Constructing Cospectral and Comatching Graphs

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

The *matching polynomial* is a graph polynomial that does not only have interesting mathematical properties, but also possesses meaningful applications in physics and chemistry. For a simple graph, the matching polynomial enumerates the number of matchings of different sizes in it. Two graphs are comatching if they have the same matching polynomial. Two vertices u, v in a graph G are comatching if $G\backslash u$ and $G\backslash v$ are comatching.

In 1973, Schwenk proved almost every tree has the same characteristic polynomial with another tree. In this thesis, we extend Schwenk's result to maximal limbs and weighted trees. We also give a construction using 1-vertex extensions for comatching graphs and graphs with an arbitrarily large number of comatching vertices. In addition, we use an alternative definition of matching polynomial for multigraphs to derive new identities for the matching polynomial. These identities are tools used towards our 2-sum construction for comatching vertices and comatching graphs.

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To My Parents and My Siblings

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Notation	Description
$H_u \cdot K_v$	The 1-sum of H and K, with respect to the vertex $u \in V(H)$ and $v \in V(K)$. 14
$u \sim v$	The vertex u is adjacent to the vertex v. 1
$\langle x^i, g(x) \rangle$	The coefficient of x^i in the power series $P(x)$. 12
$\overline{G}$	The complement of the graph G. 13
$E(G)$	The edge set of the graph G. 1
G/e	The graph formed by contracting the edge e in G. 81
$\mu(G)$	The matching polynomial of the graph G. 1
$p(G, k)$	The number of matchings with k edges in the graph G. 1
$f\|_A$	The restriction of the function f to the set A. 8
$F(T)$	The forest obtained by deletion the root from the rooted tree T, where each component in this forest is rooted at the vertex adjacent to the root of T. 23
$V(G)$	The vertex set of the graph G. 1
$\phi^*(W)$	The weighted characteristic polynomial of the weighted graph W. 48
$M(x)$	The $n \times n$ diagonal matrix with diagonal entries being $x^{w(i)}$, where $w(i)$ is the weight of the vertex i, the vertex the entry corresponds to. 6, 48

Chapter 1

Introduction

For a graph G, we use $V(G)$ to denote its set of *vertices* and $E(G)$ to denote its set of *edges*. For any $u, v \in V(G)$, if $\{u, v\} \in E(G)$, we say that u and v are *adjacent*, denoted as $u \sim v$.

Let G be a graph with n vertices. Define a *matching* M in G as a set of pairwise disjoint edges. Let $p(G, k)$ denote the number of matchings with k edges in G, then we define the *matching polynomial* of G to be

$$\mu(G, x) = \sum_i (-1)^i p(G, i) x^{n-2i}.$$

When there is no ambiguity, we drop the indeterminate variable and use $\mu(G)$ to denote the matching polynomial of G.

For example, the matching polynomial of the graph $K_{1,3}$ is

$$\mu(K_{1,3}) = x^4 - 3x^2.$$

The first known use of the matching polynomial traces back to Riodian's work, where he considered permutations and defined the rook polynomial, which is an alternative version of the matching polynomial for bipartite graphs [30]. Riodian used the rook polynomial to study permutations with restrictions.

Not only used in mathematics, the matching polynomial originally emerged from various contexts in physics and chemistry research. A number of different names for $\mu(G)$ were used by researchers, including reference polynomial, acyclic polynomial, and matching polynomial [1, 12, 13]. Mathematically speaking, the polynomial $\mu(G)$ enumerates matchings of different sizes in a graph G, so we refer to it as the *matching polynomial* in our writing.

In 1972, Heilmann and Lieb used graphs as a tool to model monomer-dimer systems: Given a matching of a graph, monomers correspond to unsaturated vertices in a matching and dimers correspond to edges in a matching [18]. This model allowed them to formulate the matching polynomial, which was used in their study. They found recursive relationships for the matching polynomial of paths, cycles, complete graphs, and Bethe graphs, which is a family of rooted regular trees constructed recursively. Further, they discovered a vertex-deletion recurrence for the matching polynomial, and used it to prove the roots of the matching polynomial are real. In this thesis, we use their vertex-deletion recurrence to prove many of our results.

Meanwhile, also in the 1970s, the matching polynomial was also studied by chemists such as Aihara, Gutman, Milun, and Trinajstić as well, to model the resonance energy of conjugated systems and to study Hückel molecular orbital theory [1, 11]. In particular, Hosoya derived an edge-deletion recurrence for the matching polynomial [21], which serves as a fundamental tool in this thesis. He also proved the matching polynomial and the characteristic polynomial coincide for all trees. We will define the characteristic polynomial of a graph later in this Chapter. This result was later confirmed and extended to acyclic graphs by several others, including Graovac et al. and Godsil and Gutman [15, 8].

Gutman and Hosoya were some of the first individuals who studied our version of the matching polynomial from a purely mathematical perspective. Their work in [14] gave a proof to a derivative formula, which we will introduce in Chapter 2. They also derived specific recursive relationships for the matching polynomial of paths, complete bipartite graphs, and complete graphs. Gutman proved a union formula in his work later [13]. It is worth noting that Trinajstić[33] and Gutman et al.[15] defined the matching polynomial for graphs with loops as well, which is used later in this thesis.

With the matching polynomial being a research interest of physicists, chemists, and mathematicians, it is important to consider its computability. In fact, it is generally hard to compute the matching polynomial of a graph. We say a problem is in $\#P$ if it counts the number of accepting answers to a problem that can be computed by a nondeterministic polynomial time Turning machine. Consequently, a problem in #P is at least as hard as the corresponding NP problem. In 1979, Valiant proved that the complexity of computing the permanent of a matrix is #P-complete [34]. Since any $(0, 1)$-matrix can be treated as the bi-adjacency matrix of a bipartite graph G, and computing its permanent is to count the number of perfect matchings in G, we can see that it is #P-complete to count the number of perfect matchings in G. This is one way to see why computing the matching polynomial of a graph can be a hard problem. There is no known efficient algorithm to compute the matching polynomial of general graphs.

Some research involving the matching polynomial was motivated from its shared properties with the characteristic polynomial. The characteristic polynomial is another graph polynomial that is widely applied in chemistry [1]. For a graph G, let A be its adjacency matrix, then the *characteristic polynomial* of G is defined as

$$\phi(G, x) = \det(xI - A).$$

Similarly, we use $\phi(G)$ to denote the characteristic polynomial of G when there is no ambiguity. The characteristic polynomial is related to the matching polynomial in a number of ways. As we mentioned earlier, the matching polynomial of a graph G is enumerating matchings in G, or subgraphs of G that only contains disjoint copies of K_2. Similarly, the characteristic polynomial of G counts the number of subgraphs of G consisting of disjoint copies of K_2 and cycles [10, Theorem 2.1.3]. Notice that when G is a tree, every such subgraph would be formed by disjoint copies of K_2, which means the edges in such a subgraph form a matching. This is one way to intuitively understand a result we mentioned earlier.

1.1 Lemma ([21, 15, 8])**.** *The matching polynomial of a graph coincides with the characteristic polynomial if and only if it is a forest.*

This lemma gives an important reason for the $(-1)^i$ term to exist in the definition of the matching polynomial. Without this alternating term, the matching polynomial and the characteristic polynomial of a forest would not coincide.

Two graphs are *cospectral* if they have the same characteristic polynomial. An important open problem in the study of characteristic polynomials is: Which graphs are determined by their characteristic polynomials? Originated from chemistry, this question has been open for about 70 years [35]. Van Dam and Haemer's paper [35] gives an overview of the development and progress on this question. However, for most graphs, this question remains open.

One of the most significant results in this direction was due to Schwenk [32], who proved almost every tree is cospectral to another tree. Here, by "almost every", we mean that, for graphs over n vertices, the limit of the proportion of graphs over n vertices approaches 1, as n approaches infinity. We will use this meaning of "almost every" throughout this thesis. In this thesis, we extend Schwenk's results to some other types of trees. This is one of our main results.

Figure 1.1: The smallest pair of comatching graphs

Meanwhile, since the matching polynomial and the characteristic polynomial coincide for trees, we could say almost every tree has the same matching polynomial as another tree, or almost every tree is *comatching* to another tree. In other words, two graphs are *comatching* if and only if they have the same matching polynomial. We know that there are graphs that are not trees but are still comatching. In fact, the smallest pair of comatching graphs are $K_{1,3}$ and $C_3 \cup K_1$, shown in Figure 1.1, where one of them is not a tree. It is then natural to ask, which graphs are not determined by their matching polynomials? Is almost every graph comatching with another graph? These are some of the main questions of interest in our research.

Although it might be generally difficult to determine whether a graph has a comatching mate, several constructions for specific sets (mostly pairs) of comatching graphs were given [5, 20, 28]. Farrell and Wahid proved a construction of a pair of comatching graphs from a graph with a pair of comatching vertices for their bivariate version of the matching polynomial. They also found two families of pairs of comatching graphs formed by paths and cycles [5]. Holland and Whitehead proved that a pair of θ-graphs, which are connected graphs with two vertices of degree 3 and all remaining vertices being degree 2, are comatching when they satisfy certain conditions [20]. Using this, they also proved some subdivisions of K_4 are comatching with each other. Pranesachar constructed a set of 2^{n-1} bipartite graphs, each of which are comatching to $K_{n,n}$ [28]. Yan and Yeh proved that, given a pair of d-regular comatching graphs, if we subdivide every one of their edges exactly once, then the resulting pair of graphs after all the subdivisions are still comatching [37]. However, more general constructions for sets of comatching graphs are yet to be found. In this thesis, we give two constructions for comatching graphs via operations called 1-vertex extension and 2-sum, respectively. We will define these two terms later in this chapter.

One way of constructing comatching graphs is through constructing graphs with comatching vertices. Given a graph G, we say that $u, v \in V(G)$ are *comatching vertices* if $G \backslash u$ and $G \backslash v$ have the same matching polynomial. Therefore, if we have a graph with a set of S comatching vertices, then by definition we have $|S|$ (possibly isomorphic) comatching graphs obtained by deleting one of the vertices in S from G. Similarly, for a graph G, we say that $u, v \in V(G)$ are *cospectral vertices* if $G \backslash u$ and $G \backslash v$ have the same characteristic polynomial. Therefore, finding constructions for graphs with cospectral or comatching vertices is another one of our research interests. The 1-vertex extension construction will be applied to construct connected graphs with an arbitrarily large number of comatching and cospectral vertices. The 2-sum construction will also be used to construct graphs with comatching vertices.

Below, we give an introduction to each of our three main results in this thesis.

1.1 Extension of Schwenk's Results

In Schwenk's proof of almost every tree is cospectral to another tree, he defined a concept called a limb [32]. For a tree T, suppose B is a subtree of T. Notice that this implies there exists a vertex $v \in V(B)$ such that every path from a vertex in $V(B)$ to a vertex in $V(T)\backslash V(B)$ contains v. We say that B is a *branch* of T at v if v is a degree 1 vertex in B. A branch B at v is a maximal subtree of T under the degree restriction on v. A *limb* L at v is a rooted subtree of T with v being the root, such that for each branch B at v, either $V(L) \cap V(B) = \{v\}$ or $V(L) \cap V(B) = V(B)$. Using this definition, Schwenk then proved that, given any ℓ-vertex rooted tree L, almost every tree contains L as a limb.

In Chapter 3, we discuss a similar concept called a maximal limb, and extend Schwenk's results to it. For a rooted tree T and any vertex v in $V(T)$, the *maximal limb* at v is the limb at v that contains exactly all descendants of v. In a rooted setting, the defined limb is maximal because all limbs at v are its subtrees. We prove the following result as Theorem 3.9.

Theorem (3.9)**.** *For any given rooted tree L, almost every rooted tree contains L as a maximal limb.*

Moreover, in Chapter 4, we extend Schwenk's results to weighted trees, both rooted and unrooted. We say that a tree is *weighted* if each of its vertices is assigned a positive integer weight. The following results are Theorem 4.5 and Theorem 4.11, respectively.

Theorem (4.5)**.** *For any given weighted rooted tree L, almost every weighted rooted tree has L as a limb.*

Theorem (4.11)**.** *For any given weighted rooted tree L, almost every weighted tree has L as a limb.*

Observe that the concept of characteristic polynomial and cospectrality were undefined for weighted trees. Therefore, to further extend Schwenk's results, we need to extend the definition of characteristic polynomial to weighted trees. For a weighted tree W, we use $A(W)$ to denote the adjacency matrix of W. Suppose $M(x)$ is an $n \times n$ diagonal matrix, such that its rows and columns are each indexed by the vertices of W, and the ii-entry of $M(x)$ is $x^{w(i)}$, where $w(i)$ is the weight of the vertex i and x an indeterminate. Let $A(W)$ be the adjacency matrix of W. The *weighted characteristic polynomial* $\phi^*(W, x)$ of W is defined as

$$\phi^*(W, x) = \det(M(x) - A(W)).$$

Two weighted graphs are *weighted cospectral* if they have the same weighted characteristic polynomial. With this definition, we will prove Theorem 4.18, which is stated below.

Theorem (4.18)**.** *Almost every weighted tree is weighted cospectral with another weighted tree.*

1.2 Constructing Cospectral and Comatching Graphs and Vertices by 1-Vertex Extension

Given a graph G and a set of vertices $S \subseteq V(G)$, we define the 1-*vertex extension* of G with respect to S to be the graph obtained by adding a vertex to G and connecting the added vertex to all vertices in S and no other vertex. Using this operation, we give a construction for cospectral and coMoreatching graphs by applying 1-vertex extension twice in a row to a graph with certain properties. The following two results containing the constructions are Theorem 5.2 and Theorem 5.9, respectively.

Theorem (5.2)**.** *Let F be a graph with c components that are pairwise cospectral. For some integer $m \geq 1$, suppose we have two distinct sets $A_1 = \{S_1^1, S_2^1, \ldots, S_m^1\}$ and $A_2 = \{S_1^2, S_2^2, \ldots, S_m^2\}$, both containing m sets of pairwise cospectral vertices from F, such that for all $1 \leq i \leq m$, each S_i^1 or S_i^2 contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$ and $j = 1, 2$, let F_i^j be the 1-vertex extension of F with respect to S_i^j, with the added vertex being v_i^j. Let H_j be the 1-vertex extension of $\bigcup_{i=1}^m F_i^j$ with respect to $v_1^j, \ldots, v_m^j$, with the added vertex being r_j. Then H_1 and H_2 are cospectral.

Theorem (5.9)**.** *Let F be a graph with c components that are pairwise comatching. For some integer $m \geq 1$, suppose we have two distinct sets $A_1 = \{S_1^1, S_2^1, \ldots, S_m^1\}$ and $A_2 = \{S_1^2, S_2^2, \ldots, S_m^2\}$, both containing m sets of pairwise comatching vertices from F, such that for all $1 \leq i \leq m$, each S_i^1 or S_i^2 contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$ and $j = 1, 2$, let F_i^j be the 1-vertex extension of F with respect to S_i^j, with the added vertex being v_i^j. Let H_j be the 1-vertex extension of $\bigcup_{i=1}^m F_i^j$ with respect to $v_1^j, \ldots, v_m^j$, with the added vertex being r_j. Then H_1 and H_2 are comatching.

Notice that these results are applicable only if a graph F with the properties stated in the theorem statement exists. In Chapter 5, we show the existence of such a graph F by providing an example of a graph satisfying the stated properties, followed by a discussion of how such a graph could be constructed.

Similarly, using the 1-vertex extension construction, we will also show that connected graphs with an arbitrarily large number of cospectral and comatching vertices could be constructed. This construction is recursive, with each iteration of the construction strictly increases the number of comatching and cospectral vertices in the resulting graph. Theorem 5.3 and Theorem 5.10 prove that each step of the construction produces cospectral and comatching vertices, respectively.

Theorem (5.3)**.** *Let F be a graph with c components that are pairwise cospectral. Suppose there exists distinct sets $S_1, S_2, \ldots, S_m \subseteq V(F)$ of pairwise cospectral vertices for some integer $m \geq 1$, such that for all $1 \leq i \leq m$, each S_i contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$, let F_i be the 1-vertex extension of F with respect to S_i, with the added vertex being v_i. Let G be the 1-vertex extension of $\bigcup_{i=1}^m F_i$ with respect to $v_1, \ldots, v_m$, with the added vertex being r. Then

(a) $\bigcup_{i=1}^m N(v_m) \backslash r$ is a set of pairwise cospectral vertices in G; and

(b) $\bigcup_{i=1}^m N(v_m) \backslash r$ is a set of pairwise cospectral vertices in $G \backslash r$.

Theorem (5.10)**.** *Let F be a graph with c components that are pairwise comatching. Suppose there exists distinct sets $S_1, S_2, \ldots, S_m \subseteq V(F)$ of pairwise comatching vertices for some integer $m \geq 1$, such that for all $1 \leq i \leq m$, each S_i contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$, let F_i be the 1-vertex extension of F with respect to S_i, with the added vertex being v_i. Let G be the 1-vertex extension of $\bigcup_{i=1}^m F_i$ with respect to $v_1, \ldots, v_m$, with the added vertex being r. Then

(a) $\bigcup_{i=1}^m N(v_m) \backslash r$ is a set of pairwise comatching vertices in G; and

(b) $\bigcup_{i=1}^m N(v_m) \backslash r$ is a set of pairwise comatching vertices in $G \backslash r$.

Combining the theorem above and Schwenk's results, we prove the following results, Theorem 5.6 and Theorem 5.13, which are two of the most important results in this thesis.

Theorem (5.6)**.** *For any $k \geq 2$, almost every tree has k cospectral vertices that are pairwise non-similar.*

Theorem (5.13)**.** *For any $k \geq 2$, almost every tree has k comatching vertices that are pairwise non-similar.*

These two results are significant, not only because they showed the large proportion of trees with cospectral and comatching vertices, but also because our proof gave a construction for them. Also note that the construction relies on 1-vertex extensions, not the fact that the underlying graphs are trees. Therefore, the construction could also be applied to general graphs. However, the construction does result in a cut-vertex, while most graphs do not have a cut-vertex, so our construction would not give any indications about the proportion of general graphs with an arbitrarily large number of cospectral and comatching vertices.

1.3 Constructing Comatching Graphs by 2-Sums

Our last main result, which will be discussed in detail in Chapter 6, is a construction for comatching vertices and comatching graphs using 2-sums of specific graphs. In general, the k-sum of two graphs would be a *multigraph*, which is defined as $G = (V, E, f)$, such that the function f maps from E to 1-subsets and 2-subsets of V. If f maps an edge $e \in E$ to a 1-subset in V, then that e is a loop on one vertex, otherwise e is mapped to a 2-subset of V, and it is an edge connecting the two vertices in this subset. Also, the definition of multigraphs allows multiple edges between two vertices.

For any function f, we use $f|_A$ to denote the restriction of f to a set A, where A is a subset of the domain of f. Suppose $G = (V(G), E(G), f_G)$, $H = (V(H), E(H), f_H)$, $K = (V(K), E(K), f_K)$ are multigraphs such that

(a) $V(G) = V(H) \cup V(K)$;

(b) $|V(H) \cap V(K)| = k$;

(c) $E(G) = E(H) \cup E(K)$;

(d) $|E(H) \cap E(K)| = 0$;

(e) $f_G|_{E(H)} = f_H$;

(f) $f_G|_{E(K)} = f_K$;

then G is a k-*sum* of H and K, with respect to the set $V(H) \cap V(K)$.

Intuitively, a k-sum of G_1 and G_2 is the graph obtained by "merging" each of the chosen vertex in G_1 with a distinct chosen vertex in G_2, where a total of k vertices are chosen in G_1 and G_2. In other words, the two graphs share exactly k vertices.

To discuss our 2-sum construction, we first generalize the definition of matching polynomial to multigraphs, using the definition provided in [15] and [33]. Let $\mathcal{M}(G)$ be the set of all matchings in the multigraph G. By using $\beta(M)$ for the number of edges in M that are loops, the *matching polynomial* of a multigraph G is defined as

$$\mu(G; x, h) = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|-\beta(M)} h^{\beta(M)} x^{n-2|M|+\beta(M)}.$$

Observe that the h variable counts the number of loops in M, while the x variable counts the number of vertices that are not saturated by M.

Using the generalized definition of the matching polynomial, we will prove Theorem 6.10, which uses two graphs with comatching vertices to construct a larger graph with comatching vertices via 2-sum.

Theorem (6.10)**.** *Let G be the 2-sum of the multigraphs G_1 and G_2 with $V(G_1) \cap V(G_2) = \{u, v\}$. Suppose u and v are comatching vertices in both G_1 and G_2. Then u and v are comatching vertices in G.*

Moreover, we will prove the following recurrence for the matching polynomial. This recurrence plays a crucial role in our 2-sum construction of comatching graphs.

Corollary (6.9)**.** *Let H be a multigraph such that u and v are non-adjacent vertices in H. Let G be the multigraph obtained by identifying u and v in H. Then*

$$\mu(G; x, h) = \mu(H \backslash u; x, h) + \mu(H \backslash v; x, h) - x\mu(H \backslash \{u, v\}; x, h).$$

Using the recurrence above, Theorem 6.11 will be proved. This is another one of our main results giving a construction for comatching graphs. Unlike the 1-vertex extension, the 2-sum construction would not result in additional cut-vertices in the new graph.

Theorem (6.11)**.** *Let* G_1 *and* G_2 *be multigraphs with* $V(G_1) \cap V(G_2) = \{u, v\}$. *Let* G_2' *be a graph isomorphic to* G_2*, such that*

$$V(G_2') = V(G_2),$$

and

$$E(G_2') = \left(\left(E(G_2) \setminus \bigcup_{\substack{i \sim u \\ \textit{in } G_2}} \{i, u\} \right) \setminus \bigcup_{\substack{j \sim v \\ \textit{in } G_2}} \{j, v\} \right) \bigcup \left(\bigcup_{\substack{i \sim u \\ \textit{in } G_2}} \{i, v\} \right) \bigcup \left(\bigcup_{\substack{j \sim v \\ \textit{in } G_2}} \{j, u\} \right).$$

Then the 2-sum of G_1 *and* G_2 *and the 2-sum of* G_1 *and* G_2' *have the same matching polynomial if and only if* u *and* v *are comatching vertices in at least one of* G_1 *and* G_2*.*

Chapter 2

Generating Functions and Recurrences

In this chapter, we give a quick overview of generating functions. Then we introduce some basic formulas that the matching polynomial and the characteristic polynomial satisfy. We will keep referring back to these recurrences for the rest of this thesis, as they are fundamental tools for our research. We also provide a 1-sum formula for both the matching polynomial and the characteristic polynomial.

2.1 Generating Functions

Generating functions are one of the most fundamental mathematical objects in enumerative combinatorics and combinatorial analysis. Given a set S and a weight function

$$w : S \to \mathbb{Z}_+ \cup \{0\},$$

the *generating function* g_S of the set S is

$$g_S(x) = \sum_{s \in S} x^{w(s)}.$$

For example, if $S = \{(1,3),(2,1),(3,4)\}$, and $w(a,b) = |a| + |b|$, then

$$g_S(x) = x^4 + x^3 + x^7.$$

In the context of enumerative graph theory, it is common to consider the generating function of a specific set of isomorphism classes of graphs, with the number of vertices being the weight of each graph. In other words, the coefficient of the x^n term in such a generating function would be the number of graphs in the set with exactly n vertices. Moreover, sometimes such a generating function could be expressed recursively, so that we do not have to know all its coefficients to write down an expression for it. A basic example would be the generating function $T(x)$ for $\mathcal{T}$, the set of all rooted trees. It is well known that

$$T(x) = x \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} T(x^i)\right).$$

Here we omit the derivation of this expression since we will derive similar expressions for the trees we are interested in later in this thesis. For more details of the derivation, please refer to [17].

Observe that a generating function $g(x)$ is a formal power series. Moreover, recall that the *radius of convergence* r of a power series $g(x)$ is a non-negative real number or ∞ such that $g(x)$ converges when $|x| < r$, and $g(x)$ diverges when $|x| > r$. In later chapters, we will use this concept to compare the asymptotic behaviors of the generating functions of specific sets of trees. For any power series $g(x)$, we use $\langle x^i, g(x)\rangle$ to denote the coefficient of x^i.

2.2 Basic Recurrences for the Matching Polynomial

Given a graph G, there are many ways to modify it and obtain a new graph. Some of the most common graph operations include adding or deleting a vertex or an edge. In this section, we introduce some formulas that describe the change of the matching polynomial under certain graph operations.

As mentioned in the Chapter 1, one of the earliest applications of the matching polynomial was to due to Heilmann and Lieb, when they studied monomer-dimer systems [18]. They proved several important properties of the matching polynomial, including that its roots are real. Below is a vertex-deletion recurrence they proved, which is a fundamental tool in this thesis.

2.1 Lemma ([18])**.** *Let G be a graph and $u \in V(G)$, then*

$$\mu(G) = x\mu(G\backslash u) - \sum_{i\sim u} \mu(G\backslash\{u, i\}).$$

This identity was later proved by Gutman and Hosoya as well [14].

Meanwhile, in Hosoya's study of the resonance energy of monocyclic conjugated systems [21], he proved an *edge-deletion recurrence* and a *derivative formula* for the matching polynomial, the former of which is also heavily applied in this thesis. These two recurrences are stated blow, respectively.

2.2 Lemma ([21])**.** *Let G be a graph and $v \in V(G)$, and let $e = \{u, v\}$ be an edge of G, then*

$$\mu(G) = \mu(G\backslash e) - \mu(G\backslash\{u, v\}).$$

Note that $G\backslash e$ denotes the graph obtained by only deleting the edge e, without deleting the end vertices of e. On the other hand, $G\backslash\{u, v\}$ denotes the graph obtained by deleting the vertices u and v, as well as all edges incident to u or v. These two notations are used throughout our discussions in this thesis.

2.3 Lemma ([21])**.** *Let G be a graph with at least one vertex, then*

$$\frac{\mathrm{d}}{\mathrm{d}x}\mu(G) = \sum_{i \in V(G)} \mu(G\backslash i).$$

Gutman also proved the following *union formula* of the matching polynomial later in his work.

2.4 Lemma ([13])**.** *Let G and H be graphs, then the graph $G \cup H$ formed by the disjoint union of G and H*

$$\mu(G \cup H) = \mu(G)\mu(H).$$

Observe that, by using the vertex-deletion recurrence and the edge-deletion recurrence, the matching polynomial of any graph can be computed recursively. Sage is the main computational tool used in this research, and in fact it mostly uses the edge-deletion recurrence to compute the matching polynomial of any given graph, with the following complement formula by Godsil used occasionally [10]. For a graph G, we follow the convention that $\overline{G}$ to denote its *complement*, such that $\overline{G} = (V(G), E(K_{|V(G)|})\backslash E(G))$.

2.5 Theorem ([10]). *For any graph G over n vertices,*

$$\mu(G) = \sum_{i=0}^{\lfloor n/2 \rfloor} p(\overline{G}, i)\mu(K_{n-2i}).$$

This theorem tells us that, the matching polynomial of a graph G is determined by the matching polynomial of its complement $\overline{G}$. In other words, suppose we have a graph G over n vertices and suppose G has more than $\lfloor \frac{n(n-1)}{4} \rfloor$ edges, which is more than half of the number of the edges in K_n. Then, if we use the edge-deletion recurrence, it takes fewer steps to compute the matching polynomial of $\overline{G}$ than to compute the matching polynomial of G.

Meanwhile, for every edge in G, the edge-deletion recurrence converts the problem of computing one matching polynomial to the problem of computing two polynomials. Therefore, the Sage algorithm is exponential. As we mentioned in Chapter 1, it is generally hard to compute the matching polynomial of a graph, so this is not very surprising to see.

