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In Part I, we study the noncrossing bond poset of a graph. The partition lattice and noncrossing partition lattice are well studied objects in combinatorics. Given a graph G on vertex set $\{1, 2, \ldots, n\}$, its bond lattice, L_G, is the subposet of the partition lattice formed by restricting to the partitions whose blocks induce connected subgraphs of G. In this article, we introduce a natural noncrossing analogue of the bond lattice, the noncrossing bond poset, NC_G, obtained by restricting to the noncrossing partitions of L_G. Both the noncrossing partition lattice and the bond lattice have many nice combinatorial properties. We show that, for several families of graphs, the noncrossing bond poset also exhibits these properties. We present simple necessary and sufficient conditions on the graph to ensure the noncrossing bond poset is a lattice. Additionally, for several families of graphs, we give combinatorial descriptions of the Möbius function and characteristic polynomial of the noncrossing bond poset. These descriptions are in terms of a noncrossing analogue of non-broken circuit (NBC) sets of the graphs and can be thought of as a noncrossing version of Whitney's NBC theorem for the chromatic polynomial. We also consider the shellability and supersolvability of the noncrossing bond poset, providing sufficient conditions for both.

In Part II, we study topological indices of finite graphs. A *topological index* is a function from the set of graphs to $\mathbb{C}$ which is invariant under graph isomorphism. We study indices such as the Randić index, the radius, and the largest eigenvalues of the adjacency, Laplacian, and signless Laplacian matrices of graphs; i.e., *spectral radii*. We aim to find the extremal graphs of the ratio of the Randić index against the other indices listed above and present two new theorems as well as our work on an open problem relating the Randić index to the radius of a graph. We also study a known open problem involving the Randić index of a graph and the graph theoretic radius of a graph.

THE NONCROSSING POSET AND TOPOLOGICAL INDICES OF FINITE
GRAPHS

by

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PREFACE

I have participated in original research since my time at Winthrop University as an undergraduate. Each research project has been centered around the topic of finite graphs. During my time at Wake Forest University, I took my first course in graph theory and fell in love with the subject. I pursued a master's project on the noncrossing bond poset, in which I studied poset and order theory, where topics in graph theory remained present. This fruitful project continued into my doctoral work and led to a very successful paper in the Electronic Journal of Combinatorics. My academic advisors, Clifford Smyth (UNC Greensboro) and Joshua Hallam (Loyola Marymount University), were invaluable in this process. I continued to study topics in graph theory. For the sake of fulfilling the computational component to my doctoral work, I chose to study the topic of topological indices on finite graphs. This presented an amazing opportunity to use computational methods and analysis on finite graphs. Moving forward, I know that I will always want to keep graph theory and combinatorics at the center of my research.

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Part I

The Noncrossing Bond Poset of a Graph

Chapter 1: Introduction

We'll begin by defining a widely studied family of objects in combinatorics known as *partially ordered sets* (or *posets*). These play a critical role in the field of enumerative and algebraic combinatorics. In particular, Möbius inversion on partially ordered sets can be viewed as a generalization of the Principle of Inclusion-Exclusion. Posets have a strong presence not only in combinatorics, but also in many other fields.

In 1972, Kreweras [40] introduced the *noncrossing set partition lattice* on $[n] := \{1, 2, \ldots, n\}$, denoted by NC_n. Figure 1.1 shows all the noncrossing and crossing set partitions of the five element set[1]. NC_n has received considerable attention from the combinatorial community. As a partially ordered set, it enjoys several interesting combinatorial and order-theoretic properties. Among the properties we define in this thesis, NC_n is graded, EL-shellable [10], self-dual (hence rank-symmetric) [40], and supersolvable [33]. It is also know that NC_n has size $C_n = \frac{1}{n+1}\binom{2n}{n}$, the nth Catalan number. Stanley described over 200 different combinatorial interpretations of C_n in [67]. It is also known that maximal chains of NC_n are equinumerous with spanning tress of the complete graph K_n. We refer the reader to McCammond's [43] and Simion's [62] surveys for more information on the many beautiful properties of noncrossing set partitions, both within and outside of combinatorics. These surveys show some of the amazing connections that NC_n has in areas outside of combinatorics, such as low-dimensional topology, geometric group theory, mathematical biology, and noncommutative probability.

The noncrossing set partition lattice has been studied and generalized in several ways (see [3,4,7,13–16,46,57]). In Part I of this thesis, we introduce a new generalization of the noncrossing set partition lattice on $[n]$ which is based on the structure of finite graphs of order n. Given a graph G with vertex set $[n]$, its bond lattice is a subposet of the partition lattice obtained by restricting it to the set of partitions such that for each block B in the partition, the induced subgraph of G with vertex set B is connected. The *noncrossing bond poset* of a graph is the intersection of the noncrossing partition lattice and its bond lattice.

We will see that while the noncrossing bond poset of a graph of order n is

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[1]This image comes from `https://en.wikipedia.org/wiki/Noncrossing_partition` with no author provided.
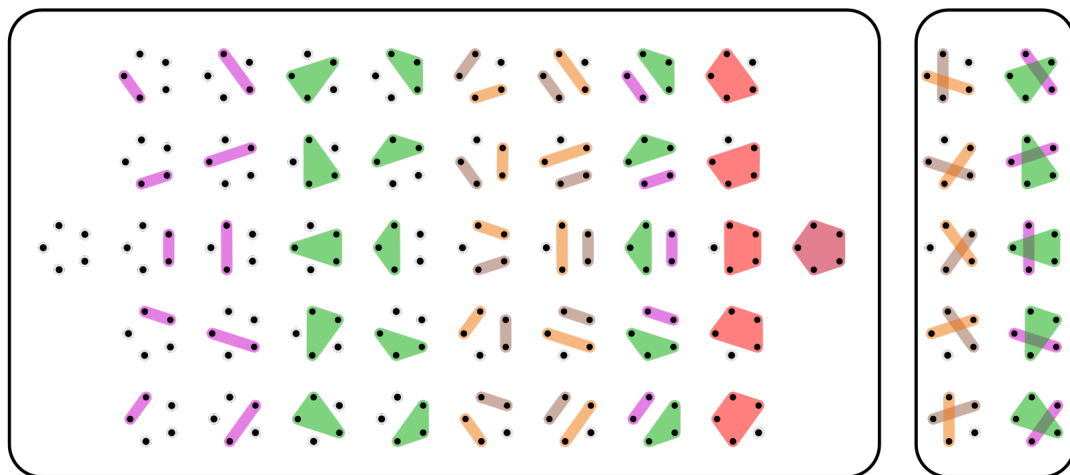
Figure 1.1. Noncrossing partitions on [5]

a generalization of NC_n, it does not necessarily have all the nice order theoretic properties listed above. This is not surprising since the structure of graphs can vary widely. Hence, one of the main goals of this project is to identify families of graphs for which some of these nice properties still hold. We will present necessary and sufficient condition on the graph for the noncrossing bond poset to be a lattice (see Theorem 3.11). We provide a combinatorial interpretation of the Möbius function and characteristic polynomial of the noncrossing bond poset when it is graded in terms on an analogue of non-broken circuit (NBC) sets (see Theorem 3.28). We then present conditions which imply that noncrossing bond poset is EL-shellable (see Theorem 3.41).

We also give two algorithms for non-crossing bond posets in the appendix. Algorithm A.1 determines if the noncrossing bond poset of a graph is a lattice. Algorithm A.6 determines if a graph belongs to a family of graphs for which the noncrossing NBC interpretation of the Möbius function and characteristic polynomial hold. Our algorithms both run in time polynomial in n, the number of vertices of the graph. This is of interest because brute-force algorithms that do not take advantage of the theory we develop can, in the worst case, take time super-exponential in n. Our work on the noncrossing bond poset was published in the Electronic Journal of Combinatorics in 2020 [23]. This was joint work with Joshua Hallam.[2]

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[2]Loyola Marymount University.

Chapter 2: Preliminaries

2.1 Partially Ordered Sets

For a finite set S, we use the notation $\#(S)$ to denote the size, or cardinality, of S.

Definition 2.1. A **partially ordered set** (or **poset**) P is a set with a partial ordering "$\leq$" such that the following hold for all $x, y, z \in P$:

1. $x \leq x$;

2. if $x \leq y$ and $y \leq x$, then $x = y$;

3. if $x \leq y$ and $y \leq z$, then $x \leq z$.

   Note that a relation satisfying Property 1 (respectively, Property 2, Property 3) is said to be reflexive (respectively, antisymmetric, transitive).

   We say that two elements x and y of a poset P are *incomparable* if $x \nleq y$ and $y \nleq x$; otherwise, we say that x and y are *comparable*. We write $x < y$ to mean $x \leq y$ and $x \neq y$. If P is a poset with elements x and y, laws of trichotomy need not apply. That is, it need not be the case that at least one of the following hold: $x < y$, $y < x$, or $x = y$. This is what merits the name of "partial order." If P is a poset for which every pair of elements is comparable, then we say P is *totally ordered.*

Example 2.2. If T is any totally ordered set (e.g., $\mathbb{R}$ or $[n]$) then it is easy to show that T satisfies the above axioms. Let W be the set of all English words where if $x, y \in W$, $x \leq y$ if and only if every letter of x is a letter of y. It is easy to show that this is a poset. Further, it is easy to show that W is not totally ordered. The words $x = $ math and $y = $ number are incomparable.

   We say that x is a *minimal* element of a poset P if there is no $y \in P$ such that $y < x$. Likewise, we say that x is a *maximal* element of P if there is no $y \in P$ such that $x < y$. We say that x is the *bottom element* of a poset P if $x \leq y$ for all $y \in P$. We say that x is the *top element* of a poset P if $x \geq y$ for all $y \in P$. If P has a bottom element, it is unique by asymmetry, and we denote it by $\hat{0}$. Likewise, if P has a top

element, then it too is unique, and we denote it by $\hat{1}$. If P is a poset which contains both a $\hat{0}$ and a $\hat{1}$, then we say that P is a *bounded poset*.

If s and t are elements of a poset P, we say that t *covers* s (or that s is *covered by* t) if $s < t$ and there is no element $x \in P$ such that $s < x < t$; we denote this by $s \lessdot t$. If P is a poset with a $\hat{0}$, then $x \in P$ is called an *atom* if $\hat{0} \lessdot x$. Similarly, if P is a poset with $\hat{1}$, then $x \in P$ is called a *coatom* if $x \lessdot \hat{1}$. We will later use $A(P)$ to denote the set of atoms of a poset, and $\mathrm{CA}(P)$ to denote the set of coatoms of P.

The *Hasse Diagram* of a poset P is a graphical representation of a poset P. The Hasse diagram is a directed graph whose vertices are the elements of P such that there is a directed edge from s to t if and only if $s \lessdot t$. This relationship is captured not by drawing an arrow on the edge, but rather by drawing s some distance below t on the page. Such diagrams are particularly useful illustrating various order theoretic properties of posets.

We call subset Q of P a *subposet* of P if $s \leq t$ in Q implies that $s \leq t$ in P, in which case we'll call P a *refinement* of Q. We call Q an *induced subposet* of P if for all $s, t \in Q$, $s \leq t$ in Q if and only if $s \leq t$ in P. In this case, we say Q has the order induced by P. In this thesis, we only consider induced subposets when we mention subposets. Let P and Q be posets. We say that P and Q are isomorphic if there exists a bijection $\varphi : P \to Q$ such that $x \leq y$ in P if and only if $\phi(x) \leq \phi(y)$ in Q.

Let C be a subposet of a poset P. If for all $x, y \in C$ we have that x and y are comparable, then we call C a *chain* of P. If C is a chain such that there is no $z \in P$ with $x < z < y$ for any $x, y \in C$, then C is called a *saturated chain*. Furthermore, C is called a *maximal chain* of P if it is not properly contained in any other chain of P. It's easy to see that maximal chains are saturated, but a saturated chain need not be maximal.

If s and t are elements of a poset P and $s \leq t$, then the interval from s to t in P is the set $[s, t] := \{x \in P : s \leq x \leq t\}$. Figure 2.1 displays an example of an interval which is not a chain. The set of all intervals of a poset P is denoted by $\mathrm{Int}(P) := \{[s, t] : s, t \in P \text{ and } s \leq t\}$. If $\mathrm{Int}(P)$ contains only finite sets, then P is said to be *locally finite*. The set of integers is an example of an infinite poset which is locally finite.

The length of a finite chain C is denoted by $\ell(C)$ and is defined by $\ell(C) = \#(C) - 1$. We call P a *graded poset of rank n* if all maximal chains of P are of length n. There is a natural function associated with graded posets called the *rank function*, $\rho : P \to \mathbb{Z}_{\geq 0}$ where $\rho(x) = 0$ if x is a minimal element of P and $\rho(x) = \rho(y) + 1$ whenever $x \lessdot y$. If $[s, t]$ is an interval in a ranked poset with rank function ρ then the length of $[s, t]$ is defined to be $\ell(s, t) := \rho(t) - \rho(s)$.

Example 2.3. The poset P in Figure 2.1 is clearly graded. If a poset P is graded, one can draw the Hasse diagram so that all elements of equal rank are drawn at the same height; i.e., the Hasse diagram will appear "level." An example of a poset which
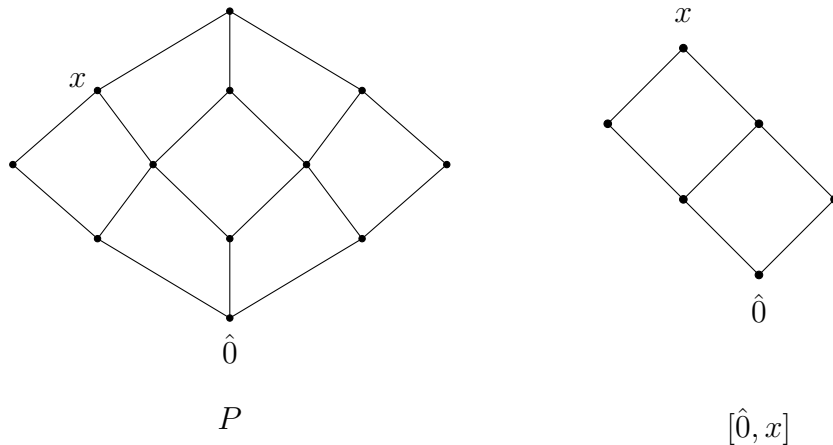
Figure 2.1. A graded poset P and an interval in P.

is not graded is $Q = \{\hat{0}, x_1, x_2, x_3, \hat{1}\}$ where $x_1 < x_2$ and x_3 is not comparable with either x_1 or x_2. Q has two maximal chains; one of length 3 and one of length 2. Note that a graded poset can have more than one minimal element and/or more than one maximal element. For instance, deleting $\hat{0}$ and $\hat{1}$ from the poset P in Figure 2.1 leaves behind a graded poset with no $\hat{0}$ or $\hat{1}$. Also note that a poset with a bottom and/or top element need not be graded (as in our example Q).

The *direct product* of P and Q is the poset $P \times Q$ on the set $\{(s, t) : s \in P, t \in Q\}$ such that $(s, t) \leq (s', t')$ if and only if $s \leq s'$ and $t \leq t'$. If P is a poset, then the *dual of P* is the poset P^* such that $s \leq t$ in P^* if and only if $t \leq s$ in P. In other words, P^* is P "upside down". We say that P is *self dual* when $P \cong P^*$.

Example 2.4. Let $\mathbf{1} := \{0, 1\}$ be the poset with two elements 0 and 1 with $0 < 1$. Then $\mathbf{1}^n$ is the poset on the set $\{(\epsilon_1, \epsilon_2, \ldots, \epsilon_n) : \epsilon_i \in \{0, 1\}\}$ such that $(\epsilon_1, \epsilon_2, \ldots, \epsilon_n) \leq (\delta_1, \delta_2, \ldots, \delta_n)$ if and only if $\epsilon_i \leq \delta_i$ for each $1 \leq i \leq n$. Now let B_n be the poset, known as the Boolean algebra, on the set of all subsets of $[n]$ ordered by inclusion. It's easy to see that $B_n \cong \mathbf{1}^n$ since the function $\varphi : B_n \to \mathbf{1}^n$ where $S \mapsto (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)$ such that $e_i = 1$ if $i \in S$ and 0 otherwise is a bijection.

Example 2.5. Consider the Boolean algebra B_n. The function $\varphi : B_n \to B_n^*$ defined by $\varphi(S) = [n] \backslash S$ is easily seen to be an order preserving isomorphism; hence, B_n is self dual.

Definition 2.6. Let P be a poset and let $\mathcal{E}(P)$ denote the set of edges in the Hasse diagram of P; that is, $\mathcal{E}(P) := \{(x \lessdot y) : x, y \in P \text{ and } x \lessdot y\}$. A function $\lambda : \mathcal{E}(P) \to \Lambda$ for some poset Λ is called an **edge labelling** of P and Λ is the set of labels. Now let

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$c = x_1 \lessdot x_2 \lessdot \cdots \lessdot x_k$ be some saturated chain of P. We say that c is **increasing** with respect to λ if

$$\lambda(x_1 \lessdot x_2) < \lambda(x_2 \lessdot x_3) < \cdots < \lambda(x_{k-1} \lessdot x_k).$$

Likewise, we say a saturated chain c is **decreasing** with respect to λ when

$$\lambda(x_1 \lessdot x_2) \geq \lambda(x_2 \lessdot x_3) \geq \cdots \geq \lambda(x_{k-1} \lessdot x_k).$$

When it is clear from the context that the chains under discussion are saturated, we may refer to some of those chains as simply being increasing or decreasing.

Let P be a poset with elements s and t. We say that an element y of P is an *upper bound* of s and t if $s, t \leq y$. We say that y is the least upper bound or *join* of s and t if $s, t \leq y$ and $y \leq z$ for all upper bounds z of s and t. It is not always the case that s and t have a join, but if they do, the join is unique. If the join of s and t exists, it is denoted by $s \vee t$. We say that an element y of P is a *lower bound* of s and t if $y \leq s, t$. We say that y is the greatest lower bound or *meet* of s and t if $y \leq s, t$ and $z \leq y$ for all lower bounds z of s and t. It is not always the case that s and t have a meet, but if they do, the meet is unique. If the meet of s and t exists, it is denoted by $s \wedge t$.

Remark. The notation "$\vee$" is motivated by the fact that the join of sets S and T in the Boolean algebra B_n is $S \cup T$ (and similarly for "$\wedge$").

