup_{\beta \in B} \{\beta\}_{\text{int}}. \quad (2.12)$$

That is, $\mathcal{U}$ is the set of interior vertices of the branches $\beta \neq \{\beta^1, \dots, \beta^m\}$ in $\mathcal{B}_S(\mathcal{Y}_S(G))$.

Set

$$\mathcal{Z}'_S(G) = \mathcal{Y}_S(G)|_{\mathcal{V}-\mathcal{U}}.$$

Recall that the branches of $\mathcal{B}_S(\mathcal{Y}_S(G))$ are mutually independent. Therefore, the graph $\mathcal{Z}'_S(G)$ is equal to $(\mathcal{V} - \mathcal{U}, \mathcal{E}', v')$, where $e \in \mathcal{E}'$ if and only if e belongs to some β^j . Furthermore, the edge weights of $\mathcal{Z}'_S(G)$ are given by the restriction $v' = v|_{\mathcal{E}'}$.

If e is an edge from the vertex a to the vertex b , we will denote this by $e = (a, b)$. Suppose the branch β^j is equal to $v_1^j, \dots, v_k^j$. For each

$$\beta \in \mathcal{B}_{ij}(\mathcal{Y}_S(G); S) - \beta^j,$$

we add an edge $(v_i, v_{k-|\beta|+2}^j)$ to the graph $\mathcal{Z}'_S(G)$. The edge $(v_i, v_{k-|\beta|+2}^j)$ is given the weight of the first edge belonging to β in $\mathcal{Y}_S(G)$. If this is done over all $1 \leq i, j \leq m$, we call the resulting graph $\mathcal{Z}''_S(G)$.

It is important to note that the graph $\mathcal{Z}''_S(G)$ may have parallel edges under this construction. By *parallel edges*, we mean that there may be multiple edges in the edges set of $\mathcal{Z}''_S(G)$ of the form (a, b) . In particular, if there are two branches $\beta_1, \beta_2 \in \mathcal{B}_{ij}(\mathcal{Y}_S(G); S)$ that have the same length, i.e., $|\beta_1| = |\beta_2| = \ell$, then there are (at least) two edges in $\mathcal{Z}''_S(G)$ of the form $(v_i, v_{\ell-|\beta|+2}^j)$.

If the graph $\mathcal{Z}''_S(G)$ has parallel edges $e_1, \dots, e_N$ of the form (v_i, v_j) with weights $w_1, \dots, w_N$, we replace the edges $e_1, \dots, e_N$ in $\mathcal{Z}''_S(G)$ with the single edge e_{ij} having weight $w_1 + \dots + w_N$. If this is done for each set of parallel edges in $\mathcal{Z}''_S(G)$, we denote the resulting graph by $\mathcal{Z}_S(G)$.

Note that our construction of $\mathcal{Z}_S(G)$ depends on the initial choice of each β^j . We therefore write $\mathcal{Z}_S(G) = \mathcal{Z}_S(G; \beta^1, \dots, \beta^m)$.

Definition 2.11. If $S \in st_0(G)$, then we call the graph $\mathcal{Z}_S(G)$ the *merged graph* of G over S .

Because each operation of expanding, reweighting, and merging does not modify the underlying branch structure of a graph or any of its branch products, the following holds.

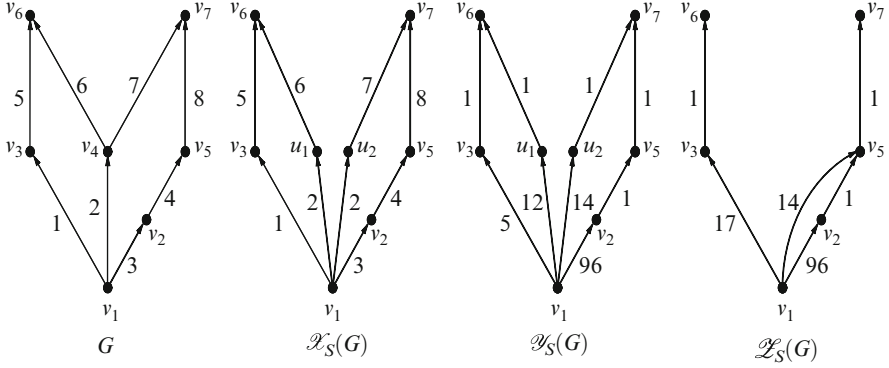


Fig. 2.11 The isospectral transformation $\mathcal{Z}_S(G)$ of G over $S = \{v_1, v_2, v_3\}$