2.3 The 1-Sum Formula

In the previous section, we discussed vertex-deletion, edge-deletion, the union of two graphs, and how they affect the matching polynomial. For this section, recall the definition of k-sum we introduced in Chapter 1. We will provide a 1-sum formula for the matching polynomial.

Suppose $u \in V(H)$ and $u \in V(K)$, then we use $H_u{\cdot}K_v$ to denote a 1-sum of H and K, which is the graphs obtained by having $u \in V(H)$ and $v \in V(K)$ as the shared vertex. When u and v are known in the context, we may denote the one-sum as $H{\cdot}K$.

For example, Figure 2.1 gives an example of a 1-sum of the two graphs G_1 and G_2, assuming that their shared vertex is the one that is rectangular in shape. Then their 1-sum is the graph G.

As a graph operation, taking a k-sum interests us because of how it affects the matching polynomial. In particular, the following 1-*sum formula* holds.

2.6 Lemma. *Let H and K be multigraphs with $u \in V(H)$ and $v \in V(K)$, then*

$$\mu(H_u{\cdot}K_v) = \mu(H\backslash u)\mu(K) + \mu(H)\mu(K\backslash v) - x\mu(H\backslash u)\mu(K\backslash v).$$

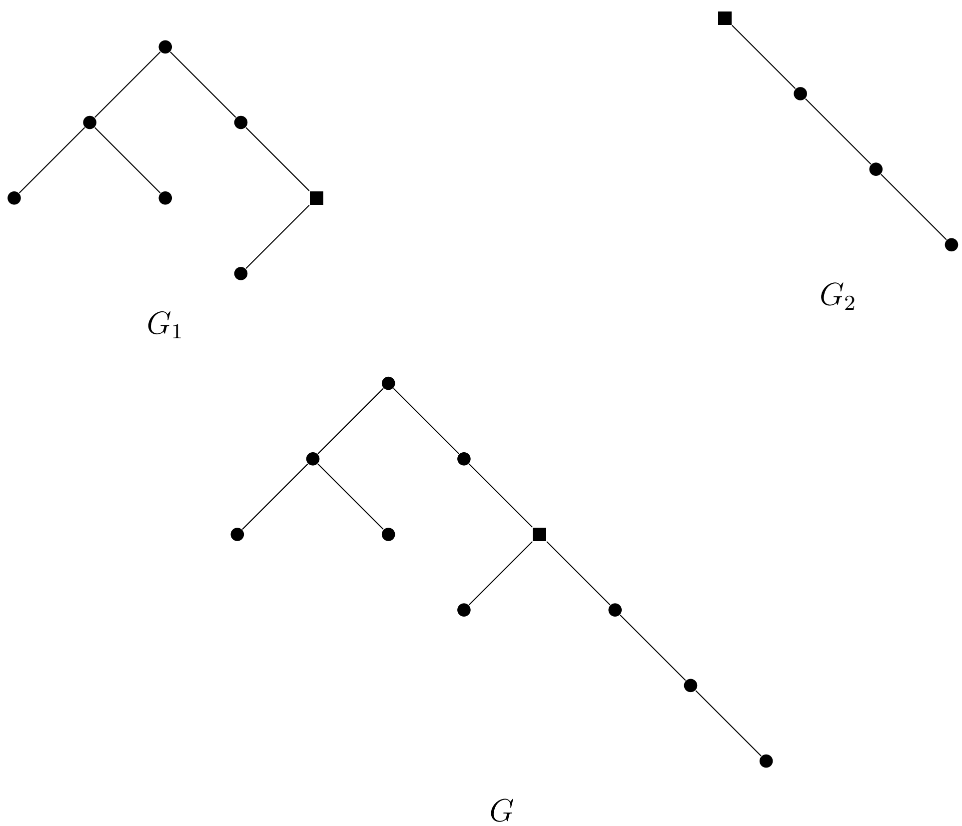


Figure 2.1: An example of a 1-sum

Proof. Use w to denote the vertex shared by H and K in $H_u{\cdot}K_v$, or $H{\cdot}K$, then observe that

$$(H{\cdot}K)\backslash w = (H\backslash u) \cup (K\backslash v).$$

Then by the union formula,

$$x\mu((H{\cdot}K)\backslash w) = x\mu(H\backslash u)\mu(K\backslash v).$$

Let $S \subseteq V(H)$ and $T \subseteq V(K)$ be the set of neighbors of u in H and the set of neighbors of v in K, respectively. Then for any $i \in S$,

$$(H{\cdot}K)\backslash\{u,i\} = (H\backslash\{u,i\}) \cup (K\backslash v),$$

and similarly for any $j \in T$,

$$(H{\cdot}K)\backslash\{v,j\} = (H\backslash u) \cup (K\backslash\{v,j\}).$$

In other words,

$$\mu((H{\cdot}K)\backslash\{u,i\}) = \mu(H\backslash\{u,i\})\mu(K\backslash v),$$

and

$$\mu((H{\cdot}K)\backslash\{v,j\}) = \mu(H\backslash u)\mu(K\backslash\{v,j\}).$$

Therefore, by the vertex deletion recurrence,

$$\begin{aligned}
\mu(H{\cdot}K) &= x\mu((H{\cdot}K)\backslash w) - \sum_{i\in S}\mu((H{\cdot}K)\backslash\{u,i\}) - \sum_{j\in T}\mu((H{\cdot}K)\backslash\{v,j\}) \\
&= x\mu(H\backslash u)\mu(K\backslash v) - \mu(K\backslash v)\left(\sum_{i\in S}\mu(H\backslash\{u,i\})\right) - \mu(H\backslash u)\left(\sum_{j\in T}\mu(K\backslash\{v,j\})\right) \\
&= x\mu(H\backslash u)\mu(K\backslash v) + \mu(K\backslash v)\left(\mu(H) - x\mu(H\backslash u)\right) + \mu(H\backslash u)\left(\mu(K) - x\mu(K\backslash v)\right) \\
&= x\mu(H\backslash u)\mu(K\backslash v) + \mu(H\backslash u)\mu(K) + \mu(H)\mu(K\backslash v) - 2x\mu(H\backslash u)\mu(K\backslash v) \\
&= \mu(H\backslash u)\mu(K) + \mu(H)\mu(K\backslash v) - x\mu(H\backslash u)\mu(K\backslash v)
\end{aligned}$$

Thus the desired formula is proven. $\square$

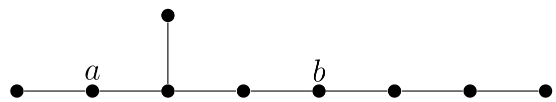


Figure 2.2: This is the smallest tree S with a pair of cospectral vertices a and b, such that a and b are not similar vertices.

This result is fundamental in Chapter 6, where we give a 2-sum construction for comatching vertices and comatching graphs. The characteristic polynomial also satisfies a similar formula, which we will introduce in the next section.

It is natural to ask, is there a similar formula for a general k-sum? Note we cannot apply the 1-sum formula recursively to obtain the matching polynomial of a k-sum, since the 1-sum formula only applies to two graphs that share exactly one vertex, whereas a k-sum is formed by two graphs sharing exactly k vertices. We need a method to obtain the matching polynomial while identifying any number of vertices in two disjoint graphs. At the end of Chapter 6, we will describe a way to compute the matching polynomial of a k-sum.

2.4 Basic Formulas for the Characteristic Polynomial

In this section, we introduce similar formulas for the characteristic polynomial and some preliminary results about cospectral vertices. Recall the characteristic polynomial $\phi(G)$ from the introduction. In Chapter 1, we defined that for a graph G, we say that $u, v \in V(G)$ are *cospectral vertices* if $\phi(G\backslash u) = \phi(G\backslash v)$.

Given any tree T, we consider $\text{Aut}(T)$, the group of automorphisms of T. For any two vertices $u, v \in V(T)$, we say that u and v are *similar* if there exists an automorphism $f \in \text{Aut}(T)$ such that $f(u) = v$. If u and v are two similar vertices, then they are cospectral. Therefore, we are more interested in finding pairs of non-similar cospectral vertices.

Figure 2.2 is the smallest tree S with a pair of cospectral vertices a and b, such that $S\backslash a$ is not isomorphic to $S\backslash b$. Note that this is the tree Schwenk used to perform his limb replacement proof that almost every tree has a cospectral mate [32]. The pair of non-similar cospectral vertices are exactly the pair of vertices he chose as the roots of his limbs. In fact, any time there is a set of pair-wise cospectral vertices in the tree L, we can use different rootings of L as a limb to build cospectral trees. This is a consequence of Lemma 2.8.

To further discuss cospectral vertices, the following identities from Godsil's book are useful [10, Theorem 2.1.5].

2.7 Lemma. *(a)* $\phi(G \cup H) = \phi(G)\phi(H)$.

(b) $\phi(G) = \phi(G\backslash e) - \phi(G\backslash\{u, v\})$ *if* $e = uv$ *is a cut-edge of* G.

(c) $\frac{d}{dx}\phi(G) = \sum_{i\in V(G)} \phi(G\backslash i)$.

Any tree T that contains L as a limb can be constructed by taking a 1-sum of the limb and the rest of the tree containing the root of the limb, which was an idea applied in Schwenk's proof. Just like the matching polynomial, the characteristic polynomial satisfies the following 1-sum identity [10, Corollary 4.3.3].

2.8 Lemma. *Let* $G = H_u{\cdot}K_v$, *with* $u \in V(H)$ *and* $v \in V(K)$. *Then*

$$\phi(G) = \phi(H\backslash u)\phi(K) + \phi(H)\phi(K\backslash v) - x\phi(H\backslash u)\phi(K\backslash v).$$

The identities in Lemma 2.7 and Lemma 2.8 play an important role in the Chapter 3, when we discuss Schwenk's work in detail. Schwenk used the 1-sum formula for the characteristic polynomial extensively to prove almost every tree has a cospectral mate. His results will be extended to weighted graphs and weighted rooted trees in Chapter 4. Moreover, in Chapter 5, they will be used in our proof for that almost every tree contains k cospectral vertices for any positive integer $k \geq 2$.

Chapter 3

Extending Limb Replacement to Rooted Trees and Maximal Limbs

In this chapter, we start with a description of Schwenk's proof that almost every tree has a cospectral mate. Then we also introduce an alternative result by McAvaney, which gives an intermediate result about rooted trees that is useful to us later [25]. After that, we will then extend Schwenk's limb replacement operation to a special type of limbs called maximal limbs, which we will define in this chapter.

The results in this chapter are joint work with Karen Yeats and are under review [36]. In particular, Theorem 3.5, Lemma 3.6, Theorem 3.7, and Theorem 3.9 are joint work.

3.1 Almost Every Tree Has A Cospectral Mate

Recall our definition of branch in Chapter 1: Let T be a tree and let B be a subtree of T. Notice that this implies there exists a vertex $v \in V(B)$ such that every path from a vertex in $V(B)$ to a vertex in $V(T)\backslash V(B)$ contains v. We say that B is a *branch* of T at v if v is a degree 1 vertex in B. A branch B at v is a maximal subtree of T under the degree restriction on v.

Observe that if B is a branch of T at v, then T is the 1-sum of B and $T\backslash(B\backslash v)$, with v being the identified vertex. An example of a branch is shown in Figure 3.1, where the part of T in the black box is a branch of T at v_1. However, the part of T in the smaller box on the right is not a branch of T at v_1 because it is not maximal, and the part of T in the box on the left is not a branch of T at v_2 because v_2 has degree 2 in it.

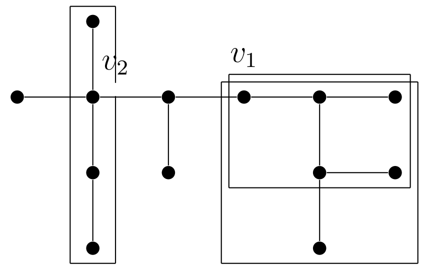


Figure 3.1: A tree T with a branch B at the vertex v in the black box

As we defined in Chapter 1, a *limb* L at v is a rooted subtree of T with v being the root, such that for each branch B at v, either $V(L) \cap V(B) = \{v\}$ or $V(L) \cap V(B) = V(B)$. Similarly, if L is a limb of T at v, then T is the 1-sum of L and $T \backslash (L \backslash v)$. Note that T is not a rooted tree while L is.

For example, consider T, L_1, L_2, and L_3 as shown in Figure 3.2, where T is a tree, and L_1, L_2, and L_3 are rooted trees with the rectangular vertices being their roots, respectively. Observe that L_1 is a limb of T, as shown in the box on the right in T. Now we consider L_2, whose underlying unrooted trees is P_4. It is clear that P_4 is a subtree of T - the box on the left of T is an occurrence of it. Based on the choice of the root in L_2, either degree 1 vertices in the box on the left in T could be considered as the root. However, this occurrence of P_4 does not include a branch at either of these root vertices entirely. This is true for other occurrences of P_4 in T as well. Therefore, L_2 is not a limb of T. Meanwhile, L_3 has the exactly the same underlying unrooted tree (which is P_4) as L_2, but the root in L_3 is different from that in L_2. We observe that L_3 is a limb of T, as shown in the box on the left of T. Note that the corresponding branches of L_3 in T are not cyclically next to each other, as they are in L_3. Cyclic ordering of branches is not being considered when deciding whether a rooted tree is a limb of a tree.

For all trees over n vertices, given a ℓ-vertex rooted tree L, how many of them have L as a limb? Does the number vary when n and ℓ remain the same but the structure of the limb changes? In Schwenk's paper, he considered the enumeration of limbs. Below is one of his main results.

3.1 Theorem ([32]). *If R and S are two rooted trees with ℓ vertices, and r_n, s_n are the numbers of n-vertex trees which do not have R or S as a limb, respectively, then $r_n = s_n$.*

In other words, given an ℓ-vertex rooted tree L, the number of n-vertex trees that contains L as a limb is a constant that only depends on n and ℓ. Given any ℓ-vertex

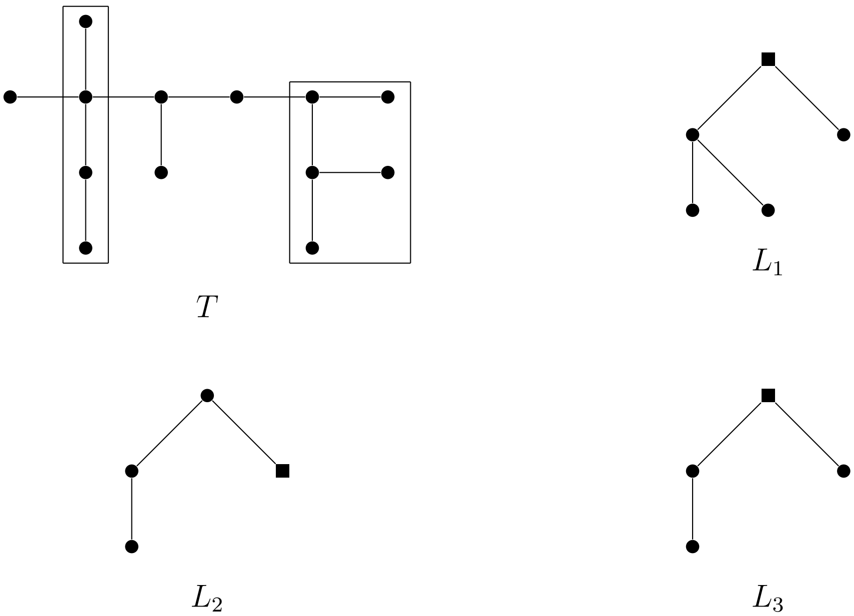


Figure 3.2: L_1 is a limb of T, L_2 is not, and L_3 is.

rooted tree L, the structure of L is irrelevant when counting the number of n-vertex trees containing L as a limb. Using this structure-less property from Theorem 3.1, the rooted tree L can be replaced as $K_{1,\ell-1}$ for the purpose of counting the number of containing L as a limb in n-vertex trees. By this limb replacement technique, Schwenk derived the following recursive equation that the generating function $S(x)$ of trees without L as a limb must satisfy [32, Theorem 5].

$$S(x) = (x - x^\ell) \sum_{i=1}^{\infty} \frac{1}{i} S(x^i)$$

It is worth noting that just one year later, McAvaney [25] derived this recursive equation using more direct enumerative arguments. We will go over this derivation in detail in the next section. In 1996, Lu [24] provided an alternative proof of Theorem 3.1 using a dissimilarity argument, which we will discuss more in the next chapter.

By performing an asymptotic analysis, Schwenk showed the radius of convergence of $S(x)$ is greater than the radius of convergence of the generating function of trees [32]. This implies that, for any ℓ-vertex rooted tree L, almost every tree contains L as limb.

In particular, Schwenk considered the tree S in Figure 2.2. In this case, $\ell = 9$. We can create two distinct rooted trees, L_1 and L_2, from S, by making a the root and b the root, respectively. Schwenk proved that, for any tree T and any vertex $v \in V(T)$, the 1-sum $T_v{\cdot}(L_1)_a$ and the 1-sum $T_v{\cdot}(L_2)_b$ are cospectral [32]. Therefore, for any tree with a copy of L_1 as a limb, we can replace that copy of L_1 with a copy of L_2 and obtain another tree cospectral to the original tree. Since almost every tree contains at least one of L_1 or L_2 as a limb, we get almost every tree is cospectral to another tree.

3.2 Theorem ([32])**.** *Almost every tree has a cospectral mate.*

For the rest of this chapter, we will give an introduction of McAvaney's result [25], and then extend several of Schwenk's results, such as Theorem 3.1 and Theorem 3.2, to a special type of limbs called maximal limbs. At the end of this chapter, we prove that, for any given ℓ-vertex rooted tree L, almost every rooted tree contains L as a maximal limb.

3.2 Limb Replacement in Rooted Trees

Limb replacement is a key technique Schwenk used to achieve his result about cospectral trees. He was able to use this technique due to the structure-less property of unrooted trees from Theorem 3.1. In this section, we discuss McAvaney's proof of that, given any ℓ-vertex rooted tree L, the number of rooted trees on n vertices containing L as a limb also does not depend on the structure of the limb [25]. This is analogous to, yet different from, Schwenk's result for unrooted trees in Theorem 3.1.

For a rooted tree T and some vertex $v \in V(T)$, we define a *branch* B at v to be a rooted subtree of T, such that v is the root of B, v has degree 1 in B, and if v' is a children of v and v' is in T, then all descendants of v' are in T. A *limb* at v is a rooted subtree of T with root v that consists of a collection of branches at v. We consider the same example as the one in the last section, with T being a rooted tree with the rectangular vertex being its root, as shown in Figure 3.3. Observe that L_1 is no longer a limb of T with the rooting of T, because there is no vertex in T with two or more children such that one of the children has degree 1 and another one of the children has exactly two children of degree 1. However, L_2 is still a limb of T, as shown in the box.

Similar to what Schwenk did in the unrooted case, for any ℓ-vertex rooted tree L, we consider the number of n-vertex rooted trees without L as a limb. In particular, when ℓ is too small, there are no n-vertex rooted trees without L as a limb, so we may assume $\ell \geq 3$. McAvaney's discussion in his paper [25] implied this number does not depend on the structure of the given limb. This implication is from his derivation of the generating

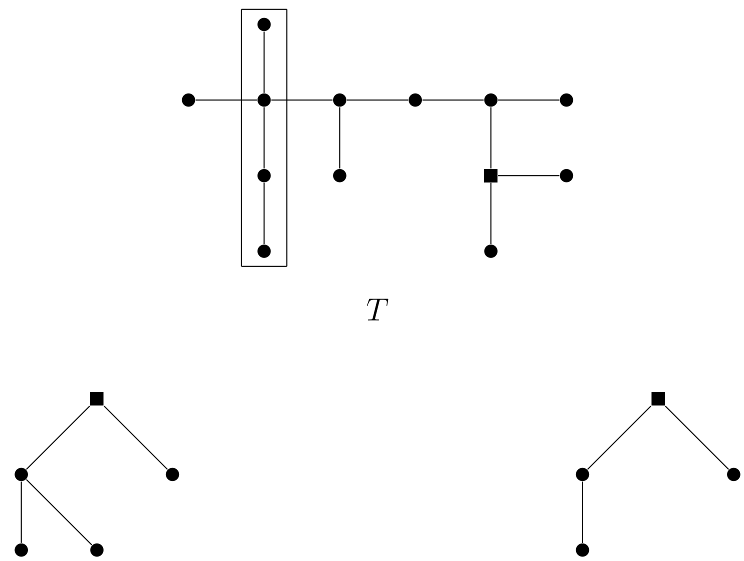


Figure 3.3: L_1 is a not limb of the rooted tree T, but L_2 is.

function of rooted trees without some rooted trees L as a limb. Here, we state this result formally and prove it. Note the proof is a rewording of McAvaney's discussion.

3.3 Theorem ([25]). *Let $\mathcal{S}$ be the set of rooted trees without some ℓ-vertex rooted tree L as a limb, and let $S(x) = \sum_{i=0}^{\infty} S_i x^i$ be its generating function, then*

$$S(x) = (x - x^{\ell}) \left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i) \right).$$

Proof. We use $F(T)$ to denote the rooted forest obtained by first deleting the root of a rooted tree T and then letting the vertex that is the neighbor of the original root serve as the new root of each component. Therefore, the number of root vertices in $F(T)$ is the number of components in it. If T is in $\mathcal{S}$, then $F(T)$ does not contain $F(L)$ as a subgraph.

We can enumerate all rooted trees R where each component of R deleting its root is in $\mathcal{S}$ using the following expression.

$$x \left(\prod_{i=1}^{\infty} \left(1 + x^j + x^{2j} + \dots\right)^{S_j} \right).$$

In this expression, the x corresponds to the root of R, and the product counts all possible combinations of components in $F(T)$. Note that R is not necessarily in $\mathcal{S}$ since the rooted trees in $F(L)$ are in $\mathcal{S}$. Therefore, L could be a limb of R at the root of R.

We can also enumerate all rooted trees R' such that each component of R' is in $\mathcal{S}$, and L is a limb of R' at the root of R'. The expression is as follows.

$$x \cdot x^{\ell-1} \left(\prod_{j=1}^{\infty} \left(1 + x^j + x^{2j} + \dots\right)^{S_j} \right).$$

Comparing to the previous expression, the only difference is the multiplication of the $x^{\ell-1}$ term, which guarantees there is a copy of every component of $F(L)$ at the root of R'. Therefore, the generating function for all rooted trees without L as a limb is the difference between these two expressions.

$$S(x) = (x - x^\ell) \exp \left(\prod_{j=1}^{\infty} \left(1 + x^j + x^{2j} + \dots\right)^{S_j} \right).$$

Taking the logarithm of both sides, we get

$$\log(S(x)) = \log(x - x^\ell) + \sum_{j=1}^{\infty} S_j \log\left(\frac{1}{1 - x^j}\right) = \log(x - x^\ell) - \sum_{j=1}^{\infty} S_j \log(1 - x^j).$$

We expand $\log(1 - x^i)$ to get

$$\begin{aligned}
\log(S(x)) &= \log(x - x^\ell) + \sum_{j=1}^{\infty} S_j \sum_{i=1}^{\infty} \frac{x^{ij}}{i} \\
&= \log(x - x^\ell) + \sum_{i=1}^{\infty} \frac{1}{i} \sum_{j=1}^{\infty} S_j x^{ij} \\
&= \log(x - x^\ell) + \sum_{i=1}^{\infty} \frac{1}{i} S(x^i).
\end{aligned}$$

By taking the exponential on both sides, we found that the generating function for rooted trees without an ℓ-vertex rooted tree L as a maximal limb satisfies the following recursive equation.

$$S(x) = (x - x^{\ell}) \left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i) \right).$$

□

From this result, we have obtained the generating function for rooted trees without a given rooted tree L as a limb. The variable ℓ is the only quantity about L in this generating function, so the number of rooted tree over n vertices without L as a limb is a fixed constant that only depends on n and ℓ, but not the structure of L. In other words, this derivation process implies the following result, which is a rooted version of Theorem 3.1.

3.4 Theorem. *Let L_1 and L_2 be two distinct rooted trees with ℓ vertices, where $\ell \geq 3$. Let $\ell_{1,n}$ and $\ell_{2,n}$ denote the number of n-vertex rooted trees without L_1 or L_2 as a limb, respectively. Then $\ell_{1,n} = \ell_{2,n}$.*

Notice that it is also possible to prove Theorem 3.4 using a combinatorial argument as well, by building a bijection between all trees without L_1 as a limb and all trees without L_2 as a limb [31].

This result coincides with what Schwenk derived in [32]. Therefore, this is an enumerative way to derive the generating function for unrooted trees without a given ℓ-vertex limb.

3.3 Maximal Limb Replacement

So far, the limbs we have considered are generic, in the sense that the branches they contain are not chosen in any specific way. In this section, we consider a particular type of limbs named maximal limbs, and extend Schwenk's results to them. For a rooted tree T and any vertex v in T, the *maximal limb* at v is the limb at v that contains exactly all descendants of v. In a rooted setting, the defined limb is maximal because all limbs at v are its subtrees.

For example, consider rooted trees T, L_1, and L_2 in Figure 3.4, where the rectangular vertices are the roots, respectively. Both L_1 and L_2 are limbs of T. However, as the box shows, the occurrence of L_2 in T does not include all branches at the vertex corresponding

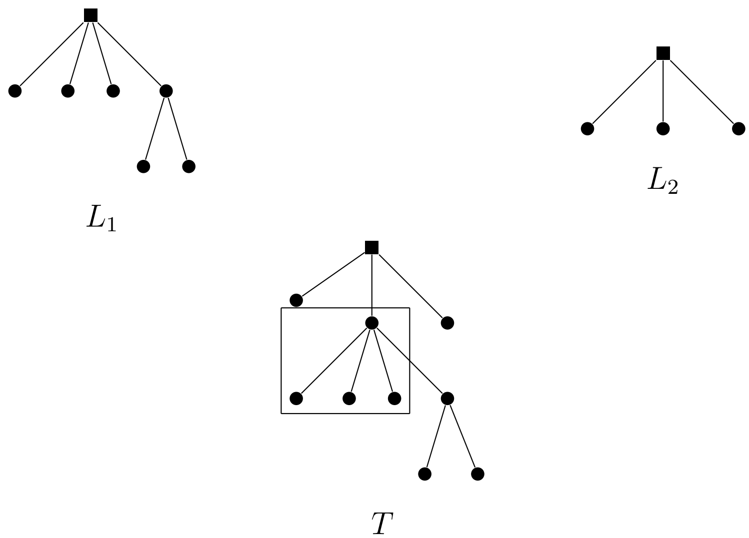


Figure 3.4: An example of a maximal limb

to the root of L_2, so L_2 is not a maximal limb of T. Meanwhile, L_1 is a limb and a maximal limb of T.

In this section, we prove a result that is similar to Theorem 3.4, but for maximal limbs.

3.5 Theorem. *Let L_1 and L_2 be two distinct rooted trees with ℓ vertices with $\ell \geq 3$. Use $\ell_{1,n}$ and $\ell_{2,n}$ to denote the number of n-vertex rooted trees without L_1 or L_2 as a maximal limb, respectively. Then $\ell_{1,n} = \ell_{2,n}$.*

Proof. When $n < \ell$, the statement is trivially true because no rooted tree with n vertices can have a limb with ℓ vertices. For the rest of this proof, we assume $n \geq \ell$.