If L is a poset such that every pair of elements has a meet and a join, then we say that L is a *lattice*. Note that lattices may be defined by a set of axioms(see Section 3.3 of [66]). We will not take this approach and will instead consider "being a lattice" as a property that a poset may or may not have. Note that a finite lattice always has $\hat{0}$ and $\hat{1}$; $\hat{0}$ will be meet of all elements in L and $\hat{1}$ will be the join of all elements in L. A *meet-semilattice* is a poset P for which any two elements have a meet. Likewise, a *join-semilattice* is a poset P for which any two elements have a join.

Proposition 2.7. *[66] A finite meet-semilattice L with a top element $\hat{1}$ is a lattice. Dually, a finite join-semilattice L with a unique minimal element $\hat{0}$ is a lattice.*

This proposition easily follows from the observation that the meet of all elements that lie above two elements s and t is necessarily the join of s and t.

A lattice L is said to be *atomic* if for each x in L there exists a set $S \subseteq A(L)$ such that $x = \bigvee_{a \in S} a$, i.e. each element of L is a join of atoms. This will also hold for $\hat{0}$ as we adopt the convention that $\hat{0}$ is the join of the empty set of atoms. We say that a lattice L is *(upper) semimodular* if it is graded with rank function ρ such that for each $x, y \in L$, $\rho(x \vee y) + \rho(x \wedge y) \leq \rho(x) + \rho(y)$. Similarly, L is lower semimodular, if $\rho(x \vee y) + \rho(x \wedge y) \geq \rho(x) + \rho(y)$ for all $x, y \in L$.

Example 2.8. Note that the posets on the left and on the right in Figure 2.2 are lattices. The left poset is graded while the right is not. The middle poset is graded but is not a lattice because a and c do not have a join. In that poset, both b and d are upper bounds of a and c, but there is no upper bound y of a and c with $y \leq b, d$. Similarly, b and d do not have a meet. These examples show that being graded is neither necessary nor sufficient for being a lattice.
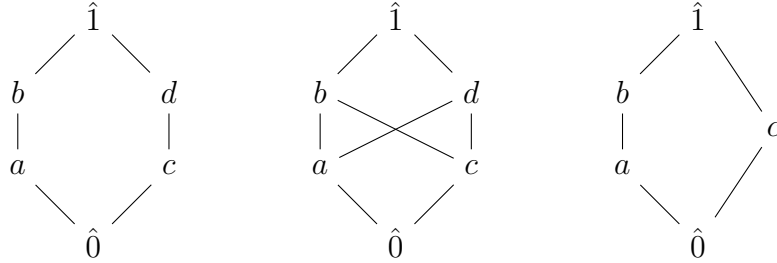
Figure 2.2. A lattice (left), a non-lattice (middle), and a non-graded lattice (right).

Definition 2.9. A **set partition** of $[n]$ is a collection of non-empty, disjoint subsets of $[n]$ whose union is $[n]$. We refer to the subsets of a partition as the **blocks** of the partition. A partition π of $[n]$ will written as $B_1/B_2/\ldots/B_k$ where the blocks are ordered lexicographically. Note that the lexicographic order on the subsets of $[n]$ is the total order defined by setting $S = \{s_1 < s_2 < \cdots\} < \{t_1 < t_2 < \cdots\} = T$ if and only if there is an index k such that for all $i < k$ we have $s_i = t_i$ and then $t_k > s_k$ or s_{k-1} is the largest element of S.

The **set partition lattice of** $[n]$, denoted by Π_n, is the poset obtained by ordering all set partitions of n by refinement. That is, if $\sigma, \tau \in \Pi_n$, then $\sigma \leq \tau$ if and only if every block of σ is contained in a block of τ.

Example 2.10. Note that $1/23/4$ and $13/24$ are partitions in Π_4 that are are incomparable, whereas $1/2/34 \leq 12/34$.

The number of set partitions of $[n]$ into k blocks is called the *Stirling number of the second kind* and is denoted by $S(n, k)$. We adopt the conventions that $S(0, 0) = 1$ and $S(n, 0) = 0$ for $n > 0$. The Bell number, $B_n = \sum_{k=0}^{n} S(n, k)$, is the total number of set partitions of $[n]$.

The main objects of study in this chapter will be Π_n and various subposets of Π_n. Figure 2.3 shows the Hasse diagrams of Π_3 and Π_4. It is known that Π_n is a graded lattice for $n \geq 1$ with both a bottom element (the partition $1/2/\cdots/n$) and a top element (the partition with exactly one block, $12\cdots n$.) In a later section, we will present a well-studied subposet of Π_n known as the *noncrossing partition lattice*, as well as a new subposet of Π_n we introduce called the *noncrossing bond poset*.

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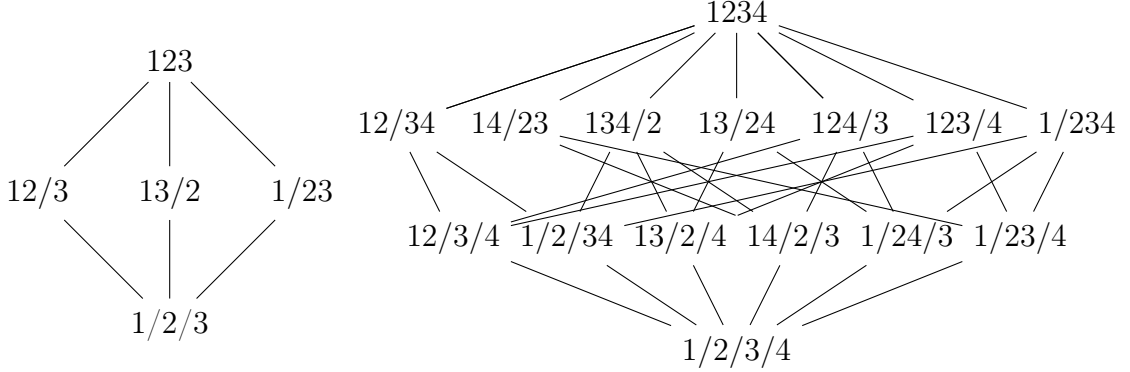
Figure 2.3. The Hasse diagrams of Π_3 and Π_4.

Let P be a locally finite poset and K be a field. Let $I(P, K)$ denote the set of all functions f such that $f : \text{Int}(P) \to K$. For ease of notation we write $f([x, y]) = f(x, y)$ for all $x, y \in P$ with $x \leq y$.

Given $f, g \in I(P, K)$ and $a \in K$ we define the scalar multiple af and sum $f + g$ in $I(P, K)$ by $(af)(x, y) = af(x, y)$ and $(f + g)(x, y) = f(x, y) + g(x, y)$ for all $x \leq y$. We also define the multiplication of f and g to be the function $f * g$ in $I(P, K)$ defined by

$$(f * g)(x, y) := \sum_{x \leq z \leq y} f(x, z)g(z, y),$$

for all $x \leq y$. The multiplication $*$ is also called *convolution*.

The set $I(P, K)$ together with these operations of scalar multiplication, addition, and convolution, is a K-algebra called the **incidence algebra** of P over K.

The following function δ is the multiplicative identity of $I(P, K)$:

$$\delta(x, y) := \begin{cases} 1, & x = y \\ 0, & \text{otherwise.} \end{cases} \tag{2.1}$$

If $f, g \in I(P, K)$ and $f * g = \delta$, then we say that f is a *left-inverse* of g and that g is a *right-inverse* of f. If we have $f * g = g * f = \delta$, then we say that f is *invertible* and that $f^{-1} = g$ is the *two-sided inverse* (or just *inverse*) of f. (Likewise, g is also invertible and the inverse of g is $g^{-1} = f$.)

In our work, we will always take K to be either $\mathbb{R}$ or $\mathbb{C}$.

Proposition 2.11 ([66]). *Let $f \in I(P, K)$. Then the following conditions are equivalent:*

1. f has a left inverse;

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2. *f has a right inverse;*

3. *f has a two-sided inverse (which is necessarily the unique left and right inverse).*

4. $f(t,t) \neq 0$ *for all* $t \in P$

Define the function ζ in $I(P, K)$ by $\zeta(x, y) = 1$ for all $x \leq y$. Since $\zeta(x, x) = 1 \neq 0$ for all x, Theorem 2.11 implies that ζ has a unique multiplicative inverse in $I(P, K)$. We define the *Möbius* function μ to be the multiplicative inverse of ζ, i.e. $\mu = \zeta^{-1}$. The zeta function enjoys many nice combinatorial properties. For instance, if P is a poset with $x \leq y \in P$, then

$$\zeta^2(x, y) = \sum_{x \leq z \leq y} \zeta(x, z)\zeta(z, y)$$

$$= \sum_{x \leq z \leq y} 1$$

$$= \#[x, y].$$

Hence, the zeta function can be used to count the number of elements in an interval of a poset P. The reader can see [66] for more uses of ζ.

Note that μ may also be defined "recursively" as in the following proposition.

Proposition 2.12. *The Möbius function μ may be defined by*

$$\mu(x, y) = \begin{cases} 1, & x = y \\ -\sum_{x \leq z < y} \mu(x, z), & x < y, \end{cases} \tag{2.2}$$

for all $x \leq y$.

Proof. By Theorem 2.11, $\mu = \zeta^{-1}$ is equivalent to $\mu * \zeta = \delta$. This in turn is equivalent to $\mu(x, x) = \mu(x, x)\zeta(x, x) = (\mu * \zeta)(x, x) = \delta(x, x) = 1$ for all x and $\sum_{x \leq z \leq y} \mu(x, z) = \sum_{x \leq z \leq y} \mu(x, y)\zeta(z, y) = (\mu * \zeta)(x, y) = \delta(x, y) = 0$ for all $x < y$. The second equation may be rewritten as $\mu(x, y) = -\sum_{x \leq z < y} \mu(x, z)$ for all $x < y$. $\square$

For a poset P, Equation 2.2 is often called the *two variable Möbius* function for some $x \leq y \in P$. If P contains $\hat{0}$ and $\hat{1}$, then we define $\mu(P) := \mu(\hat{0}, \hat{1})$. If P is a poset with $\hat{0}$, then for $x \in P$, we may define the *one variable Möbius* function $\mu(x) := \mu(\hat{0}, x)$. We often refer to the values $\mu(x)$ and $\mu(P)$, collectively, as the *Möbius values* of P.

Some posets allow for the computation of their Möbius values with nice closed formulas. We now demonstrate this phenomenon with the poset B_n. It's a standard result that for posets P and Q, we have

$$\mu_{P \times Q}((s, t), (s', t')) = \mu_P(s, t)\mu_Q(s', t'). \tag{2.3}$$

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We saw in Example 2.4 that $B_n \cong \mathbf{1}^n$. In $\mathbf{1}$, it is easy to compute $\mu(0,0) = \mu(1,1) = 1$ and $\mu(0,1) = -1$. Now, let $T \le S$ in B_n. Observe that the interval $[T, S]$ in B_n has length $\ell(T, S) = \#(S - T)$. This is because $x \lessdot y$ in B_n if and only if $y = x \cup \{i\}$ for some $i \in [n]$ where $i \notin x$. We can identify T and S with the unique n-tuples $(t_1, \dots, t_n)$ and $(s_1, \dots, s_n)$ where $t_i = 1$ (respectively $s_i = 1$) if $i \in T$ (respectively if $i \in S$). Then $\ell((t_1, \dots, t_n), (s_1, \dots, s_n)) = \ell(T, S)$ and by 2.3 we get that

$$
\begin{aligned}
\mu_{B_n}(T, S) &= \mu_{\mathbf{1}^n}((t_1, \dots, t_n), (s_1, \dots, s_n)) \\
&= \mu_{\mathbf{1}}(t_1, s_1)\mu_{\mathbf{1}}(t_2, s_2) \cdots \mu_{\mathbf{1}}(t_n, s_n) \\
&= (-1)^{f(n)},
\end{aligned}
$$

where $f(n)$ is the number of times $\mu_{\mathbf{1}}(t_i, s_i) = -1$. This only occurs when $\mu_{\mathbf{1}}(t_i, s_i) = \mu_{\mathbf{1}}(0,1)$; i.e., when $t_i < s_i$ if and only if $i \notin T$ and $i \in S$. Hence, $f(n) = \#(S - T)$ so $\mu_{B_n}(T, S) = (-1)^{\#(S-T)}$.

The reader may refer to Section 3.8 of [66] for techniques on computing $\mu(P)$ for various posets. Such techniques can involve counting chains $\hat{0} = t_0 < t_1 < \cdots < t_i = \hat{1}$ of length i. One of our goals is determining classes of graphs for which the noncrossing bond poset allows for easy computation of its Möbius values. We will also utilize the following.

Definition 2.13. Let P be a finite, graded poset with $\hat{0}$. Then the **characteristic polynomial** of P in the variable t is denoted and defined as

$$
\chi(P, t) = \sum_{x \in P} \mu(x) t^{\rho(P) - \rho(x)}.
$$

Characteristic polynomials often provide very useful information about posets. Namely, the coefficients may encode information about poets. We will see more of this concept in Chapters 3 and 4.

2.2 Poset Topology and Shellability

Definition 2.14. Let P be a finite set. We say that Δ is an *abstract simplicial complex on P* (or just a *simplicial complex on P*) if Δ is a family of subsets of P such that

1. $\{v\} \in \Delta$ for all $v \in P$;

2. if $G \in \Delta$ and $F \subseteq G$, then $F \in \Delta$ (closed under taking subsets).

The elements of Δ are called *simplices* (or *faces*) of Δ. For ease of notation, we'll denote a simplex $S = \{v_1, v_2, \ldots, v_k\}$ as $v_1 v_2 \ldots v_k$. We say that a simplex F has dimension k and write $\dim(F) = k$ when $\#F = k + 1$. The dimension of a simplicial complex Δ is defined as $\dim(\Delta) := \max_{F \in \Delta} \dim(F)$. If a simplex is not properly contained in another simplex of Δ, then it is called a *maximal simplex of* Δ. Maximal simplices need not have equal dimension in Δ. If Δ is a simplicial complex whose maximal faces all have equal dimension though, we say that Δ is *pure*. If F is a simplex of some complex Δ, then the subcomplex generated by F is defined as $\langle F \rangle := \{f : f \subseteq F\}$.

Before we discuss how abstract simplicial complexes can be drawn, we require additional definitions.

Definition 2.15. ([70]) A d-dimensional **geometric simplex** in $\mathbb{R}^n$ is defined to be the convex hull of $d + 1$ affinely independent points in $\mathbb{R}^n$ called **vertices**. The convex hull of any subset of the vertices in a geometric simplex is called a **face** of the simplex. A **geometric simplicial complex** K in $\mathbb{R}^n$ is a nonempty collection of geometric simplices in $\mathbb{R}^n$ such that

1. every face of a simplex in K is in K;

2. the intersection of any two simplices of K is a face of both of them.

Let K be a geometric simplicial complex. One gets an abstract simplicial complex, denoted by $\Delta(K)$, by letting the faces of $\Delta(K)$ be the vertex set of the simplices of K.

Every abstract simplicial complex Δ may be obtained in the way described by Definition 2.15. That is, there is a geometric simplicial complex K such that $\Delta(K) = \Delta$. Even though K is not necessarily unique, the underlying topological space, which is obtained by taking the union of the simplices of K under the usual topology on $\mathbb{R}^n$, is unique up to homeomorphism. We refer to this space as the *geometric realization* of Δ and denote it by $||\Delta||$. Though, we will usually drop the $|| \, ||$ and let Δ denote an abstract simplicial complex as well as its geometric realization. For more details, see [70].

Example 2.16. For example, let $\Delta_1 = \langle 124 \rangle \cup \langle 234 \rangle \cup \langle 245 \rangle$ and let $\Delta_2 = \langle 124 \rangle \cup \langle 234 \rangle \cup \langle 45 \rangle$. Figure 2.4 displays possible geometric realizations for each simplicial complex. Observe that Δ_1 and Δ_2 are pure and non-pure respectively.

We remark that a finite graph (to be formally defined in a later section) may be identified with an abstract simplicial complex whose faces have dimension less than or equal to 1. In this sense, an abstract simplicial complex can be viewed as a generalization of a graph.

The concept of a geometric realization of an abstract simplicial complex Δ allows us to provide a visual representation of Δ, provided that $\dim(\Delta) \leq 3$. If, for instance, Δ contains a face F of dimension 4, it would be impossible to draw.
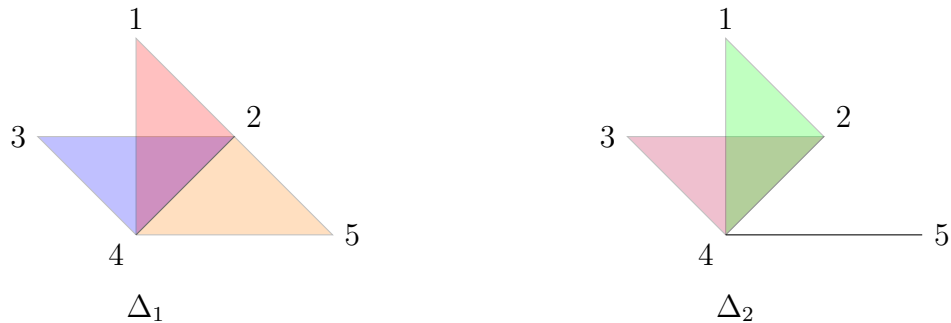
Figure 2.4. Pure and Non-Pure Simplicial Complexes

Definition 2.17. Let P be a poset. The **order complex** of P, denoted by $\Delta(P)$, is the abstract simplicial complex whose vertices are the elements of P and whose simplices are the chains of P.

It is easy to see that $\Delta(P)$ satisfies the axioms on Definition 2.14 since subsets of chains are totally ordered.
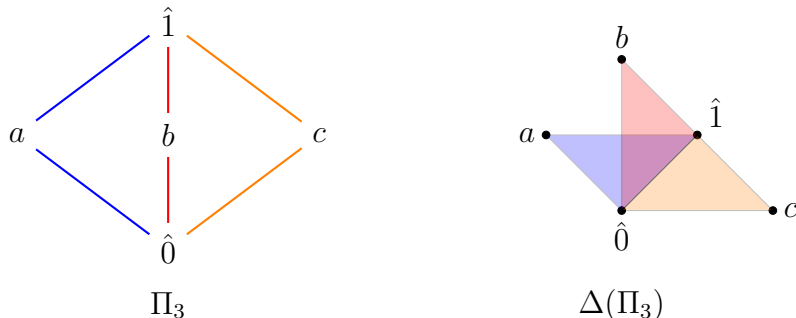
Figure 2.5. Order Complex $\Delta(\Pi_3)$

Definition 2.18. Let Δ be a simplicial complex and let $F_1, \ldots, F_n$ be the maximal simplices of Δ. We say that Δ is **shellable** if the F_i can be linearly ordered in such a way that the subcomplex $\left(\bigcup_{i=1}^{k-1} \langle F_i \rangle \right) \cap \langle F_k \rangle$ is both pure and $(\dim F_k - 1)-$dimensional for all $k = 2, \ldots, n$. Such an ordering on maximal simplices is called a **shelling** of Δ.