Theorem 2.9. For $G \in \mathbb{G}$ and $S \in st_0(G)$, suppose the edge weights of G are in the semiring $\mathbb{U} \subseteq \mathbb{W}$. Then

- (i) $\mathcal{Z}_S(G)$ has edge weights in the set $\mathbb{U}$;
- (ii) the nonzero eigenvalues $\sigma_0(\mathcal{Z}_S(G))$ are equal to $\sigma_0(G)$; and
- (iii) the spectral radius $\rho(\mathcal{Z}_S(G))$ is equal to $\rho(G)$.

Proof. The fact that $\mathcal{Z}_S(G)$ and G have weights in the semiring $\mathbb{U}$ follows from the fact that the weights of $\mathcal{Z}_S(G)$ are sums and products of the weights of G . The nonzero spectrum and spectral radius of $\mathcal{Z}_S(G)$ and G follow from Corollary 2.4, since by construction, $\mathcal{R}_S(G) = \mathcal{R}_S(\mathcal{Z}_S(G))$. $\square$

Example 2.11. Let $G = (V, E, \omega)$ be the graph shown in Fig. 2.11 (far left). Note that the vertex set $S = \{v_1, v_2, v_3\}$ is a complete structural set of G , since G has no cycles (including loops). The branches of G with respect to S are then $\beta_1 = v_1, v_3, v_6$, $\beta_2 = v_1, v_4, v_6$, $\beta_3 = v_1, v_4, v_7$, and $\beta_4 = v_1, v_2, v_5, v_7$. Observe that only β_2 and β_3 share an interior vertex.

The isospectral expansion $\mathcal{Z}_S(G)$, shown in Fig. 2.11 (middle left), is then the graph in which the branches β_2 and β_3 have been replaced with the independent branches $\tilde{\beta}_2 = v_1, u_1, v_6$ and $\tilde{\beta}_3 = v_1, u_2, v_7$ respectively. Thus, the expansion $\mathcal{Z}_S(G)$ has the vertex set $\mathcal{V} = \{v_1, v_2, v_3, v_5, v_6, v_7, u_1, u_2\}$.

Note that the products of the weights along the branches $\beta_1, \tilde{\beta}_2, \tilde{\beta}_3, \beta_4$ are 5, 12, 14, 96 respectively. By construction, these are the first edge weights of each of the branches $\beta_1, \tilde{\beta}_2, \tilde{\beta}_3, \beta_4$ in $\mathcal{Y}_S(G)$, respectively (see Fig. 2.11, middle right). Each other edge of $\mathcal{Y}_S(G)$ has unit weight.

To construct $\mathcal{Z}'_S(G)$, note that $\beta^1 = \emptyset$, $\beta^7 = \beta_4$, and β^6 is either β_1 or $\tilde{\beta}_2$. Here we make the arbitrary choice of letting $\beta^6 = \beta_1$. Since $\{\beta_2\}_{\text{int}} = \{u_1\}$ and $\{\beta_3\}_{\text{int}} =$

$\{u_2\}$, we have that $\mathcal{Z}'_S(G)$ has vertex set $\mathcal{V} - \{u_1, u_2\} = \{v_1, v_2, v_3, v_5, v_6, v_7\}$. Given that the branch set

$$\mathcal{B}_S(\mathcal{Z}'_S(G)) - \{\beta^6, \beta^7\} = \{\tilde{\beta}_2, \tilde{\beta}_3\},$$

constructing $\mathcal{Z}''_S(G)$ amounts to adding two edges to $\mathcal{Z}'_S(G)$, one for $\tilde{\beta}_2$ and one for $\tilde{\beta}_3$.