Use $\mathcal{T}_1$ to denote the set of n-vertex rooted trees with L_2 as a maximal limb but without L_1 as limb, and $\mathcal{T}_2$ to denote the set of n-vertex rooted trees with L_1 as a maximal limb but without L_2 as limb. It suffices to show that $|\mathcal{T}_1| = |\mathcal{T}_2|$. We prove this bijectively.

Let $T \in \mathcal{T}_1$, and consider the occurrences of the maximal limb L_2 in T. By definition of maximal limbs, these occurrences must be rooted at distinct vertices. If two occurrences of L_2 rooted at two distinct vertices v_1, v_2 with $i \neq j$ share a vertex u, then the union of the paths $v - v_1 - u$ and $v - v_2 - u$ contains a cycle, which is a contradiction. Therefore, no two of these occurrences of L_2 share a vertex. To obtain a tree in $\mathcal{T}_2$ from T, we simply replace each occurrence of the limb L_2 with the limb L_1. A similar argument can be applied to the trees in $\mathcal{T}_2$.

Therefore, this process is reversible, and we have constructed a bijection between $\mathcal{T}_1$ and $\mathcal{T}_2$, which completes the proof. □

As a result, we have proved that, just as with generic limbs, for any ℓ-vertex rooted tree L, the number of n-vertex trees with L as a maximal limb is independent of the structure of L. In the next section, we show that almost every rooted tree contains such a maximal limb L by proving a number of more general statements.

3.4 Maximal Limb in Rooted Trees

In the previous section, we extended Schwenk's limb replacement result to maximal limbs. Moreover, we can also ask, given any ℓ-vertex rooted tree L, would almost every rooted tree contains it as a maximal limb? In this section, we show that, this answer to this question is yes.

Similar to the approach Schwenk used, we start by deriving a recursion for the generating function of the set of rooted trees without L as a maximal limb. Due to the structure-less property shown in Theorem 3.5, we may assume $L = K_{1,\ell-1}$. Let $\mathcal{S}$ be the set of rooted trees without L as a maximal limb, and let $S(x) = \sum_{i=0}^{\infty} S_i x^i$ be the generating series of $\mathcal{S}$.

Suppose we have a rooted tree T in $\mathcal{S}$. If we delete the root of T, we can see that $F(T)$ is a rooted forest $\mathcal{S}$ that is not identical to $F(L)$, where $F(L)$ is a rooted forest consisting of $(\ell-1)K_1$, with the vertex in each copy of K_1 being a root. Therefore, we get the following expression for $S(x)$.

$$\begin{aligned} S(x) &= x\left(\prod_{j=1}^{\infty}\left(1 + x^j + x^{2j} + \dots\right)^{S_j} - x^{\ell-1}\right) \\ &= x\left(\prod_{j=1}^{\infty}\left(\frac{1}{1-x^j}\right)^{S_j}\right) - x^{\ell} \end{aligned}$$

Using a derivation process that is similar to that in the proof of Theorem 3.3, we get

$$S(x) = x\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}S(x^i)\right) - x^{\ell}.$$

To compare this generating function with the generating function of all rooted trees, one way is to compare their radii of convergence. We denote the radius of convergence of $S(x)$ as α_S, and in the following lemma we prove $S(\alpha_S) = 1$.

3.6 Lemma. *The series $S(x)$ satisfies $S(\alpha_S) + (\alpha_S)^\ell = 1$.*

Proof. Define a multivariate function: for $x, y \in \mathbb{C}$,

$$F_S(x, y) = x \exp\left(y + \sum_{i=2}^{\infty} \frac{1}{i} S(x^i)\right) - x^\ell - y.$$

Observe that $y = S(x)$ is a solution to the equation $F(x, y) = 0$. We can see that $F(x, y)$ is analytic in each variable separately in the neighborhoods of α_S and $S(\alpha_S)$.

Moreover, consider the following partial derivative:

$$\frac{\partial F_S}{\partial y}(x, y) = x \exp\left(y + \sum_{i=2}^{\infty} \frac{1}{i} S(x^i)\right) - 1 = F(x, y) + x^l + y - 1.$$

If $\frac{\partial F_S}{\partial y}(\alpha_S, S(\alpha_S)) \neq 0$, then by the Implicit Function Theorem (see Appendix 7.4 for more details), there is a unique function $f(x)$ such that $F_S(x, f(x)) = 0$, so this function must be $S(x)$. Moreover, the Implicit Function Theorem also gives that this function is analytic in the neighborhood of α_S. However, since α_S is the radius of convergence of $S(x)$, we know that $S(x)$ has a singularity at $x = \alpha_S$, which is a contradiction. Therefore, we must have

$$\frac{\partial F_S}{\partial y}(\alpha_S, S(\alpha_S)) = 0,$$

and as a result $S(\alpha_S) + (\alpha_S)^\ell = 1$. □

Meanwhile, recall that the generating function for rooted trees satisfies

$$T(x) = x \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} T(x^i)\right).$$

Let α_T be the radius of convergence of $T(x)$. Note that it is known that $T(\alpha_T) = 1$ [17].

3.7 Theorem. *The radius of convergence of $S(x)$ is greater than the radius of convergence of $T(x)$.*

Proof. Note that $T(r_T) = 1$, while Lemma 3.6 gives $S(\alpha_S) + (\alpha_S)^\ell = 1$.

By definition, $S(x)$ is coefficient-wise bounded above by $T(x)$, which implies $\alpha_S \geq \alpha_T$. Moreover, since the trees $T(x)$ counts include trees with L as a maximal limb while the trees $S(x)$ counts do not, we get $\langle x^i, S(x) + x^\ell \rangle = \langle x^i, T(x) \rangle$ for all $i \leq \ell$, and $\langle x^i, S(x) + x^\ell \rangle < \langle x^i, T(x) \rangle$ for all $i > \ell$. Therefore, $S(\alpha_T) + (\alpha_T)^\ell < T(\alpha_T) = 1$, which means $\alpha_S \neq \alpha_T$. Consequently, we obtain $\alpha_S > \alpha_T$. □

The following theorem on Page 211 in the book by Harary and Palmer relates the radius of convergence of series with their coefficients.

3.8 Theorem ([17]). *Let $F(x, y)$ be analytic in each variable separately in some neighborhood of (x_0, y_0) and suppose that the following conditions are satisfied:*

(a) $F(x_0, y_0) = 0$;

(b) $y = f(x)$ *is analytic in* $|x| \leq |x_0|$ *and* x_0 *is the unique singularity on the circle of the convergence;*

(c) *if* $f(x) = \sum_{n=0}^{\infty} f_n x^n$ *is the expansion of* f *at the origin, then* $y_0 = \sum_{n=0}^{\infty} f_n x_0^n$;

(d) $F(x, f(x)) = 0$ *for* $|x| < x_0$;

(e) $\frac{\partial F}{\partial y}(x_0, y_0) = 0$;

(f) $\frac{\partial^2 F}{\partial y^2}(x_0, y_0) \neq 0$.

Then $f(x)$ *may be expanded about* x_0:

$$f(x) = f(x_0) + \sum_{k=1}^{\infty} a_k (x_0 - x)^{k/2}$$

and if $a_1 \neq 0$,

$$f_n \sim \frac{-a_1}{2\sqrt{\pi}} x_0^{-n+1/2} n^{-3/2}$$

and if $a_1 = 0$ *but* $a_3 \neq 0$

$$f_n \sim \frac{3a_3}{4\sqrt{\pi}} x_0^{-n+3/2} n^{-5/2}.$$

Using the theorem above, we obtain the following result.

3.9 Theorem. *For any given rooted tree L, almost every rooted tree contains L as a maximal limb.*

Proof. We define

$$F_S(x,y) = x\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}S(x^i)\right) - x^{\ell} - y$$

and

$$F_T(x,y) = x\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}T(x^i)\right) - y.$$

It is easy to see that both of these bivariate functions satisfy the conditions of Theorem 3.8, with $S_(x)$ and $T(x)$ being the corresponding univariate functions, respectively. The radii of convergence α_S and α_T serve as the point x_0 in the statement of Theorem 3.8. To see why $F_S(x,y)$ and $F_T(x,y)$ satisfy the conditions for Theorem 3.8, we consider $F_S(x,y)$ and $S(x)$ as an example.

It is clear that $F_S(x,y)$ satisfies condition (a) in Theorem 3.8.

To see why $S(x)$ satisfies condition (b) in Theorem 3.8, we consider a point p on the circle of the convergence of $S(x)$ such that $p \neq \alpha_S$. We know that

$$\frac{\partial F_S}{\partial y}(x,y) = x\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}S(x^i)\right) - 1.$$

Moreover, observe that

$$\left|x\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}S(x^i)\right) - 1\right| \geq 1 - \left|x\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}S(x^i)\right)\right| > 1 - F(\alpha_S, S(\alpha_S)) = 0.$$

Therefore, for any point p with $|p| = \alpha_S$ and $p \neq \alpha_S$, we have that $\frac{\partial F_S}{\partial y}(p, S(p)) \neq 0$. (Note that $S(p)$ is bounded since $S(\alpha_S)$ is bounded.) Then by the Implicit Function Theorem, $S(x)$ is analytic at p for $|p| = \alpha_S$ and $p \neq \alpha_S$.

Condition (c) in Theorem 3.8 follows from Lemma 3.6. Conditions (d) and (e) are clearly satisfied. For condition (f), we have

$$\frac{\partial^2 F_S}{\partial y^2}(x,y) = x\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}S(x^i)\right),$$

so $\frac{\partial^2 F_S}{\partial y^2}(\alpha_S, S(\alpha_S)) \neq 0$.

In the neighborhood of $x = \alpha_S$, we match the coefficients of the defining power series of $S(x)$ and the expansion given by Theorem 3.8.

$$S(x) = S(\alpha_S) + \sum_{k=1}^{\infty} a_k(\alpha_S - x)^{k/2} \text{ for some constants } a_k.$$

By taking the derivative of this expansion in the neighborhood of α_S, we get

$$S'(x) = \frac{-a_1}{2(\alpha_S - x)^{1/2}} + O(\alpha_S - x),$$

Meanwhile, if we take the derivative of the recursion definition of $S(x)$, we get

$$S'(x) = \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right) + \left(\sum_{i=1}^{\infty} x S(x^i)\right) \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right) - \ell x^{l-1}.$$

We consider $S'(x)(1 - S(x) - x^\ell)$ using these two different expressions of $S'(x)$, where $x < \alpha_S$ and x is in the neighborhood of α_S. For the first expression, we get

$$\begin{aligned} &S'(x)(1 - S(x) - x^\ell) \\ &\quad = \left(\frac{-a_1}{2(\alpha_S - x)^{1/2}} + O(\alpha_S - x)\right)(1 - S(\alpha_S) - (\alpha_S)^\ell - a_1(\alpha_S - x)^{1/2} + O(\alpha_S - x)). \end{aligned}$$

Recall that Lemma 3.6 gives $1 - S(\alpha_S) - (\alpha_S)^\ell = 0$. After omitting the $O(\alpha_S - x)$ terms, the expression above becomes

$$S'(x)(1 - S(x) - x^\ell) = \frac{1}{2} a_1^2.$$

On the other hand, if we compute $S'(x)(1 - S(x) - x^\ell)$ using the other expression of $S'(x)$, we get

$$\begin{aligned} &S'(x)(1 - S(x) - x^\ell) \\ &= \left(\left(\exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right) - \ell x^{l-1}\right) + \left(\sum_{i=1}^{\infty} x S(x^i)\right) \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right)\right)(1 - S(x) - x^\ell). \end{aligned}$$

Since both $S(x)$ and x^ℓ are monotone increasing and $S(\alpha_S) + (\alpha_S)^\ell = 1$, we can see that $(1 - S(x) - x^\ell) > 0$ when $x < \alpha_S$ and x is in the neighborhood of α_S. Observe that

$$\langle x^{\ell-1}, \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right) \rangle = \langle x^\ell, x \exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right) \rangle = \langle x^\ell, S(x) + x^\ell \rangle,$$

which is simply one plus the number of ℓ-vertex rooted trees without a specific ℓ-vertex rooted tree as a maximal limb. This number is clearly greater than ℓ, so $\exp\left(\sum_{i=1}^{\infty} \frac{1}{i} S(x^i)\right) - \ell x^{l-1}$ is a series with all positive coefficients, which implies the first term in the product above is positive when $x < \alpha_S$ and x is in the neighborhood of α_S. Thus $S'(x)(1 - S(x) - x^\ell) = \frac{1}{2} a_1^2 > 0$, which implies $a_1 \neq 0$. By Theorem 3.8, we conclude that

$$S_n \sim \frac{-a_1}{2\sqrt{\pi}} \alpha_S^{-n+1/2} n^{-3/2}.$$

By a similar argument, we can also see that

$$T_n \sim \frac{-a_1'}{2\sqrt{\pi}} \alpha_T^{-n+1/2} n^{-3/2},$$

where a_1' is a non-zero constant. Therefore, the ratio between S_n and T_n approaches 0 as n approaches infinity, which implies that for any given rooted tree L, almost every rooted tree contains L as a maximal limb. □

It is important to note that Schwenk's result does imply Theorem 3.9. Consider a rooted tree L with root r. We construct the rooted tree L' by adding a leaf r' to r and make r' the root of L'. Schwenk proved that almost every tree contains L' as a limb, which implies almost every tree contains L as a maximal limb. Our contribution is to study the generating series for trees without a specific maximal limb and therefore providing an alternative proof to Theorem 3.9.

Chapter 4

Cospectral Weighted Trees

In this chapter, the main mathematical objects of interest are weighted trees, both rooted and unrooted. As defined in Chapter 1, a tree is *weighted* if each of its vertices is assigned a positive integer weight. Weighted trees are widely studied in the field of combinatorics, mathematics, and computer science. Specifically, the interpretation of limbs in quantum field theorem inspired us to study them. For more details, please refer to [4].

The results in this chapter are joint work with Karen Yeats and are under review [36]. In particular, Lemma 4.2, Lemma 4.3, Theorem 4.4, Theorem 4.5, Lemma 4.11, Lemma 4.12, Lemma 4.14, Lemma 4.15, Lemma 4.16, Lemma 4.17, and Theorem 4.18 are joint work.

4.1 Limb Replacement in Weighted Rooted Trees

We start by considering weighted rooted trees in this section. In particular, we define *weighted rooted trees* as rooted trees where each vertex is assigned a positive integer weight. In this context, we say a weighted rooted tree L is a *limb* of a weighted rooted tree T if the unweighted version of L is a limb of the unweighted version of T, and there exists an occurrence of the unweighted version of L in T such that the weights assigned to each of the vertices in this occurrence are exactly the same as the weights in the corresponding vertices in L. We extend Schwenk's limb replacement technique and asymptotic analysis to weighted rooted trees.

An example of limbs for weighted rooted trees is shown in Figure 4.1. In the figure, we have three weighted rooted trees, T, L_1 and L_2, with the rectangular vertices being their

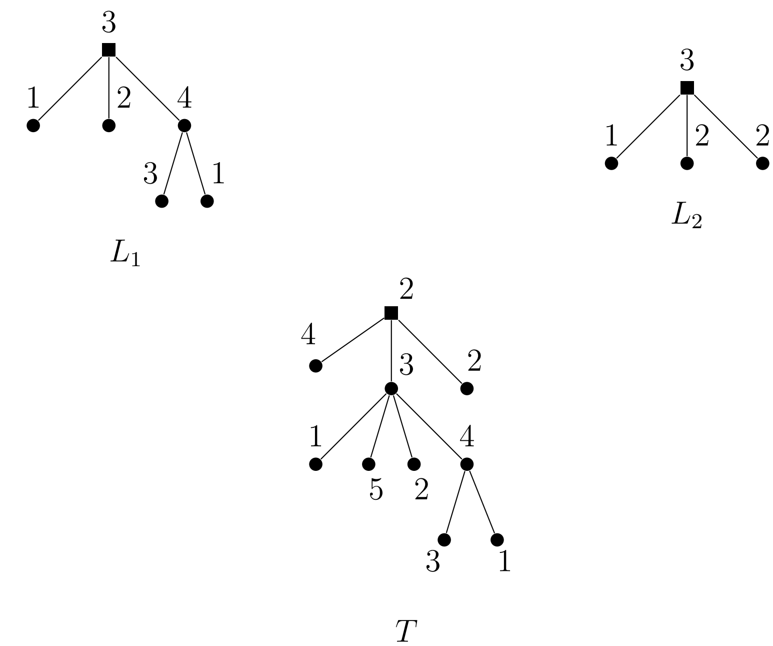


Figure 4.1: An example of a limb in weighted rooted trees

roots, respectively. Observe that L_1 is a limb of T. Meanwhile, even though L_2 has the same underlying unweighted tree as L_1, it is not a limb of T. This is because we cannot find a vertex of weight 3 in T as the root of an occurrence of L_2, such that it has three degree 1 children vertices having the same degrees as the three children vertices of the root in L_2. The vertex of degree 3 in T has three neighboring vertices of degree 1 with the same degrees as the ones in L_2, but one of those neighboring vertices is its parent vertex, so it would not work.

We apply the generating function argument that Schwenk used to analyze weighted rooted trees without a given limb. To utilize this argument, we need to first derive a recursion for the generating function of the set of weighted rooted trees. For the purpose of generating functions, the *weight* of a weighted graph, rooted or unrooted, is the sum of the weights of all its vertices. Let $\mathcal{T_W}$ be the set of all weighted rooted trees, and let $T_W(x) = \sum_{i=0}^{\infty} T_{w,i}x^i$ be its generating function, where a weight of a tree is the sum of the weights of all its vertices. Like for the rooted trees, given a weighted rooted tree T_W, we use $F(T_W)$ to denote the weighted rooted forest obtained by first deleting the root of T_W and then letting the vertex that was adjacent to the root of T_W serve as the new root of each component, and the weight on each of the remaining vertices is unchanged. Similarly to unweighted rooted trees, consider what happens to a weighted rooted tree T_W if its root r with weight w_r is deleted. We see that $F(T_W)$ is a forest, where each component of $F(T_W)$ is an element of $\mathcal{T}_R$. Therefore, we can obtain the following equation.

$$\begin{aligned} T_W(x) &= \left(\sum_{k=1}^{\infty} x^k\right)\left(\prod_{j=1}^{\infty}(1+x^j+x^{2j}+\dots)^{T_{w,j}}\right) \\ &= \left(\sum_{j=1}^{\infty} x^j\right)\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}T(x^i)\right) \\ &= \frac{x}{1-x}\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}T_W(x^i)\right) \end{aligned} \tag{4.1}$$

The simplification process from the first line to the second line is similar to the simplification process for $S(x)$ in the proof of Theorem 3.3. Observe that rooted trees can be considered as a specific case of weighted rooted trees where all vertices have weight 1.

Analogous to Schwenk's proof, we start by considering the radius of convergence of $T_W(x)$, denoted as α_T.

4.1 Lemma. *The radius of convergence of $T_W(x)$ is at least $\frac{1}{16}$.*

Proof. Define the sequence $\{T_n\}$ such that

$$T_W(x) = \sum_{n=1}^{\infty} T_n x^n.$$

Let

$$A(x) = \frac{T_W(x)}{x}$$

and

$$B(x) = \sum_{i=1}^{\infty}\frac{1}{i}T_W(x^i).$$

Note that, by Equation (4.1), $A(x) = \frac{1}{1-x}\exp B(x)$. Moreover, we have

$$\begin{aligned}
\frac{d}{dx}A(x) &= \frac{1}{1-x}\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}T_W(x^i)\right)\cdot\frac{d}{dx}B(x) \\
&\quad + \frac{1}{(1-x)^2}\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}T_W(x^i)\right) \\
&= A(x)\cdot\frac{d}{dx}B(x) + \frac{1}{1-x}A(x).
\end{aligned}$$

Therefore,

$$\begin{aligned}
T_{n+1} &= \frac{1}{n}\langle x^{n-1}, \frac{d}{dx}A(x)\rangle \\
&= \frac{1}{n}\langle x^{n-1}, A(x)\cdot\frac{d}{dx}B(x)\rangle + \frac{1}{n}\sum_{i=0}^{n-1}\langle x^{n-1-i}, A(x)\rangle \\
&= \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{d|i} dT_d\right)T_{n-i+1} + \frac{1}{n}\sum_{i=1}^{n}T_{n-i+1} \\
&= \frac{1}{n}\sum_{i=1}^{n}\left(iT_i\cdot\sum_{i\le ci\le n}T_{n-ci+1} + T_{n-i+1}\right)
\end{aligned}$$

For every weighted rooted tree of weight n, by adding 1 to the weight of its root, we can create a distinct weighted rooted tree corresponding to it with weight $n+1$. Therefore, the sequence $\{T_n\}$ is weakly increasing, and so for any c such that $i \le ci \le n$, we have $T_{n-ci+1} \le T_{n-i+1}$. Then $\sum_{i\le ci\le n}T_{n-ci+1} \le nT_{n-i+1}$. Additionally, since $T_1 = 1$, it is clear that $T_i \ge 1$ for any $i \ge 1$, so $\frac{T_{n-i+1}}{iT_i} \le T_{n-i+1}$ for any $1 \le i \le n$. Thus,

$$\begin{aligned}
&= \frac{1}{n}\sum_{i=1}^{n}iT_i\cdot\left(\sum_{i\le ci\le n}T_{n-ci+1} + \frac{T_{n-i+1}}{iT_i}\right) \\
&\le \frac{1}{n}\sum_{i=1}^{n}iT_i\cdot\frac{n+i}{i}T_{n-i+1} \\
&\le 2\sum_{i=1}^{n}T_iT_{n-i+1}.
\end{aligned}$$

Now, we define a power series $f(x) = \sum_{i=1} f_i x^i$, where $f_1 = 1$ and

$$f_n = 2\sum_{i=1}^{n} f_i f_{n-i-1}.$$

Since $f(x)$ bounds $T_W(x)$ above, the radius of convergence of $f(x)$ is a lower bound for the radius of convergence of $T_W(x)$. Moreover,

$$\langle x^{n+1}, (f(x))^2\rangle = \sum_{i=1}^{n} f_i f_{n-i+1} = \frac{1}{2} f_{n+1}$$

for all $n \geq 2$, and $\langle x, (f(x))^2\rangle = 0$. Then we have

$$(f(x))^2 - \frac{1}{2} f(x) + x = 0.$$

By the quadratic formula and the fact that $f(0) = 0$, we get

$$f(x) = \frac{1}{4}\left(1 - \frac{1}{\sqrt{1-16x}}\right).$$

The radius of convergence of $f(x)$ is $\frac{1}{16}$, so the radius of convergence of $T_W(x)$ is at least $\frac{1}{16}$. □

The following lemma shows that $T_W(\alpha_T)$ is bounded, where α_T the radius of convergence of $T_W(x)$. We will use this to compare α_T and the radius of convergence of the generating series of weighted trees with a forbidden limb. The general approach used to prove this lemma is described in Section 9.5 of Harary and Palmer [17].

4.2 Lemma. *The series $T_W(x)$ converges to 1 at $x = \alpha_T$.*

Proof. We begin by proving $T_W(x)$ converges at $x = \alpha_T$.

Observe that, for all $x \in (0, \alpha_T)$,

$$\log\left(\frac{T_W(x)}{x/(1-x)}\right) = T_W(x) + \sum_{i=2}^{\infty} T_W(x^i).$$

Consequently, we get

$$T_W(x) \leq \log\left(\frac{T_W(x)}{x/(1-x)}\right).$$

Since $T_W(x)$ has positive coefficients, $\log\left(\frac{T_W(x)}{x/(1-x)}\right)$ must be positive as well. We divide both sides of the inequality above by $\frac{x}{1-x}\log\left(\frac{T_W(x)}{x/(1-x)}\right)$ to obtain

$$\frac{T_W(x)/(x/(1-x))}{\log\left(\frac{T_W(x)}{x/(1-x)}\right)} \leq \frac{1-x}{x}.$$

Observe that

$$\frac{T_W(x)}{x/(1-x)} = \exp\left(\sum_{i=1}^{\infty}\frac{1}{i}T_W(x^i)\right),$$

which is monotone increasing and is greater than 1 on $(0, \alpha_T)$. As $x \to \alpha_T^-$, we have $\frac{1-x}{x}$ approaching the constant $\frac{1-\alpha_T}{\alpha_T}$. The function $f(x) = \frac{x}{\log(x)}$ is continuous on the interval $(1, \infty)$, and this is the only interval for which the value of $f(x)$ is positive. It strictly decreases on $(1, e)$ and strictly increases on (e, ∞). Therefore, since $\frac{T_W(x)/(x/(1-x))}{\log\left(\frac{T_W(x)}{x/(1-x)}\right)} \leq \frac{1-x}{x}$ on $(0, \alpha_T)$, the left hand side of this inequality is positive, we get the value of $\frac{T_W(x)}{x/(1-x)}$ is bounded above by either $f(1)$ or $\frac{1-\alpha_T}{\alpha_T}$. So $T_W(x)$ is bounded on $(0, \alpha_T)$.

Since $T_W(x)$ is monotone increasing, $\lim_{x\to\alpha_T} T_W(x)$ exists, and its value is $T_W(\alpha_T)$.

Now we show that the value that $T_W(x)$ converges to at $x = \alpha_T$ is 1. Define a multivariate function: for $x, y \in \mathbb{C}$,

$$G(x,y) = \frac{x}{1-x}\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}T_W(x^i)\right) - y.$$

Observe that $y = T_W(x)$ is a solution to the equation $G(x,y) = 0$. We can see that $G(x,y)$ is analytic in each variable separately in the neighborhoods of α_T and $T_W(\alpha_T)$.

Moreover, consider the following partial derivative:

$$\frac{\partial G}{\partial y}(x,y) = \frac{x}{1-x}\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}T_W(x^i)\right) - 1 = G(x,y) - 1 + y.$$

Then

$$\frac{\partial G}{\partial y}(\alpha_T, T_W(\alpha_T)) = G(\alpha_T, T_W(\alpha_T)) + T_W(x) - 1 = T_W(\alpha_T) - 1.$$

If $\frac{\partial G}{\partial y}(\alpha_T, T_W(\alpha_T)) \neq 0$, then by the Implicit Function Theorem, there is a unique function $f(x)$ such that $G(x, f(x)) = 0$, so this function must be $T_W(x)$. Moreover, the Implicit Function Theorem also gives that this function is analytic in the neighborhood of α_T. However, since α_T is the radius of convergence of $T_W(x)$, we know that $T_W(x)$ has a singularity at $x = \alpha_T$, which is a contradiction. Therefore, we must have

$$\frac{\partial G}{\partial y}(\alpha_T, T_W(\alpha_T)) = 0,$$

and as a result $T_W(\alpha_T) = 1$. □

Now we have established the groundwork to discuss weighted rooted trees, let us define what a limb is in this case. Let T be a weighted rooted tree and suppose $v \in V(T)$. A *branch* B at v is a weighted rooted subtree of T, such that v is the root of B, v has degree 1 in B, and if v' is a child of v and v' is in T, then all descendants of v' are in T. A *limb* at v is a weighted rooted subtree of T with root v that consists of a collection of branches at v.

It is useful to observe that Theorem 3.4 applies to weighted rooted trees. The reason is simple: Consider two weighted rooted trees L_1 and L_2 with the weights for each of their vertices already assigned. By Theorem 3.4, the number of n-vertex rooted trees without the unweighted version L_1 as a limb is the same as the number of n-vertex rooted trees without the unweighted version of L_2 as a limb. Since the weight for each vertex is already fixed, taking the weights into consideration does not affect the equality of these two numbers. Therefore, the number of weight n weighted rooted trees without the L_1 as a limb is the same as the number of weight n weighted rooted trees without L_2 as a limb.