A typical explanation of shellablity refers to the easiest way to take a simplicial complex apart so that it can be put back together again. For the intuitive idea, a shelling is a way of gluing an abstract simplicial back together from its maximal simplices in a well-behaved manner.

Example 2.19. Let $\Delta = \langle 123 \rangle \cup \langle 124 \rangle \cup \langle 134 \rangle \cup \langle 234 \rangle$ be the 3-simplex with vertices $1, 2, 3,$ and 4, seen in Figure 2.6. When drawn, Δ takes the shape of a tetrahedron.

Note that this tetrahedron is "hollow" because Δ does not include the 3-dimensional face 1234. Order the maximal faces of Δ as follows: $F_1 = 123$, $F_2 = 124$, $F_3 = 134$, and $F_4 = 234$. One can show explicitly that for each $i \in [4]$, the intersections considered in Definition 2.18 are indeed pure and have the correct dimension. The order complex of Π_3 is also known to be shellable.
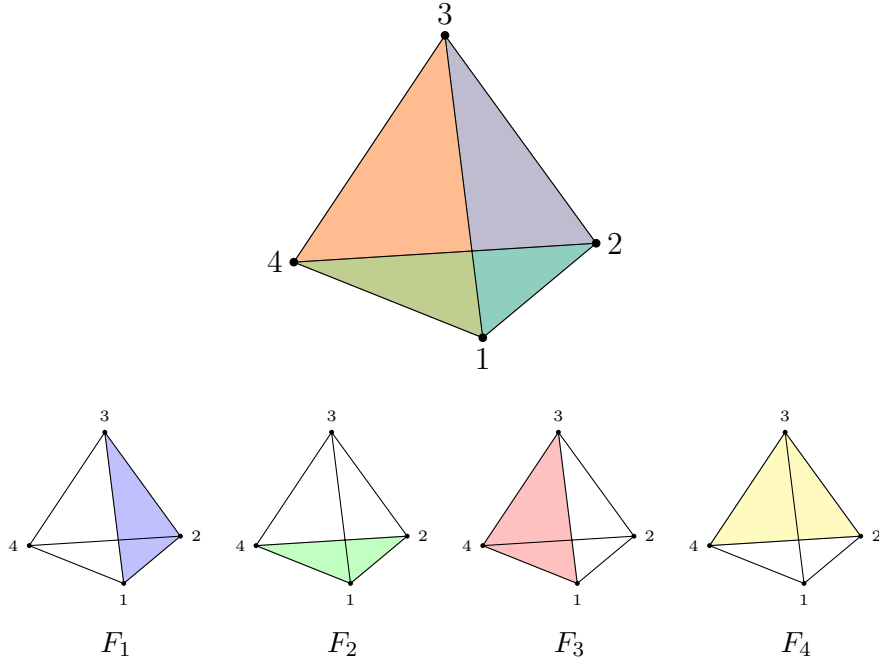
Figure 2.6. The shelling of a 3-simplex

Example 2.20. To see a less obvious example, consider the simplicial complex Δ drawn in Figure 2.7. In this example, we've picked labels for our maximal faces. In the second half of this figure, we list and draw the subcomplexes prescribed by Definition 2.18 and draw the corresponding geometric representation of each. Each subcomplex has exactly one face, so they are all pure. Furthermore, we can see that the dimension condition of Definition 2.18 is satisfied. Each subcomplex is a single vertex and is dimension zero. Each F_i for $i \geq 2$ has dimension 1. Hence, we have a valid shelling of the given simplicial complex.

Example 2.21. We will also present a simplicial complex which is not shellable. Consider the simplicial complex given in Figure 2.8, which appears to be the same as in Figure 2.7, but with the rightmost triangle filled in. More precisely, this complex contains two maximal faces of dimension 2. Though, as we compute the subcomplexes

$$\langle F_1 \rangle \cap \langle F_2 \rangle, \qquad \left(\bigcup_{i=1}^{2} \langle F_i \rangle \right) \cap \langle F_3 \rangle, \qquad \left(\bigcup_{i=1}^{3} \langle F_i \rangle \right) \cap \langle F_4 \rangle, \qquad \left(\bigcup_{i=1}^{4} \langle F_i \rangle \right) \cap \langle F_5 \rangle$$
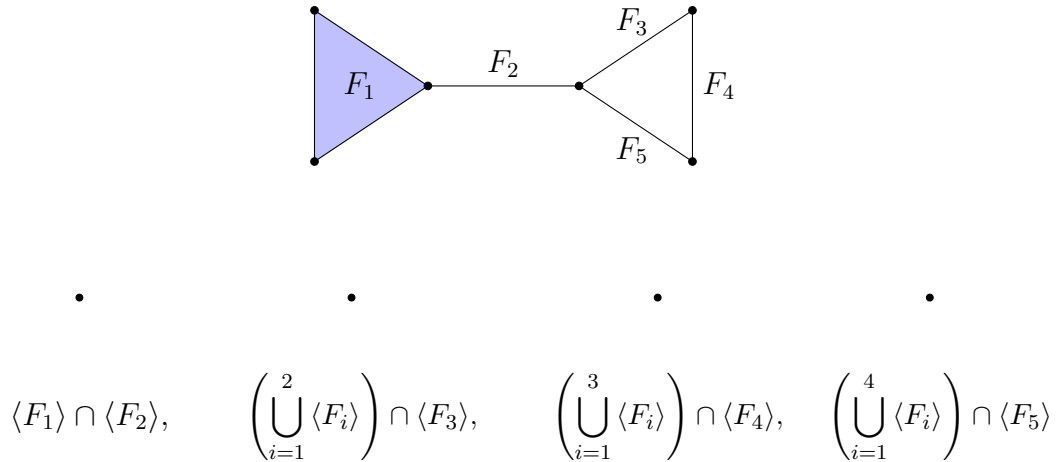
Figure 2.7. A less obvious shellable simplicial complex

prescribed by Definition 2.18, we observe that the subcomplex $\left(\bigcup_{i=1}^{2} \langle F_i \rangle \right) \cap \langle F_3 \rangle$ is a single vertex with dimension 0, but F_3 has dimension 2. This simplicial complex has only three maximal faces, and it is easy to see that any choice of labelling will not result in a shelling.

Definition 2.22. Let $\lambda : \mathcal{E}(P) \to \Lambda$ where $\mathcal{E}$ is the set of edges in the Hasse diagram of P and Λ is some totally ordered set. We say that λ is an **edge-lexicographical labelling** (or an **EL-labelling**) of P if for each closed interval $[x, y]$ of P, there is a unique increasing maximal chain, which lexicographical precedes all other maximal chains of $[x, y]$.

Example 2.23. In Figure 2.9, we show a poset $P \cong \Pi_3$ which has an EL-labelling. The poset Q does not have an EL-labelling. If Q had an EL-labelling, then the chains $\{\hat{0}, c, d\}$ and $\{c, d, \hat{1}\}$ would be increasing. This means that $\{\hat{0}, c, d, \hat{1}\}$ would be increasing. Similarly, $\{\hat{0}, a, b, \hat{1}\}$ would also be increasing. Then $[\hat{0}, \hat{1}]$ would not have a unique increasing maximal chain, a contradiction.

As may be seen by the previous examples, determining whether or not a simplicial complex is shellable is in general a difficult task. However, the following theorems give useful criteria for determining shellability.

Theorem 2.24 (Björner and Wachs [70]). *The product of bounded posets is shellable if and only if each of the posets is shellable.*

Theorem 2.25 (Björner [10], Björner and Wachs [9]). *Suppose that P is a bounded poset (contains $\hat{0}$ and $\hat{1}$) with an EL-labelling. Then the lexicographic order of the maximal chains of P is a shelling of $\Delta(P)$. Moreover, the corresponding order of the maximal chains of $\overline{P}$ is a shelling of $\Delta\overline{P}$, where $\overline{P} := P - \{\hat{0}, \hat{1}\}$.*

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$$\langle F_1 \rangle \qquad\qquad \langle F_1 \rangle \cap \langle F_2 \rangle \qquad\qquad \left(\bigcup_{i=1}^{2} \langle F_i \rangle \right) \cap \langle F_3 \rangle$$
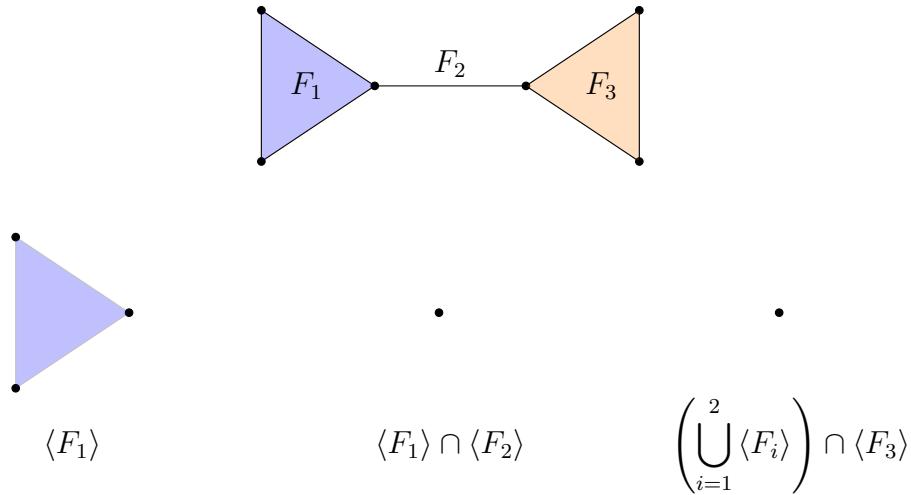
Figure 2.8. A non-shellable simplicial complex
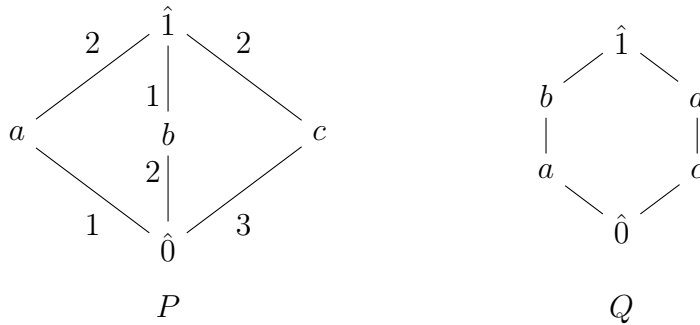
Figure 2.9. A poset with an EL-labelling and a poset with no EL-labelling

2.3 Finite Graphs

Definition 2.26. A **finite simple graph** (or simply a **graph**) is an ordered pair $G = (V, E)$ comprising of the following:

1. $V(G)$, the set of **vertices** of G where $\#V(G) < \infty$;

2. $E(G) \subseteq \big\{ \{i, j\} : i, j \in V(G), i \neq j \big\}$, the set of **edges** of G. When $V(G)$ is totally ordered, we denote an edge $\{i, j\}$ of G by ij where $i < j$.

When a graph G is clear from context, we will write V and E for the vertex and edge set of G respectively.

We say that two edges e and f of a graph are *adjacent* if they have a vertex in common. Likewise, we say that vertices u and v are *adjacent* or *neighbors* if there is an edge $e = uv \in E(G)$. For $v \in V(G)$, denote the *neighborhood of v* by $N(v) := \{u \in V(G) : \exists\, e \in E(G)$ with $e = uv\}$. For a vertex v, the *degree of v* is defined as $\#N(v)$ and is denoted by $\deg(v)$. If $e = uv \in E(G)$, we say that u and e are *incident* to one another (as well as v and e). A *walk* from vertices u to v is a sequence of vertices in G, beginning with u and ending at v such that consecutive vertices in the sequence are adjacent. A walk is called a *path* if no vertices are repeated in the sequence. Note that it is often common to define a path by a sequence of edges of a graph G so that no vertex is repeated. We say a graph G is *connected* if for every $u, v \in V(G)$, there is a path from u to v. Otherwise, we say a graph is *disconnected*. An acyclic graph is called a *forest*, and a connected forest is called a *tree*. A vertex of degree 1 is called a *leaf* and an edge incident to a leaf is called a *pendant edge*.

Definition 2.27. Suppose that G and H are graphs on $[n]$. If there exists a bijection $\varphi : V(G) \to V(H)$ such $uv \in E(G)$ if and only if $\varphi(u)\varphi(v) \in E(H)$, we say that φ is a **graph isomorphism** (or an **isomorphism** when clear from context) and that G is **isomorphic** to H, denoted by $G \cong H$.

In this thesis, we will take $V(G) := [n] = \{1, 2, \ldots, n\}$ and will say that *G is a graph on $[n]$*. When discussing the noncrossing bond poset in Chapter 3 - 5 and Appendix A, we will embed (or draw) these graphs in the plane in the so-called *graphical representation* where the vertices lie on a circle with 1 at the top and the remaining vertices appearing in clockwise ascending order and the edges are drawn as straight-line line segments (or chords) connecting their endpoints.

Example 2.28. Figure 2.10 shows two graphs G and H which are isomorphic with isomorphism φ defined by $\varphi(1) = 2, \varphi(2) = 1, \varphi(3) = 3$, and $\varphi(4) = 4$. Many properties of graphs are preserved under isomorphism (e.g., connectivity and degree of vertices). We say such properties are *invariant under graph isomorphism*.

Definition 2.29. We say that two edges of G **cross** if their respective line segments intersect in the graphical representation, i.e., edges $a_1 a_2$ and $b_1 b_2$ cross if and only if $a_1 < b_1 < a_2 < b_2$ or $b_1 < a_1 < b_2 < a_2$. We also refer to such edges as **crossing edges.**

Figure 2.10 shows isomorphic graphs G and H drawn in their graphical representations. Note that G has a pair of crossing edges while H does not. This demonstrates having crossing edges is not invariant under graph isomorphism.

Definition 2.30. A **subgraph** of G is a graph H such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. We say that H is a **spanning subgraph of** G when $V(H) = V(G)$. We say that H is an **induced subgraph of** G if whenever u and v are vertices in H and $uv \in E(G)$, then $uv \in E(H)$.
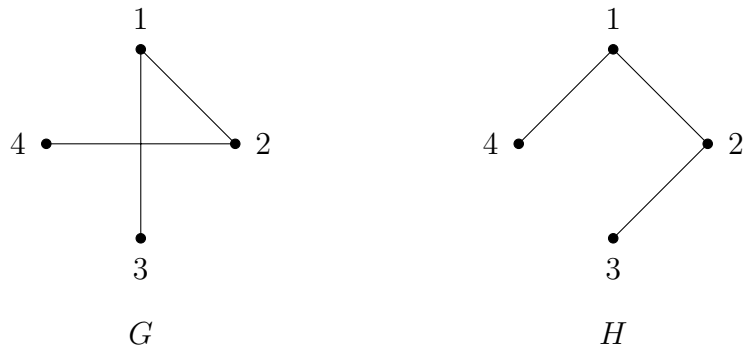
Figure 2.10. Graphs drawn in the graphical representation

A *connected component* of a graph G is a subgraph H of G such that for any vertices $u, v \in H(G)$, there exists a path P in $V(H)$ beginning at u and ending at v. Hence, a finite graph may be regarded as a union of its connected components. An *isolated vertex* of G is a vertex with no neighbors in G. A *trivial connected component* of G is an isolated vertex of G. Later in this chapter, we will use $cc(G)$ to denote the number of connected components of a graph G.
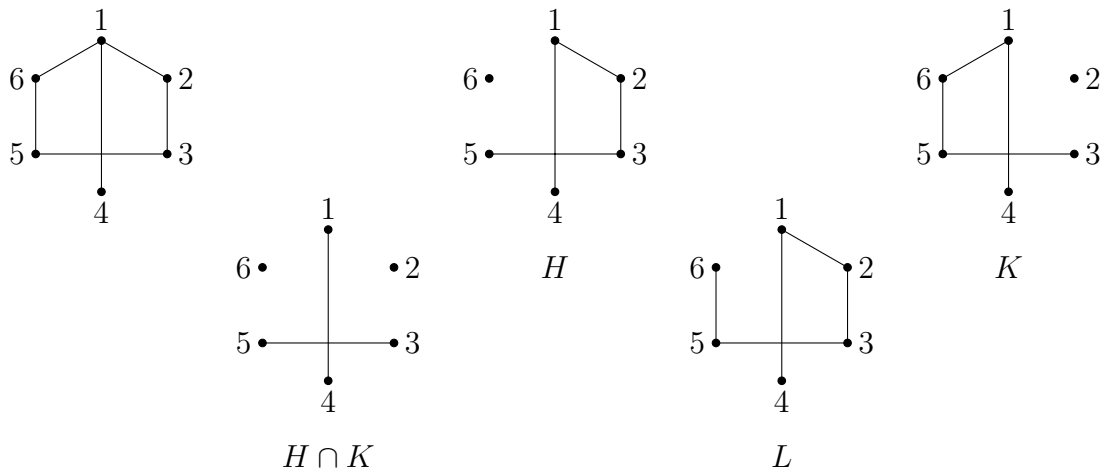
Figure 2.11. A graph and several spanning subgraphs

2.4   Matroids

Matroids have been a topic of study since the 1930's, notably in "Moderne Algebra" by van der Waerden [61] and by Hassler Whitney in 1933 [72]. Whitney presented matroids as an abstract generalization of matrices, as the name might suggest. His work in graph theory lead to beautiful connections between matroids and graphs. We present some basic definitions and terminology of matroids to help motivate Definition 2.40 in Section 2.5. For more information on matroids, and for references on the following definitions, see [5, 49, 52, 68].

Definition 2.31. Given some finite set E, a **matroid** M is a pair $M = (E, \mathcal{I})$ where E is a set (often called a *ground* set) and $\mathcal{I}$ is a family of subsets of E called **independent sets** which satisfy the following axioms:

1. $\varnothing \in \mathcal{I}$:

2. if $X \in \mathcal{I}$ and $Y \subseteq X$, then $Y \in \mathcal{I}$;

3. if $X, Y \in \mathcal{I}$ and $\#X > \#Y$, then there exists $x \in X - Y$ such that $Y \cup \{x\} \in \mathcal{I}$.