Observe that $\tilde{\beta}_2 \in \mathcal{B}_{16}(\mathcal{Y}_S(G); S)$ with first edge weight 12 and $|\tilde{\beta}_2| = 3$. Since $|\beta^6| = 3$, we add to the graph $\mathcal{Z}'_S(G)$ a parallel edge from v_1 to v_3 with weight 12. For the branch $\tilde{\beta}_3 \in \mathcal{B}_{17}(\mathcal{Y}_S(G); S)$, note that it has first edge weight 14 and $|\tilde{\beta}_3| = 3$. Since $|\beta^7| = 4$, we add to the graph $\mathcal{Z}'_S(G)$ an edge from v_1 to v_5 with weight 14. The result is the graph $\mathcal{Z}''_S(G)$.

Note that the two parallel edges from v_1 to v_3 in $\mathcal{Z}''_S(G)$ have weights 5 and 12 respectively. Hence, in $\mathcal{Z}_S(G) = \mathcal{Z}_S(G; \beta_1, \beta_4)$, shown in Fig. 2.11 (far right), the edge e_{13} has weight 17.

Since the edge weights of G are $\omega(E) = \{1, \dots, 8\}$, these weights belong to the semiring of nonnegative integers $\mathbb{Z}^+ = \{0, 1, 2, \dots\}$. As guaranteed by Theorem 2.9, the graph $\mathcal{Z}_S(G)$ also has edge weights in $\mathbb{Z}^+$. Moreover, one can also compute that $\sigma_0(\mathcal{Z}_S(G)) = \sigma_0(G)$ and $\rho(\mathcal{Z}_S(G)) = \rho(G)$.

By first expanding a graph and then merging its branches, we will typically change the size of the graph. To determine the size of the resulting graph, we will use the following notation. For a graph $G = (V, E, \omega)$, let $|G| = |V|$, i.e., the number of vertices in V .

Proposition 2.1. *For $G = (V, E, \omega)$, let $S = \{v_1, \dots, v_m\} \in st_0(G)$. Then*

$$|\mathcal{Z}_S(G)| = |S| + \sum_{i=1}^m (|\beta^j| - 2),$$

where $|\beta^j| = 2$ if $\beta^j = \emptyset$.

Proof. Let $\mathcal{Y}_S(G) = (\mathcal{V}, \mathcal{U}, \nu)$, where we suppose $\alpha, \beta \in \mathcal{B}_S(\mathcal{Y}_S(G))$ and $\alpha \neq \beta$. Note that the branches of $\mathcal{B}_S(\mathcal{Y}_S(G))$ are pairwise independent and each vertex of $\mathcal{V}$ belongs to a branch of $\mathcal{B}_S(\mathcal{Y}_S(G))$. Hence, $\{\alpha\}_{\text{int}} \cap \{\beta\}_{\text{int}} = \emptyset$ and $\{\beta\}_{\text{int}} \cap S = \emptyset$. Therefore, $\mathcal{V}$ is the disjoint union

$$\mathcal{V} = S \cup \left(\bigcup_{\beta \in \mathcal{B}_S(\mathcal{Y}_S(G))} \{\beta\}_{\text{int}} \right).$$

Recall that the set $\mathcal{U}$, given by (2.12), is the set of interior vertices of the branches $\mathcal{B}_S(\mathcal{Y}_S(G)) - \{\beta^1, \dots, \beta^m\}$. Thus, the vertex set $\mathcal{V} - \mathcal{U}$ is given by

$$\mathcal{V} - \mathcal{U} = S \cup \left(\bigcup_{i=1}^m \{\beta^i\}_{\text{int}} \right),$$