Given a rooted tree L, let $\mathcal{S}_W$ be the set of all weighted rooted trees without L as a limb. We derive its generating series $S_W(x)$ by an argument similar to Schwenk's [32]. Suppose the weight of L is ℓ, and the weight of its root vertex is w. If L is too small, $\mathcal{S}_W$ would be trivial. So, assume L contains at least three vertices, which implies $\ell \geq 3$.

We construct the generating function $S_W(x) = \sum_{i=0}^{\infty} s_{w,i} x^i$ using the recursive relationship among the trees in the set $\mathcal{S}_W$. Given a weighted rooted tree T_W in $\mathcal{S}_W$, observe that $F(T_W)$ is a weighted rooted forest in S_W that does not contain $F(L)$ as a subset. Assume the root of L has weight w, then the total weight of the vertices in $F(L)$ is $\ell - w$. The generating function $S_W(x)$ is the difference between the generating function for weighted rooted trees with a root of any weight attached to any forest where each component is an element of $\mathcal{S}_W$ and the generating function for weighted rooted trees U with root of weight w while $F(L)$ is a subgraph of $F(U)$. Consequently, the generating function for weighted rooted trees without a given weighted limb L satisfies the following equation.

$$
\begin{aligned}
S(x) &= \left(\sum_{k=1}^{\infty} x^k\right)\left(\prod_{j=1}^{\infty}(1+x^j+x^{2j}+\dots)^{s_{w,j}}\right) - x^w \cdot x^{\ell-w}\left(\prod_{j=1}^{\infty}(1+x^j+x^{2j}+\dots)^{s_{w,j}}\right)\\
&= \frac{x}{1-x}\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}S(x^i)\right) - x^w \cdot x^{\ell-w}\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}S(x^i)\right)\\
&= \left(\frac{x}{1-x} - x^{\ell}\right)\exp\left(\sum_{i=1}^{\infty}\frac{1}{i}S(x^i)\right)
\end{aligned}
$$

Since the number of weighted rooted trees without a given limb increases as a function of the number of vertices, it is easy to see that the radius of convergence of S, denoted as α_S, is finite. Meanwhile, by definition, $\langle x^i, S_W(x)\rangle \leq \langle x^i, T_W(x)\rangle$ for any non-negative integer i, so $\alpha_S \geq \alpha_T > 0$. To further compare these two quantities, in the following lemma, we prove $S(\alpha_S) = 1$.

4.3 Lemma. *The series $S_W(x)$ satisfies $S_W(\alpha_S) = 1$.*

Proof. Define a multivariate function: for $x, y \in \mathbb{C}$,

$$
F(x,y) = \left(\frac{x}{1-x} - x^l\right)\exp\left(y + \sum_{i=2}^{\infty}\frac{1}{i}S_W(x^i)\right) - y.
$$

By the Implicit Function Theorem (see Appendix 7.4 for more details), $y = S_W(x)$ is the unique analytic solution of $F(x,y) = 0$. Moreover, it has a singularity at $x = \alpha_S$, and $F(\alpha_S, S_W(\alpha_S)) = 0$.

Therefore,

$$
\frac{\partial F}{\partial y}(\alpha_S, S_W(\alpha_S)) = F(\alpha_S, S_W(\alpha_S)) + S_W(x) - 1 = S_W(\alpha_S) - 1 = 0,
$$

due to the singularity. Thus $S_W(\alpha_S) = 1$. □

Now we are ready to prove $\alpha_S > \alpha_T$.

4.4 Theorem. *The radius of convergence of $S_W(x)$ is greater than the radius of convergence of $T_W(x)$.*

Proof. By definition, $S_W(x)$ is coefficient-wise bounded above by $T_W(x)$, which implies $\alpha_S \geq \alpha_T$, and $S_W(x) \leq T_W(x)$ for any $x > 0$. Moreover, since $\mathcal{T}_{\mathcal{W}}$ contains all weighted rooted trees with weight ℓ while $L \notin \mathcal{S}_{\mathcal{W}}$, the coefficient of x^l in S_W is strictly less than the coefficient of that in T_W. Meanwhile, Lemma 4.3 and Lemma 4.2 imply $S_W(\alpha_S) = T_W(\alpha_T)$. Therefore, $\alpha_S \neq \alpha_T$, so $\alpha_S > \alpha_T$. □

A direct consequence of the theorem is the following result analogous to Schwenk's main result in [32].

4.5 Theorem. *For any given weighted rooted tree L, almost every weighted rooted tree has L as a limb.*

Proof. By Theorem 4.4, $S_W(x)$ converges on a larger disk than $T_W(x)$. In other words, the coefficients of $T_W(x)$ have a larger order of growth that those of $S_W(x)$. Since $S_W(x)$ is the generated series of weighted rooted trees without L as a limb, we can conclude that for any rooted weighted tree L, almost every weighted rooted tree has L as a limb. □

Therefore, we have successfully extended Schwenk's results to weighted rooted trees.

4.2 The Dissimilarity Theorem

The dissimilarity theorem is an important result by Otter [27] that can be used to relate the number of rooted trees and the number of trees. In this section, we provide a summary of the dissimilarity theorem, preparing for our discussion about the relationship between the number of weighted rooted trees and the number of weighted unrooted trees in the next section.

Given any tree T, we consider $\mathrm{Aut}(T)$, the group of automorphisms of T. For any two edges $e_1, e_2 \in E(T)$, we say that e_1 and e_2 are *similar* if there exists an automorphism $f \in \mathrm{Aut}(T)$ such that $f(e_1) = e_2$. An *orbit* of a vertex u (an edge e) is the largest set of pairwise similar vertices (edges) in T that contains the vertex u (the edge e). We say an edge is a *symmetry edge* if its two end-vertices are a pair of similar vertices.

In his well-known paper, Otter considered the relationship between orbits of vertices and orbits of edges [27]. In particular, he proved the famous dissimilarity theorem for trees. The following is a rewording of the original theorem statement.

4.6 Theorem ([27]). *Suppose T is a tree with p orbits for vertices, q orbits for edges, and s symmetry edges. Then $p - q + s = 1$.*

Moreover, the following simple result tells us any tree has at most one symmetry edge.

4.7 Lemma. *Let T be a tree, then T has either zero or one symmetry edge.*

Proof. For any tree T, either T has no symmetry edge, or it has at least one symmetry edge. In the first case, we are done, so we only consider the latter.

Suppose T has at least two symmetry edges $e_1 = \{u_1, v_1\}$ and $e_2 = \{u_2, v_2\}$. Then by definition $T\backslash u_1 = T\backslash v_1$ and $T\backslash u_2 = T\backslash v_2$. In particular, the component in $T\backslash u_1$ containing v_1 and the component in $T\backslash v_1$ containing u_1 are isomorphic. Moreover, observe that each vertex of T is in exactly one of these components, and these two components form exactly $T\backslash e_1$. In other words, $T\backslash e_1$ consists of exactly two isomorphic components.

By the same logic, $T\backslash e_2$ also consists of exactly two isomorphic components, C_1 and C_2. Without loss of generality, assume $e_1 \in E(C_1)$. We can obtain $T\backslash e_1$ by deleting e_1 from C_1 and add the edge e_2 to $(C_1\backslash e_1) \cup C_2$. However, one of the components of $(C_1\backslash e_1) \cup C_2$ must be a proper subtree of C_1, which has fewer vertices than C_1 does. Recall C_1 and C_2 are isomorphic and therefore have the same number of vertices, then a proper subtree of C_1 has less than $|V(T)|/2$ vertices. This contradicts the fact that $T\backslash e_1$ consists of exactly two isomorphic components. Thus, it is impossible for T to have two or more symmetry edges. □

Therefore, by Theorem 4.6, the difference between the number of orbits of vertices and the number of orbits of edges in any tree is either 0 or 1. Let

$$t(x) = \sum_{i=0}^{\infty} t_i x^i$$

be the generating function for all trees, and

$$T(x) = \sum_{i=0}^{\infty} T_i x^i$$

be the generating function for all rooted trees. Using Theorem 4.6, a proof in Harary's book [16] showed that

$$t(x) = T(x) - \frac{1}{2}[T^2(x) - T(x^2)].$$

We provide a version of the full proof here, since similar ideas will be discussed for weighted trees later.

4.8 Theorem ([16])**.** *Let $T(x) = \sum_{i=0}^{\infty} T_i x^i$ be the generating function for all trees, and $T^{\bullet}(x) \sum_{i=0}^{\infty} T_i^{\bullet} x^i$ be the generating function for all rooted trees, then*

$$T(x) = T^{\bullet}(x) - \frac{1}{2}[(T^{\bullet}(x))^2 - T^{\bullet}(x^2)].$$

Proof. This proof is based on the proof of Theorem 15.11 in Harary's book [16].

Use $\mathcal{T}$ to denote the set of all trees, $\mathcal{T}^{\bullet}$ to denote the set of all rooted trees, and $\mathcal{T}_n$ to denote the set of all tree with n vertices. For any tree $T \in \mathcal{T}_n$, suppose T has p orbits for vertices, q orbits for edges, and s symmetry edges.

Theorem 4.6 gives $1 = p - q + s$. Summing both sides of this equation over all trees over n vertices, we get

$$T_n = \sum_{T \in \mathcal{T}_n} p - \sum_{T \in \mathcal{T}_n} (q - s).$$

If we were to convert the unrooted tree T into a rooted tree, then we need to pick a root out of the n vertices of T. There are p distinct choices up to isomorphism. Therefore, if we were to sum the number of orbits of all trees over n vertices, then we get

$$\sum_{T \in \mathcal{T}} p = T_n^{\bullet},$$

the number of rooted trees over n vertices.

Similarly, we could consider $\sum_{T \in \mathcal{T}_n} (q - s)$ as the number of trees over n vertices rooted at an edge that is not its symmetry edge. In particular, suppose we pick $e \in E(T)$ that is not a symmetry edge of T. Then $T \backslash e$ can be considered as two non-isomorphic rooted trees. In other words, each term in this sum corresponds to an unordered pair of distinct rooted trees with a total of n vertices.

Let $\mathbf{SET}_2(\mathcal{T})$ be the set of all subsets of size 2 of $\mathcal{T}$. Based on the discussion above, we get the following equation.

$$|\mathcal{T}| = |\mathcal{T}^{\bullet}| - |\mathbf{SET}_2(\mathcal{T})|. \tag{4.2}$$

Define $D(\mathcal{T} \times \mathcal{T}) := \{(T, T) | T \in \mathcal{T}\}$, then

$$2|\mathbf{SET}_2(\mathcal{T})| = |(\mathcal{T} \times \mathcal{T})| - |D(\mathcal{T} \times \mathcal{T})|.$$

Observe that the generating function for $D(\mathcal{T} \times \mathcal{T})$ is $T^2(x)$. As a result, we can see that the generating function of $\mathbf{SET}_2(\mathcal{T})$ is

$$\frac{1}{2}((T^\bullet(x))^2 - T^\bullet(x^2)).$$

Using this and Equation 4.2, we get

$$T(x) = T^\bullet(x) - \frac{1}{2}[(T^\bullet(x))^2 - T^\bullet(x^2)],$$

as desired. □

In the next section, we use the ideas in the proof above to discuss the relationship between weighted rooted trees and weighted unrooted tress.

4.3 Limb Replacement in Weighted Trees

Using the underlying relationships between corresponding rooted and unrooted structures, we extend the discussion from the previous section to weighted trees that are unrooted. Similar to weighted rooted trees, a *weighted tree* is defined as a tree where each vertex is assigned a positive integer weight, but with no distinguished root vertex. The following result relates the generating functions of weighted trees and weighted rooted trees.

4.9 Theorem. *Let $\mathcal{W}$ be the set of all weighted trees, and $W(x)$ be the generating function of $\mathcal{W}$. Let $\mathcal{T}_{\mathcal{W}}$ be the set of all weighted rooted trees, and $T_W(x)$ be the generating function of $\mathcal{T}_{\mathcal{W}}$. Then*

$$W(x) = T_W(x) - \frac{1}{2}((T_W(x))^2 - T_W(x^2)).$$

Proof. Let $\mathcal{T}_{\mathcal{W}}$ be the set of weighted rooted trees. Let $\mathbf{SET}_2(\mathcal{T}_{\mathcal{W}})$ denote the set of all subsets of size 2 of $\mathcal{T}_{\mathcal{W}}$. Define $D(\mathcal{T}_{\mathcal{W}} \times \mathcal{T}_{\mathcal{W}}) := \{(T,T) | T \in \mathcal{T}_{\mathcal{W}}\}$, then

$$2|\mathbf{SET}_2(\mathcal{T}_{\mathcal{W}})| = |(\mathcal{T}_{\mathcal{W}} \times \mathcal{T}_{\mathcal{W}})| - |D(\mathcal{T}_{\mathcal{W}} \times \mathcal{T}_{\mathcal{W}})|.$$

Observe that the generating function of $D(\mathcal{T}_{\mathcal{W}} \times \mathcal{T}_{\mathcal{W}})$ is $T_W(x^2)$. Consequently, the generating function for $\mathbf{SET}_2(\mathcal{T}_{\mathcal{W}})$ is

$$\frac{1}{2}((T_W(x))^2 - T_W(x^2)).$$

Meanwhile, observe that the dissimilarity theorem for trees still holds for weighted trees as we simply ignore the weights for the constructions of the dissimilarity theorem. Specifically, the dissimilarity theorem says that

$$|\mathcal{W}| = |\mathcal{T}_{\mathcal{W}}| - |\mathbf{SET}_2(\mathcal{T}_{\mathcal{W}})|.$$

Based on the combinatorial equivalence above, we get

$$W(x) = T_W(x) - \frac{1}{2}((T_W(x))^2 - T_W(x^2)),$$

as desired. □

There is an equation relating the generating functions of weighted trees without a given limb and weighted rooted trees without a given limb. However, the proof of the previous theorem does not directly apply.

Lu [24] proved this analogous equation for the unweighted versions of trees without a given limb. Below is a rewording of his result and its proof.

4.10 Lemma ([24])**.** *Suppose L is an ℓ-vertex rooted tree. Let $\mathcal{R}$ be the set of rooted trees without L as a limb. Let $\mathcal{S}$ be the set of unrooted trees without L as a limb. Use $R(x)$ and $S(x)$ to denote the generating functions of $\mathcal{R}$ and $\mathcal{S}$, respectively. Then $R(x)$ and $S(x)$ satisfy the following equation.*

$$S(x) = R(x) + \frac{1}{2}((R(x))^2 - R(x^2)).$$

Proof. Let $\mathcal{R}_1$ be the set of unrooted trees with L as a limb, such that each of them has a vertex v and L is not a limb of the rooted tree obtained by setting v as the root of this tree. Let $R_1(x)$ be the generating function of $\mathcal{R}_1$.

Note that the trees in $\mathcal{R}_1$ could have multiple occurrences of L as a limb. However, these occurrences must be rooted at the same vertex, and no two of them are disjoint, for otherwise the definition of $\mathcal{R}_1$ is violated. Therefore, the vertex orbit containing the root of L is T has size 1.

For any unrooted tree $T \in \mathcal{S}$, use p, q, s to denote the number of vertex orbits, the number of edge orbits, and the number of symmetry edges in T, respectively. By Otter's formula [27], we get $p - q + s = 1$. Summing this over all trees over n vertices in S, we get

$$\sum_{\substack{T' \in \mathcal{S} \\ |V(T')|=n}} p - \sum_{\substack{T' \in \mathcal{S} \\ |V(T')|=n}} (q - s) = \sum_{\substack{T' \in \mathcal{S} \\ |V(T')|=n}} 1 = \langle x^n, S(x) \rangle.$$

(Recall that we use $\langle x^n, S(x)\rangle$ to denote the coefficient of x^n in $S(x)$.)

Similarly, for a unrooted tree $T' \in \mathcal{R}_1$, use p', q', s' to denote the number of vertex orbits, the number of edge orbits, and the number of symmetry edges in T', respectively. Otter's formula gives $(p'-1)-(q'-s')=0$. Summing this over all trees over n vertices in $\mathcal{R}_1$, we get

$$\sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} (p'-1) - \sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} (q'-s') = 0.$$

Observe that for a unrooted tree $T' \in \mathcal{R}_1$, we can consider $p'-1$ as the number of ways of picking a vertex in a specific vertex orbit in T' to create a rooted version of T', such that the picked vertex is not the root of an occurrence of L in T'. Let x be the number of vertex orbits in T', such that the vertices in these orbits can be chosen as a root of T' to get a rooted tree without L as a limb, and let x' be an integer such that $p'-1 = x + x'$. Since each rooted tree without L as a limb corresponds to a unrooted tree in $\mathcal{R}_1$ or a unrooted tree without L as a limb, we get

$$\langle x^n, R(x)\rangle = \sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} x + \sum_{\substack{T'\in\mathcal{S}\\|V(T')|=n}} p.$$

Meanwhile, for a unrooted tree $T' \in \mathcal{R}_1$, let y be the number of edge orbits in T' that do not contain the symmetry edge, such that if an edge-rooted tree is created by setting e as the root edge of T', the resulting edge-rooted tree does not have L as a limb. Let y' be an integer such that $q'-s' = y + y'$.

Recall that $p'-1 = x+x'$, so x' counts the number of vertex orbits that do not contain the root of occurrences of L in T', yet picking a root vertex from any of these vertex orbits would give a rooted tree with L as a limb. Meanwhile, since $q'-s' = y+y'$, we see that y' counts the number of edge orbits that contain edges that are not symmetry edges, yet picking a root edge from any of these edge orbits would give an edge-rooted tree with L as a limb. Suppose v is in an orbit counted by x', then v is not the root of any occurrences of L. Moreover, since T' is a tree, there exists a unique path between v and the root r of any occurrences of L in T. This path does not use any vertices except for r in at least one occurrence of L or edges in at least one occurrence of L, since L is a limb in the rooted tree created by setting v as the root vertex. Let e be the edge incident to v in this path. Since $T' \in \mathcal{R}_1$, it cannot contain two disjoint occurrences of L as limbs, so v is not in the same orbit as the other end-vertex of e'. Then e is not a symmetry edge, and therefore it is an edge in an orbit counted by y'. For each such vertex v, we have a unique edge e corresponding to it. Therefore, $y' \geq x'$.

On the other hand, if we pick an edge e from an orbit counted by y', then both of its end vertices v_1 and v_2 must be counted by x'. Note that there is a unique path from each of v_1 and v_2 to the the root r of any occurrences of L in T, and one of these two paths contains e. Without loss of generality, suppose v_1 is further away to r than v_2, then the edge orbit of each such e corresponds to the vertex orbit of such a v_1. So we have $x' \geq y'$. Therefore, $x = y$.

Consequently, we get

$$\begin{aligned}\langle x^n, S(x)\rangle &= \sum_{\substack{T\in\mathcal{S}\\|V(T)|=n}} p - \sum_{\substack{T\in\mathcal{S}\\|V(T)|=n}} (q-s)\\ &= \langle x^n, R(x)\rangle - \sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} x - \sum_{\substack{T\in\mathcal{S}\\|V(T)|=n}} (q-s)\\ &= \langle x^n, R(x)\rangle - \left(\sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} y + \sum_{\substack{T\in\mathcal{S}\\|V(T)|=n}} (q-s)\right).\end{aligned}$$

Observe that

$$\sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} y + \sum_{\substack{T\in\mathcal{S}\\|V(T)|=n}} (q-s)$$

counts the number of weighted edge-rooted trees over n vertices in S obtained by joining two distinct weighted rooted trees on the two ends of the root edge. So

$$\sum_{\substack{T'\in\mathcal{R}_1\\|V(T')|=n}} y + \sum_{\substack{T\in\mathcal{S}\\|V(T)|=n}} (q-s) = \frac{1}{2}\langle x^n, (R(x))^2 - R(x^2)\rangle.$$

Thus the desired equation holds. $\square$

The proof for the corresponding result for weighted trees and weighted rooted trees is identical since the proof only involves the structure of trees without needing to consider their vertex weights.

Let $\mathcal{S}_U$ be the set of all weighted trees without a given rooted tree L as a limb, let $S_U(x)$ be the generating function of $\mathcal{S}_U$, and let S_W be the generating function for weighted rooted trees without L as a limb, then

$$S_U(x) = S_W(x) - \frac{1}{2}((S_W(x))^2 - S_W(x^2)).$$

Suppose the radius of convergence of a power series $A(x)$ is less than 1. Then the radius of convergence of $A(x^2)$ is less than 1 but strictly greater than that of $A(x)$, and the radius of convergence of $(A(x))^2$ is the same as that of $A(x)$. Therefore, the radius of convergence of $S_W(x) - \frac{1}{2}((S_W(x))^2 - S_W(x^2))$ is the same as that of $S_W(x)$. Consequently, the radius of convergence of $T_W(x)$ is α_T and the radius of convergence of $S_U(x)$ is α_S. Theorem 4.4 proved $\alpha_S > \alpha_T$. Similarly to Corollary 4.5, we get the following result.

4.11 Theorem. *For any given weighted rooted tree L, almost every weighted tree has L as a limb.*

Therefore, we have extended one of Schwenk's main results to weighted trees.

4.4 Cospectrality of Weighted Graphs

Recall that, in Chapter 1, we defined the weighted characteristic polynomial for a weighted graph W over n vertices in the following way: Let $M(x)$ be an $n \times n$ diagonal matrix, such that its rows and columns are each indexed by the vertices of W, and the ii-entry of $M(x)$ is $x^{w(i)}$, where $w(i)$ is the weight of the vertex i and x is an indeterminate. Let $A(W)$ be the adjacency matrix of W. The *weighted characteristic polynomial* $\phi^*(W, x)$ of W is

$$\phi^*(W, x) = \det(M(x) - A(W)).$$

When there is no ambiguity, we drop the indeterminate variable and use

$$\phi^*(W) = \det(M - A(W))$$

to denote the weighted characteristic polynomial of W.

This definition of weighted characteristic polynomial is consistent with our previous definitions. In particular, we choose to put the weight of each vertex to be the power of their corresponding term, because that was how we enumerated the weighted trees and weighted rooted trees. For any weighted graph G, the term of the highest power of the weighted characteristic polynomial is exactly x to the weight of G. This is not necessarily the only possible definition for the weighted characteristic polynomial, and we choose it here because it works well with the results which we apply this definition to. It is worth noting that some of the following results could still hold with some other sensible definition of the weighted characteristic polynomial.

If two weighted graphs have the same weighted characteristic polynomial, we say that they are *weighted cospectral*. Similarly, two vertices u and v in a weighted graph G are *weighted cospectral* if $G\backslash u$ and $G\backslash v$ are weighted cospectral graphs. For the rest of this section, we prove that almost every weighted rooted tree is weighted cospectral with another weighted rooted tree.

We start by proving the weighted characteristic polynomial satisfies identities that are analogous to the union formula, the edge-deletion recurrence, the derivative formula, and the 1-sum formula for the characteristic polynomial, discussed in Section 2.2 and Section 2.3.

Below, we consider the union formula for the weighted characteristic polynomial, which is fairly straight-forward.

4.12 Lemma. *Suppose W_1 and W_2 are weighted graphs. Then*

$$\phi^*(W_1 \cup W_2) = \phi^*(W_1)\phi^*(W_2).$$

Proof. For square matrices A and B, note that $\det \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} = \det(A)\det(B)$. Therefore,

$$\begin{aligned} \phi^*(W_1 \cup W_2) &= \det(M(x) - A(W_1 \cup W_2)) \\ &= \det \begin{bmatrix} M_1(x) - A(W_1) & 0 \\ 0 & M_2(x) - A(W_2) \end{bmatrix} \\ &= \phi^*(W_1)\phi^*(W_2), \end{aligned}$$

where $M_1(x)$ and $M_2(x)$ are the corresponding diagonal matrices for W_1 and W_2 in the definition of the weighted characteristic polynomial. $\square$

It is a little more complex to prove the edge-deletion recurrence for the weighted characteristic polynomial. To do so, we need to use the following two intermediate results. The first result is a theorem about the determinant of the sum of two matrices. For more information about this theorem, please refer to Godsil [10, Theorem 2.1.1].

4.13 Theorem ([10])**.** *Let X and Y be any $n \times n$ matrices. Then $\det(X+Y)$ is equal to the sum of the determinants of the 2^n matrices obtained by replacing each subset of the columns of X by the corresponding subset of the columns of Y.*

Meanwhile, the following lemma discusses a specific type of block matrix and shows its determinant is zero.

4.14 Lemma. *Let M be a $n \times n$ block matrix of the form*

$$\begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix},$$

where 0 represents all-zero matrices of appropriate dimensions, C is a $\ell \times m$ matrix with $\ell \neq m$, and D is a $(n-\ell) \times (n-m)$ matrix. Then $\det(M) = 0$.

Proof. Without loss of generality, we may assume that $\ell > m$. Suppose $D = [D_1|D_2]$ where D_1 is a $(n-\ell) \times (\ell - m)$ matrix and D_2 is a $(n-\ell) \times (n-\ell)$ matrix. Then we can view M as a block lower triangular matrix

$$\begin{bmatrix} C' & 0 \\ E & D_2 \end{bmatrix},$$

where $C' = [C|0]$ is a $\ell \times \ell$ matrix, $E = [0|D_1]$ is a $(n-\ell) \times \ell$ matrix, with 0 again representing all-zero matrices of appropriate dimensions. Clearly, $\det(C') = 0$. Then $\det(M) = \det(C')\det(D_2) = 0$. □

Now we have all the necessary tools to prove the following result for the weighted characteristic polynomial, analogous to the edge-deletion recurrence for the characteristic polynomial.

4.15 Lemma. *Let W be a weighted graph. Suppose $e = \{u, v\}$ is a cut-edge in W. Then*

$$\phi^*(W) = \phi^*(W \backslash e) - \phi^*(W \backslash \{u, v\}),$$

where $W \backslash e$ denotes the weighted graph obtained by deleting the edge e from the weighted graph W, but not the end vertices of e, while $W \backslash \{u, v\}$ denotes the weighted graph induced by $V(W) \backslash \{u, v\}$.

Proof. Suppose W has n vertices. Let E_{uv} be the $n \times n$ matrix, all of whose entries are zeros except that the uv-entry and vu-entry are 1's. Recall that e is a cut-edge, so deleting it would separate the graph into two components. We may assume the $n \times n$ matrices in our discussion are arranged in a way where the first ℓ rows and columns correspond to the component C_1 with u in it, with the ℓ-th row and column corresponding u, and the $(\ell + 1)$-st row and column corresponding to v. The other component is C_2. Observe that

$$\phi^*(W) = \det(M - A(W)) = \det(M - A + E_{uv} - E_{uv}).$$

Let

$$X = M - A(W) + E_{uv} = \begin{bmatrix} M_1 - A(C_1\backslash u) & \cdots & 0 & 0 \\ \vdots & x^{w(u)} & 0 & 0 \\ 0 & 0 & x^{w(v)} & \vdots \\ 0 & 0 & \cdots & M_2 - A(C_2\backslash v) \end{bmatrix},$$

where the matrices M_1 and M_2 are diagonal matrices of appropriate dimensions, whose diagonal entries are $x^{w(i)}$, such that i is the vertex corresponding to the respective row and column. Notice that each entry represented by dots above and to the left of the $x^{w(u)}$ term or the dots below and to the right of the $x^{w(v)}$ term could be either 0 or -1, depending on their adjacency relationship with the vertex u of v, respectively.

Let $Y = -E_{uv}$. Then we can apply Theorem 4.13 to compute $\det(M - A(W))$, or $\det(X + Y)$. Since any matrix with an all zero column has determinant 0, when using Theorem 4.13 to replace columns of $M - A(W) + E_{uv}$, only three cases need to be considered:

1. Do not replace column u or column v at all.
2. Replace both column u and column v.
3. Replace exactly one of column u and column v.