These axioms are often called the **independence axioms.** We will also say M is a matroid on E.

It's worth remarking that if we remove axiom (3) from the above definition, we obtain an equivalent definition for an abstract simplicial complex (also called an *independence system*). Axiom (3) is not a consequence of items (1) and (2), so matroids are not identical to abstract simplicial complexes.

Definition 2.32. Let G be a graph on n vertices. The *cycle matroid* (also called the *graphic matroid*) M of G is defined as the family of subsets of $E(G)$ which contain no cycles; i.e., the set of forests of G. Denote the cycle matroid of a graph by $M(G)$.

It's easy to see that this family satisfies the independence axioms. The maximal independent sets of a cycle matroid of G are the spanning forests of G. This matroid will be of particular importance for our purposes.

Definition 2.33. Let M be a matroid on E with independent sets $\mathcal{I}$. A basis of M is an independent set of maximal size.

It is a basic result of matroid theory, directly analogous to a similar theorem of bases in linear algebra, that any two bases of a matroid M have the same number of elements (see Lemma 3.1 of [52]).

Definition 2.34. Let M be a matroid on E with independent sets $\mathcal{I}$. The **rank function** of M is the function $rk : 2^E \to \mathbb{Z}_{\geq 0}$ given by $rk(A) := \max\{\#I : I \subseteq A, I \in \mathcal{I}\}$ for any $A \subseteq E$, i.e., $rk(A)$ is the size of the largest independent set contained in A.
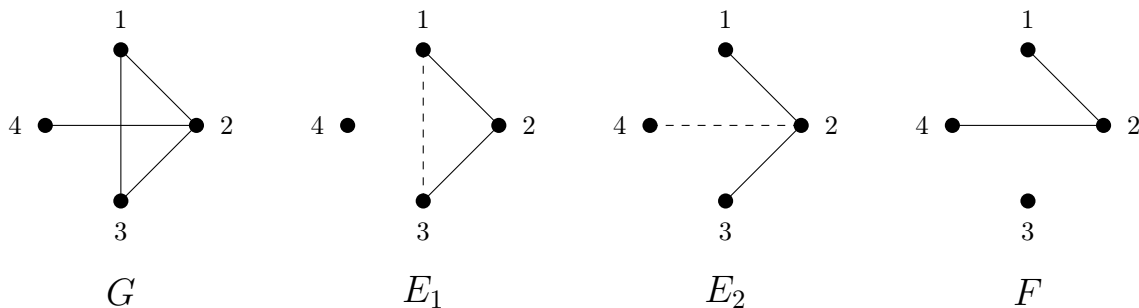
Figure 2.12. Example of a flat in the cycle matroid of a graph.

Remark. Note that the rank function had domain 2^E, the set of all subsets of E, not just $\mathcal{I}$.

Definition 2.35. Given a matroid M on E with independent sets $\mathcal{I}$, the **closure operator** is a set function $cl : 2^E \to 2^E$ defined by $cl(A) = \{y \in E : rk(A \cup \{y\}) = rk(A)\}$ for all $A \subseteq E$. It follows from the definition that if $A \subseteq E$, then $A \subseteq cl(A)$.

It is also important to remark that the closure operator takes as input any $A \subseteq E$ and output an independent set. Though, because the closure operator depends on the rank function of M, it depends on the set of independent sets.

Definition 2.36. If $A \subseteq E$ has the property that $cl(A) = A$, we say that A is a **flat** of M.

Example 2.37. Consider the graph G in Figure 2.12. The set $E = \{12, 23\}$ is an independent set of $M(G)$ of rank 2. We aim to compute it's closure. Since $E \subseteq cl(E)$, we need only compute the ranks of $E_1 = \{12, 23, \mathbf{13}\}$ and $E_2 = \{12, 23, \mathbf{24}\}$. We show in bold-face the edges which are being added to E, and use dashed lines to represent the same thing in Figure 2.12. Observe that E_1 is a cycle and E_2 is a forest. Adding the edge 13 to E didn't increase its rank, while adding 24 to E did increase its rank. Thus, $cl(E) = \{12, 13, 23\}$.

Example 2.38. Use the graph G from Example 2.37 and let $F = \{12, 24\}$, also shown in Figure 2.12. It is relatively straightforward to show that $cl(F) = F$, since the addition of edges 13 or 23 will result in a larger independent set (i.e., the rank will increase). One may observe that the edges 12 and 24 so not belong to a cycle of G whereas in Example 2.37, the edges of E did belong to a cycle. By adding the edge 13 to E, we closed this cycle and resulted in a non-independent set of $M(G)$, hence it would have been impossible for E_1 to contain an independent set of larger size than E.

For a matroid M, let $\mathcal{L}(M)$ denote the set of all flats of M. This set forms a poset where flats are ordered by inclusion.

Theorem 2.39 ([68]). *Let M be a matroid. Then the poset of flats of M, $\mathcal{L}(M)$, is a lattice.*

It is known that the intersection of two flats is also a flat (see Section 3.1 of [68]). Hence, $\mathcal{L}(M)$ is a meet-semilattice. If M has ground set E, then E is a flat, so $\mathcal{L}(M)$ has a top element $\hat{1} = E$. So Theorem 2.39 follows from Proposition 2.7.

If L is a finite semimodular lattice with $\hat{0}$, then we call L a *geometric lattice*. A *matroid lattice* is a geometric lattice without the assumption of finiteness. It is a known fact that the class $\mathcal{L}(M)$, the set of all flats of a matroid M, is a partially ordered set ordered by inclusion. This poset forms a matroid lattice, and in the case that $\mathcal{L}(M)$ is finite, it forms a geometric lattice (see [5]). Hence, the set of all flats of the cycle matroid of a graph forms a geometric lattice. This will be come particularly relevant in Section 2.5.

2.5 The Bond Lattice of a Graph

Before we define the noncrossing bond poset, we need to discuss the *bond lattice* of a graph G.

Let $\mathcal{SS}_n(G)$ be the set of all spanning subgraphs of an order n graph G. Then let $\pi : \mathcal{SS}_n \to \Pi_n$ be the function which maps a spanning subgraph H of G to the set partition $\pi(H)$ whose blocks are the vertex sets of the connected components of H. That is, vertices i and j of H are in the same block of $\pi(H)$ if and only if they are in the same connected component of H. We will refer to $\pi(H)$ as the *corresponding set partition* of H

Given a set partition $\pi = B_1/B_2/\cdots/B_k$, the associated spanning subgraph $G[\pi]$ is the graph whose edge set is the disjoint union of the edges in $G[B_1], G[B_2], \ldots, G[B_k]$. See Figure 2.13 for some examples. It's important to note that $G[B_1/B_2/\cdots/B_k]$ is not always a bond since each $G[B_i]$ need not be connected.

Definition 2.40. Let G be a graph. Call a subgraph H of G a **bond** if H is a spanning subgraph such that every connected component of H is induced. That is, if i and j are in the same connected component of H and $ij \in E(G)$, then $ij \in E(H)$.

Definition 2.41. Let G be a graph on $[n]$. The **bond lattice** of G is the set of all bonds of G where $H \leq K$ if and only if $E(H) \subseteq E(K)$.

There are a few ways to approach the definition of a bond (and the bond lattice) in the literature. Stanley discusses in [68] how L_G is isomorphic to an intersection lattice derived from hyperplane arrangements. It is known that the bond lattice of a
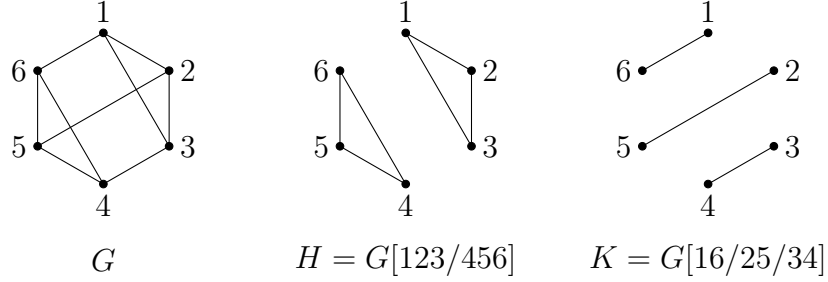
Figure 2.13. Graphs from set partitions

graph is a graded lattice that is EL-shellable (see [59, 68]). We will discuss how bonds can be derived from the cycle matroid of a graph, and how they can be realized by comparing graphs to their corresponding set partitions.

The following is a known result. While we were unable to locate an explicit statement in the literature, we present the result with our own proof.

Proposition 2.42. *Let G be an order n graph and let L_G be the bond lattice of G. Then L_G is the lattice of flats of the cycle matroid of G.*

Proof. First we note that since bonds are spanning subgraphs of G, each bond is uniquely determined by its edge set. The claim of the result is thus more precisely worded as saying $\{E(H) : H \in L_G\}$ is the lattice of flats of the cycle matroid of G.

We also claim that the rank of a set $A \subseteq E(G)$ in the cycle matroid is $rk(A) = n - cc(A)$ where $cc(A)$ is the number of connected components of the spanning subgraph G' of G with edge set A. Recall that the rank of A is defined to be the size of the largest independent set which is the edge set of a spanning forest F', that is contained in A. Each component F'' of F' must be a spanning tree of a component G'' of G'. If not, F'' could be enlarged to a spanning tree of G'', thus enlarging F'. Thus $\#F'' = \#V(G'') - 1$. Summing this over all components of F' we get $\#F' = \#V(G) - cc(F') = \#V(G) - cc(G') = \#V(G) - cc(A)$.

We claim that for each $H \in L_G$, $E(H)$ is a flat of M. Let e be some edge of G not contained in $E(H)$. Then e is not in any connected component of H. Otherwise, H would not be a bond. Thus, e must connect two components of H. That is, if H' is the bond obtained by adding e to H, then $cc(H') = cc(H) - 1$. Hence, $rk(E(H')) = rk(E(H)) + 1$ in the cycle matroid. Thus, $E(H)$ is a flat in the cycle matroid.

Next, we claim that each flat E of M corresponds to a bond. Let H be the spanning subgraph of G with $E = E(H)$. By way of contradiction, suppose that H is not a bond; i.e., not all connected components of H are induced. This would mean that there is some edge e not yet in E, such that e belongs to a connected component of H. Let $E' = E \cup \{e\}$. Then $cc(E') = cc(E)$ and so $rk(E') = rk(E)$ in the cycle

matroid. This shows that E is not closed. We have just shown that there exists an edge e that, when added to E, does not increase the rank of E in the cycle matroid. Hence, E is not a flat, which is a contradiction. Therefore, every connected component of H must be induced, which implies that H is a bond. □

If E is a flat of the cycle matroid M, we see that one cannot add an edge to E without increasing its rank. Similarly, one may not add an edge to a bond without decreasing the number of connected components. In Figure 2.12, we see that by adding the edge 13 to E_1, we are not increasing the size of a largest acyclic subgraph of G contained in E_1; i.e., we are not increasing its rank. We are also forcing being an induced subgraph.

One may also arrive at Definition 2.40 in the following way. In Figure 2.11, we see a graph G and four spanning subgraphs of G. Its easy to see that the subgraphs H, K, and $H \cap K$ are bonds, since all connected components inherit all edges from G. The same cannot be said about the subgraph L since $16 \in E(G)$ and 1 and 6 are in the same connected component of L. Observe that $\pi(G) = \pi(L) = 123456$. Hence, π is not necessarily an injective map. However, $\pi : L_G \to \Pi_n$ will be an injective map. To see this, let G be an order n graph with bonds H_1 and H_2, and let $\pi(H_1) = B_1/\cdots/B_k$ and $\pi(H_2) = C_1/\cdots/C_\ell$. Suppose that $\pi(H_1) = \pi(H_2)$. Then $k = \ell$ and $B_i = C_i$ for each $1 \leq i \leq k$. B_i is a block which contains the vertices $V = \{v_1, \ldots, v_{m_i}\}$. Then H_1 and H_2 have a connected component with the vertices V and edges induced from G. Since this is true for all $1 \leq i \leq k$, $H_1 = H_2$.

The set of all bonds of a graph G are exactly the spanning subgraphs of G for which there is a unique corresponding set partition. One observation is that if G is a tree, then all spanning subgraphs are bonds of G. Further the edge sets of all spanning subgraphs of G are independent sets in the cycle matroid; hence, every spanning subgraph of G is a flat. It is also easy to see that if $G = K_n$, then $L_G = \Pi_n$. Hence, one may regard the bond lattice of an order n graph G as a generalization of Π_n.

See Figure 2.14 for an example of a graph and its corresponding bond lattice. In some of our examples, we will show the bond lattice by drawing each bond as a node in the Hasse diagram. In most examples, we will draw $\pi(H)$ as the nodes of the Hasse diagram (see Figure 3.2).
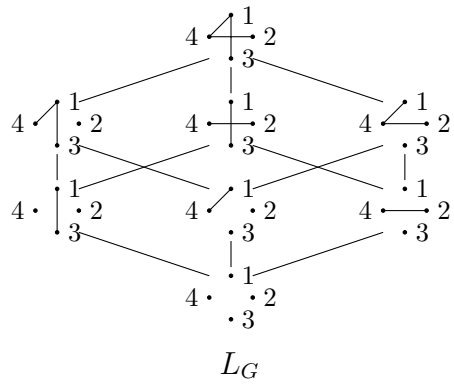
Figure 2.14. L_G for $G = ([4], \{13, 14, 24\})$

Chapter 3: The Structure of the Noncrossing Bond Poset

3.1 Introducing the Noncrossing Bond Poset

Definition 3.1. Let $\pi \in \Pi_n$ where $\pi = B_1/B_2/\cdots/B_k$. We say that π is **crossing** if there exists $a, c \in B_i, b, d \in B_j$ with $i \neq j$ such that $a < b < c < d$. Otherwise, π is said to be *noncrossing.*

The set of all noncrossing set partitions, denoted by NC_n, is a lattice with the same partial ordering as Π_n; i.e. NC_n is an induced subposet of Pi_n. It is known that NC_n is a lattice for all n and that noncrossing set partitions of $[n]$ are counted by the Catalan numbers $C_n = \frac{1}{n+1}\binom{2n}{n}$ (see [40]). This lattice is well known in combinatorics, and we refer the reader to [3, 4, 7, 13–16, 46, 57] for more information. The noncrossing set partition lattice will lead us into our main topic of study in this Part I of this thesis.

Definition 3.2. Let G be a graph and let H be a bond of G. Then H is called a **crossing bond** if and only if $\pi(H)$ is a crossing partition. Otherwise, H is called a **noncrossing bond.**

Proposition 3.3. *A bond H is crossing if and only if there exists two distinct connected components H_1 and H_2 of H and edges $e_1 \in H_1$ and $e_2 \in H_2$ such that e_1 and e_2 cross.*

Proof. We'll first prove the forward direction. Suppose $\pi(H)$ is crossing. Let B_1 and B_2 be the crossing blocks of $\pi(H)$ and let H_1 and H_2 be the corresponding components of H with vertex sets B_1 and B_2. Let a, c be in B_1 and b, d be in B_2 with $a < b < c < d$. It's not necessarily true that a, c are the endpoints of an edge e_1 in H_1 or that b, d are the endpoints of an edge e_2 in H_2. However, H_1 and H_2 are connected components of H. So there is a path P_1 in H_1 connecting a and c. Let I_2 and J_2 be the two cyclically contiguous subsets of $[n] \setminus \{b, d\}$. Without loss of generality we may assume a is in I_2 and c is in J_2. So there must be an edge $e_1 = \{a', c'\}$ of P_1 (and hence in H_1) with a' in I_2 and c' in J_2. The pairs $\{a', c'\}$ and $\{b, d\}$ must cross each other. Now let I_1
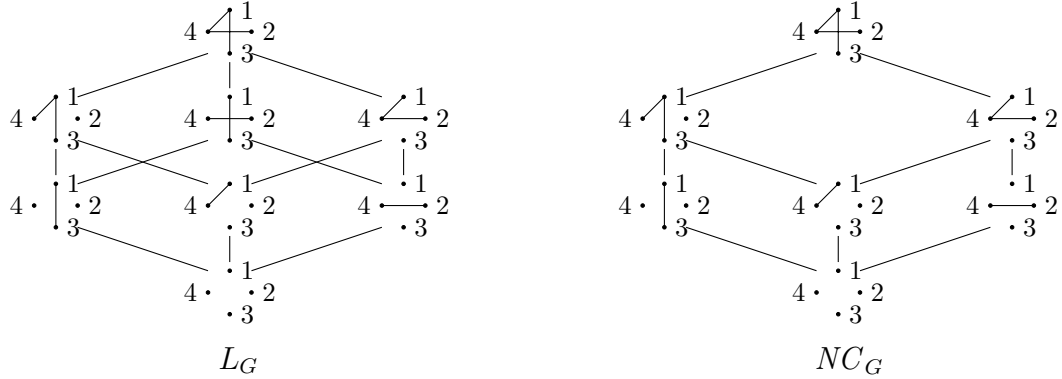
Figure 3.1. L_G and NC_G for $G = ([4], \{13, 14, 24\})$

and J_1 be the cyclically contiguous subsets of $[n] \setminus \{a', c'\}$. Without loss of generality, we may assume b is in I_1 and d is in J_1. Thus there must be an edge $e_2 = \{b', d'\}$ of P_2 (and hence in H_2) with b' in I_1 and $d' \in I_2$. So the pairs $\{a', c'\}$ and $\{b', d'\}$ must cross each other and so e_1 and e_2 cross.

Conversely, suppose H is a bond satisfying the conditions of the theorem. We show that $\pi(H)$ is crossing. Let B_1 and B_2 be the blocks of $\pi(H)$ that are the vertex sets of the graph H_1 and H_2 respectively. Let a, c with $a < c$ be the endpoints of e_1 and b, d with $b < d$ be the endpoints of e_2. Since e_1 and e_2 cross, we must have $a < b < c < d$ or $b < a < d < c$. Thus B_1 and B_2 cross. $\square$

Definition 3.4. Let G be a graph. The **noncrossing bond poset** of G, denoted by NC_G, is the the set of all noncrossing bonds of G, ordered by inclusion.

Example 3.5. An example of the noncrossing bond poset of the graph G on $[4]$ with edge set $\{13, 14, 24\}$ is shown in Figure 3.1. Clearly, NC_G is a subposet of L_G for all graphs G. Examples of when $NC_G \neq L_G$ are shown in Figure 3.1 and Figure 3.2.