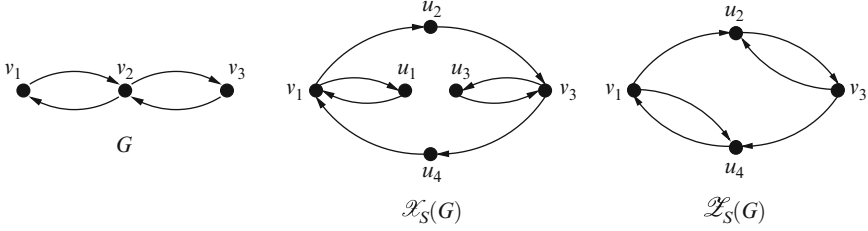


Fig. 2.12 The graphs $\mathcal{X}_S(G)$ and $\mathcal{Z}_S(G)$ for $S = \{v_1, v_3\}$, both of which are larger than G

where each $\{\beta^i\}_{\text{int}} \cap \{\beta^j\}_{\text{int}}$ is the empty set and $\{\beta^i\}_{\text{int}} \cap S = \emptyset$ for $i \neq j$. Therefore,

$$|\mathcal{V} - \mathcal{W}| = |S| + \sum_{i=1}^m (|\beta^i| - 2),$$

since each branch β^j has $|\beta^j| - 2$ interior vertices. If $\beta^j = \emptyset$, then this branch has no interior vertices, which is compensated by the assumption $|\beta^j| = 2$.

Note that $|\mathcal{Z}'_S(G)| = |\mathcal{Y}_S(G)|_{\mathcal{V}-\mathcal{W}} = |\mathcal{V} - \mathcal{W}|$. Since constructing $\mathcal{X}_S''(G)$ from $\mathcal{Z}'_G(S)$ involves only the addition of edges, and constructing $\mathcal{Z}_S(G)$ from $\mathcal{X}_S''(G)$ involves only the removal of parallel edges, it follows that $|\mathcal{Z}_S(G)| = |\mathcal{V} - \mathcal{W}|$. This completes the proof. $\square$

In Example 2.11, we considered the construction of the graph $\mathcal{Z}_S(G)$ in Fig. 2.11 over the complete structural set $S = \{v_1, v_6, v_7\}$. From Proposition 2.1, it follows that $|\mathcal{Z}_S(G)| = |S| + |\beta^1| + |\beta^6| + |\beta^7|$. Since $\beta^1 = \emptyset$, $\beta^6 = v_1, v_3, v_6$, and $\beta^7 = v_1, v_2, v_5, v_7$, we have $|\mathcal{Z}_S(G)| = 6$.

Note that in this example, $|G| > |\mathcal{Z}_S(G)|$. Hence $\mathcal{Z}_S(G)$ can be considered a *reduction* of G over the weight set $\mathbb{Z}^+$ having the same nonzero spectrum. However, we note that it may happen that $|\mathcal{Z}_S(G)| > |G|$ for a particular graph G , as shown in the following example.

Example 2.12. Consider the unweighted graph G in Fig. 2.12 (left) with the complete structural set $S = \{v_1, v_3\}$. The graph $\mathcal{Z}_S(G)$ shown in Fig. 2.12 (right) is strictly larger than the original graph G , i.e., $\mathcal{Z}_S(G)$ has more vertices than G . Therefore, even though the branches of the expansion $\mathcal{X}_S(G)$, shown in Fig. 2.12 (center), have been merged to form $\mathcal{Z}_S(G)$, this resulting graph is still larger than the original graph G . At this point, it is yet unknown whether there is a general construction (algorithm) that allows one to reduce an arbitrary graph $G \in \mathbb{G}$ in size while preserving the semiring of its edge weights and (nonzero) spectrum.

As a final remark for this chapter, we note that it is possible to define a merged graph $\mathcal{Z}_S(G)$ over a general structural set S rather than a complete structural set. This more general construction is analogous to the procedure described in this

section in that $\mathcal{L}_S(G)$ is still constructed by expanding, reweighting, and merging the branches of G . The major difference, though, is that if S is a structural set, then these branches may have loops.

The reason we consider merged graphs over complete structural sets is for the sake of simplicity. We leave it as an exercise to the reader to apply these techniques over structural sets that are not complete.

Isospectral Transformations

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