In the first case, the determinant of the resulting matrix is $\det(M - A(W) + E_{uv})$, which is $\phi^*(W\backslash e)$.

In the second case, by Laplace's formula (cofactor expansion) along the ℓ-th and $(\ell+1)$-st columns we see that the determinant of the resulting matrix is $-\phi^*(W\backslash\{u, v\})$.

Now we consider the last case. Assume first that the ℓ-th column in $M - A(W) + E_{uv}$ is replaced by the ℓ-th column of $-E_{uv}$. We call the resulting matrix is B, which is the following.

$$B = \begin{bmatrix} M_1 - A(C_1\backslash u) & 0 & 0 & 0 \\ \vdots & 0 & 0 & 0 \\ 0 & -1 & x^{w(v)} & \vdots \\ 0 & 0 & \cdots & M_2 - A(C_2\backslash v). \end{bmatrix}$$

Then we consider the determinant of B. Let B' be the matrix obtained from B by deleting its $(\ell + 1)$-st row and ℓ-th column, so

$$B' = \begin{bmatrix} M_1 - A(C_1 \backslash u) & 0 & 0 \\ \vdots & 0 & 0 \\ 0 & \cdots & M_2 - A(C_2 \backslash v). \end{bmatrix}$$

By cofactor expansion along the ℓ-th column of B, we get $\det(B) = \pm \det(B')$. Note that the entries in the ℓ-th column of B' come from the $(\ell+1)$-st column of B. In particular, the first ℓ entries in this column are zeros, and all other entries in this column can be 0 or -1. Therefore B' is a block matrix of the form

$$\begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix}$$

where C is $\ell \times (\ell - 1)$ and D is $(n - \ell - 1) \times (n - \ell)$. By Lemma 4.14, $\det(B') = 0$. An analogous argument applies when replacing only the $(\ell + 1)$-st column. Therefore, the last case simply gives a determinant of 0.

Summing the determinants from all three cases, we get

$$\phi^*(W) = \phi^*(W \backslash e) - \phi^*(W \backslash \{u, v\}).$$

□

Just like the proof for the edge-deletion recurrence for the weighted characteristic polynomial, our proof for the derivative formula for the weighted characteristic polynomial is also more complex than the proof for the corresponding identity for the characteristic polynomial presented in the book by Godsil [10, Theorem 2.1.5]. The addition of vertex weights requires more careful manipulation of the terms when expanding the weighted characteristic polynomial as the determinant of a matrix, especially when taking derivatives of the diagonal entries.

4.16 Lemma. *Let W be a weighted graph with weight function w, such that W has at least one vertex, then*

$$\frac{d}{dx}\phi^*(W) = \sum_{i \in V(W)} w(i) x^{w(i)-1} \phi^*(W \backslash i).$$

Proof. Let S_n be the set of all permutations of $\{1, 2, \ldots, n\}$. Recall that for a matrix M, if m_{ij} is its ij-entry, then its determinant can be computed by the Leibniz formula:

$$\det(M) = \sum_{\sigma \in S_n} \left(\operatorname{sgn}(\sigma) \prod_{i=1}^{n} m_{i,\sigma(i)} \right),$$

where $\mathrm{sgn}(\sigma)$ is the sign of the permutation. Use $c_{i,j}$ to denote the ij-entry of $M - A$. Then we get

$$\begin{aligned}
\frac{d}{dx}\phi^*(W) &= \frac{d}{dx}\sum_{\sigma\in S_n}\left(\mathrm{sgn}(\sigma)\prod_{i=1}^{n} c_{i,\sigma(i)}\right) \\
&= \sum_{\sigma\in S_n}\left(\mathrm{sgn}(\sigma)\frac{d}{dx}\prod_{i=1}^{n} c_{i,\sigma(i)}\right) \\
&= \sum_{\sigma\in S_n}\left(\mathrm{sgn}(\sigma)\sum_{j\in\mathrm{fix}(\sigma)} w(j)x^{w(j)-1}\left(\prod_{\substack{i=1\\ i\neq j}}^{n} c_{i,\sigma(i)}\right)\right),
\end{aligned}$$

by the chain rule, where $\mathrm{fix}(\sigma)$ is the set of fixed points of σ. We can switch the order of the summations, but note the permutation must skip the vertex j, so it would be a permutation of $\{1, 2, \ldots, j-1, j+1, \ldots, n\}$, although we fix the values of the sign func.

$$\begin{aligned}
&= \sum_{j\in V(W)}\sum_{\sigma\in S_{n-1}}\left(\mathrm{sgn}(\sigma)w(j)x^{w(j)-1}\left(\prod_{i\neq j}^{n} c_{i,\sigma(i)}\right)\right) \\
&= \sum_{j\in V(W)} w(j)x^{w(j)-1}\phi^*(W\backslash j)
\end{aligned}$$

□

Last but not least, we show that the 1-sum formula holds for the weighted characteristic polynomial as well.

4.17 Lemma. *Suppose W_1 and W_2 are weighted graphs with weight functions w_1 and w_2, such that their underlying unweighted graphs share exactly one vertex, v. Observe that it is possible that $w_1(v) \neq w_2(v)$. Let W be the weighted graph on n vertices such that*

(a) the underlying unweighted graph of W is the 1-sum of the underlying unweighted graphs of W_1 and W_2; and

(b) the weight function w for W satisfies $w(x) = w_1(x)$ for $x \in V(W_1)\backslash V(W_2)$ and $w(x) = w_2(x)$ for $x \in V(W_1)\backslash V(W_2)$, and the value of $w(v)$ is a positive integer.

Then

$$\phi^*(W) = \phi^*(W_1\backslash v)\phi^*(W_2) + \phi^*(W_1)\phi^*(W_2\backslash v) \\ + (x^{w(v)} - x^{w_1(v)} - x^{w_2(v)})\phi^*(W_1\backslash v)\phi^*(W_2\backslash v).$$

Proof. Let $A(W)$ be the adjacency matrix of W. We may assume that the $n \times n$ matrix $M - A(W)$ is organized so that its first ℓ rows/columns correspond to W_1, with the ℓ-th row/column corresponding v, and the remaining rows/columns correspond to vertices in $W_2\backslash v$. Use a_{ij} to denote the ij-entry of $M - A(W)$, and $M_{i,j}$ to denote the ij-cofactor of $M - A(W)$.

We first consider the right hand side of the equation in the lemma statement. Observe $\phi^*(W_1\backslash v)\phi^*(W_2)$ is the product of the determinant of two matrices, namely $M_1 - A(W_1\backslash v)$ and $M_2 - A(W_2)$, where M_1 and M_2 are diagonal matrices of appropriate dimensions, whose diagonal entries are $x^{w(i)}$, such that i is the vertex corresponding to the respective row and column. The product $\phi^*(W_1\backslash v)\phi^*(W_2)$ can also be viewed as the determinant of an $n \times n$ matrix B defined as

$$B := \begin{bmatrix} M_1 - A(W_1\backslash v) & 0 \\ 0 & M_2 - A(W_2) \end{bmatrix},$$

In other words, B is much like the matrix $M - A(W)$, with the only differences being that, in B, the entries above and to the left of the $\ell\ell$-entry are all zeros, and the $\ell\ell$-entry of B is $x^{w_2(v)}$, while the $\ell\ell$-entry of $M - A(W)$ is $x^{w(v)}$. Therefore, if we compute $\phi^*(W_1\backslash v)\phi^*(W_2)$ by applying Laplace's formula to the ℓ-th column of B, the result would be

$$\left(\sum_{j>\ell}(-1)^{\ell+j}a_{j\ell}M_{j,\ell}\right) + x^{w_2(v)}M_{\ell,\ell}.$$

Note the latter term of the sum is simply $x^{w_2(v)}\phi^*(W_1\backslash v)\phi^*(W_2\backslash v)$.

Similarly, $\phi^*(W_1)\phi^*(W_2\backslash v)$ can be considered as the determinant of a corresponding $n \times n$ matrix as well. So

$$\phi^*(W_1)\phi^*(W_2\backslash v) = \left(\sum_{i<\ell}(-1)^{\ell+i}a_{i\ell}M_{i,\ell}\right) + x^{w_1(v)}\phi^*(W_1\backslash v)\phi^*(W_2\backslash v).$$

Likewise

$$\phi^*(W) = \left(\sum_{k\neq\ell}(-1)^{\ell+k}a_{k\ell}M_{k,\ell}\right) + x^{w(v)}\phi^*(W_1\backslash v)\phi^*(W_2\backslash v).$$

Therefore,

$$\begin{aligned}
&\phi^*(W_1\backslash v)\phi^*(W_2) + \phi^*(W_1)\phi^*(W_2\backslash v) \\
&\qquad = \phi^*(W) + (x^{w_1(v)} + x^{w_2(v)})\phi^*(W_1\backslash v)\phi^*(W_2\backslash v) - x^{w(v)}\phi^*(W_1\backslash v)\phi^*(W_2\backslash v).
\end{aligned}$$

□

Just as Schwenk did, we could use the 1-sum formula for the weighted rooted trees to perform the limb replacement action. With the limb replacement results we proved in previous sections, we show that almost every weighted tree has a weighted cospectral mate.

4.18 Theorem. *Almost every weighted tree is weighted cospectral with another weighted tree.*

Proof. Consider the tree L as shown in Figure 2.2. Let L_1 and L_2 be the weighted rooted trees obtained by assigning weight 1 to all vertices in L and assigning a and b as the root, respectively. Observe that $\phi^*(L_1) = \phi^*(L_2)$, and $\phi^*(L_1\backslash a) = \phi^*(L_2\backslash b)$.

If L_1 is a limb of some weighted rooted tree W, then it indicates the weight of a in W is 1 as well. We could replace L_1 in W by L_2, and Lemma 4.17 implies the resulting weighted rooted tree is weighted cospectral to W. By Corollary 4.5, almost every weighted rooted tree has L_1 as a limb. Since the rooting of the weighted tree does not affect its weighted characteristic polynomial, we conclude that almost every weighted tree is weighted cospectral with another weighted tree. □

Therefore, we have extended Schwenk's result to weighted rooted trees through analyzing the corresponding generating series and defining the weighted characteristic polynomial.

Chapter 5

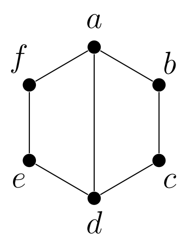
Constructing Graphs with Many Cospectral Vertices and Graphs with Many Comatching Vertices

In this chapter, our first topic of discussion is cospectral vertices within the same graph. In particular, we will use the various characteristic polynomial recurrences and identities to provide a step-by-step construction of trees with an arbitrarily large number of cospectral vertices that are not similar. Further, we will prove that, for any integer $k \geq 2$, there exists a graph that contains k cospectral vertices such that no two of them are pairwise similar, and almost every tree has a set of k cospectral vertices such that no two of them are pairwise similar. We also show that the same construction works for creating graphs with comatching vertices. In addition, one of the intermediate results in the main construction will be generalized to construct comatching graphs.

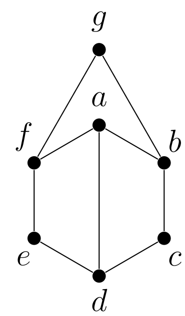
The results in this chapter are joint work with Karen Yeats and are under review [36]. In particular, Theorem 5.1, Theorem 5.2, Theorem 5.3, Corollary 5.4, Theorem 5.5, Theorem 5.6, Theorem 5.7 are joint work.

5.1 1-Vertex Extension

As defined in Chapter 1, for a graph G and a set $S \subseteq V(G)$, the 1-*vertex extension* of G with respect to S is the graph obtained by adding a vertex to G and connecting the added vertex to all vertices in S and no other vertex.



G



1-vertex extension of G with respect to $\{b, f\}$

Figure 5.1: An example of a graph G and one of its 1-vertex extensions

Figure 5.1 gives an example of a graph G and its 1-vertex extension with respect to the set $S = \{b, f\}$. In the 1-vertex extension, we added a new vertex g, and then connected it to exactly the vertices in the set S.

1-vertex extension is a practical graph operation that can be used to construct cospectral graphs. Specifically, we prove the following result, which is an important step in our main construction.

5.1 Theorem. *Let G be a graph with a set of cospectral vertices $A = \{a_1, a_2, \cdots, a_k\}$. Let S_1 and S_2 be non-empty subsets of A such that $|S_1| = |S_2|$, and each component of G contains at most one vertex in S_1 and at most one vertex in S_2. For $i = 1, 2$, let G_i be the 1-vertex extension of G with respect to S_i. Then G_1 and G_2 are cospectral.*

Proof. We prove this theorem by induction on the size of S_1 and S_2. Suppose $|S_1| = |S_2| = 1$. Without loss of generality, let v be connected to a_i in G_i, for $i = 1, 2$. Use $e_{a_i v}$ to denote the edge with a_i and v being its endpoints. Each $e_{a_i v}$ is a cut-edge and so

$$\begin{aligned}
\phi(G_1) &= \phi(G_1 \backslash e_{a_1 v}) - \phi(G_1 \backslash \{a_1, v\}) \\
&= x\phi(G) - \phi(G \backslash a_1) \\
&= \phi(G_2 \backslash e_{a_2 v}) - \phi(G \backslash a_2) \\
&= \phi(G_2).
\end{aligned}$$

Now assume the theorem statement holds for all $|S_1| = |S_2| \leq \ell - 1$, where $1 < \ell \leq k$. Without loss of generality, suppose $|S_1| = |S_2| = k$, $a_1 \in S_1$, $a_2 \in S_2$. Since each component

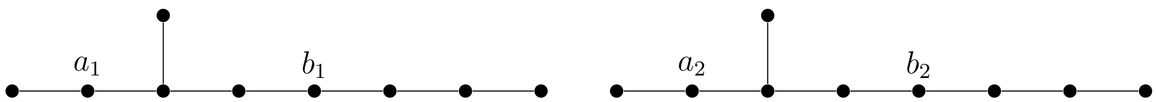


Figure 5.2: The graph F with a_1, b_1, a_2, and b_2 as cospectral vertices

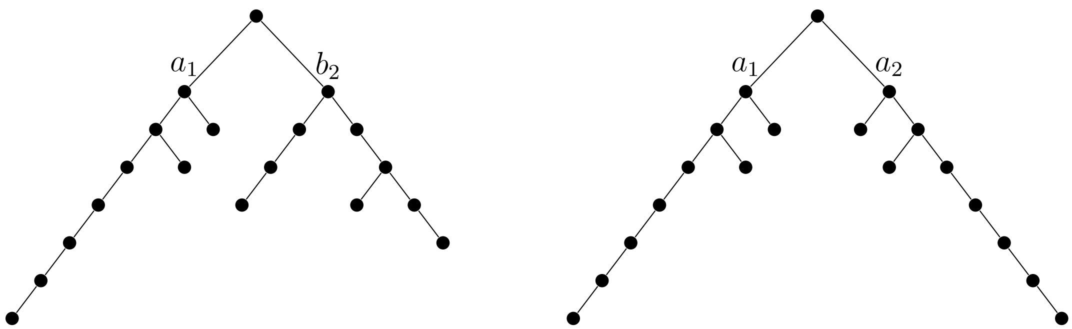


Figure 5.3: An example of F and its 1-vertex extensions

of G contains at most one vertex in A, e_{a_iv} is a cut-edge. By the induction hypothesis, $\phi(G_1\backslash e_{a_1v}) = \phi(G_2\backslash e_{a_2v})$.

Note that

$$\begin{aligned}\phi(G_1) &= \phi(G_1\backslash e_{a_1v}) - \phi(G_1\backslash\{a_1, v\}) \\ &= \phi(G_1\backslash e_{a_1v}) - \phi(G\backslash a_1) \\ &= \phi(G_2\backslash e_{a_2v}) - \phi(G\backslash a_2) \\ &= \phi(G_2).\end{aligned}$$

Hence the theorem statement is true. □

Theorem 5.1 applies to any graph with cospectral vertices in different components. Figure 5.2 gives a forest F with a_1, b_1, a_2 and b_2 being cospectral vertices, which is formed by two copies of Schwenk's tree shown in Figure 2.2. Based on this F, we construct a pair of cospectral graphs using Theorem 5.1. Each of the two graphs in Figure 5.3 is a 1-vertex extension of the graph F in Figure 5.2, where the extension is done on different but cospectral vertices.

For the rest of the chapter, we use Theorem 5.1 and 1-vertex extensions to give a construction of cospectral graphs and a construction of connected graphs with an arbitrarily large number of cospectral vertices.

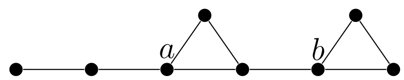


Figure 5.4: A graph with a pair of cospectral vertices a and b

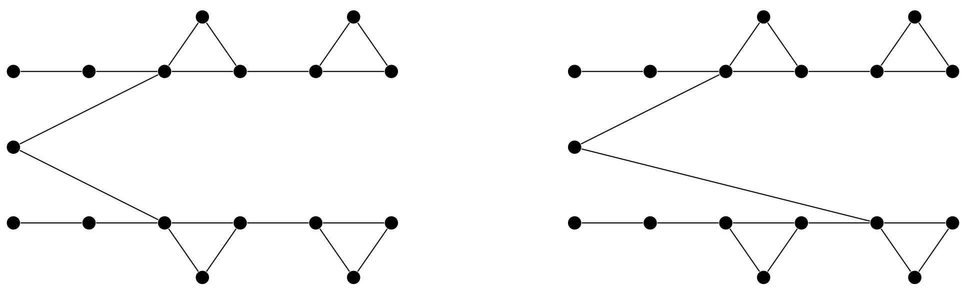


Figure 5.5: A pair of cospectral graphs constructed from the graph in Figure 5.4 using Theorem 5.1

5.2 1-Vertex Extension Construction for Cospectral Graphs

In this section, we provide another construction for cospectral graphs using 1-vertex extensions, by applying it twice in a row. Although it might not be as widely applicable as the construction in the previous section, this construction results in a graph for us to use in order to construct connected graphs with an arbitrary large number of cospectral vertices in the next section.

Suppose we have a graph F satisfying the following conditions.

- F has exactly c components.
- The components of F are pairwise cospectral.
- There exists distinct sets $S_1, S_2, \dots, S_m \subseteq V(F)$ of pairwise cospectral vertices for some integer $m \geq 1$, such that for all $1 \leq i \leq m$, each S_i contains exactly one vertex from each component of F.

Observe that such a graph F exists. For example, as shown in Figure 5.3, we could take two disjoint copies of Schwenk's tree in Figure 2.2 as F, with the two isomorphic components being C_1, C_2. If we call the pair of cospectral vertices in C_i as a_i, b_i for $i = 1, 2$. Let $S_1 = \{a_1, a_2\}$, $S_2 = \{b_1, a_2\}$, and $S_3 = \{b_1, b_2\}$. This graph satisfies the condition listed in the paragraph above with $c = 2$ and $m = 3$. Moreover, in this example, the graphs $F\backslash S_i$ are pairwise non-isomorphic. This fact will be further discussed later in this section.

In general, given a graph G and two vertices $u, v \in G$, if $G\backslash u \cong G\backslash v$, and u and v are not in the same orbit, then u and v are a pair of *pseudosimilar* vertices. Any graph G with a pair of pseudo-similar vertices can be used to construct F, where F consists of two copies of G. In this case, $c = 2$ and $m = 3$ as well. Herndon and Ellzey gave a construction for graphs with pairs of pseudo-similar vertices in 1975 [19]. Later, Godsil and Kocay proved all graphs with a pair of pseudo-similar vertices can be constructed by Herndon and Ellzey's construction [9]. Therefore, other than our example in the previous paragraph, there exists a construction for even more graphs satisfying the conditions of F, with $c = 2$ and $m = 3$. Later in this section, we show our construction can create F with greater values of c and m.

The reason why we want such a graph F is so that we could do 1-vertex extensions of F with respect to each set S_i, for $1 \leq i \leq m$. In our construction, these sets would give a total of m graphs that are 1-vertex extensions of F. By Theorem 5.1, these resulting graphs are cospectral. Therefore, the existence of such F gives a quick way to construct m cospectral graphs.

Moreover, the following theorem uses two distinct sets of such $S_i's$ to create two cospectral graph that are even larger, by applying the 1-vertex extension twice in a row.

5.2 Theorem. *Let F be a graph with c components that are pairwise cospectral. For some integer $m \geq 1$, suppose we have two distinct sets $A_1 = \{S_1^1, S_2^1, \ldots, S_m^1\}$ and $A_2 = \{S_1^2, S_2^2, \ldots, S_m^2\}$, both containing m sets of pairwise cospectral vertices from F, such that for all $1 \leq i \leq m$, each S_i^1 or S_i^2 contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$ and $j = 1, 2$, let F_i^j be the 1-vertex extension of F with respect to S_i^j, with the added vertex being v_i^j. Let H_j be the 1-vertex extension of $\bigcup_{i=1}^m F_i^j$ with respect to $v_1^j, \ldots, v_m^j$, with the added vertex being r_j. Then H_1 and H_2 are cospectral.

Proof. We prove this result by induction on m.

When $m = 1$, let e_1 be the only edge r_1 is incident to, and let e_2 be the only edge r_2 is incident to. Then v_1^1 and v_1^2 are the other end-vertices of e_1 and e_2, respectively. Figure 5.6 gives a demonstration of the resulting graphs H_1 and H_2 for the base case.

Note that by Theorem 5.1,

$$\phi(H_1\backslash e_1) = \phi(H_2\backslash e_2),$$

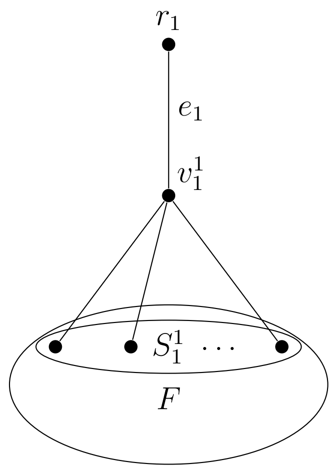


Figure 5.6: An example demonstrating H_1 and H_2 constructed during the base case in the proof of Lemma 5.2

and by construction,

$$\phi(H_1 \backslash \{r_1, v_1^1\}) = \phi(H_2 \backslash \{r_2, v_1^2\}).$$

Since e_1 and e_2 are cut-edges in their corresponding graphs, the edge-deletion recurrence for the characteristic polynomial gives $\phi(H_1) = \phi(H_2)$.

Now suppose the lemma holds when $m = n - 1$ for some $n \geq 1$. We consider the case where $m = n$. Let e_1 and e_2 be edges that connect r_1 and r_2 to v_1^1 and v_1^2, respectively. Figure 5.7 gives a demonstration of the resulting graphs H_1 and H_2 in the induction step.

Note that by the induction hypothesis and Theorem 5.1,

$$\phi(H_1 \backslash e_1) = \phi(H_2 \backslash e_2),$$

and by the construction,

$$\phi(H_1 \backslash \{r_1, v_1^1\}) = \phi(H_2 \backslash \{r_2, v_1^2\}).$$

Then once again Lemma 2.7 (b) gives $\phi(H_1) = \phi(H_2)$. □

In the lemma above, note that even though A_1 and A_2 are distinct, they are not necessarily disjoint. Let us consider the graph in Figure 5.2 as F again. We set $A_1 = \{\{a_1, b_2\}, \{a_1, a_2\}\}$ and $A_2 = \{\{a_1, b_2\}, \{b_1, b_2\}\}$. Applying the construction in Theorem 5.2, we obtain the two graphs in Figure 5.8.

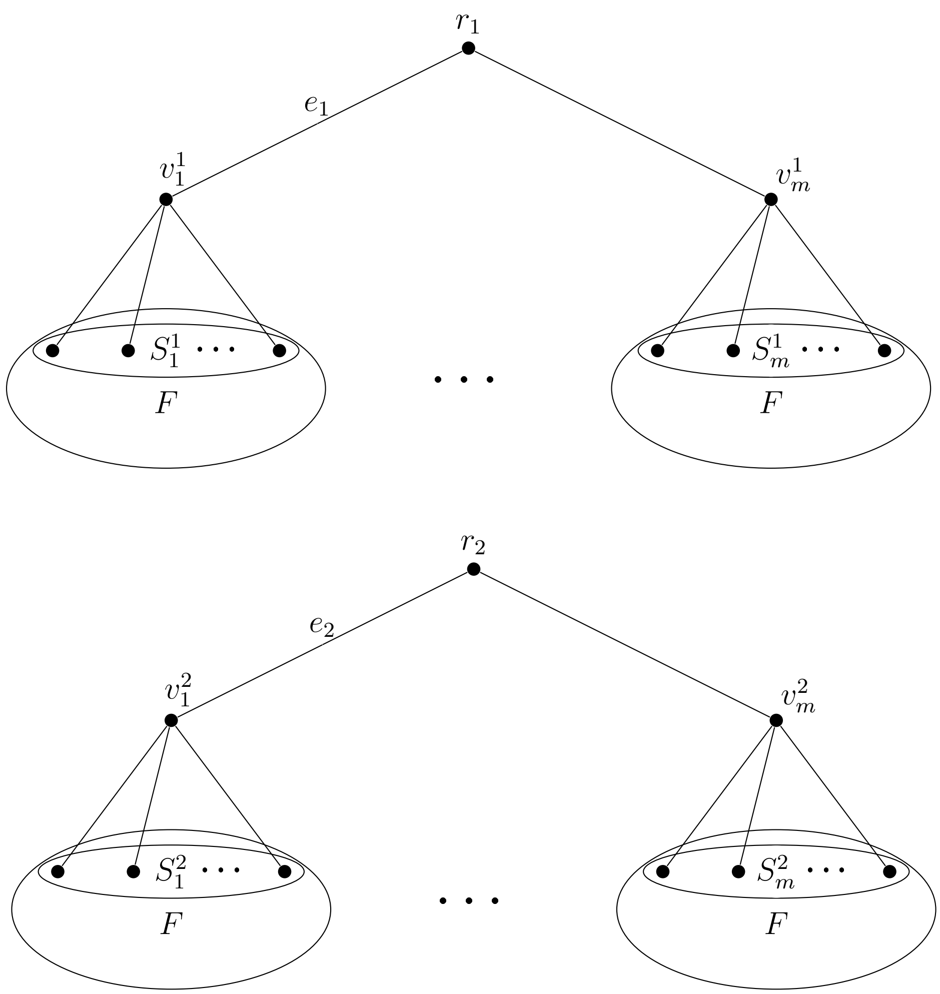


Figure 5.7: An example demonstrating H_1 and H_2 constructed during the inductive step in the proof of Lemma 5.2

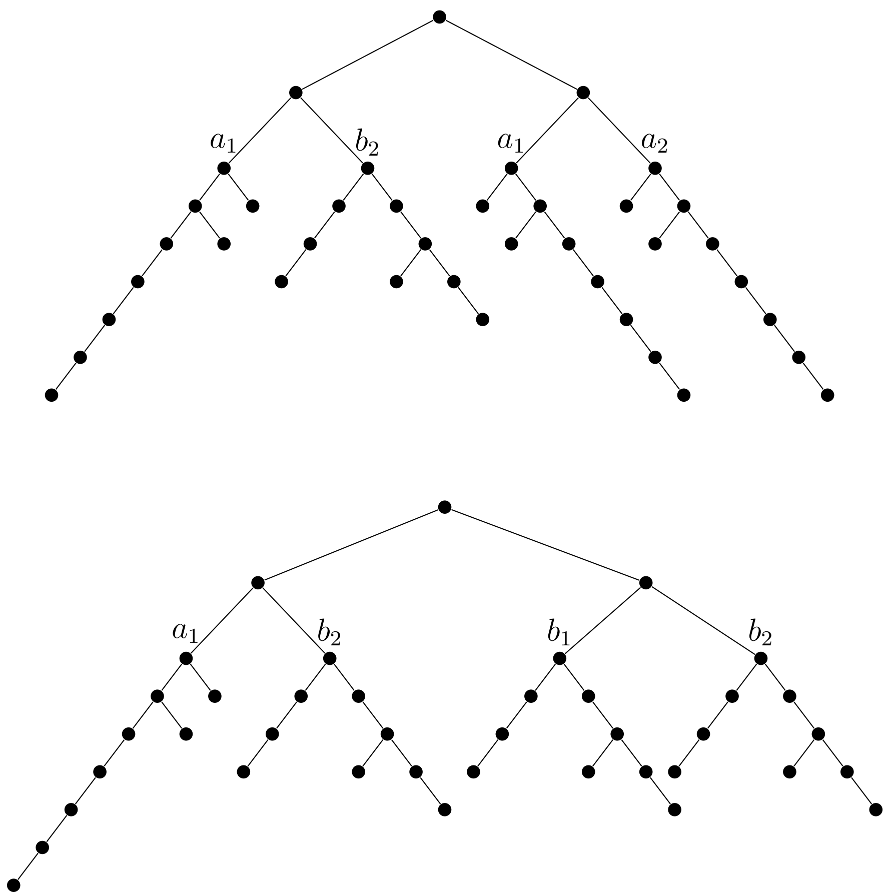


Figure 5.8: A pair of cospectral graphs constructed using Theorem 5.2

Meanwhile, if $A_1 = \{\{a_1, b_2\}\}$ and $A_2 = \{\{b_1, a_2\}\}$, then the two graphs resulting from the construction in Theorem 5.2 would be the same. Just like the previous example, the original graph L that serves as the components of F is still Schwenk's tree in Figure 2.2. It is important to recognize these components (copies of L) are indistinguishable, so the sets $A_1 = \{\{a_1, b_2\}\}$ and $A_2 = \{\{b_1, a_2\}\}$ would result in isomorphic graphs. In this example, $m = 1$ and the underlying graph F has two components, each with two cospectral vertices. In this case, our construction gives at most three cospectral graphs, using the sets $\{a_1, a_2\}$, $\{a_1, b_2\}$, and $\{b_1, b_2\}$. This is the same as the number of ways of picking two balls from a bag with two labeled balls with replacement happening each time before the picking happens. We will revisit this idea after the discussion in the next section, which is about constructing cospectral vertices.