The goal of this project is to study the order theoretic and combinatorial properties of NC_G. Note that L_G is a graded, shellable lattice (see [59, 68]). Hence, we endeavor to determine which graphs G yield noncrossing bond posets with these properties. Since there are some known interesting theorems about the Möbius function and characteristic function of L_G (see [66, 68, 71]), it is natural to try to extend some of those results to NC_G, if only for certain classes of graphs G.

3.2   New Families of Graphs

Definition 3.6. Let G be a graph and let e and f be two crossing edges of G. We say e and f are **crossing closed** if there exists a unique induced connected subgraph

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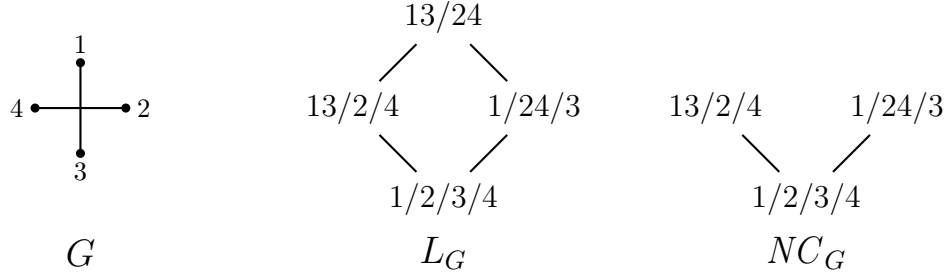
Figure 3.2. A graph and its bond lattice and noncrossing bond poset.

of G containing e and f that is minimal among all such subgraphs with respect to containment. If such a subgraph exists, we denote it by $J(e, f)$. We say G is **crossing closed** if every pair of crossing edges in G are crossing closed.

Let G be a graph with crossing edges e and f. We view e as the bond that is the spanning subgraph of G with edge set consisting only of e. We consider f to be a bond in the same way. The "J" in the notation $J(e, f)$ is chosen because, as we shall see in Theorem 3.10, if it exists, it yields the join of the bonds e and f in the noncrossing bond poset. Note that $J(e, f)$ is not a bond by definition. We will clarify in various proofs that we consider a bond whose edge set is that of $J(e, f)$. In Figure 3.3, $J(13, 25)$ is given for crossing edges 13 and 25 for the graph G, and the bond H whose edge set is $E(J(13, 25))$.
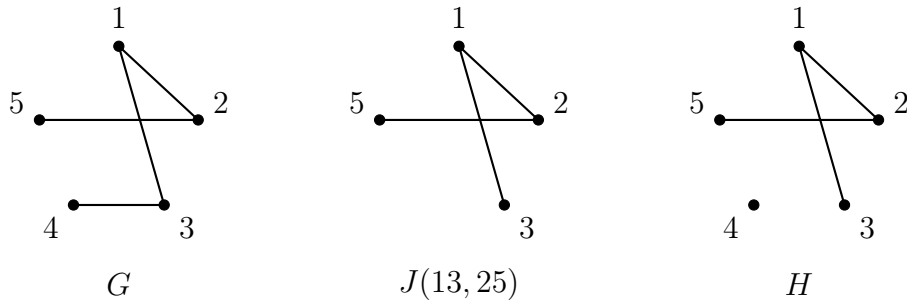
Figure 3.3. Distinction between $J(e, f)$ and the bond whose edge set is $E(J(e, f))$

We explain why we chose the name "crossing closed." When we introduced matroids, we discussed what it meant for an independent set to be closed, and what the closure of a set is in this context. There are many ways to define matroids, and one way is through a closure operator. In terms of the lattice of flats, the closure of a subset of the ground set is the join of the elements in the lattice of flats. As fore-mentioned, crossing closed edges are exactly the crossing edges which have a join in the graph's

noncrossing bond poset and crossing closed graphs are exactly the graphs whose noncrossing bond poset is a lattice. Therefore, if a graph is crossing closed, it implies the existence of a closure operator on the crossing edges that behaves in a similar way that the closure operator does in the cycle matroid. It should be noted, however, that this does not imply a matroid structure as our closure operator is not the same as the one for matroid.

Example 3.7. The crossing edges of in Figure 3.4 are not crossing closed because the noncrossing bonds $H = G[12345/6]$ and $K = G[13456/2]$ are incomparable and both contain 14 and 35.
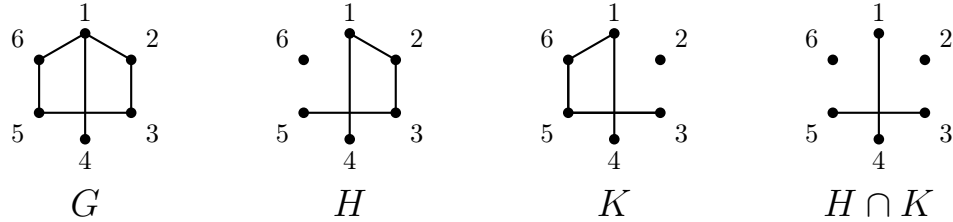
Figure 3.4. Crossing edges that are not crossing closed

Lemma 3.8. *The clique K_n is crossing closed.*

Proof. Let e and f be any pair of crossing edges. Let C be the clique on 4 vertices defined by $C = G[e \cup f]$. Clearly, C is connected and induced and contains e and f. Since there is no smaller induced subgraph of G that contains $e \cup f$, $J(e, f)$ exists and is $J(e, f) = C = G[e \cup f]$. Since e and f were an arbitrary pair of crossing edges, G is crossing closed.

$\square$

In the example we present in Figure 3.4, we are showing edges which are not crossing closed. It can be difficult to visualize what $J(e, f)$ looks like (should it exist) for crossing edges e and f from the definition alone. We present the following lemma to resolve this issue. Lemma 3.9 asserts that if $J(e, f)$ exists, it can take on one of two possible forms.

Lemma 3.9. *Let G be a graph and let e and f be two crossing closed edges of G. Then $J(e, f)$ is of one of the following two forms, depending on whether or not there is an edge in G connecting a vertex of e to a vertex of f.*

1. *There is an edge in G connecting a vertex of e to a vertex of f. In this case, $J(e, f) = G[e \cup f]$ and $J(e, f)$ is a subgraph of K_4.*

2. There does not exist an edge between a vertex of e and a vertex of f. In this case, $J(e, f)$ has the form of the graph depicted in Figure 3.5. Moreover, all vertices in $J(e, f)$ not on e or not on f are cut vertices of G that separate e and f.

Before we begin the proof, the form that the second item in Lemma 3.9 is what we've often referred to as a "dumbbell" (see Figure 3.5). $J(e, f)$ need not always assume this exact shape though; i.e., it need not contain two 3-cycles.

Proof. Let G be a graph with crossing edges e and f so that $J(e, f)$ exists. First assume that there exists an edge x which connects a vertex of e with a vertex of f. Then $G[e \cup f]$ is connected and induced. Since there is no possible smaller induced subgraph that contains e and f, we must have $J(e, f) = G[e \cup f]$, which is necessarily a subgraph of K_4.

Next, we assume that G contains no edge which connects e and f. Let T be some spanning tree of $J(e, f)$ which contains e and f. We know T exists because e and f are crossing and $J(e, f)$ has e and f within the same connected component. We claim that T must be a path. To show this, assume that T is a tree which is not a path. Then there must be some vertex with degree at least 3. This implies that T has at least three leaves (vertices of degree 1). Since e and f are crossing edges in the same connected component, e itself contains at most one leaf (the same is true for f). So there is a third leaf ℓ which is not in e nor f. Notice that $J(e, f) \backslash \ell$ is connected (since it contains spanning tree $T \backslash \ell$), induced, and contains both e and f. This contradicts the minimality of $J(e, f)$. Therefore T must be a path. Observe that e and f must contain the two endpoints of T. Otherwise, at least one end-vertex of T, say ℓ would not be on either e or f and $J(e, f) \backslash \ell$ would again contradict the minimality of $J(e, f)$.

Next, order the vertices of $J(e, f)$ as $v, v', x_0, \ldots, x_k, w', w$, seen in Figure [?]. These vertices come along the spanning tree T so that $e = vv'$ and $f = ww'$, where $k \geq 0$ since e and f are crossing. Recall that $E(J(e, f))$ is the set of edges induced by the vertices of $J(e, f)$, which need not be equal to $E(G)$. We claim that besides the edges in T, there are no additional edges in $E(J(e, f))$ except possibly for the edges $x_0 v$ and $x_k w$ should either of them be present in G. Note that we mention these edges specifically because of how we've chosen to label our vertices with respect to T.

We will prove this claim by way of contradiction, so suppose the above is not true, and assume we have some additional edge ℓ. Then $k > 0$. To see this, suppose that $k = 0$, as shown in Figure 3.6. The additional edge cannot be adjacent to e or f since they are the pendant edges of T. So ℓ must be indecent to x_0. However, this would imply that any spanning tree T of $J(e, f)$ would have a vertex of degree 3 or more, a contradiction. Hence, $k > 0$.

The edge ℓ cannot be incident to a vertex of both e and f by initial assumption. Then ℓ can only be an edge between x_i and a vertex from e or f, except for $v' x_0$ and $x_k w'$ since these edges are in T already. In the case that $\ell = v x_i$ with $i > 0$, then

we have the path $v'vx_ix_{i+1}\cdots v_kw'w$ which contains e and f, and whose vertex set is contained in $V(J(e,f))$. This is a contradiction, because this vertex set induces a noncrossing bond properly contained in $J(e,f)$. If $\ell = v'x_i$ for $i \geq 1$, then we arrive at the same contradiction. This implies there is only one possible case remaining, where $\ell = x_ix_j$ where $j - i \geq 2$. If this were the case, then we have the path $v'vx_0\cdots x_ix_j\cdots x_kv_kw'w$ which would contradict the minimality of $J(e,f)$ for reasons similar to the previous contradiction. Hence, the claim about having no additional edge is proven. This proves the first half of the second part of the lemma.

To prove that each vertex in $J(e,f)$ not in e or f is a cut vertex of G which separates e and f, suppose that there exists some connected component C in $G\backslash x_i$ containing e and f. Then $J(e,f)$ must be contained by C. This contradicts the minimality of $J(e,f)$, so such a connected component cannot exist. This ends the proof of the lemma. $\qquad\square$
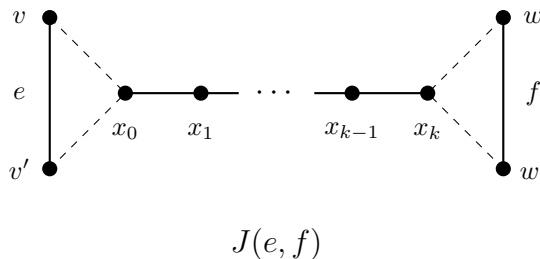
Figure 3.5. At least one of the dotted edges incident to x_0 and at least of the dotted edges incident to x_k exist in $J(e,f)$.
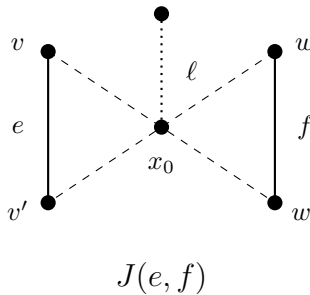
Figure 3.6. Why is $k > 0$?

In the following theorem, we establish a condition for which crossing edges e and f are crossing closed.

Theorem 3.10. *Let G be a graph. Let e and f be two crossing edges of G. Then e and f are crossing closed if and only if $e \vee f$ exists in NC_G. In the case e and f are crossing closed, $J(e, f)$ is the unique non-trivial component of $e \vee f$ and $e \vee f$ is the bond with edge set $E(J(e, f))$. Furthermore, G is crossing closed if and only if $e \vee f$ exists for every pair of crossing edges e and f.*

Proof. Suppose that G is a graph with crossing closed edges e and f. Then $J(e, f)$ exists. Denote by e and f the bonds of G with edge sets $\{e\}$ and $\{f\}$ respectively. Also let H denote the bond with edge set $E(J(e, f))$. We claim that $H = e \vee f$ in NC_G. To show this, let H' be a noncrossing bond such that $e, f \leq H'$ in NC_G. Then H' contains e and f. Further, since H' is noncrossing, e and f must be in the same connected component of H', so we'll call this component C. By definition, $J(e, f)$ is a subgraph of C. And since H is the bond with edges from $J(e, f)$, we get that $H \leq H'$. Thus, H is the unique minimal element of NC_G that contains bonds e and f, which also proves that $H = e \vee f$.

Conversely, assume that $e \vee f$ is a noncrossing bond of G. Let $H = e \vee f$. Since H is the join of e and f in NC_G, there is some connected component C of H which contains e and f. Since $e \vee f$ is the unique minimal noncrossing bond of G containing e and f, C must be the unique non-trivial component of H. Let C' be any connected induced subgraph of G which contains e and f. Then let H' be the bond with edge set $E(C')$. Since C' is connected, $H' \in NC_G$. It's clear that the bonds e and f are contained in H'. Thus, $H \leq H'$ in NC_G. Moreover, this implies that C is a subgraph of H' so C is a subgraph of C'. Hence, C is the unique induced minimal connected component of G which contains e and f; i.e., $C = J(e, f)$. Therefore, e and f are crossing closed edges of G.

It immediately follows that G is a crossing closed graph if and only if $e \vee f$ exists and is a noncrossing bond of G for each pair of crossing edges of G. $\qquad \square$

Let G be a graph with crossing edges e and f. Now that we understand when $e \vee f$ exists in NC_G, we can hope to answer the previously stated question: "For which graphs is the noncrossing bond poset a lattice?" To do this, we use the previous theorem, and address whether the meet of two noncrossing bonds exists in NC_G.

Theorem 3.11. *Let G be a graph. Then NC_G is a lattice if and only if G is crossing closed. Moreover, if G is crossing closed and $H, K \in NC_G$, then $H \wedge K = H \cap K$. Thus NC_G is a meet semi-lattice of L_G.*

Proof. We'll prove the forward direction and assume that NC_G is a lattice. Then every pair of noncrossing bonds has a join in NC_G. Hence, for each pair of crossing edges e and f, $e \vee f \in NC_G$. So by Theorem 3.10, $J(e, f)$ exists and there is a noncrossing bond with edge set $E(J(e, f))$. Thus, G must be crossing closed.

Now assume that G is a crossing closed graph. Notice that G cannot be a crossing bond itself. If G was a crossing bond, then it would contain crossing edges e and f in

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distinct connected components. So there would be no induced connected subgraph of G which contained e and f. Hence, it is enough to show that G is a meet semi-lattice. Since G is a noncrossing bond, $G = \hat{1}$ in NC_G. The noncrossing bond poset is a finite poset, so it will be enough to show that NC_G is a meet semi-lattice, by Proposition 2.7. We aim to show that for noncrossing bonds H and K that $H \wedge K = H \cap K$; i.e. the bond with edges $E(H) \cap E(K)$. It is known that $H \wedge K = H \cap K$ in L_G, so we must show that $H \cap K$ is noncrossing. By way of contradiction, suppose that $H \cap K$ is a crossing bond. Then this bond contains crossing edges e and f in distinct connected components. Since G is crossing closed, $J(e, f)$ exists and we know there is a bond L whose edge set is $E(J(e, f))$. Then L is an upper bound of bonds e and f and $H \cap K \leq L$ since $H \cap K$ is the meet of H and K. But by definition, $J(e, f)$ is a subgraph of H and K these noncrossing bonds both contain e and f. This gives us a contradiction. Hence, $H \cap K$ must be a noncrossing bond, proving that $H \wedge K = H \cap K$ in NC_G. $\qquad\square$

Proposition 3.12. *Let G be a crossing closed graph. Then we have the following:*

(a) NC_G *is atomic.*

(b) NC_G *is a meet-sublattice of L_G.*

(c) *If e and f cross in G, then $J(e, f)$ is the unique non-trivial connected component of $e \vee f$ (namely, the component that contains e and f).*

(d) NC_G *is semimodular if and only if G has no crossing edges.*

(e) NC_G *has a $\hat{1}$.*

Proof. (a) Let H be a noncrossing bond and suppose that $E(H) = \{e_1, \ldots, e_k\}$. Let e_i, denote the bond with edge set $\{e_i\}$. It's clear that $e_1, \ldots, e_k \leq H$. We claim that $\bigvee_{i=1}^{k} e_i = H$. Let $H' \in NC_G$ be any upper bound of $e_1, \ldots, e_k$. Then H' contains each e_i, so $H \leq H'$. Hence, NC_G is an atomic poset.

Both (b) and (c) follow from the proof of Theorem 3.11.

(d) First, assume that G has no crossing edges. Then NC_G is exactly the bond lattice of G which is known to be upper semimodular. Now assume that NC_G is upper semimodular. By way of contradiction, assume that G has crossing edges e and f. Since G is crossing closed, $J(e, f)$ exists. Since e and f cover their meet, which is $\hat{0}$, then $e \vee f \lessdot H$. Since $J(e, f)$ is minimal by definition, $J(e, f)$ must be a connected component of H.

(e) If $J(e, f)$ exists for each pair of crossing edges e and f, then G must be a graph for which all pairs of crossing edges appear in the same connected component of G. Hence, G is a noncrossing bond of itself, implying that NC_G has a $\hat{1}$. $\qquad\square$

Proposition 3.13. *Let G be a graph. Then the following are equivalent.*

(a) NC_G has a $\hat{1}$.

(b) Whenever e and f are crossing edges of G, they are in the same connected component of G.

(c) G is a noncrossing bond of itself.

Proof. First, assume that NC_G has a $\hat{1} = G$ and we will prove (b). If e and f cross in G and if $G \in NC_G$, then (b) follows immediately. It's clear that (b) implies (c) and that (c) implies (a) by definition. $\square$

Lemma 3.14. *Suppose that G consist of connected components $C_1 \ldots, C_k$ such that no edges of C_i and C_j cross for all $i \neq j$. Then $NC_G \cong NC_{C_1} \times NC_{C_2} \times \cdots \times NC_{C_k}$.*

Proof. We'll proceed by induction, and it will be enough to show that the result holds for $k = 2$. Consider the map $\varphi : NC_G \to NC_{C_1} \times NC_{C_2}$ where $H \mapsto (H \cap E(C_1), H \cap E(C_2))$. It's very straightforward to show that φ is a well-defined bijection. Be definition, it's clear that φ is an order preserving map, so it is an isomorphism of posets, which proves the result. $\square$

There was a large period of time for which we erroneously believed the noncrossing poset was always graded. A simple reason for this was that graphs of order $n \leq 5$ yielded noncrossing bond posets whose structure was "accidentally nice." In other words, there weren't enough poset elements to allow for missing properties. The following example demonstrates a case where the noncrossing bond poset of a graph is not graded. Hence, we require Proposition 3.16 to provide conditions for which a graph does yield a graded noncrossing bond poset. Further, it also tells us the rank of a noncrossing bond poset H in terms of its number of connected components.

Example 3.15. The graph G in Figure 3.7 yields a noncrossing bond poset which is not graded. This figure displays two maximal chains of different lengths. The chain on the left is $1/2/3/4/5 \lessdot 1/26/3/4/5 \lessdot 1/26/35/4 \lessdot 123456$ and the chain on the right is $1/2/3/4/5/6 \lessdot 14/2/3/5/6 \lessdot 124/3/5/6 \lessdot 1246/3/5 \lessdot 12456/3 \lessdot 123456$. The drawing of the shorter maximal chain makes it clear that any additional edge added to the bond $1/26/35/4$ will result in a crossing bond. Hence, it is covered by $\hat{1}$. The maximal chain of greater length shows a sequence of bonds with edges that graphically cross, but each pair of crossing edges is in the same connected component.

Proposition 3.16. *Let G be a graph on $[n]$ which is a noncrossing bond of itself. Then, NC_G is graded if and only if for every cover relation $H \lessdot K$, there are exactly two blocks of H that merge to get K. Moreover, in the case that NC_G is graded, the rank function is given by $\rho(H) = n - cc(H)$.*
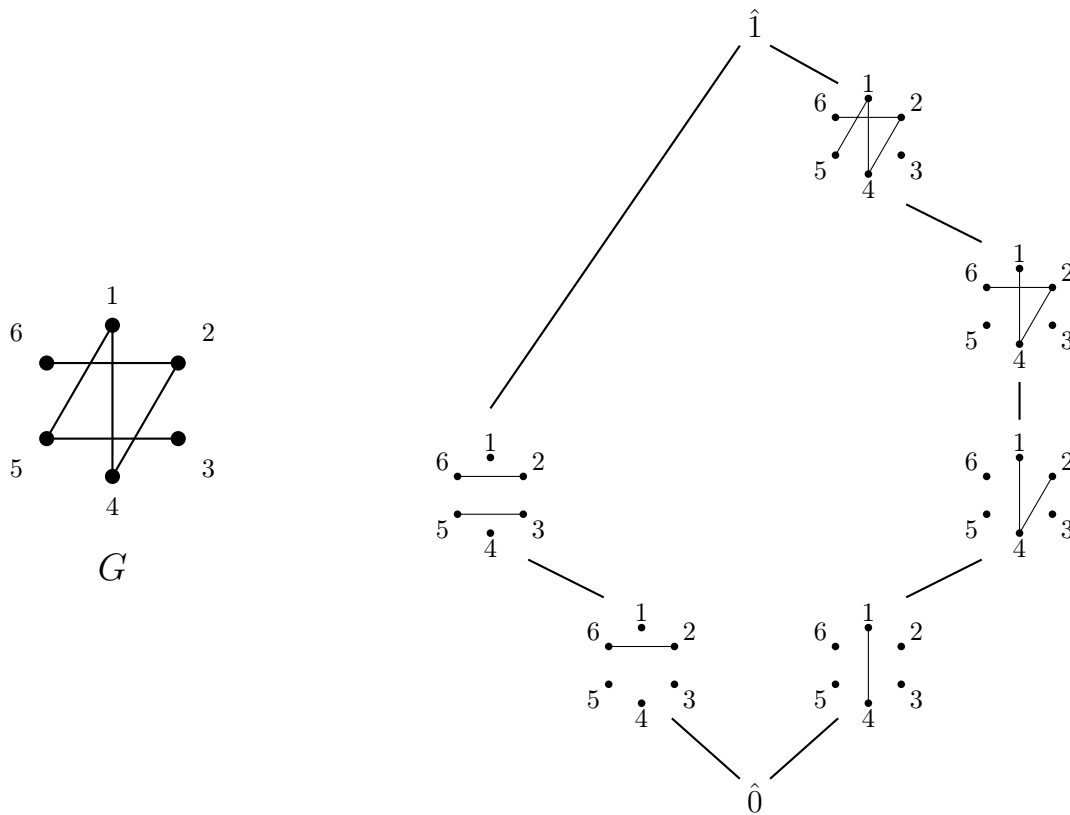
Figure 3.7. A graph whose noncrossing bond poset is not graded.
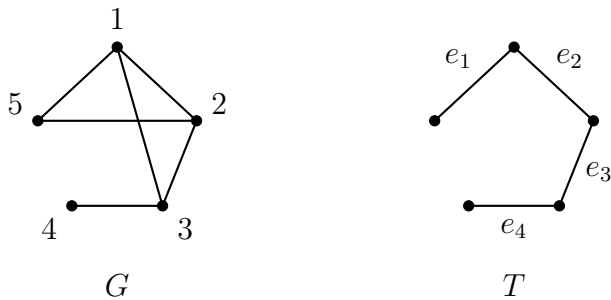
Figure 3.8. Spanning tree and edge sequence

Proof. Since G is a noncrossing bond poset of itself, then $G = \hat{1}$ in NC_G by Proposition 3.13. From this proposition, we also know that the connected components of G so not cross. Hence, Lemma 3.14 implies that NC_G is thus the product of noncrossing bonds posets of the connected components of G. It is known that the product of graded posets is graded, and that the rank function of the product is the sum of the rank

functions. Thus, it will be sufficient to show the result holds for connected graphs.

We assume that G is a connected graph of order n. Let T be a spanning tree of G. Then let $e_1, \ldots, e_{n-1}$ be a sequence of edges of T such that for each forest in the sequence $\{e_1\}, \{e_1, e_2\}, \ldots, \{e_1, e_2, \ldots, e_{n-1}\}$, there is a unique nontrivial connected component (Figure 3.8 shows an example of such a sequence). For each $1 \leq i \leq n-1$, let H_i be the induced subgraph on $\{e_1, \ldots, e_i\}$. By assumption, each H_i has a unique nontrivial connected component; hence H_i is noncrossing. This implies that $\hat{0} \lessdot H_1 \lessdot H_2 \lessdot \cdots \lessdot H_{n-1} = G$ is a maximal chain of length $n-1$. We know $\hat{0}$ of NC_G has n blocks and that $\hat{1}$ has one block, and that there is a maximal chain of length $n-1$. Hence, NC_G is a graded poset if and only if the over relation $H \lessdot H'$ implies that there are exactly two blocks in H which merge to get H'. It is for this reason that the last statement of the theorem holds since the number of connected components of a bond H decreases by one once two blocks are merged. This completes the proof. $\square$

3.3 Chromatic Polynomials and Non-Broken Circuits

In this section, we will define *broken* and *non-broken circuit sets* so that we may provide a combinatorial interpretations for the characteristic polynomial of the bond lattice, the chromatic polynomial, and the noncrossing bond poset.

Definition 3.17. Given a set S, a *coloring* of G by S is a function *proper* if $\kappa(u) \neq \kappa(v)$ whenever u and v are adjacent vertices in G.

Naturally, the combinatorial question of "How many proper colorings are there for a graph G?" George Birkhoff introduced a way of answering this question in [8] by defining the following:

Definition 3.18. Let G be a finite graph on n vertices. The *chromatic polynomial* on G as follows: given a graph G and $t \in \mathbb{N}$, $\text{ch}(P, t) := \#\{\kappa : V(G) \to [t] \mid \kappa \text{ is proper}\}$.

It does not automatically follow from the definition that the chromatic polynomial is a polynomial. Sagan shows in [60] that it is a polynomial, and provides a very nice explanation by using the method known as *deletion/contraction*.

Example 3.19. By way of example, observe the graphs G and H in Figure 3.9. This figure shows proper colorings for these graphs from the set {red, blue, green}. For G, there are t choices for vertex 1, $(t-1)$ choices for vertex 2, $(t-1)$ choices for vertex 3, and $(t-2)$ choices for vertex 4. The chromatic polynomial for H is found by the method of *deletion-contraction*. Then we obtain the following:

$$\text{ch}(G, t) = t(t-1)^2(t-1) \qquad \text{ch}(H, t) = (t-1)^4 + (t-1)(-1)^4$$

Stanley shows a very nice connection between the chromatic polynomial of a graph G and the characteristic polynomial of the bond lattice of G.
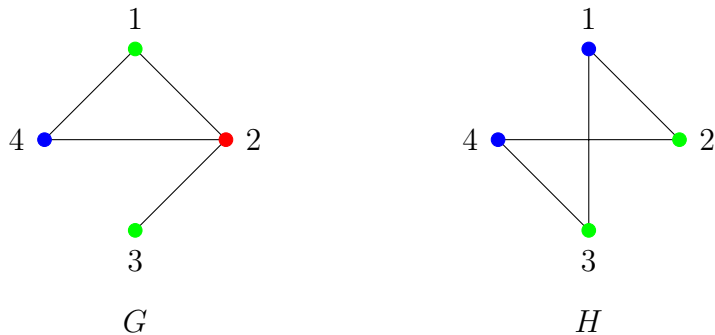
Figure 3.9. Proper Coloring

Recall from Definition 2.13 that $\chi(P, t)$ denotes the characteristic polynomial of a poset P whose coefficients are given by the Möbius values of P.

Theorem 3.20 ([65]). *For all finite graphs G, $ch(G, t) = t^{cc(G)}\chi(L_G, t)$, where $cc(G)$ denotes the number of connected components of G.*

Example 3.21. This is a very nice result in algebraic combinatorics, and it is not obvious that this should be true. For a brief example, see the graph G in Figure 3.10 with its bond lattice. Then

$$\chi(L_G, t) = t^2 - 2t + 1 \qquad\qquad \begin{aligned} ch(G, t) &= t(t-1)(t-2) \\ &= t^1(t^2 - 2t + 1) \end{aligned}$$

and $cc(G) = 1$.
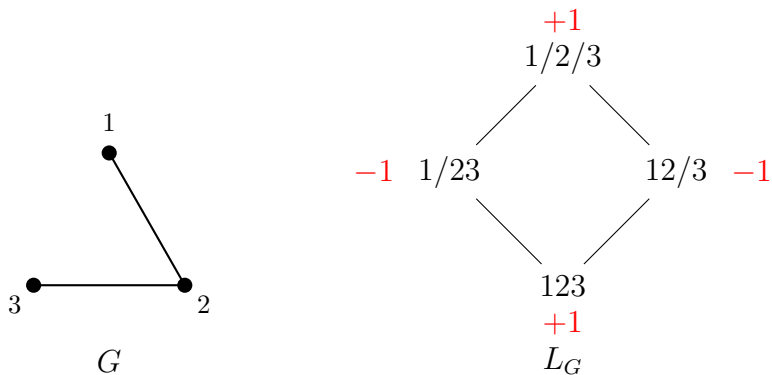
Figure 3.10. A graph and it's bond lattice, including Möbius values

Definition 3.22. Given an graph G where the edges E of G are totally ordered. A *broken circuit set* (or **broken circuit**) is set $B \subset E$ obtained by removing the smallest edge from a cycle of G. A set $N \subset E$ is called a **non-broken circuit set** (or **NBC**) if N doesn't contain any broken circuit of G. Let $\mathbf{nbc_k(G)}$ denote the number of NBC sets of size k for a graph G. It should be clear that subsets of an NBC set are also NBC sets, which can be a useful fact in practice.

Example 3.23. The following tables show the NBC sets for graphs G and H in Figure 3.9 where the edges are ordered lexicographically.

k	NBC sets of size k	$\mathrm{nbc}_k(G)$	Broken Circuits
0	$\varnothing$	1	-
1	$\{12\}, \{13\}, \{23\}, \{24\}$	4	-
2	$\{12,13\}, \{12,23\}, \{12,24\}, \{13,24\}, \{23,24\}$	5	$\{13,23\}$
3	$\{12,13,24\}, \{13,23,24\}$	2	-
4	none	0	-

k	NCB sets of size k	$\mathrm{nbc}_k(H)$	Broken Circuits
0	$\varnothing$	1	-
1	$\{13\}, \{14\}, \{23\}, \{24\}$	4	-
2	$\{13,14\}, \{13,23\}, \{13,24\}, \{14,23\}, \{14,24\}$ $\{23,24\}$	6	-
3	$\{13,14,23\}, \{13,14,24\}, \{13,23,24\}$	3	$\{14,23,24\}$
4	none	0	-

Theorem 3.24. *(Whitney [71]) Let G be a finite graph on $[n]$. Then for any total ordering $\trianglelefteq$ on $E(G)$,*

$$\mathrm{ch}(G,t) = \sum_{k \geq 0} (-1)^k nbc_k(G) t^{n-k}.$$

and

$$\chi(L_G, t) = \sum_{k \geq 0} (-1)^k nbc_k(G) t^{\rho(L_G)-k}$$

3.4 The Möbuis function and Combinatorial Interpretations

Theorem 3.24 shows us how we can use NBC of a graph G sets to compute characteristic polynomial of the bond lattice G. In a similar spirit, we are in search of analogous

result for the noncrossing bond poset. To do this, we present a very natural subset of NBC sets which will certainly aid out endeavors. The following serves as a very nice motivating example which further explains out intuition.

Example 3.25. Consider the graph G, the twisted 4-cycle, whose noncrossing bond poset is shown in Figure 3.11. It's straightforward to show that

$$\chi(L_G, t) = t^3 - 4t^2 + 6t - 3.$$

Let $\trianglelefteq$ be the lexicographic order on $E(G)$; i.e., $12 \triangleleft 13 \triangleleft 24 \triangleleft 34$. Observe that since G is a cycle, we can look for broken circuits. The only broken circuit set is $\{13, 24, 34\}$ since it was obtained by removing the smallest edge 12 from the 4-cycle. So every subset of $E(G)$ is an NBC set except for $\{13, 24, 34\}$ and $\{12, 13, 24, 34\}$; the latter set contains a broken circuit. Then, it's easy to see that $\mathrm{nbc}_0 G = 1, \mathrm{nbc}_1(G) = 4, \mathrm{nbc}_2(G) = 6$, and $\mathrm{nbc}_3(G) = 3$. This example verifies Whitney's theorem, though on it's own, not much is being said. Though, by using the Möbius values provided in Figure 3.11, we find that

$$\chi(NC_G, t) = t^3 - 4t^2 + 5t - 2.$$

Observe that in absolute value, the coefficients of $\chi(NC_G, t)$ are less than or equal to that of $\chi(L_G, t)$. The question becomes "do the coefficients of $\chi(NC_G, t)$ count a subset of the NBC set of G? And if so, which ones?" This is where we'll introduce our noncrossing analogue of NBC sets

Definition 3.26. Let G be a graph and let $\trianglelefteq$ be a total order on $E(G)$. We say that $S \subseteq E(G)$ is a **noncrossing non-broken circuit set** with respect to this ordering if it is an NBC set of G whose edges do not cross in the graphical representation. Denote by $\mathcal{NCNBC}_k(G)$ the set of noncrossing NBC sets of size k and $\mathbf{ncnbc}_k(G)$ to be the number of such sets.

Consider Example 3.25 once again. One may observe that all NBC sets are noncrossing NBC sets except for $\{13, 24\}$ and $\{12, 13, 24\}$.

We will introduce a family of graphs which are a subset of crossing closed graphs below. The motivation is that this class of graphs that we will be able to provide a combinatorial interpretation for with respect to the Möbius functions and characteristic polynomial of the noncrossing bond poset.

Definition 3.27. We say a graph G is **upper crossing closed** if it is crossing closed and there is a total ordering $\trianglelefteq$ on $E(G)$ such that for every pair of crossing edges e and f, $J(e, f)$ contains an edge h such that $h \triangleleft e, f$. If $\trianglelefteq$ is one such ordering, we say that G is **upper crossing closed with respect to** $\trianglelefteq$ and also that $\trianglelefteq$ **is an upper crossing closed ordering** of $E(G)$.
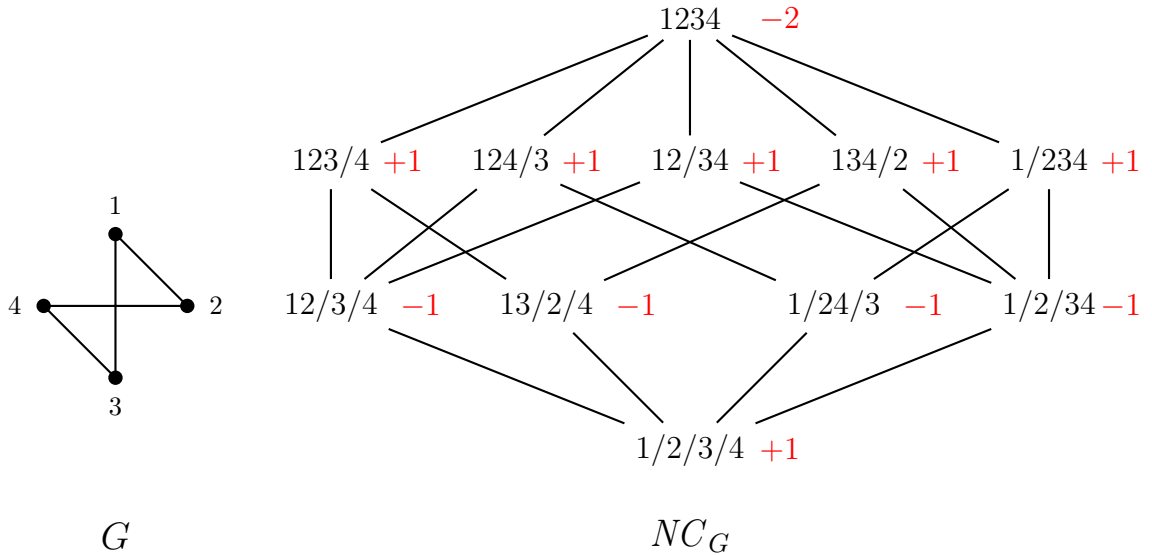
Figure 3.11. The twisted 4-cycle and its noncrossing bond poset with it's Möbius values.

Theorem 3.28. *Let G be a graph on $[n]$. If G is upper crossing closed with respect to the order $\trianglelefteq$ on $E(G)$. Then for all $H \in NC_G$,*

$$\mu(H) = (-1)^{n-cc(H)} \operatorname{ncnbc}_{n-cc(H)}(H).$$

Moreover, if NC_G is graded, then

$$\chi(NC_G, t) = \sum_{k \geq 0} (-1)^k \operatorname{ncnbc}_k(G) t^{\rho(NC_G)-k}.$$

This theorem gives an assertion of the non-obvious fact that the number of NBC sets of size k does not depend on the ordering of the edges, and that $\rho(L_G) = n - cc(G)$.