5.3 1-Vertex Extension Construction for Cospectral Vertices

In this section, we provide a construction for connected graphs with an arbitrarily large number of pairwise cospectral vertices using Theorem 5.1 and Theorem 5.2. The proof for the construction has two steps. First, we argue that if a graph F satisfies the conditions discussed in the last section, then it can be used to construct a connected graph with an arbitrarily large number of pairwise cospectral vertices. We give an example and some ways to construct the desired F to show existence of such graphs. Second, we show that taking the 1-sum of the constructed graph and some other graph would not alter the pairwise cospectrality of the cospectral vertices in F.

To start, we show that by applying the 1-vertex extension twice in a row on a graph F with some cospectral vertices and satisfying some additional conditions, a graph with potentially more cospectral vertices can be constructed.

5.3 Theorem. *Let F be a graph with c components that are pairwise cospectral. Suppose there exists distinct sets $S_1, S_2, \dots, S_m \subseteq V(F)$ of pairwise cospectral vertices for some integer $m \geq 1$, such that for all $1 \leq i \leq m$, each S_i contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$, let F_i be the 1-vertex extension of F with respect to S_i, with the added vertex being v_i. Let G be the 1-vertex extension of $\bigcup_{i=i}^{m} F_i$ with respect to $v_1, \dots, v_m$, with the added vertex being r. Then

(a) $\bigcup_{i=1}^{m} N(v_m) \backslash r$ is a set of pairwise cospectral vertices in G; and

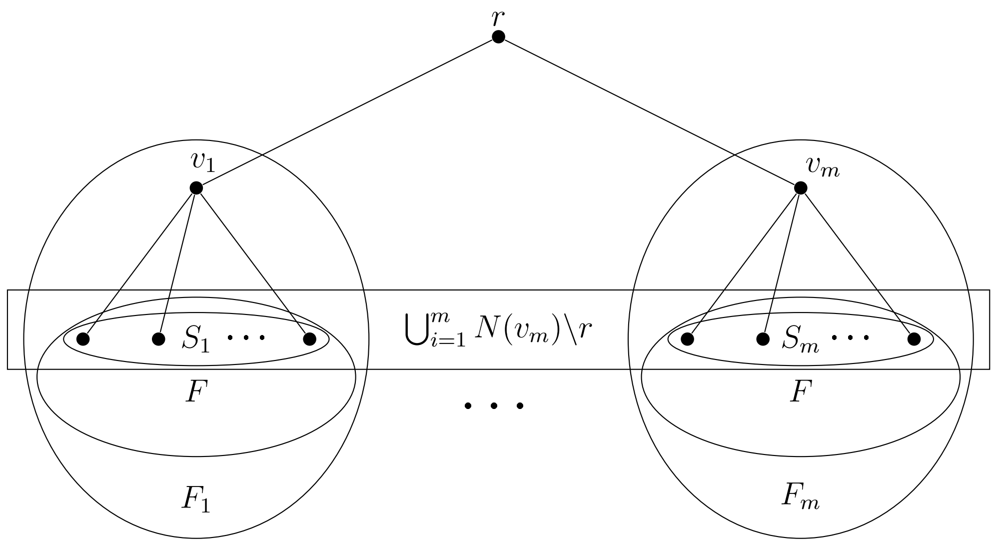


Figure 5.9: A demonstration of the graph constructed in Theorem 5.3

(b) $\bigcup_{i=1}^m N(v_m)\backslash r$ *is a set of pairwise cospectral vertices in* $G\backslash r$*.*

Proof. Let $u_1, u_2 \in \bigcup_{i=1}^m N(v_m)\backslash r$. The graph constructed using the process described in Theorem 5.3 is shown in Figure 5.9.

(a) We first show that $\phi(G\backslash u_1) = \phi(G\backslash u_2)$.

Let $1 \leq i_1, i_2 \leq m$ such that v_{i_1} is a neighbor of u_1 and v_{i_2} is a neighbor of u_2. Note it is possible for $i_1 = i_2$. Use e_1, e_2 to denote the edges between v_{i_1} and r or v_{i_2} and r, respectively. Figure 5.10 gives a visual demonstration of this, assuming $i_1 \neq i_2$.

We first compare $\phi(G\backslash\{u_1, v_{i_1}, r\})$ to $\phi(G\backslash\{u_2, v_{i_2}, r\})$. For $j = 1, 2$, observe that

$$G\backslash\{u_j, v_{i_j}, r\} = \left(\bigcup_{\substack{\ell=1 \\ \ell \neq i_j}}^{m} F_\ell \right) \cup (F_{i_j}\backslash\{v_{i_j}, u_j\}).$$

Since u_1 and u_2 originally came from cospectral vertices in F, $\phi(F_{i_1}\backslash\{v_{i_1}, u_1\}) = \phi(F_{i_2}\backslash\{v_{i_2}, u_2\})$. Moreover, by Theorem 5.1, the graphs $F_1, \ldots, F_m$ are pairwise cospec-

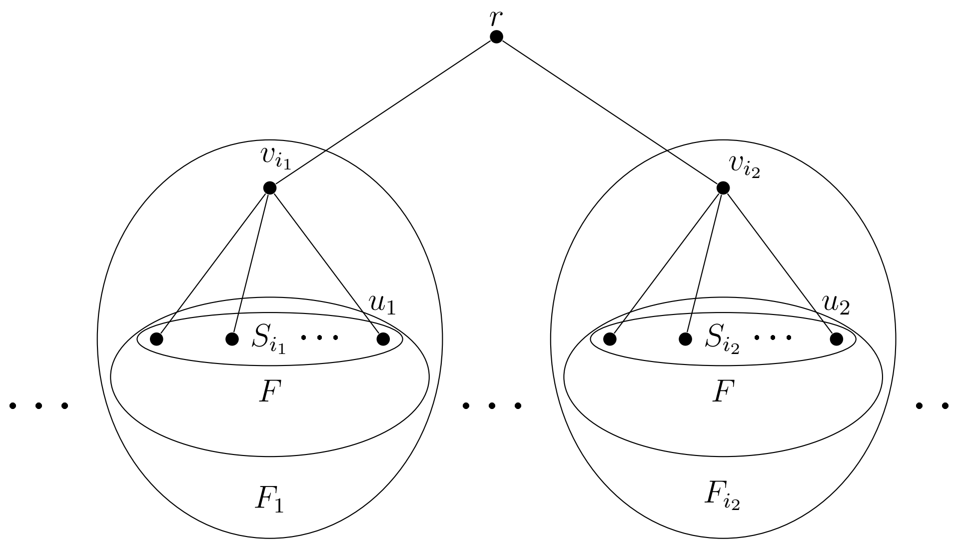


Figure 5.10: A demonstration of the choices of u_1 and u_2, assuming $i_1 \neq i_2$

tral, so $\phi\left(\bigcup_{\substack{\ell=1\\ \ell\neq i_1}}^{m} F_\ell\right) = \phi\left(\bigcup_{\substack{\ell=1\\ \ell\neq i_2}}^{m} F_\ell\right)$. Therefore,

$$\phi(G\backslash\{u_1, v_{i_1}, r\}) = \phi(G\backslash\{u_2, v_{i_2}, r\}).$$

Now we compare $\phi((G\backslash u_1)\backslash e_1)$ with $\phi((G\backslash u_2)\backslash e_2)$. For $j = 1, 2$, use C_j to represent the component of $G\backslash v_{i_j}$ containing the vertex u_j, then

$$(G\backslash u_i)\backslash e_i = (G\backslash F_{i_j}) \cup (F_{i_j}\backslash C_j) \cup (C_j\backslash u_j).$$

As discussed above, $\phi(F_{i_1}\backslash\{v_{i_1}, u_1\}) = \phi(F_{i_2}\backslash\{v_{i_2}, u_2\})$. Meanwhile, Theorem 5.1 implies $\phi(F_{i_1}\backslash C_1) = \phi(F_{i_2}\backslash C_2)$. Then $\phi(G\backslash F_{i_1}) = \phi(G\backslash F_{i_2})$ is a result of Theorem 5.2. Therefore,

$$\phi((G\backslash u_1)\backslash e_1) = \phi((G\backslash u_2)\backslash e_2).$$

By Lemma 2.7 (b), the edge-deletion recurrence for the characteristic polynomial, since $\phi(G\backslash\{u_1, v_{i_1}, r\}) = \phi(G\backslash\{u_2, v_{i_2}, r\})$ and $\phi((G\backslash u_1)\backslash e_1) = \phi((G\backslash u_2)\backslash e_2)$, we have $\phi(G\backslash u_1) = \phi(G\backslash u_2)$ after adding the edge e_1 and e_2 to $\phi((G\backslash u_1)\backslash e_1)$ and $\phi((G\backslash u_2)\backslash e_2)$ respectively.

(b) To see u_1 and u_2 are cospectral vertices in $G\backslash r$, observe that, for $j = 1, 2$, we have

$$G\backslash\{u_j, r\} = \left(\bigcup_{\substack{\ell=1 \\ \ell\neq i_1}}^{m} F_\ell\right) \cup (F_{i_j}\backslash u_j) = \left(\bigcup_{\substack{\ell=1 \\ \ell\neq i_1}}^{m} F_\ell\right) \cup (F_{i_j}\backslash C_j) \cup (F_{i_j}\backslash\{v_{i_j}, u_j\}).$$

In Part (a), we have already proven $\phi\left(\bigcup_{\substack{\ell=1 \\ \ell\neq i_1}}^{m} F_\ell\right) = \phi\left(\bigcup_{\substack{\ell=1 \\ \ell\neq i_2}}^{m} F_\ell\right)$, $\phi(F_{i_1}\backslash C_1) = \phi(F_{i_2}\backslash C_2)$, and $\phi(F_{i_1}\backslash\{v_{i_1}, u_1\}) = \phi(F_{i_2}\backslash\{v_{i_2}, u_2\})$. Therefore u_1 and u_2 are cospectral vertices in $G\backslash r$. □

Theorem 5.3 gives us a way to construct a connected graph with cospectral vertices using a disconnected graph with cospectral vertices. Moreover, if the graphs F_i are pairwise non-isomorphic for $1 \leq i \leq m$, and $u_1, u_2 \in \cup_{i=1}^{m} N(v_m)\backslash v$ do not have a common neighbor, then u_1 and u_2 would not be similar vertices in G.

As an example, we consider Figure 5.2 as F again, where each of its components is a copy of L shown in Figure 2.2. As discussed earlier in this section, when $c = 2$, we can get three sets of two vertices S_1, S_2, and S_3 such that the resulting F_1, F_2, and F_3 are pairwise non-isomorphic. Therefore, our extension would generate a connected graph as shown in Figure 5.11, which has six cospectral vertices lying in four distinct orbits. In general, we can treat the sets S_i as distinct multisets of cospectral vertices in the graphs F. Then if there exists a connected graph G with k non-similar cospectral vertices, for an arbitrary positive integer value $c \geq 2$ we can construct a connected graph with $c\binom{k+c-1}{c}$ cospectral vertices, where at least $\binom{k+c-1}{c}$ of them being pairwise non-similar.

This gives us a method to construct connected graphs with an arbitrarily large number of cospectral vertices, which is our next result. Moreover, since this construction does not create cycles in the graph, and there exists a tree (Schwenk's tree) with a pair of non-similar cospectral vertices, we can say that for any integer $k \geq 2$, there exists a tree with k cospectral vertices.

5.4 Corollary. *For any $k \geq 2$ there exists a connected graph with k cospectral vertices that are pairwise non-similar.*

Proof. Figure 5.11 is a graph with four cospectral vertices that are pairwise non-similar. Therefore, the statement is certainly true for $k = 2, 3$ and 4.

We prove the rest of the statement by induction. Assume the statement holds for some $k = n$ for some $n \geq 4$, we prove the statement holds for $k = n + 1$. Take the c copies of

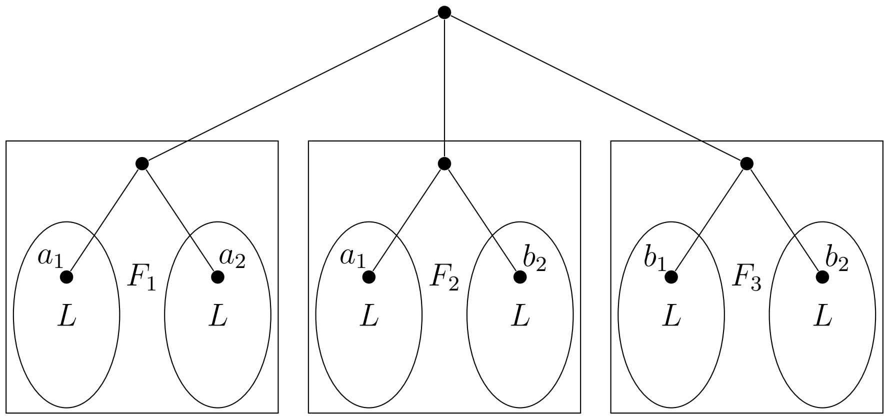


Figure 5.11: A graph obtained by applying our construction in Theorem 5.3 to the graph shown in Figure 5.2

the connected graph with n cospectral vertices that are pairwise non-similar as F, then F contains at least cn cospectral vertices. If we are to pick sets containing exactly one vertex from each of the c components of F, where that vertex is one of the n cospectral vertices in that component, there are at most $\binom{n+c-1}{c}$ choices. We use these choices as the sets $S_1, \ldots, S_m$ in the statement of Theorem 5.3, so that $m = \binom{n+c-1}{c}$.

By the construction in Theorem 5.3, we can obtain a connected graph with at least $\binom{cn+c-1}{c}$ cospectral vertices that are pairwise non-similar. Since $c = 2$ and $n \geq 4$,

$$\binom{2n+2-1}{2}\binom{n+1}{2} \geq n+1.$$

Therefore, the construction in Theorem 5.3 gives a graph with a least $n+1$ cospectral vertices that are pairwise non-similar. $\square$

Therefore, Theorem 5.3 is powerful because it gives a way to construct connected graphs with an arbitrarily large number of cospectral vertices that are pairwise non-similar. Note that even though the components of the graph F has been isomorphic in all of the examples we have shown, they do not need to be isomorphic for the construction in the previous section and this section to work.

Since the construction in Theorem 5.3 does not introduce any additional cycles to the graph, if F is a forest, then the resulting graph would be a tree. There exists a forest with at least two cospectral and non-similar vertices, so the corollary above implies there exists a tree with k cospectral vertices that are pairwise non-similar, for any $k \geq 2$. In particular, suppose a rooted tree L with k cospectral vertices that are non-similar is constructed using Theorem 5.3, such that the vertex r, the vertex added for the last 1-vertex extension in the construction, is the root of L. Then almost every tree contains the rooted tree L as a limb [32]. However, would the cospectral vertices in L still be cospectral in the trees containing L as a limb? The following theorem gives a positive answer to this question.

5.5 Theorem. *Let G be a graph. For any integer $k \geq 2$, suppose L is a graph with k cospectral vertices $a_1, a_2, \ldots, a_k$. Moreover, assume there exists a vertex $r \in L$ such that $r \notin \{a_1, a_2, \ldots, a_k\}$, and the vertices $a_1, a_2, \ldots, a_k$ are still cospectral vertices in $L \backslash r$. Let G' be the 1-sum of G and L with respect to an arbitrary vertex in G and r. Then the vertices $a_1, a_2, \ldots, a_k$ are cospectral in G'.*

Proof. For any $1 \leq i \leq k$, by Lemma 2.8, we get

$$\phi(G' \backslash a_i) = \phi(G)\phi(L \backslash \{a_i, r\}) + \phi(G \backslash v)\phi(L \backslash a_i) - x\phi(G \backslash v)\phi(L \backslash \{a_i, r\}).$$

Given any $1 \leq j \leq k$, our assumptions guarantee that

$$\phi(L \backslash a_i) = \phi(L \backslash a_j)$$

and

$$\phi(L \backslash \{a_i, r\}) = \phi(L \backslash \{a_j, r\}),$$

so we get

$$\phi(G' \backslash a_i) = \phi(G' \backslash a_j).$$

In other words, $a_1, a_2, \ldots, a_k$ are cospectral vertices in G'. □

Then we obtain the following result immediately.

5.6 Theorem. *For any $k \geq 2$, almost every tree has k cospectral vertices that are pairwise non-similar.*

Theorem 5.5 implies that we could take the 1-sum of a connected graph with an arbitrarily large number of cospectral vertices resulting from the construction in Theorem 5.3 and any general graph and obtain a larger connected graph with an arbitrarily large number of cospectral vertices. However, this construction has its limitations, since it still results in a cut-vertex, while most graphs do not have a cut-vertex. Therefore, our construction does not give any indication of whether almost every graph is cospectral with another graph.

This construction would also work for comatching graphs. Suppose a graph G has a pair of comatching vertices a and b. Recall that the matching polynomial and the characteristic polynomial coincide for forests. By the 1-sum formula, for any other graph H and $v \in V(H)$, we have $G_a{\cdot}H_v$ is comatching with $G_b{\cdot}H_v$. Since our construction gives graphs with an arbitrarily large number of comatching vertices, along with the 1-sum formula, this gives us infinite sets of arbitrarily large sets of comatching graphs as well.

In Section 4.4, we proved our definition of weighted characteristic polynomial preserved a lot of properties of the characteristic polynomial for unweighted graphs. Consequently, our construction for cospectral vertices in graphs applies to weighted graphs as well: given weighted trees or graphs as input, satisfying the hypotheses as before but with weighted cospectrality in place of cospectrality, each time a 1-vertex extension is used in the construction simply assign weight 1 to the new vertex. In particular then we can build weighted graphs L with k weighted cospectral vertices satisfying the conditions for Theorem 5.5. Then let G be a weighted graph and $v \in V(G)$ with any positive integer weight. By Lemma 4.17, the k weighted cospectral vertices in L are still weighted cospectral in a weighted graph obtained by identifying v in G and r in L, regardless of the specific weight of the identified vertex. Specifically, our results in this section apply to weighted trees as well.

5.7 Theorem. *For any $k \geq 2$ almost every weighted tree has k pairwise weighted cospectral vertices.*

5.4 Application to Comatching Graphs

Recall that in Chapter 2, we discussed the connections between the matching polynomials and the characteristic polynomial for graphs. In particular, they both satisfy similar recurrences, such as the union formula, some version of the edge-deletion recurrence, and the 1-sum formula. Notice that these are the only recurrences we used to prove most of the results in the previous sections of this chapter. Consequently, the following analogous results hold for the matching polynomial.

5.8 Theorem. *Let G be a graph with a set of comatching vertices $A = \{a_1, a_2, \cdots, a_k\}$, with each component of G containing at most one vertex in A. Let S_1 and S_2 be non-empty subsets of A such that $|S_1| = |S_2|$. For $i = 1, 2$, let G_i be the 1-vertex extension of G with respect to S_i. Then G_1 and G_2 are comatching.*

5.9 Theorem. *Let F be a graph with c components that are pairwise comatching. For some integer $m \geq 1$, suppose we have two distinct sets $A_1 = \{S_1^1, S_2^1, \ldots, S_m^1\}$ and $A_2 =$*

$\{S_1^2, S_2^2, \ldots, S_m^2\}$, both containing m sets of pairwise comatching vertices from F, such that for all $1 \leq i \leq m$, each S_i^1 or S_i^2 contains exactly one vertex from each component of F.

For $1 \leq i \leq m$ and $j = 1, 2$, let F_i^j be the 1-vertex extension of F with respect to S_i^j, with the added vertex being v_i^j. Let H_j be the 1-vertex extension of $\bigcup_{i=1}^m F_i^j$ with respect to $v_1^j, \ldots, v_m^j$, with the added vertex being r_j. Then H_1 and H_2 are comatching.

5.10 Theorem. *Let F be a graph with c components that are pairwise comatching. Suppose there exists distinct sets $S_1, S_2, \ldots, S_m \subseteq V(F)$ of pairwise comatching vertices for some integer $m \geq 1$, such that for all $1 \leq i \leq m$, each S_i contains exactly one vertex from each component of F.*

For $1 \leq i \leq m$, let F_i be the 1-vertex extension of F with respect to S_i, with the added vertex being v_i. Let G be the 1-vertex extension of $\bigcup_{i=i}^m F_i$ with respect to $v_1, \ldots, v_m$, with the added vertex being r. Then

(a) $\bigcup_{i=1}^m N(v_m)\backslash r$ is a set of pairwise comatching vertices in G; and

(b) $\bigcup_{i=1}^m N(v_m)\backslash r$ is a set of pairwise comatching vertices in $G\backslash r$.

5.11 Theorem. *For any $k \geq 2$ there exists a connected graph with k comatching vertices that are pairwise non-similar.*

5.12 Theorem. *Let G be a graph. For any integer $k \geq 2$, suppose L is a graph with k comatching vertices a_1, a_2, $\ldots$, a_k. Moreover, assume there exists a vertex $r \in L$ such that $r \notin \{a_1, a_2, \ldots, a_k\}$, and the vertices a_1, a_2, $\ldots$, a_k are still comatching vertices in $L\backslash r$. Let G' be the 1-sum of G and L with respect to an arbitrary vertex in G and r. Then the vertices a_1, a_2, $\ldots$, a_k are comatching G'.*

5.13 Theorem. *For any $k \geq 2$, almost every tree has k comatching vertices that are pairwise non-similar.*

These results imply that we have a construction for connected graphs with an arbitrarily large number of comatching vertices as well. In addition, note that the edge-deletion recurrence only applies to the characteristic polynomial when the edge being deleted is a cut-edge, while the edge-deletion recurrence applies to the matching polynomial regardless of the choice of the edge. Consequently, we have the following result, which is a stronger version of Theorem 5.8.

5.14 Theorem. *Let G be a graph with a set of comatching vertices $A = \{a_1, a_2, \cdots, a_k\}$. Let S_1 and S_2 be non-empty subsets of A such that $|S_1| = |S_2|$. For $i = 1, 2$, let G_i be the 1-vertex extension of G with respect to S_i. Then G_1 and G_2 are comatching.*

Proof. We prove this theorem by induction on the size of S_1 and S_2. Suppose $|S_1| = |S_2| = 1$. Let v be connected to a_i and a_j in G_1 and G_2, respectively. Then we have

$$\begin{aligned}\mu(G_1, x) &= \mu(G_1 \backslash \{e_{a_i v}\}, x) - \mu(G_1 \backslash \{a_i, v\}) \\ &= x\mu(G, x) - \mu(G \backslash a_i) \\ &= \mu(G_2 \backslash \{e_{a_j v}\}) - \mu(G \backslash \{a_j\}) \\ &= \mu(G_2, x),\end{aligned}$$

where $e_{a_i v}$ denotes the edge with a_i and v being its endpoints.

Now assume the theorem statement holds for all $|S_1| = |S_2| \leq l - 1$, where $1 < l \leq k$. Suppose $|S_1| = |S_2| = 1$, $a_i \in S_1$, $a_j \in S_1$. Let $S_1' = S_1 \backslash \{a_i\}$ and $S_2' = S_2 \backslash \{a_j\}$, and use G_1', G_2' to denote the graphs constructed by the process in the theorem statement, using the sets S_1' and S_2', respectively. By the induction hypothesis, $\mu(G_1', x) = \mu(G_2', x)$.

Note that

$$\begin{aligned}\mu(G_1, x) &= \mu(G_1', x) - \mu(G_1 \backslash \{a_i, v\}, x) \\ &= \mu(G_1', x) - \mu(G \backslash \{a_i\}, x) \\ &= \mu(G_2', x) - \mu(G \backslash \{a_j\}, x) \\ &= \mu(G_2, x).\end{aligned}$$

Hence the theorem statement is proven. □

Theorem 5.14 is a strong result that can be applied to construct large sets of comatching graphs. For example, all vertices in a cycles are pairwise comatching. Therefore, given a cycle C, any 1-vertex extensions of C with respect to a set of vertices S with a fixed size m are comatching graphs, regardless of the choice of elements in S. Figure 5.12 gives an example of a pair of comatching graphs using this construction.

In general, for a vertex transitive graph G, all vertices of G can be put in the set A defined in Theorem 5.14. Therefore, this result gives a construction of an infinite number of large sets containing pairwise comatching graphs without a cut-vertex. Technically, the connectivity of the resulting comatching graphs could be arbitrarily high, since we could apply Theorem 5.14 to complete graphs. This provides yet another construction for comatching graphs.

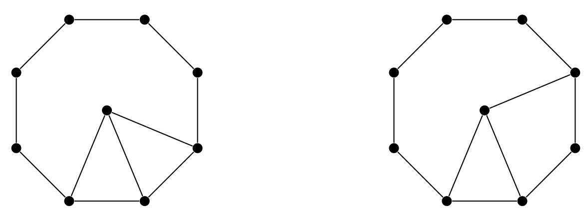


Figure 5.12: A pair of comatching graphs constructed using Theorem 5.14

Chapter 6

The 2-Sum Construction of Comatching Graphs

In this chapter, we consider another construction for pairs of comatching graphs, using 2-sums. To do so, we first provide a definition of the matching polynomial generalized to multigraphs. We prove that the basic recurrences for the matching polynomial still hold for the generalized definition. Then, we derive an edge contraction recurrence for the matching polynomial, and use this recurrence to build our 2-sum construction for comatching vertices and comatching graphs.

6.1 The Generalized Matching Polynomial

Let G be a multigraph with n vertices. Analogous to the case for simple graphs, we define a *matching* M in G as a set of pairwise disjoint edges. Note that when G is a graph with loops, a matching M could include a loop as long as the loop does not share its end-vertex with any other edge in M. A vertex $v \in V(G)$ is *saturated* by M if v is an end-vertex of an edge in M. Note that a loop can be disjoint from other edges, so by our definition of matching in Chapter 1, a matching could contain loops. The *loop order* of M, denoted as $\beta(M)$, is the number of edges in M that are loops.

Recall that, when defining the matching polynomial for simple graphs, we used $p(G, k)$ to denote the number of matchings in G with size k, and consequently we defined the matching polynomial as

$$\mu(G, x) = \sum_i (-1)^i p(G, i) x^{n-2i}.$$

In 1977, Gutman et al. and Trinajistić defined the matching polynomial for multigraphs in [15] and [33]. We adapt their definition in our discussion: Let $\mathcal{M}(G)$ be the set of all matchings in the multigraph G. Recall that in Chapter 1, we defined the *matching polynomial* of a multigraph G as

$$\mu(G;x,h) = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|-\beta(M)} h^{\beta(M)} x^{n-2|M|+\beta(M)}.$$

Observe that the h variable counts the number of loops in M, while the x variable counts the number of vertices that are not saturated by M. Note the empty set of edges is a matching, so the leading term of $\mu(G;x,h)$ is always x^n. Moreover, for any bivariate polynomial $P(x,y)$, use $\langle x^i y^j, P(x,y)\rangle$ to denote the coefficient of $x^i y^j$ in $P(x,y)$. Then the number of edges in G is

$$\langle hx^{n-1}, \mu(G;x,h)\rangle + \langle x^{n-2}, \mu(G;x,h)\rangle.$$

The first term of the equation above counts the number of loops in G while the second term counts the number of non-loop edges in G.

Also note that if $h = 0$, which implies the graph does not have any loops, then the generalized matching polynomial for multigraphs is the same as the matching polynomial for simple graphs.

Before considering the generalized matching polynomial of a given 2-sum, we show that it satisfies similar recurrences as the matching polynomial for simple graphs does, starting with the union formula.

6.1 Lemma. *Let G and H be multigraphs, then*

$$\mu(G \cup H;x,h) = \mu(G;x,h)\mu(H;x,h).$$

Proof. Given a matching $M \in \mathcal{M}(G)$, M consists of a unique matching $M_1 \in G$ with $\beta(M_1) = a$ and a unique matching $M_2 \in H$ with $\beta(M_2) = \beta(M) - a$. Then we have

$$\begin{aligned}
&\langle h^{\beta(M)} x^{|G\cup H|-2|M|+\beta(M)}, \mu(G\cup H;x,h)\rangle \\
&= \sum_{a=0}^{\beta(M)} (\langle h^a x^{|G|-2|M_1|+a}, \mu(G;x,h)\rangle \langle h^{\beta(M)-a} x^{|H|-2|M_2|+\beta(M)-a}, \mu(H;x,h)\rangle).
\end{aligned}$$

Then $\mu(G \cup H;x,h) = \mu(G;x,h)\mu(H;x,h)$. □

Similarly, the generalized matching polynomial satisfies the vertex-deletion recurrence.

6.2 Lemma. *Let G be a multigraph and let u be a vertex of G. Use ℓ to denote the number of loops at u, then*

$$\mu(G;x,h) = x\mu(G\backslash u;x,h) + \ell h\mu(G\backslash u;x,h) - \sum_{i\sim u}\mu(G\backslash\{u,i\};x,h).$$

Proof. Let S be the set of matchings in G that contain exactly $\beta(M) = a$ loops and $|M| - \beta(M) = b$ non-loops, then

$$|S| = (-1)^b\langle h^a x^{n-a-2b}, \mu(G;x,h)\rangle.$$

Meanwhile, given any matching M in S, then the vertex u is either not saturated by M, or saturated by M. In the latter case, u could be saturated by a loop in M, or saturated by a non-loop in M. Therefore, we have the following three cases.

Case 1: If u is not saturated by M, then M induces a matching in $G\backslash u$, and there are a total of

$$(-1)^b\langle h^a x^{(n-1)-a-2b}, \mu(G\backslash u;x,h)\rangle$$

such matchings in S.

Case 2: If u is saturated by a loop, the matching M would induce a matching in $G\backslash u$ as well, and there are a total of

$$(-1)^b\ell\langle h^{a-1} x^{(n-1)-(a-1)-2b}, \mu(G\backslash u;x,h)\rangle$$

such matchings in S.

Case 3: If the edge in M incident to u connects u to another vertex $i \in G$, then $M\backslash ui$ induces a matching in $G\backslash\{u,i\}$, and there are a total of

$$(-1)^{b-1}\sum_{i\sim u}\langle h^a x^{(n-2)-a-2(b-1)}, \mu(G\backslash\{u,i\};x,h)\rangle$$

such matchings in S.

Therefore,

$$\begin{aligned}(-1)^b\langle h^a x^{n-a-2b}, \mu(G;x,h)\rangle &= (-1)^b\langle h^a x^{(n-1)-a-2b}, \mu(G\backslash u;x,h)\rangle \\ &\quad + (-1)^b\ell\langle h^{a-1} x^{(n-1)-(a-1)-2b}, \mu(G\backslash u;x,h)\rangle \\ &\quad + (-1)^{b-1}\sum_{i\sim u}\langle h^a x^{(n-2)-a-2(b-1)}, \mu(G\backslash\{u,i\};x,h)\rangle.\end{aligned}$$

Summing the equation above over all possible values of a and b, we get

$$\mu(G;x,h) = x\mu(G\backslash u;x,h) + \ell h\mu(G\backslash u;x,h) - \sum_{i\sim u}\mu(G\backslash\{u,i\};x,h).$$

□

Consequently, we obtain the following corollary.

6.3 Corollary. *Let G be a graph and suppose $u,v \in V(G)$ are comatching vertices in G. Then the number of loops at u is the same as that at v.*

The edge-deletion recurrence is slightly different for the generalized matching polynomial, because a multigraph could have two types of edges: loops and non-loops. The recurrences for both of these two cases are derived.

6.4 Lemma. *Let G be a multigraph and suppose e is a loop in G at some vertex u, then*

$$\mu(G;x,h) = \mu(G\backslash e;x,h) + h\mu(G\backslash u;x,h).$$

Proof. Let S be the set of matchings in G that contain exactly $\beta(M) = a$ loops and $|M| - \beta(M) = b$ non-loops, then

$$|S| = (-1)^b\langle h^a x^{n-a-2b}, \mu(G;x,h)\rangle.$$

For any $M \in S$, if e is in M, then $M\backslash e$ is a matching in $G\backslash u$. There are

$$(-1)^b\langle h^{a-1}x^{(n-1)-(a-1)-2b}, \mu(G\backslash u;x,h)\rangle$$

such matchings in S.

If e is not in M, then M is a matching in $G\backslash e$ as well, and there are

$$(-1)^b\langle h^a x^{n-a-2b}, \mu(G\backslash e)\rangle$$

such matchings in S.

Thus

$$\begin{aligned}(-1)^b\langle h^a x^{n-a-2b}, \mu(G;x,h)\rangle = (-1)^b&\langle h^{a-1}x^{(n-1)-(a-1)-2b}, \mu(G\backslash u;x,h)\rangle \\ &+ (-1)^b\langle h^a x^{n-a-2b}, \mu(G\backslash e;x,h)\rangle.\end{aligned}$$

Summing this equation over all possible values of a and b, we get

$$\mu(G;x,h) = \mu(G\backslash e;x,h) + h\mu(G\backslash u;x,h),$$

if e is a loop on the vertex $u \in G$. □

6.5 Lemma. *Let G be a multigraph and suppose $e = \{u, v\}$ is an edge in G that is not a loop, then*

$$\mu(G; x, h) = \mu(G\backslash e; x, h) - \mu(G\backslash\{u, v\}; x, h).$$

Proof. Let S be the set of matchings in G that contain exactly $\beta(M) = a$ loops and $|M| - \beta(M) = b$ non-loops, then

$$|S| = (-1)^b \langle h^a x^{n-a-2b}, \mu(G; x, h)\rangle.$$

For any matching $M \in S$, if e is not in M, then $M\backslash e$ forms a matching in $G\backslash e$. There are

$$(-1)^b \langle h^a x^{n-a-2b}, \mu(G\backslash e; x, h)\rangle$$

such matchings in S.

If e is in M, then $M\backslash e$ forms a matching in $G\backslash\{u, v\}$. There are

$$(-1)^{b-1} \langle h^a x^{n-a-2(b-1)}, \mu(G\backslash\{u, v\}; x, h)\rangle$$

such matchings in S.

This analysis implies

$$\begin{aligned}(-1)^b \langle h^a x^{n-a-2b}, \mu(G; x, h)\rangle &= (-1)^b \langle h^a x^{n-a-2b}, \mu(G\backslash e; x, h)\rangle \\ &\quad + (-1)^{b-1} \langle h^a x^{n-a-2(b-1)}, \mu(G\backslash\{u, v\}; x, h)\rangle.\end{aligned}$$

Summing this equation over all possible values of a and b, we get

$$\mu(G; x, h) = \mu(G\backslash e; x, h) - \mu(G\backslash\{u, v\}; x, h)$$

if $e = uv$ is an edge of G that is not a loop. □

Last but not least, we prove the derivative formula for the generalized matching polynomial.

6.6 Lemma. *Let G be a multigraph with at least one vertex, then*

$$\frac{\partial}{\partial x} \mu(G; x, h) = \sum_{i \in V(G)} \mu(G\backslash i; x, h).$$

Proof. Let S be the set of matchings in G that contain exactly $\beta(M) = a$ loops and $|M| - \beta(M) = b$ non-loops, then

$$|S| = (-1)^b \langle h^a x^{n-a-2b}, \mu(G; x, h)\rangle.$$

We may assume $a + 2b < n$, then note that

$$\langle h^a x^{n-a-2b-1}, \frac{\partial}{\partial x}\mu(G; x, h)\rangle\rangle = (-1)^b (n - a - 2b)|S|.$$

Observe that $(n - a - 2b)|S|$ counts the number of ways of first choosing a matching in S, and then choose a vertex i that is not saturated by this matching. Alternatively, we could pick the vertex i first, and then pick a matching with a loops and b non-loop edges in $G\backslash i$. Therefore,

$$\langle h^a x^{n-a-2b-1}, \frac{\partial}{\partial x}\mu(G; x, h)\rangle = (-1)^b (n - a - 2b)|S| = \langle h^a x^{n-a-2b-1}, \sum_{i \in V(G)} \mu(G\backslash i; x, h)\rangle.$$

So we have

$$\frac{\partial}{\partial x}\mu(G; x, h) = \sum_{i \in V(G)} \mu(G\backslash i; x, h).$$

□

We also observe that the 1-sum formula still holds for the generalized matching polynomial, because its proof only requires the vertex-deletion recurrence.

6.7 Lemma. *Let G_1, G_2 be multigraphs. Suppose G is the* 1*-sum of G_1 and G_2 with the shared vertex being v. Then*

$$\mu(G; x, h) = \mu(G_1\backslash v; x, h)\, \mu(G_2; x, h) + \mu(G_1; x, h)\, \mu(G_2\backslash v; x, h) - x\mu(G_1\backslash v; x, h)\, \mu(G_2\backslash v; x, h).$$

Therefore, we can see that the generalized matching polynomial has a lot of properties in common with the matching polynomial. For the rest of this chapter, we will use some of these recurrences to work towards our 2-sum construction of comatching vertices and comatching graphs.

Figure 6.1: An edge contraction on a simple graph could result in a multigraph.

6.2 Edge-Contraction Recurrence

In this section, we discuss what happens to the matching polynomial of a graph G when an edge e in G is contracted. Specifically, we provide an edge-contraction recurrence for the matching polynomial. We use G/e to denote the graph formed by contracting the edge e in G.

Even though we are discussing the matching polynomial in the context of multigraphs in this chapter, this recurrence applies to simple graphs as well. However, it is necessary to discuss multigraphs, because when an edge $e = \{u, v\}$ in a simple graph G is contracted, if u and v have a common neighbor w, then there would be two edges connecting w to the new vertex uv formed due to the contraction. The simplest example of this is shown in Figure 6.1. Since edge contraction of simple graphs could result in multigraphs, this must be discussed in the context of multigraphs.

Below is the edge-contraction recurrence we derived.

6.8 Theorem. *Let G be a multigraph and $u, v \in V(G)$ such that there is an edge e between u and v. Suppose there are a total of ℓ edges between vertices u and v, then*

$$\mu(G/e; x, h) = \mu(G\backslash u; x, h) + \mu(G\backslash v; x, h) - x\mu(G\backslash\{u, v\}; x, h) + (\ell - 1)h(\mu(G\backslash\{u, v\}; x, h)).$$

Proof. Use $w \in G/e$ to denote the new vertex formed by the two end vertices of e during the contraction of e. For each matching M in G, we consider the set of edges M' in G/e, such that M' contains all edges in M, where the edges with one of u and v as an end-vertex now has w as that end-vertex instead, and edges between u and v (other than the contracted edge) become a loop on w. In other words, each matching in G corresponds to such a set of edges M' in G/e (not necessarily a matching), although this correspondence is not necessarily one-to-one since a set of edges in G/e could correspond to multiple matchings that contain e in G. We consider when M' would be a matching in G/e.

For every matching M in G/e, there are two cases: either both u and v are saturated by e, or at most one of u and v is saturated. In the first case, the corresponding M' is a matching in G/e only if there exists an edge $e' \neq e$ in M that connects u to v. In the second case, the corresponding set M' is a matching in G/e. Moreover, note that all matchings in G/e can be obtained by this correspondence from at least one matching in G.

When both u and v are saturated by the matching M, observe that the edge e' in M that connects u to v would become a loop on w in G/e. Since there are a total of ℓ edges between u and v, there are $\ell - 1$ choices for e' in G/e. Any matching in G/e that include such a loop is a matching in $H\backslash w$, which is the same multigraph as $G\backslash\{u, v\}$. Therefore, these matchings can be counted as $(\ell - 1)h(\mu(G\backslash\{u, v\}; x, h))$.

Now we do the counting for the second case. In G, the matchings with u saturated can be counted by

$$\mu(G; x, h) - x\mu(G\backslash u; x, h),$$

the matchings with v saturated can be counted by

$$\mu(G; x, h) - x\mu(G\backslash v; x, h),$$

and the matchings with at least one of u and v saturated can be counted by

$$\mu(G; x, h) - x^2\mu(G\backslash\{u, v\}; x, h).$$

By the inclusion-exclusion principle, the matchings with both u and v saturated in G can be counted by

$$\begin{aligned}\mu(G; x, h) - x\mu(G\backslash u; x, h) + \mu(G; x, h) - x\mu(G\backslash v; x, h) - (\mu(G; x, h) - x^2\mu(G\backslash\{u, v\}; x, h))\\ = \mu(G; x, h) - x\mu(G\backslash u; x, h) - x\mu(G\backslash v; x, h) + x^2\mu(G\backslash\{u, v\}; x, h).\end{aligned}$$

Then the matchings in G where u and v are not both saturated can be counted by

$$\begin{aligned}\mu(G; x, h) - (\mu(G; x, h) - x\mu(G\backslash u; x, h) - x\mu(G\backslash v; x, h) + x^2\mu(G\backslash\{u, v\}; x, h))\\ = x\mu(G\backslash u; x, h) + x\mu(G\backslash v; x, h) - x^2\mu(G\backslash\{u, v\}; x, h).\end{aligned}$$

Consequently, the matching polynomial of G/e is

$$\begin{aligned}&\mu(G/e; x, h)\\ &= \frac{1}{x}(x\mu(G\backslash u; x, h) + x\mu(G\backslash v; x, h) - x^2\mu(G\backslash\{u, v\}; x, h)) + (\ell - 1)h(\mu(G\backslash\{u, v\}; x, h))\\ &= \mu(G\backslash u; x, h) + \mu(G\backslash v; x, h) - x\mu(G\backslash\{u, v\}; x, h) + (\ell - 1)h(\mu(G\backslash\{u, v\}; x, h)).\end{aligned}$$

□

Moreover, using this edge-contraction recurrence, we easily obtain the following vertex-identification recurrence.

6.9 Corollary. *Let H be a multigraph such that u and v are non-adjacent vertices in H. Let G be the multigraph obtained by identifying u and v in H. Then*

$$\mu(G; x, h) = \mu(H\backslash u; x, h) + \mu(H\backslash v; x, h) - x\mu(H\backslash\{u, v\}; x, h).$$

Proof. Add an edge between u and v, then apply Theorem 6.8. □

Note that when u and v are in different components in G, Corollary 6.9 gives the 1-sum formula, as expected. In the next section, we use the vertex-identification recurrence in our 2-sum construction for comatching vertices and comatching graphs.

6.3 Comatching Constructions by 2-Sum

In this section, we give a 2-sum construction for comatching graphs. To begin, we show that, if we have a pair of graphs each with a pair of comatching vertices, then by taking a 2-sum with respect to the pair of comatching vertices, we would create a new graph with a pair of comatching vertices.

6.10 Theorem. *Let G be the 2-sum of the multigraphs G_1 and G_2 with $V(G_1) \cap V(G_2) = \{u, v\}$. Suppose u and v are comatching vertices in both G_1 and G_2. Then u and v are comatching vertices in G.*

Proof. Observe that $G\backslash u$ is the 1-sum of $G_1\backslash u$ and $G_2\backslash u$ with respect to v. Then by the 1-sum formula,

$$\begin{aligned}\mu(G\backslash u; x, h) = \mu(G_1\backslash u; x, h)\,\mu(G_2\backslash\{u, v\}; x, h) + \mu(G_1\backslash\{u, v\}; x, h)\,\mu(G_2\backslash u; x, h)\\ - \mu(G_1\backslash\{u, v\}; x, h)\,\mu(G_2\backslash\{u, v\}; x, h).\end{aligned}$$

Moreover, since u and v are comatching vertices in G_1 and G_2, by definition we have $\mu(G_1\backslash u; x, h) = \mu(G_1\backslash v; x, h)$ and $\mu(G_2\backslash u; x, h) = \mu(G_2\backslash v; x, h)$, so

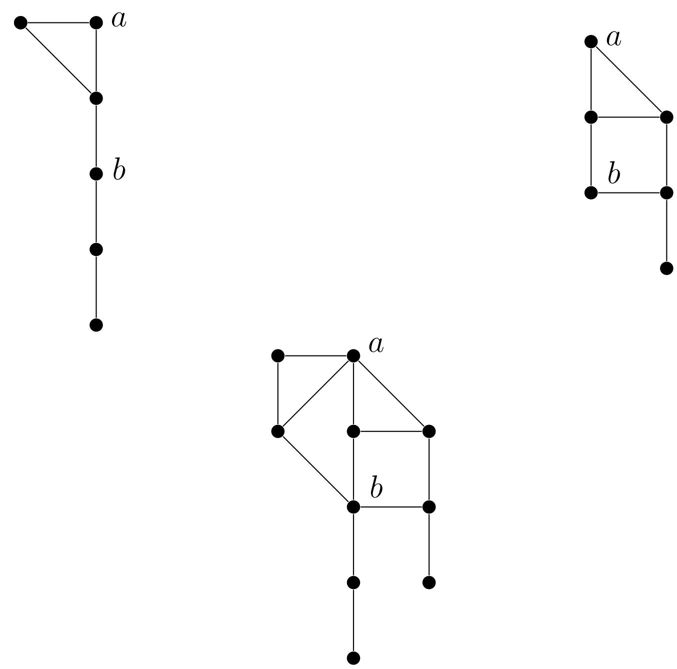


Figure 6.2: The 2-sum construction for cospectral vertices

$$\mu(G\backslash u;x,h) = \mu(G_1\backslash v;x,h)\,\mu(G_2\backslash\{u,v\};x,h) + \mu(G_1\backslash\{u,v\};x,h)\,\mu(G_2\backslash v;x,h) \\ - \mu(G_1\backslash\{u,v\};x,h)\,\mu(G_2\backslash\{u,v\};x,h) = \mu(G\backslash v;x,h).$$

□

Figure 6.2 gives an example of the construction in Theorem 6.10. The original two graphs each have a pair of comatching vertices a and b. By taking their 2-sum with respect to a and b, we constructed a bigger graph where a and b are still comatching vertices.

Next, we show that if the two vertices being summed in the 2-sum are switched in one of the subgraphs, the resulting 2-sum is comatching with the original 2-sum.

6.11 Theorem. *Let G_1 and G_2 be multigraphs with $V(G_1) \cap V(G_2) = \{u,v\}$. Let G_2' be a graph isomorphic to G_2, such that*

$$V(G_2') = V(G_2),$$

and

$$E(G_2') = \left(\left(E(G_2) \backslash \bigcup_{\substack{i \sim u \\ \text{in } G_2}} \{i, u\} \right) \backslash \bigcup_{\substack{j \sim v \\ \text{in } G_2}} \{j, v\} \right) \bigcup \left(\bigcup_{\substack{i \sim u \\ \text{in } G_2}} \{i, v\} \right) \bigcup \left(\bigcup_{\substack{j \sim v \\ \text{in } G_2}} \{j, u\} \right).$$

Then the 2-sum of G_1 and G_2 and the 2-sum of G_1 and G_2' have the same matching polynomial if and only if u and v are comatching vertices in at least one of G_1 and G_2.

Proof. Let G be the 2-sum of G_1 and G_2 and G' be the 2-sum of G_1 and G_2'. Let H be the 1-sum of G_1 and G_2 with respect to the vertex u, such that we refer to the vertex v in G_1 and G_2 as v_1 and v_2 in H, respectively.

Apply Lemma 6.9 to H, and we see that

$$\begin{aligned}
\mu(G; x, h) &= \mu(H \backslash v_1; x, h) + \mu(H \backslash v_2; x, h) - x\mu(H \backslash \{v_1, v_2\}; x, h) \\
&= [\mu(G_1 \backslash v; x, h)\mu(G_2 \backslash u; x, h) + \mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2; x, h) \\
&\quad - x\mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2 \backslash u; x, h)] \\
&\quad + [\mu(G_1; x, h)\mu(G_2 \backslash \{u, v\}; x, h) + \mu(G_1 \backslash u); x, h\mu(G_2 \backslash v; x, h) \\
&\quad - x\mu(G_1 \backslash u; x, h)\mu(G_2 \backslash \{u, v\}; x, h)] \\
&\quad - x[\mu(G_1 \backslash v; x, h)\mu(G_2 \backslash \{u, v\}; x, h) + \mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2 \backslash v; x, h) \\
&\quad - x\mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2 \backslash \{u, v\}; x, h)].
\end{aligned}$$

Similarly, the matching polynomial of G' is

$$\begin{aligned}
\mu(G'; x, h) &= [\mu(G_1 \backslash v; x, h)\mu(G_2 \backslash v; x, h) + \mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2; x, h) \\
&\quad - x\mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2 \backslash v; x, h)] \\
&\quad + [\mu(G_1; x, h)\mu(G_2 \backslash \{u, v\}; x, h) + \mu(G_1 \backslash u; x, h)\mu(G_2 \backslash u; x, h) \\
&\quad - x\mu(G_1 \backslash u; x, h)\mu(G_2 \backslash \{u, v\}; x, h)] \\
&\quad - x[\mu(G_1 \backslash v; x, h)\mu(G_2 \backslash \{u, v\}; x, h) + \mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2 \backslash u; x, h) \\
&\quad - x\mu(G_1 \backslash \{u, v\}; x, h)\mu(G_2 \backslash \{u, v\}; x, h)].
\end{aligned}$$

Figure 6.3: These two graphs are comatching.

Taking the difference of $\mu(G; x, h)$ and $\mu(G'; x, h)$, we get

$$\begin{aligned}
&\mu(G; x, h) - \mu(G'; x, h) \\
&= \mu(G_1\backslash v; x, h)[\mu(G_2\backslash u; x, h) \\
&\qquad - \mu(G_2\backslash v; x, h)] - x\mu(G_1\backslash\{u, v\}; x, h)[\mu(G_2\backslash u; x, h) - \mu(G_2\backslash v; x, h)] \\
&\qquad + \mu(G_1\backslash u; x, h)[\mu(G_2\backslash v; x, h) - \mu(G_2\backslash u; x, h)] \\
&\qquad - x\mu(G_1\backslash\{u, v\}; x, h)[\mu(G_2\backslash v; x, h) - \mu(G_2\backslash u; x, h)] \\
&= [\mu(G_1\backslash v; x, h) - \mu(G_\backslash u; x, h)][\mu(G_2\backslash u; x, h) - \mu(G_2\backslash v; x, h)].
\end{aligned}$$

Thus $\mu(G; x, h) - \mu(G'; x, h) = 0$ if and only if $\mu(G_1\backslash v; x, h) - \mu(G_1\backslash u; x, h) = 0$ or $\mu(G_2\backslash u; x, h) - \mu(G_2\backslash v; x, h) = 0$. □

Therefore, if the two shared vertices u and v are switched in one of the subgraphs forming the 2-sum, the resulting 2-sum would be comatching to the original 2-sum. In other words, we have found a construction for pairs of comatching graphs using 2-sums.

An example of this construction is shown in Figure 6.3. The two underlying subgraphs are the same as the two underlying subgraphs in Figure 6.2, with a and b being comatching vertices in both of these subgraphs. There are two ways of forming the 2-sum using the pair of comatching vertices in these two subgraphs. The two resulting 2-sums are not isomorphic because the pairs of comatching vertices are not similar in either of the two subgraphs. These two 2-sums are comatching.

Observe that this construction could be used along with Theorem 5.3, which is one of our main results in Chapter 5 giving a construction for connected graphs with an arbitrarily large number of comatching vertices that are not pairwise similar. With two of such graphs constructed, we could pick any combination of pairs of comatching vertices from each of them and take the 2-sum accordingly. This gives a construction for arbitrarily large sets of comatching graphs.

The idea used in Theorem 6.11 can be applied to compute the matching polynomial of a k-sum recursively. In particular, suppose G is a k-sum of G_1 and G_2 with respect to the set $\{v_1, v_2, \cdots, v_k\}$. To compute the matching polynomial of G, we first consider the graphs H, a $(k-1)$-sum of G_1 and G_2 with respect to the set $\{v_1, v_2, \cdots, v_{k-1}\}$. We refer to the vertices in G_1 and G_2 corresponding to v_k as u_1 and u_2, respectively. If the matching polynomial of H, $H\backslash u_1$, $H\backslash u_2$, and $H\backslash\{u_1, u_2\}$ are known, then we could apply the vertex-identification recurrence to u_1 and u_2 and obtain the matching polynomial of G. Observe that H, $H\backslash u_1$, $H\backslash u_2$, and $H\backslash\{u_1, u_2\}$ are $(k-1)$-sums of known graphs. Therefore, if we have the matching polynomials of some specific $(k-1)$-sums, we can compute the matching polynomial of a k-sum accordingly. This implies that the matching polynomial of a k-sum can be computed recursively.