Before we prove Theorem 3.28, we need to introduce a concept that was presented by Bass and Sagan below.

Definition 3.29 (Bass and Sagan [11])**.** Let L be a lattice with partial order $\leq$, and and let $A(L)$ be the set of atoms of L, with partial order $\trianglelefteq$. A set $S \subseteq A(L)$ is said to be **bounded below** if there exists an atom $a \in A(L) \setminus S$ such that

(a) $a \triangleleft s$ for all $s \in S$

(b) $a < \bigvee S$.

We say that $B \subseteq A(L)$ is a **non-bounded below** set (or an **NBB** set) if B does not contain any S which is bounded below. In this case, we will call B an **NBB base** for $x = \bigvee B$.

In Definition 3.29, a is a lower bound for each s in S with respect to the partial order $\trianglelefteq$ for $A(L)$ while simultaneously being a lower bound for $\bigvee S$ with respect to the partial order $\leq$ for L. The partial order $\trianglelefteq$ on $A(L)$ can be anything from a total ordering to totally incomparable order induced by $\leq$. It might be tempting to conclude that condition (b) is trivially met, so consider the following example.

Example 3.30. Consider the lattice L in Figure 3.12, and order the atoms of L by $a \triangleleft s_1 \triangleleft s_2 \triangleleft s_3$. Let $S = \{s_1, s_2\}$ and $T = \{s_2, s_3\}$. S is a bounded below set since $a \triangleleft s_1, s_2$ and $a \leq \bigvee S = s_1 \vee s_2$. However, $a \not< \bigvee T$. It's easy to see that T does not contain a bounded below set, so T is an NBB set.
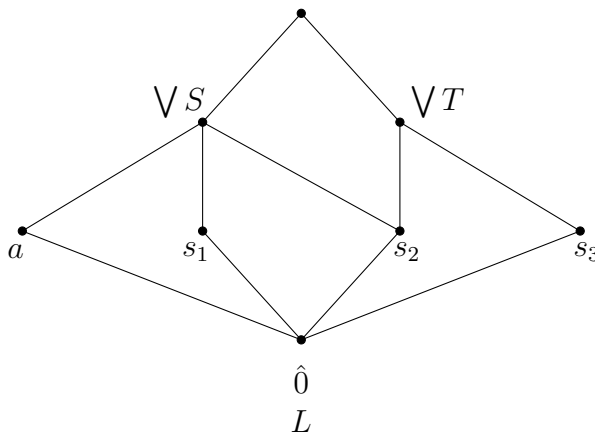
Figure 3.12. Examples of BB and NBB sets.

Theorem 3.31 (Blass and Sagan [11]). *Let L be any finite lattice and let $\trianglelefteq$ be a partial order on $A(L)$. Then for all $x \in L$, we have*

$$\mu(x) = \sum_B (-1)^{\#B}$$

where the sum is over NBB bases of x.

Here, we provide the proof of this theorem since it shows some nice techniques in working with Möbius values. This proof comes from [11] with some additional details and elaboration.

Proof. Let $x \in L$ and define $\overline{\mu}(x) = \sum_B (-1)^{\#B}$ where B runs over all NBB bases B of x. Since L is a finite lattice it has a $\hat{0}$ so the same recursive definition of the Möbius function applies: namely,

$$\mu(x) = \begin{cases} 1 & \text{if } x = \hat{0} \\ -\sum_{y<x} \mu(y) & \text{if } x > \hat{0} \end{cases}$$

Note that μ is the unique $\mathbb{Z}$-valued function on L such that $\sum_{y \le x} \mu(u) = \delta_{\hat{0}x}$ (it's the weak inequality which gives this relation).

To prove the result, we must show that $\overline{\mu}(x) = \mu(x)$ for all such x. Then it suffices to show that $\sum_{y \le x} \overline{\mu}(x) = \delta_{\hat{0}x}$ (the Kronecker Delta). If $x = \hat{0}$, then $x = \bigvee B$ is only true if $B = \varnothing$, which is clearly an NBB set. So

$$\sum_{y \le \hat{0}} \overline{\mu}(y) = \overline{\mu}(\hat{0}) = (-1)^{\#\varnothing} = 1$$

as desired. Suppose now that $x \ne \hat{0}$. If x is an atom, then $x = \bigvee B$ only if $B = \{x\}$. So

$$\sum_{y \le \hat{x}} \overline{\mu}(y) = \overline{\mu}(\hat{0}) + \overline{\mu}(x) = (-1)^{\#\varnothing} + (-1)^{\#\{x\}} = 0$$

as desired.

Now let $x > \hat{0}$ so that $x \notin A(L)$. We aim to show that $\sum_{y \le x} \overline{\mu}(y) = 0$. To do this, let $\mathcal{S} = \{B : B \text{ is an NBB base for some } y \le x\}$; the purpose of which is to set up a corresponding signed set for x. The sign of $B \in \mathcal{S}$ will be defined as $\epsilon(B) = (-1)^{\#B}$, so that from the definitions,

$$\sum_{y \le x} \overline{\mu}(y) = \sum_{B \in \mathcal{S}} \epsilon(B) = \sum_{B \in \mathcal{S}} (-1)^{\#B}.$$

The goal now is to find a sign-reversing involution on $\mathcal{S}$, and if we can do this, the last sum will be zero. From all $a \in A(L)$ with $a < x$, pick one which is minimal with respect to $\trianglelefteq$ and denote it by a_0. The consider the map on $\mathcal{S}$ defined by $\varphi(B) = B \triangle \{a_0\}$ where $\triangle$ is the symmetric difference. Observe that $\varphi^2(B) = (B \triangle \{a_0\}) \triangle \{a_0\} = B$, so this map is an involution. The order of B changes by exactly one once it passes through φ, so $\epsilon(\phi(B)) = -\epsilon(B)$. We should also check that this map is well defined; i.e., that B being an NBB set implies that $\varphi(B)$ is NBB as well.

If B is an NBB set such that $\varphi(B) = B - \{a_0\}$, then $\varphi(B)$ is clearly still NBB. Next, we'll assume the case that $\varphi(B) = B \cup \{a_0\}$ and show that $B' = B \cup \{a_0\}$ by contradiction. If B' is not an NBB set, then there is a subset $D \subseteq B'$ which is bounded below. Then $a_0 \in D$ since B itself is still NBB. Let a be the corresponding element guaranteed by the definition of a bounded below set. So $a \triangleleft a_0$ and $a \bigvee B' \le x$ which contradicts the definition of a_0. Hence, B' must be an NBB set. This shows that φ

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is well defined. It is clear that φ is a bijection of sets in $\mathcal{S}$. Hence, we obtain the following:

$$\sum_{B \in \mathcal{S}} \epsilon(B) = \sum_{B \in \mathcal{S}} \epsilon(\varphi(B)) = -\sum_{B \in \mathcal{S}} \epsilon(B).$$

This implies that $\sum_{B \in \mathcal{S}} \epsilon(B) = \sum_{y \leq x} \overline{\mu}(y) = 0$ as desired. Hence, $\sum_{y \leq x} \overline{\mu}(y) = 0 = \delta_{\hat{0}x}$, and since there is only one $\mathbb{Z}$-values function with properly, we get that $\overline{\mu}(x) = \mu(x)$ for each $x \in L$. This completes the proof. $\qquad\square$

Remark. For any graph G, $A(NC_G)$ is the set of all bonds whose edge sets consist of a single edge of G.

In order to utilize this result to prove Theorem 3.28, we need to draw a connection between NBB and NCNBC sets under the right circumstances. We will illustrate this connection by continuing with our running example of the twisted 4-cycle G in Figure 3.11. We know that with the lexicographic ordering $\trianglelefteq$ that this graph is upper crossing closed. We also saw in the previous proof that the empty set and any singleton subset of atoms are NBB. One can also see that any subset of two noncrossing edges of G is NBB since their joins have only themselves below them. Let's now consider the edges which do cross, 13 and 24. $J(13, 24) = G$, and since $12 \triangleleft 13, 24$ and $12/3/4 \triangleleft 1234$, $\{13, 24\}$ is a bounded-below set. If we take subsets of $E(G)$ of size three, then the join of three edges will also be the entire graph since G is a 4-cycle. All three element subsets of $E(G)$ are NBB except for $\{13, 24, 34\}$ (same argument as before) and $\{12, 13, 34\}$ since it contains $\{13, 24\}$ and itself. So all NBB sets of of the G are the following:

$$\varnothing, \{12\}, \{13\}, \{24\}, \{34\}, \{12, 13\}, \{12, 14\}, \{12, 34\}, \{13, 34\}, \{24, 34\},$$

$$\{12, 13, 34\}, \{12, 14, 34\}.$$

Observe that these are exactly the noncrossing NBC sets of G under the lexicographical order. We will prove in Lemma 3.4 that this is true for all upper crossing closed graphs under the correct ordering $\trianglelefteq$.

Lemma 3.32. *Let G be a crossing closed graph, and let $S \in \mathcal{NCNBC}_k(G)$. Then the join of the elements in S is the same in L_G and NC_G*

Remark. By "the elements in S," we mean the edges of the NCNBC set. The join of these elements is taken to mean the join of the bonds whose edge sets are $\{e\}$ for each $e \in S$.

Proof. Let S be a noncrossing NBC set of G with $\#S = k$. In this proof, we will use $\bigvee_{L_G}$ and $\bigvee_{NC_G}$ to denote the join operators in L_G and NC_G respectively. First, let us show that $\bigvee_{L_G} S$ is a noncrossing bond. Assume to the contrary that this is not the case. We will contradict the fact that S is a noncrossing NBC set. Then

let C_1 and C_2 be connected components of $\bigvee_{L_G} S$ which have crossing edges e and f. Let $S_1 = S \cap E(C_1)$ and $S_2 = S \cap E(C_2)$. Then S_1 is spanning tree of C_1 and S_2 is a spanning tree of C_2. Since C_1 and C_2 cross, there exists edges $ac \in E(C_1)$ and $bd \in E(C_2)$ with $a < b < c < d$ which cross. In S_1 there is a path from a to c, but this path must be separate b and d. Similarly, in S_2 there is a path between b and d. This path must cross the path between a and c. However, these two paths are in different connected components. This implies that S_1 and S_2 must cross, but then S is crossing which is impossible.

Since S is a collection of edges of G and contains no broken circuits, it forms a spanning forest of G. It's not hard to see that $\bigvee_{L_G} S$ is the bond whose induced connected components are the connected components of S. As we saw, since S is noncrossing, $\bigvee_{L_G} S$ is a noncrossing bond in L_G and hence is an element of NC_G. It follows that the partition associated with $\bigvee_{L_G} S$ is noncrossing. It is not hard to see that this is exactly the same partition associated with $\bigvee_{NC_G} S$. Thus, the result holds. $\qquad\square$

Lemma 3.33. *Let G be an upper crossing closed graph with total ordering $\trianglelefteq$ on $E(G)$. Suppose G is upper crossing closed with respect to $\trianglelefteq$. Order the atoms of NC_G by $\trianglelefteq$. Then $\mathcal{NBB}_k(G) = \mathcal{NCNBC}_k(G)$, where $\mathcal{NBB}_k(G)$ is the set of non-bounded below sets of NC_G with k elements.*

Proof. By way of contradiction, suppose that $S \in \mathcal{NBB}_k(G)$, but that $S \notin \mathcal{NCNBC}_k(G)$. If S is a size j set which is not an NBC set, then it contains a broken circuit C. Let e be the edge removed from the cycle to obtain C. Then e is minimal with respect to $\trianglelefteq$, so it follows that that C is a bounded below set with e as the atom which is below all the elements of C; e is an atom because it is the bond with a single edge. This would imply that $S \notin \mathcal{NBB}_k(G)$. Thus, S must be an NBC set. Now suppose that S has crossing edges. Let S' be a set consisting of two such crossing edges. Since G is upper crossing closed, $\bigvee S'$ contains an edge smaller than all the edges of S'. It follows that S' is a bounded below set, but then S is not an NBB set as it contains S'. Thus $S \in \mathcal{NCNBC}_k(G)$.

Next, suppose that $S \in \mathcal{NCNBC}_k(G)$, but that $S \notin \mathcal{NBB}_k(G)$. Then S contains a bounded below set, T. Note that since $T \subseteq S$, T is a noncrossing NBC set. Moreover, since T is bounded below, there exists an atom e such that $e \triangleleft t$ for all $t \in T$ and $e < \bigvee T$. By Lemma 3.4, $\bigvee T$ is the same in L_G and NC_G. Thus, $e < \bigvee T$ and $e \notin T$, implies that e must be in some cycle C of $\bigvee T$. To see why, note that $\bigvee T$ is the induced subgraph on T. The fact that $e < \bigvee T$, implies e is in $\bigvee T$. So if $e = uv$, there is a path from u to v in $\bigvee T$. The set T must contain a spanning tree for the component containing u and v. But since $e \notin T$, e is not on this spanning tree, so e must be on a cycle. Moreover, since e is smaller than all the elements of T, $C \setminus e$ would be a broken circuit of T. But then S is not an NBC set which is impossible. $\quad\square$

Now that we have defined NBB sets, we can use Lemmas and , and Theorem 3.31 to prove the Theorem 3.28.

(Proof of Theorem 3.28). Let G be a graph on $[n]$ that is upper crossing closed with respect to the order $\trianglelefteq$ on E(G). We won't need to assume that NC_G is graded for the first part of the proof since we are showing a result regarding Möbius values. Denote by $A(NC_G)$ the atoms of G. Since $\trianglelefteq$ is a total ordering on $E(G)$, we have $A(NC_G)$ is totally ordered. Using the fact that G is upper crossing closed, Lemma 3.4 asserts that any subset of $A(NC_G)$ is NBB if and only if it is a noncrossing NBC set of G. Then using Blass and Sagan's result, we have that for each $H \in NC_G$,

$$\mu(H) = \sum_B (-1)^{|B|}$$

where the sum is over all the noncrossing NBC sets B such that $\bigvee B = H$. Since B is a noncrossing NBC set, Lemma 3.4 implies that $\bigvee B$ is the same in L_G and NC_G. We claim that for a fixed H, all the NBC sets whose join is H in L_G have the same size, namely $n - cc(H)$. To see why, suppose that S is an NBC set and $\bigvee S = H$. It must be the case that the edges in S form a subgraph of G so that its connected components are exactly the connected components of H. Moreover, since NBC sets cannot contain cycles, S must be minimal with respect to spanning the connected components. So each connected component of S must be a tree. Thus the number of edges in S is $n - cc(S) = n - cc(H)$. It now follows that

$$
\begin{aligned}
\mu(H) &= \sum_B (-1)^{|B|} \\
&= \sum_B (-1)^{n-cc(H)} \\
&= (-1)^{n-cc(H)} \#(\text{noncrossing NBC sets of } G \text{ whose join is } H) \quad (3.1) \\
&= (-1)^{n-cc(H)} \operatorname{ncnbc}_{n-cc(H)}(H).
\end{aligned}
$$

To prove the latter half, assume now that NC_G is graded. Since G is crossing closed, it has a $\hat{1}$ by Proposition 3.12. Then Proposition 3.16 implies that the rank function of NC_G is $\rho(H) = n - cc(H)$. By definition, $\chi(NC_G, t) = \sum_{H \in NC_G} \mu(H) t^{\rho(NC_G)-\rho(H)}$,

then by Equation 3.1, we obtain the following:

$$\chi(NC_G, t) = \sum_{H \in NC_G} (-1)^{n-cc(H)} \#(\text{noncrossing NBC sets of } G \text{ with join } H) t^{\rho(NC_G)-\rho(H)}$$

$$= \sum_{k \geq 0} \sum_{\rho(H)=k} (-1)^k \#(\text{noncrossing NBC sets of } G \text{ with join } H) t^{\rho(NC_G)-k}$$

$$= \sum_{k \geq 0} (-1)^k \left(\sum_{\rho(H)=k} \#(\text{noncrossing NBC sets of } G \text{ with join } H) \right) t^{\rho(NC_G)-k}$$

$$= \sum_{k \geq 0} (-1)^k \, \text{ncnbc}_k(G) t^{\rho(NC_G)-k}$$

which completes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

We showed that the graph in Figure 3.7 NC_G need not be graded; hence the distinction in Theorem 3.28. This distinction is vital since the characteristic polynomial of a poset requires that poset to be graded. We'll continue using the graph in Figure 3.7 in concert with the concept of being upper crossing closed.

Example 3.34. Observe that in the graph G shown in Figure 3.13, is not upper crossing closed. To see this, notice that every edge in G is a crossing edge, including the smallest edge 14. That is, 14 crosses two edges, but $J(14, 26)$ and $J(14, 35)$ cannot contain an edge e such that $14 \lhd e$.

To address this problem, we will subdivide the graph G into the graph H in Figure 3.13. We divide the edges 15 and 14 and label the new vertices $6'$ and $2'$. G is a tree, H inherits this property from G. Thus by Lemma 3.8, H is crossing closed.

Observe that this subdivision provides us with noncrossing edges. It's straightforward to see that any ordering $\unlhd$ for which $16'$ and $22'$ are the smallest edges will result in an upper crossing closed ordering. To see this, notice that for any crossing edges e and f where $J(e, f)$ must contain at least one of these edges. For example in NC_H, $J(14, 26) = H$ and $16', 22' \lhd 14, 26$.

To see that H, however, is not graded, take the bond whose corresponding set partition is $16'/22'6/35/4$, shown in Figure 3.14. Since H is a tree, the addition of any edge would merge two blocks of $16'/22'6/35/4$, but this would result in adding a single edge which would produce a crossing of edges in distinct connected components. Hence, by Proposition 3.16, H cannot have a graded noncrossing bond poset.

3.5 Edge Labellings and Shellability

Recall that a map $\lambda : \mathcal{E}(P) \to \Lambda$ is called an *edge labelling* of P when Λ is some totally ordered set and $\mathcal{E}(P)$ is the set of all edges of the Hasse diagram of P; i.e., the set of
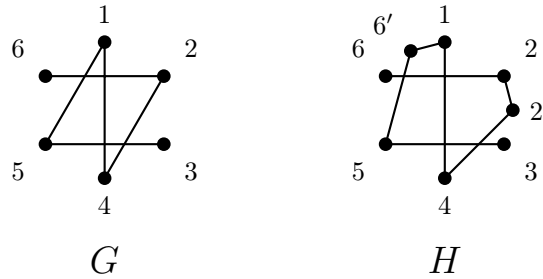
Figure 3.13. NC_G and NC_H are not ranked. H is upper crossing closed (G is not).