One might ask, could we use this to extend the 2-sum construction for comatching graphs to a k-sum construction for comatching graphs? The answer is no. To see why, let us assume the set of vertices $\{v_1, v_2, \cdots, v_k\}$ are pairwise comatching in both G_1 and G_2. Suppose all the $(k-1)$-sums H of G_1 and G_2, produced by summing all $(k-1)$-subsets $\{v_1, v_2, \cdots, v_k\}$, are pairwise comatching graphs. As we discussed, the matching polynomial of G depends on H, $H\backslash u_1$, $H\backslash u_2$, and $H\backslash\{u_1, u_2\}$. In particular, $H\backslash u_1$ can be considered as the $(k-1)$-sum of $G_1\backslash u_1$ and G_2. There is no guarantee that the vertices in the set $\{v_1, v_2, \cdots, v_{k-1}\}$ are still pairwise comatching in $G_1\backslash u_1$. Therefore, the assumption for this argument no longer holds if we were to apply this recursively. Consequently, this recursive way to computing the matching polynomial of k-sums does not lead to a construction for comatching graphs.

Even though we discussed the 2-sum construction for comatching vertices and comatching graphs in the context of multigraphs, we could still apply these constructions to simple graphs. In fact, if we take the 2-sum of two simple graphs G_1 and G_2 with respect to the vertex set $\{a, b\}$, then the resulting 2-sum is a simple graph as long as a and b are not adjacent in at least one of G_1 and G_2. Understanding this is important in our exploration of the proportion of graphs that are comatching to some other graphs, because this big question can only be considered in the context of simple graphs. Therefore, with a small restriction, our construction can be applied to simple graphs and it gives larger simple graphs than the ones we start with.

Chapter 7

Future Directions

In this chapter, we conclude our discussion of cospectral and comatching graphs and vertices by pointing out several directions for future research.

7.1 Other Known Recurrences

Recall that we used a number of recurrences of the matching polynomial to obtain our main constructions. We found the vertex-identification recurrence, which was particularly powerful in our discussion of 2-sums. In our research, we have also found the following recurrences: The vertex-splitting recurrence and the edge-subdivision recurrence.

Figure 7.1 illustrates the vertex splitting operation by showing a graph G and a graph H obtained from splitting the vertex v in G into vertices v_1 and v_2 in H.

7.1 Lemma. *Let G be a connected graph with vertex v. Let H be the graph constructed from splitting the vertex v into two vertices v_1, v_2, such that $N(v_1) \cup N(v_2) = N(v)$ and $N(v_1) \cap N(v_2) = \emptyset$. v_1 and v_2 are not neighbors. Then*

$$\mu(H) = \sum_{a \in N(v_1)} \sum_{b \in N(v_2)} \mu(G \backslash \{v, a, b\}) + x\mu(G).$$

Proof. All matchings in G are still matchings in H, so they contribute the term

$$x\mu(G)$$

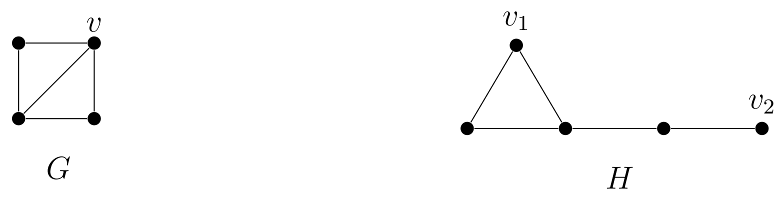


Figure 7.1: A graph G and a graph H obtained from splitting a vertex in G.

to the matching polynomial of H.

Any matching M in H that are not a matching in G must saturate both v_1 and v_2. Then v, as well as two neighbors of v in G, one is a neighbor of v_1 in H and the other a neighbor of v_2 in H, are not saturated by $M\backslash e$ in G. These matchings contribute

$$\sum_{a\in N(v_1)}\sum_{b\in N(v_2)}\mu(G\backslash\{v,a,b\})$$

to the matching polynomial of H. Thus with these possibilities being disjoint we get

$$\mu(H)=\sum_{a\in N(v_1)}\sum_{b\in N(v_2)}\mu(G\backslash\{v,a,b\})+x\mu(G).$$

□

7.2 Lemma. *Let G be a graph and $e=uv$ be an edge in G. Let G' be the graph obtained from subdividing the edge e. Then*

$$\mu(G')=x\mu(G)+x\mu(G\backslash\{u,v\})-\mu(G\backslash\{u\})-\mu(G\backslash\{v\}).$$

Proof. Let e_u and e_v be the two edges in G' that connect v_e to u and v, respectively. Note that any matching in G' is formed by lifting matchings in G in exactly one of the following three ways.

(a) A matching in G containing the edge e could form a matching in G' by replacing e with e_u or e_v. Such matchings in G are counted by $\mu(G)-\mu(G\backslash e)=-\mu(G\backslash\{u,v\})$. Accounting for the one additional vertex in G', we get that these matchings contribute

$$-2\mu(G\backslash\{u,v\})$$

to $\mu(G')$.

(b) Consider a matching in G that does not contain e, and u and v are both saturated or both unsaturated. These matchings still form matchings in G', and they contribute

$$x(\mu(G\backslash e) - x\mu(G\backslash\{u\}) - x\mu(G\backslash\{v\}) + 2x^2\mu(G\backslash\{u,v\})$$

to $\mu(G')$.

(c) The only matchings in G that have not been considered are the ones where exactly one of u and v saturated. They can be lifted to matchings in G' in two ways, because they already form matchings in G, and one of the edges e_u and e_v can be added to these matchings to obtain a proper matching in G'. These matchings contribute $x\mu(G\backslash\{u\}) + x\mu(G\backslash\{v\}) - 2x^2\mu(G\backslash\{u,v\})$ to $\mu(G)$, so they contribute

$$(x\mu(G\backslash\{u\}) + x\mu(G\backslash\{v\}) - 2x^2\mu(G\backslash\{u,v\}))(x - \frac{1}{x})$$

to $\mu(G')$.

Summing the contributions of the three cases together, we obtain that

$$\mu(G') = x\mu(G) + x\mu(G\backslash\{u,v\}) - \mu(G\backslash\{u\}) - \mu(G\backslash\{v\}).$$

□

Just like the other recurrences used in this thesis, the vertex-splitting recurrence and the edge-subdivision recurrence are results that can be applied to obtain the matching polynomial after a certain graph operation. The edge-subdivision recurrence is particularly interesting because Yan and Yeh has a construction for comatching graphs using pairs of d-regular comatching graphs and edge subdivisions [37]. My question is, could we use these recurrences to create more constructions for comatching graphs?

7.2 Graphs Comatching with Their Complements

Other than finding constructions for sets of comatching graphs, we also computed specific examples of pairs of comatching graphs. In particular, we computed the matching polynomial for all graphs over no more than nine vertices. For each $n = 4$ to 9, we partition the set of graphs over n vertices to sets of comatching graphs. We give the percentage of graphs with a comatching mate in Table 7.1. For $n = 4 - 9$, the percentage of graphs with

n	4	5	6	7	8	9
Number of graphs	11	34	156	1044	12346	274668
Number of graphs with a comatching mate	2	16	100	884	11388	269125
Persentage of graphs with a comatching mate	18%	47%	64%	85%	92%	98%

Table 7.1: For $n = 4$ to 9, we computed the percentage of graphs with a comatching mate.

n	4	5	6	7	8	9
Size of largest comatching sets	2	2	4	13	32	188
Number of largest sets	1	8	2	2	1	1

Table 7.2: For each of $n = 4 - 9$, we computed the size of largest sets of comatching graphs over n vertices, and the number of largest sets.

a comatching mate increases as n increases. The size of largest sets of comatching graphs for each of the n values are also shown in Table 7.2.

For any graph G, recall that Theorem 2.5 tells us the matching polynomial of G can be determined by the matching polynomial of its complement. Moreover, if two graphs G_1 and G_2 are comatching, then their complements $\overline{G_1}$ and $\overline{G_2}$ are comatching as well. Therefore, if there exists a set of k graphs that are pairwise-comatching, then their complements form a set of k pairwise comatching graphs as well. However, observe that in Table 7.2 there is only one largest set of comatching graphs for $n = 8$ and $n = 9$. This implies that each graph in these two sets is comatching to its complement, and therefore must have $\frac{n(n-1)}{4}$ edges. There are only 10 self-complementary graphs over 8 vertices and 36 self-complementary graphs over 9 vertices [22]. Therefore, most of the graphs in these largest comatching sets are not self-complementary yet are comatching to their complements. On the other hand, there are 1646 graphs over 8 vertices with 14 edges and 34040 graphs over 9 vertices with 18 edges [26], so the graphs in the largest comatching set(s) for $n = 8$ and $n = 9$ are only a small proportion of graphs with $\frac{n(n-1)}{4}$ edges.

Based on this data, it would be interesting to further explore the following questions:

- For any $n \geq 8$ such that $n \equiv 0$ or $1 \bmod 4$, is there always exactly 1 largest set of pairwise comatching graphs, with $\frac{n(n-1)}{4}$ edges? Note that a graph could possibly have same number of edges as its complement only if $n \equiv 0$ or $1 \bmod 4$, which is why we are considering only these n values.
- When is a non-self-complementary graph comatching with its complement?
- What is the proportion of graphs comatching with its complement out of all non-self-complementary graphs with n vertices and $\frac{n(n-1)}{4}$ edges, for $n \equiv 0$ or $1 \bmod 4$?
- For any $n \equiv 0$ or $1 \bmod 4$, do proportions of graphs with $\frac{n(n-1)}{4}$ edges being in the largest comatching set(s) increase or decrease as n approaches infinity?
- Does this lead to a construction for comatching graphs?

7.3 1-Vertex Extensions and the Matching Coefficient Matrix

To construct comatching pairs of graphs, one method we introduced was through 1-vertex extension, i.e. extending a graph by one vertex in two different ways. In particular, for a given graph G, suppose there exist two disjoint sets $V_1, V_2 \in V(G)$ such that

$$\sum_{i \in V_1} \mu(G \backslash i) = \sum_{i \in V_2} \mu(G \backslash i).$$

Let G_1 and G_2 be 1-vertex extensions of G with respect to V_1 and V_2, respectively. We can see that G_1 and G_2 are comatching by applying the vertex-deletion recurrence to their matching polynomials. In other words, if the sets V_1 and V_2 exist, we could use 1-vertex extensions of G to construct a pair of comatching graphs.

For a graph G with n vertices, its *matching coefficient matrix*, a concept suggested by Chris Godsil, is the $n \times \lfloor \frac{n}{2} \rfloor$ matrix such that the rows correspond to the vertices of G. For row i, the $\lfloor \frac{n}{2} \rfloor$ are the coefficients of $\mu(G \backslash i)$, sorted from coefficient of x^n to the constant term. This matrix is unique up to permutations of rows.

For any graph G, use M_G to denote its matching coefficient matrix and r_G to denote the rank of M_G. When the graph under discussion is clear from context, the subscript is omitted. Observe that the sets V_1 and V_2 exist for G if and only if $M_G\mathbf{x} = \mathbf{0}$ has a non-trivial solution, where each entry of that solution are one of 1, -1, or 0.

n	9	10	11	12	13	14	15	16
Number of Graphs with Solution(s)	61	56	18	10	4	3	0	0
Number of Graphs with Extension(s)	60	55	18	10	4	3	0	0

Table 7.3: Number of graphs with $1, -1, 0$ solutions and number of graphs with comatching extensions for $n = 9 - 16$.

Even though V_1 and V_2 are disjoint, the extensions based on them could still be isomorphic to each other. Therefore, if a graph G has a pair of non-isomorphic comatching extensions, then $M_G\mathbf{x} = \mathbf{0}$ necessarily has a non-trivial solution with each entry being 1, -1, or 0, although it is not sufficient. For each such solution, let A be the set of vertices with entries 1, B be the set of vertices with entries -1, and C be the set of vertices with entries 0. Then form V_1 and V_2 by setting $V_1 = A \cup S$ and $V_2 = B \cup S$ for some $S \subseteq C$. Observe that each 1, -1, 0 solution corresponds to $2^{|C|}$ choices for V_1 and V_2.

We experimented to explore the proportion of graphs with non-isomorphic one vertex extensions. For $n = 9 - 16$, we generated 100 graphs from all graphs over n vertices at random. Computations were performed to see how many of their matching coefficient matrices have non-trivial 1, -1, 0 solutions, and how many such solutions would give a pair of non-isomorphic comatching graphs. The results are shown in Table 7.3.

As n increases, the computation results suggest the proportion of graphs whose matching coefficient matrices with non-trivial $1, -1, 0$ solutions decreases. It indicates that, if almost every graph has a comatching mate, then these comatching pairs are unlikely to be formed by one-vertex extensions. However, due to computational limitations, the experiment can only be performed on relatively small graphs, so these results may not be representative of larger graphs. Even so, it would be interesting to explore if there is a specific type of graphs that this construction applies to.

Meanwhile, the matching coefficient matrix is still interesting to consider because it is a tool to learn about matching-related properties of a graph. Let $A(x)$ be a $n \times n$ matrix polynomial over $\mathbb{C}$ with rank $r \leq n$. Let $d_i(x)$ be the greatest common divisor of all $i \times i$ minors of $A(x)$. Define $d_0 \equiv 1$. Since any minor of order $i \geq 2$ can be expressed as a linear combinations of minors of order $i - 1$, $d_{i-1}(x)$ is a factor of $d_i(x)$. Consider the quotients $\alpha_i = \frac{d_i(x)}{d_{i-1}(x)}$ for $1 \leq i \leq r$. They are called the *elementary divisors* of $A(x)$. For simplicity, we refer to the elementary divisors of the matching coefficient matrix of a graph G as the *matching elementary divisors* of G. Then we have the simple observation below.

7.3 Observation. *Let G be a vertex transitive graph, then its matching elementary divisors are $\alpha_1 = 1$ and $\alpha_i = 0$ for $2 \leq i \leq r$.*

Other than vertex transitive graphs, the matching elementary divisors of the matching coefficient matrices of several classes of graphs are known. Consider the star graphs $K_{1,n-1}$, $n \geq 2$. Their coefficient matrices M has the form

$$M = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & n-2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & n-2 & 0 & \cdots & 0 \end{bmatrix}.$$

Clearly, any $i \times i$ minor with $i \geq 3$ is zero, so the i-th determinant divisor and matching elementary divisor are 0 for $i \geq 3$. Observe that $d_1 = (M) = 1$, and $d_2(M) = n-2$, since only the upper left 2×2 minor is non-zero. Therefore, the matching elementary divisors of $K_{1,n-1}$ are 1 and $n-2$.

Moreover, for $m > n$, we can prove that the matching elementary divisors of $K_{m,n}$ are 1 and $m-n$.

7.4 Lemma. *For $m > n$, the matching elementary divisors of $K_{m,n}$ are 1 and $m-n$.*

Proof. The argument above easily generalizes to $K_{m,n}$ with $m > n$. Note that $K_{m-1,n}$ has $i!\binom{m-1}{i}\binom{n}{i}$ matchings with size i and $K_{m,n-1}$ has $i!\binom{m}{i!}\binom{n-1}{i!}$ matchings with size i. Therefore, its coefficient matrix is

$$M = \begin{bmatrix} 1 & mn-m & \cdots & (n-1)!\binom{m-1}{n-1}\binom{n}{n} & n!\binom{m-1}{n} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & mn-m & \cdots & (n-1)!\binom{m-1}{n-1}\binom{n}{n} & n!\binom{m-1}{n} & 0 & \cdots & 0 \\ 1 & mn-n & \cdots & (n-1)!\binom{m}{n-1} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & mn-n & \cdots & (n-1)!\binom{m}{n-1} & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Since M has rank 2, $K_{m,n}$ has two non-zero matching elementary divisors, with the first being 1. To obtain its second matching elementary divisor, we consider the non-zero 2×2 minors of M.

There are two types of non-zero 2×2 minors of M. The first time contains entries from the i-th column and the $(n+1)$-th column, where $i < n$.

$$\begin{aligned}
&\det\begin{vmatrix} i!\binom{m-1}{i}\binom{n}{i} & n!\binom{m-1}{n} \\ i!\binom{m}{i}\binom{n-1}{i} & 0 \end{vmatrix} \\
= \quad & -\frac{i!(n-1)!n!(m-1)!}{i!(n-1-i)!n!(m-1-n)!}\binom{m}{i} \\
= \quad & -(n-1)\cdots(n-i)(m-1)\cdots(m-n)\binom{m}{i}
\end{aligned}$$

The other type of non-zero 2×2 minors of M takes distinct entries from the $(i+1)$-th and the $(j+1)$-th column. Without loss of generality we may assume $i < j < n$.

$$\begin{aligned}
&\det\begin{vmatrix} i!\binom{m-1}{i}\binom{n}{i} & j!\binom{m-1}{j}\binom{n}{j} \\ i!\binom{m}{i}\binom{n-1}{i} & j!\binom{m}{j}\binom{n-1}{j} \end{vmatrix} \\
= \quad & i!j!\left(\binom{m-1}{i}\binom{n}{i}\binom{n-1}{j}\binom{m}{j} - \binom{n-1}{i}\binom{m-1}{j}\binom{m}{i}\binom{n}{j}\right) \\
= \quad & \frac{(m-1)!n!(n-1)!m!}{i!j!(m-1-i)!(n-i)!(n-1-j)!(m-j)!} \\
& -\frac{(m-1)!n!(n-1)!m!}{i!j!(m-1-j)!(n-j)!(n-1-i)!(m-i)!} \\
= \quad & \frac{(m-1)!n!(n-1)!m!}{i!j!(m-1-i)!(n-i)!(n-1-j)!(m-j)!}[(n-1-i)\cdots(n-j)(m-i)\cdots(m-j+1) \\
& -(m-1-i)\cdots(m-j)(n-i)\cdots(n-j+1)] \\
= \quad & \frac{(m-1)!n!(n-1)!m!(n-1-i)\cdots(n-j+1)(m-1-i)\cdots(m-j+1)}{i!j!(m-1-i)!(n-i)!(n-1-j)!(m-j)!}[(n-j)(m-i) \\
& -(n-i)(m-j)] \\
= \quad & \frac{(m-1)!n!(n-1)!m!(n-1-i)\cdots(n-j+1)(m-1-i)\cdots(m-j+1)(i-j)(m-n)}{i!j!(m-1-i)!(n-i)!(n-1-j)!(m-j)!}
\end{aligned}$$

Note that $m-n$ is a divisor of both types of minors. Moreover,

$$\det\begin{vmatrix} 1 & mn-m \\ 1 & mn-n \end{vmatrix} = -(m-n).$$

Therefore, $m-n$ is the other matching elementary divisor of M. $\square$

Vertex transitive graphs clearly have a matching coefficient matrix with rank 1. It remains to prove or disprove that all graphs with rank 1 coefficient matrices are vertex transitive. Meanwhile, we have the following result, which says the graphs and its complement have the same matching elementary divisors.

7.5 Lemma. *Let G be a graph and use $\overline{G}$ to denote its complement. Then G and $\overline{G}$ have the same matching elementary divisors.*

Proof. We prove the lemma by showing $M_{\bar{G}} = M_G T$, where T is an $\left(\lfloor \frac{n}{2} \rfloor + 1\right) \times \left(\lfloor \frac{n}{2} \rfloor + 1\right)$ matrix with $|\det(T)| = 1$.

Recall that

$$\mu(K_n) = \sum_{a=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^a \frac{n!}{a!(n-2a)!2^a} x^{n-2a}.$$

Theorem 2.5 gives $\mu(\overline{G}) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} p(G,i)\mu(K_{n-2i})$, then we get the following.

$$\mu(\overline{G}) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} \sum_{a=0}^{\lfloor \frac{n}{2} \rfloor} p(G,i)(-1)^a \frac{(n-2i)!}{a!(n-2a-2i)!2^a} x^{n-2a-2i}.$$

Use $\langle x^\alpha, P(x)\rangle$ to denote the coefficient of x^α in $P(x)$, where $P(x)$ is a polynomial in x. For any $0 \le \lfloor \frac{n}{2} \rfloor$, consider $\langle x^{n-2j}, \mu(\overline{G})\rangle$.

$$\begin{aligned}
\langle x^{n-2j}, \mu(\overline{G})\rangle &= \sum_{i=0}^{j} (-1)^{j-i} p(G,i) \frac{(n-2i)!}{(j-i)!(n-2j)!2^{j-i}} \\
&= \sum_{i=0}^{j} (-1)^{j} p(G,i) \frac{(n-2i)!}{(j-i)!(n-2j)!2^{j-i}} \langle x^{n-2i}, \mu(G)\rangle
\end{aligned}$$

Let T be the $\left(\lfloor \frac{n}{2} \rfloor + 1\right) \times \left(\lfloor \frac{n}{2} \rfloor + 1\right)$ matrix such that

$$\begin{aligned}
&[\langle x^n, \mu(\overline{G})\rangle \quad \langle x^{n-2}, \mu(\overline{G})\rangle \quad \cdots \quad \langle x^{n-2\lfloor \frac{n}{2} \rfloor}, \mu(\overline{G})\rangle] \\
=&[\langle x^n, \mu(G)\rangle \quad \langle x^{n-2}, \mu(G)\rangle \quad \cdots \quad \langle x^{n-2\lfloor \frac{n}{2} \rfloor}, \mu(G)\rangle]T.
\end{aligned}$$

Then based on the discussion above, the ij-th entry of T is

$$T_{ij} = \begin{cases} 0 & i > j; \\ (-1)^{j-1}\frac{(n-2i+2)!}{(j-i)!(n-2j+2)!2^{j-i}} & i \leq j. \end{cases}$$

In particular, note T is upper-triangular, and all diagonal entries of T are ± 1, so $|\det(T)| = 1$. Moreover, the entries of T only depends on n, and does not depend on the structure of the graph G at all. Use T_n to denote such a matrix T for graphs over n vertices.

Let M be the matching coefficient matrix of a graph G, and let $\overline{M}$ be the matching coefficient matrix of $\overline{G}$, then $\overline{M} = MT_{n-1}$. Let $S(M)$, $S(\overline{M})$ denote the Smith Normal form of M, $\overline{M}$, respectively. Then $S(\overline{M}) = S(M)S(T)$. Since $|\det(T_{n-1})| = 1$, we may conclude $S(\overline{M}) = S(M)$, which implies G and $\overline{G}$ has the same matching elementary divisors. $\square$

This discussion about matching coefficient matrix and matching elementary divisor lead to the following questions.

- Could we characterize the graphs with two non-isomorphic comatching extensions?
- Are the ranks of the matching coefficient matrices of a pair of comatching graphs always equal?
- Do a pair of comatching graphs always have the same matching elementary divisors?
- We computed the matching coefficient matrix and matching elementary divisors for paths up to 16 vertices. All these matrices have the maximum rank possible and have all 1's as matching elementary divisors. Is this true for all paths? What about other basic graphs such as cycles or wheels?

7.4 The Rook Polynomial

As we mentioned in Chapter 1, the rook polynomial is an alternatively version of the matching polynomial for bipartite graphs. For a bipartite graph G, *the rook polynomial* of G is defined as is defined as

$$R(G, x) = \sum_i p(G, k)x^i.$$

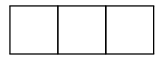


Figure 7.2: A board

This polynomial arose from Riodian's research in restricted permutations [30]. It is called the rook polynomial because Riodian originally considered such permutation problems as placing non-attacking rooks on a chess board that is not necessarily square-shaped. Note two rooks are non-attacking if they are not in the same row or the same column. Any such board corresponds to a bipartite graph, where each row and each column is a vertex, and there is an edge between a vertex representing a row and a vertex representing a column if there is a cell at a corresponding position in the map. Then each k-matching in the bipartite graph corresponds to a unique way to place k non-attacking rooks on the board. For example, the board in Figure 7.2 corresponds to the graph $K_{1,3}$. and its rook polynomial is $R(K_{1,3}, x) = 1 + 3x$. In general, we can see that

$$\mu(G) = x^{m+n} R(G, x^{-2}).$$

Two boards are *rook equivalent* if their corresponding bipartite graphs have the same rook polynomial. Note that rotation, reflection, and permutations of rows and columns are operations that preserve rook equivalence, because the corresponding bipartite graph is unchanged. As one might suspect, there exist boards that are rook equivalent such that one could not start from one of the equivalent boards, and obtain another one of the equivalent boards using these operations. The smallest non-trivial pair of rook equivalent boards B_1 and B_2 are shown in Figure 7.3. However, the bipartite graphs G_1 and G_2 corresponding to these two boards are not comatching, because one of them have five vertices and the other one has four.

Meanwhile, the fact that the two graphs G_1 and G_2 that these two boards correspond to are rook equivalent implies that $p(G_1, k) = p(G_2, k)$ for all non-negative integers k, and we say these graphs are *matching equivalent*. The difference in number of vertices caused the matching polynomials to be different, but we have $\mu(G_1) = x\mu(G_2)$. In other words, the graphs G_1 and $G_2 \cup K_1$ are comatching. Generally speaking, if we have a pair of rook equivalent boards whose corresponding graphs are not comatching, then we can obtain a pair of comatching graphs by adding an appropriate number of vertices to one of them. Therefore, understanding constructions for pairs of rook equivalent boards is of our research interest.

Being one of the first individuals to study rook equivalence, Riodian proved some basic observations about rook equivalent boards. For example, given a pair of rook equivalent

Figure 7.3: The smallest non-trivial pair of rook equivalent boards B_1(left) and B_2(right)

boards, he constructed a pair of larger rook equivalent boards by attaching a rectangular board with a number of rows that is no less than the number of rows of both of the original pair of rook equivalent boards. To understand this construction using matching polynomials, we observe that the bipartite complement of the graphs corresponding to the original pair of boards and that of the constructed pair of boards are the same. Godsil proved that the matching polynomial of a bipartite graph is determined by its bipartite complement [10, Theorem 1.3.1]. Therefore, with some additions or subtraction of vertices if necessary, we can see that, if the graphs corresponding to the original pair of boards are matching equivalent, then the constructed pair of boards are rook equivalent.

Several others have also provided various constructions for rook equivalent boards. In 1970, Foata and Schüzenberger proved that all Ferrers boards are rook equivalent to exactly one strictly decreasing Ferrers board [6]. Five years later, Goldman, Joichi, and White gave an alternative proof of the same result [29]. In 1986, Garsia and Remmel gave a characterization of rook equivalent Ferrers boards [7]. In more recent years, the more significant result in this direction was due to Bloom and Saracino's result in 2018 and 2019, where then proved rook equivalence implies Wilf equivalence and vice versa [2, 3].

Here, we would like to ask,

- What do these results imply in terms of graphs theory and comatching graphs?
- Could we extend these results to general graphs that are not necessarily bipartite?

These are some questions to be further explored.

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Implicit Function Theorem

Below is a version Implicit Function Theorem stated as Theorem 1.3.1 in [23]. For more information about the Implicit Function Theorem, please refer to [23].

Theorem ([23]). *Let $\mathcal{F}$ be a real-valued continuously differentiable function defined in a neighborhood $(X_0, Y_0) \in \mathbb{R}^2$. Suppose that $\mathcal{F}$ satisfies two conditions.*

$$\mathcal{F}(X_0, Y_0) = Z_0,$$

$$\frac{\partial \mathcal{F}}{\partial Y}(X_0, Y_0) \neq 0.$$

Then there exists open intervals U and V, with $X_0 \in U$, $Y_0 \in V$, and a unique function $F : U \to V$ satisfying

$$\mathcal{F}(X_0, F(X_0)) = Z_0, \text{ for all } X \in U,$$

and this function F is continuously differentiable with

$$\frac{\partial Y}{\partial X}(Y_0) = F'(X_0) = -\left[\frac{\partial \mathcal{F}}{\partial X}(X_0, Y_0) \Big/ \frac{\partial \mathcal{F}}{\partial Y}(X_0, Y_0)\right].$$

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