$16'/22'6/35/4$
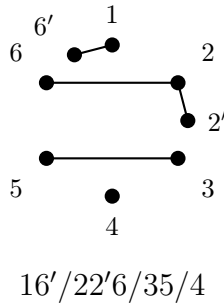
Figure 3.14. Adding any edge to this bond from H in Figure 3.13 will create a crossing

all cover relations of P. Note that this definition is still valid if Λ is partially ordered, though for our purposes, we will assume that it is totally ordered.

Also recall that a saturated chain $c : x_0 \lessdot x_1 \lessdot \cdots \lessdot x_k$ is said to be increasing if $\lambda(x_0 \lessdot x_1) < \cdots < \lambda(x_{k-1} \lessdot x_k)$ and decreasing if $\lambda(x_0 \lessdot x_1) \geq \cdots \geq \lambda(x_{k-1} \lessdot x_k)$. Definition 2.22 describes an EL-labelling, one for which every interval of a poset P has a unique maximal increasing chain which precedes every other maximal chain in the interval in the lexicographic order.

Note that in this section, we will use the term *spanning NBC set* of a graph X to mean an NBC set S of X such that the induced subgraph S is X.

Example 3.35. Consider the graphs in Figure 3.15. The spanning subgraph S has edges which make up an NBC set, and if we induce all possible edges, we obtain X itself.

T recursive nature of the Möbius function can lead to tedious computations by hand. It's natural to search for more efficient ways of computing Möbius values for general posets. The following result provides such a method using EL-labellings.
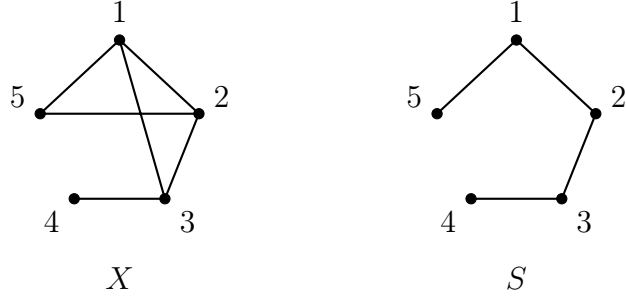
Figure 3.15. Spanning NBC set S of X

Theorem 3.36 (Björner [10]). *Let P be a graded poset with an EL-labelling. Then*

$$\mu(x) = (-1)^{\rho(x)} \#(\text{decreasing saturated chains from } \hat{0} \text{ to } x).$$

Example 3.37. We can demonstrate this with a quick example. Consider the graph G in Figure 3.16. The values in red are the Möbius values of each bond of G and the values in blue represent the edge labellings. Clearly, this is an EL-labelling.

Then

$$\mu(\hat{0}) = (-1)^0 \#(\text{decreasing saturated chains from } \hat{0} \text{ to } \hat{0}) = 1$$
$$\mu(1/23) = (-1)^1 \#(\text{decreasing saturated chains from } \hat{0} \text{ to } 1/23) = (-1)(1) = -1$$
$$\mu(12/3) = (-1)^1 \#(\text{decreasing saturated chains from } \hat{0} \text{ to } 12/3) = (-1)(1) = -1$$
$$\mu(123) = (-1)^2 \#(\text{decreasing saturated chains from } \hat{0} \text{ to } 123) = (1)(1) = 1.$$

The EL-labelling was easily chosen for this example because of the size of the Hasse diagram. This, of course, cannot work in general. Hence, need to approach this more systematically. We will use an edge labelling for the bond lattice which can be applied to the noncrossing bond poset.

Definition 3.38 (Björner [10]). Let G be a graph. Fix some total order $\trianglelefteq$ on $E(G)$. The **minimum labelling** of L_G is defined by

$$\lambda(H \lessdot H') = \min(E(H') \setminus E(H))$$

where the minimum is taken with respect to $\trianglelefteq$.

Example 3.39. Figure 3.17 shows the noncrossing poset of a given graph G with the minimum labelling applied, shown by the Hasse diagram. Once can easily check that this labelling is an EL-labelling. Hence, NC_G is a shellable poset (and in this case, a graded lattice).
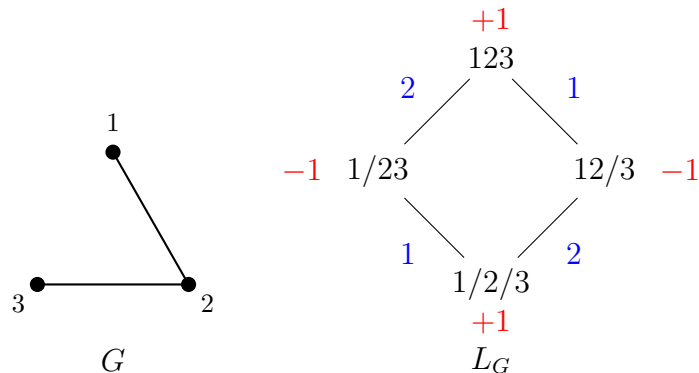
Figure 3.16. Relationship between the chromatic and characteristic polynomials
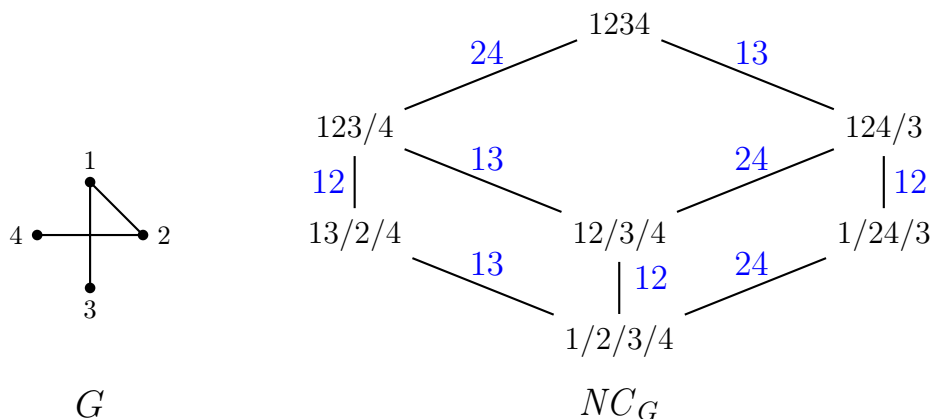
Figure 3.17. A graph and its noncrossing bond posets labeled by the minimum labelling

The following theorem from Björner can be found in [10] and will help is prove a strong result about when the noncrossing bond poset is shellable.

Theorem 3.40 (Björner [10])**.** *Let G be a graph and let $\trianglelefteq$ be a total ordering of $E(G)$. Then we have the following (where the NBC sets are taken with respect to $\trianglelefteq$).*

(a) *The minimum labelling with respect to $\trianglelefteq$ is an EL-labelling of L_G and so L_G is shellable.*

(b) *The labels along any decreasing saturated chain from $\hat{0}$ to X form a spanning NBC set of X.*

(c) *For every $X \in L_G$, each spanning NBC set of X appears exactly once as a saturated decreasing chain from $\hat{0}$ to X.*

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Theorem 3.41. *Let G be a graph on $[n]$ such that NC_G has a $\hat{1}$. Let $\trianglelefteq$ be a total ordering of $E(G)$. Suppose that whenever $H \lessdot H'$ and $e = \min E(H') \setminus E(H)$, the bond induced on $E(H) \cup \{e\}$ is noncrossing. Then we have the following (where the noncrossing NBC sets are taken with respect to $\trianglelefteq$).*

(a) *NC_G is graded and $\rho(X) = n - cc(X)$.*

(b) *The minimum labelling with respect to $\trianglelefteq$ is an EL-labelling and so NC_G is shellable.*

(c) *The labels along any decreasing saturated chain from $\hat{0}$ to X form a spanning noncrossing NBC set of X.*

(d) *For every $X \in NC_G$, each spanning noncrossing NBC set of X appears exactly once as a saturated decreasing chain from $\hat{0}$ to X.*

(e) *For $H \in NC_G$,*
$$\mu(H) = (-1)^{n-cc(H)} \operatorname{ncnbc}_{n-cc(H)}(H)$$
and
$$\chi(NC_G, t) = \sum_{k \geq 0} (-1)^k \operatorname{ncnbc}_k(G) t^{\rho(NC_G)-k}.$$

Proof. (a) Suppose that $H \lessdot H'$, and let $e = \min E(H') \setminus E(H)$. Let H'' then be the bond induced by $E(H) \cup \{e\}$, which will be a noncrossing bond by assumption. Then we have that $H \lessdot H'' \leq H$ which implies that $H' = H''$ since H' covers H. By adding a single edge to H, we are merging two blocks of the corresponding set partition. Hence, we can assert by Proposition 10 that NC_G is graded because the choice of $H \lessdot H'$ was arbitrary. Moreover, $\rho(X) = n - cc(X)$.

(b) Let λ be the minimum labelling with respect to $\trianglelefteq$. From (a) we know that NC_G is a graded subposet of L_G. Hence, the ranks of all noncrossing bonds will be the same as they are in L_G. Even though we delete crossing bonds from L_G to get NC_G, if we label the edges of the Hasse diagram of L_G by λ, all edges in $\mathcal{E}(L_G)$ which survive in $\mathcal{E}(NC_G)$ will inherit the same labels. Each interval in L_G has a unique increasing maximal chain that is minimal with respect to the lexicographical ordering in. Though, as we remove crossing bonds from L_G, we need to ensure that these chains survive in NC_G.

Consider an interval $[H, H']$ in NC_G. We will induct on the length k of $[H, H']$. If the length is 1, the result is trivial. So assume that $k > 1$ that any interval $[H, H']$ inherits it's increasing maximal chain from L_G. Then suppose that $[H, H']$ has length $k+1$. Let $e = \min E(H') \setminus E(H)$ and let H'' be the bond induced on $E(H) \cup \{e\}$. Then by our initial assumption, H'' is noncrossing, so $H'' \in [H, H']$. Then $\lambda(H \lessdot H'') = e$. By the inductive hypothesis $[H'', H']$ has an increasing maximal chain which starts

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with a label larger than e. Concatenating this chain with $H \lessdot H''$ will produce an increasing maximal chain of $[H, H']$. Hence, the unique increasing maximal chain for each interval in L_G survives in NC_G. It's follows automatically that these chains will still be minimal with respect to the lexicographical ordering. Moreover, the minimum labelling is an EL-labelling and so NC_G is shellable.

(c) Let $X \in NC_G$ and let c be some decreasing saturated chain from $\hat{0}$ to X. By Theorem 3.40, we get automatically that the labels along c form an NBC set, say S. We need to show that this is a noncrossing NBC set. We'll proceed by way of contradiction. Suppose that S is an NBC set which contains crossing edges a and b. Since the edges are totally ordered, let $a \lhd b$ without loss of generality. We'll assume that X is minimal among element of NC_G that have crossing edges in one of its NBC sets. We claim that a is the smallest edge of $E(X)$. First note that every spanning NBC set of X contains the smallest edge of $E(X)$. To see why, note that if the smallest edge was a bridge of X, it must be in this spanning set. If it is not a bridge, it is contained in some cycle and so must be in the spanning set since otherwise X would contain a broken circuit. Thus, the smallest edge of X is in every spanning NBC set of X. Hence, the labels along any saturated chain from $\hat{0}$ to X must contain the smallest edge, so the labels along all decreasing saturated chains from $\hat{0}$ to X must end with the smallest edge. We have a minimality assumption on X with respect to having a crossing. So the last label is either a or b. Though, $a \lhd b$, so a must be the smallest edge in $E(X)$. Since b is an edge of x, we know the interval $[b, X]$ exists in NC_G where b is the bond with only the edge b. We get that $a = \min E(X) \setminus \{b\}$, so by our assumption, the bond induced on a and b is a noncrossing bond. Though, a and b were assumed to crossing edges, hence they are not adjacent; i.e., they do not share an end point. So the bond induced on a and b is the bond with edge set $\{a, b\}$. But since this bond is noncrossing by initial assumption, this contradicts the face that a and b cross.

(d) Let $F = \{e_1, e_2, \ldots, e_k\}$ be a spanning noncrossing NBC set of X with $e_1 \rhd e_2 \rhd \cdots \rhd e_k$. Let $H_0 = \hat{0}$ and for $1 \leq i \leq k$, let F_i be the forest with vertex set $V(G)$ and edge set $\{e_1, e_2, \ldots, e_i\}$. Moreover, let H_i be the bond induced on F_i. We claim that each of these bonds is noncrossing. To see why, note that the partitions associated to F_j and H_j are the same for all $0 \leq j \leq k$. Since each F_j is noncrossing, Proposition 3.3 implies that the partition for F_j is noncrossing and so H_j is a noncrossing bond.

By Theorem 3.40, each spanning NBC set of X appears exactly once as a saturated decreasing chain in L_G. By construction, $H_0 \lessdot H_1 \lessdot \cdots \lessdot H_k$ is the saturated chain chain from $\hat{0}$ to X which produces the NBC set $F = \{e_1, e_2, \ldots, e_k\}$. The claim now follows since this chain also exists in NC_G.

(e) Note that by Proposition 3.16 and part (a), $\rho(H) = n - cc(H)$ for all $H \in NC_G$. Parts (c) and (d) provide a bijection between the saturated decreasing chains from $\hat{0}$ to H and noncrossing NBC sets. Then to finish, apply part (b) and Theorem 3.36. $\square$

Chapter 4: The Noncrossing Bond
Poset of Families of Graphs

Thus far, we have spent much time and attention to constructing families of graph which necessarily yield noncrossing bond posets with desired combinatorial properties and interpretations. Moving forward, we will discuss our research on known families of graphs, and explore the the consequences on the noncrossing bond poset.

4.1   Perfectly Labeled Graphs

Definition 4.1. Let G be a graph. We say G is **perfectly labeled** if whenever $ik, jk \in E(G)$ with $i < j < k$, $ij \in E(G)$.[1]

Example 4.2. In Figure 4.1, we see two isomorphic graphs G and H. Once can easily check that G is perfectly labeled, whereas H is not. Observe that H contains the edges 14 and 24 where $1 < 2 < 4$. To be perfectly labeled, it is required that 12 is an edge of H, and this is not the case.
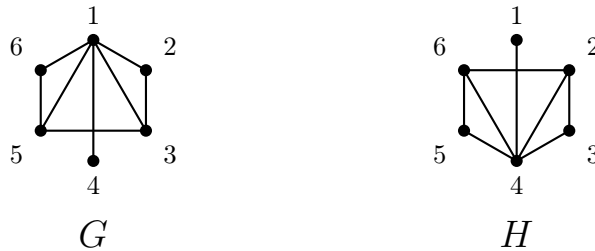
Figure 4.1. A perfectly labeled graph and a non-perfectly labeled graph.

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[1]It is common in the literature to call a labelling of a graph with this property a **perfect elimination order**.

Lemma 4.3. *Let G be a connected perfectly labeled graph. Let r be the smallest vertex in G, and let v be any other vertex of G. There exists an increasing path from r to v in G. That is, there is a path $ru_1u_2\ldots u_kv$ where $r < u_1 < u_2 < \cdots < u_k < v$.*

Proof. We'll prove this by way of contradiction. Suppose there is no such path from r to v. Then let P be a shortest path from r to v. By assumption, P is not an increasing path. Since this path contains the smallest vertex of G, it must contain contain a subsequence of vertices ikj where $i < j < k$. Though, G is a perfectly labeled graph, and since P contains ikj, this implies that ik and jk are edges of G. Hence, $ij \in E(G)$, so we may replace the edges ik, jk with ij and get a shorter path from r to v. This contradicts the minimality of P. Therefore, G must contain such a path P when it is perfectly labeled. $\square$

Lemma 4.4. *Let G be a perfectly labeled graph. Suppose that $H \leq H'$ in NC_G. Moreover, suppose that $B_1, B_2, \ldots, B_k$ where $\min B_1 < \min B_2 < \cdots < \min B_k$, are the connected components of H that are merged together to get H'. Then merging B_1 and B_2 in H creates a noncrossing bond of G.*

Proof. Assume that G is a perfectly labeled graph, and let $3 \leq i \leq k$. By definition, if we merged B_1 and B_2 in such a way that it crossed with B_i (i.e., resulted in a crossing partition), then there would exist $a, c \in B_1 \cup B_2$ and $b, d \in B_i$ or $a, c \in B_i$ and $b, d \in B_1 \cup B_2$ with $a < b < c < d$.

Assume the former case that $a, c \in B_1 \cup B_2$ and $b, d \in B_i$. Then $\min B_1 < \min B_2 < b < c < d$ which implies either B_1 and B_i cross or B_2 and B_i cross (depending on if $c \in B_1$ or $c \in B_2$). Neither is possible since H is noncrossing. The latter case is shown by similar argument, that it is not possible that there exists $a, c \in B_i$ and $b, d \in B_1 \cup B_2$ with $a < b < c < d$. Hence merging B_1 and B_2 does not cause a crossing with $B_3, B_4, \ldots, B_k$. Moreover, merging B_1 and B_2 cannot create a crossing with any of other connected components of G since that would mean that H' was crossing.

Thus it suffices to show that merging B_1 and B_2 in H forms a bond of G. It is not hard to see that any induced subgraph of a perfectly labeled graph is perfectly labeled. It follows that H' is perfectly labeled. By Lemma 4.3 there is an increasing path in H' from $\min B_1$ to $\min B_2$. Except for $\min B_2$, this path must only contain vertices from B_1 since otherwise it would not be increasing. So there is an edge, e, between a vertex in B_1 and a vertex in B_2. Then the bond induced on on $E(H) \cup \{e\}$ is exactly the spanning subgraph obtained by merging B_1 and B_2 in H. The result follows. $\square$

So far, we have been using the lexicographic ordering on edges, save for a couple small examples where we presented some ad-hoc ordering. Though, for the next lemma, we will use the *colexicographical* ordering on edges. That is, we'll say that $a_1a_2\ldots a_k \lhd b_1b_2\ldots b_k'$ if and only if $a_i < b_i$ for the last i where a_i and b_i differ. Put another way, this ordering is the regular lexicographical ordering if we write all

words in reverse order. For example, the following are ordered lexicographically and colexicographically respectively:

$$12 < 13 < 14 < 15 < 23 < 24 < 25$$
$$12 < 13 < 23 < 14 < 24 < 34 < 15$$

Lemma 4.5. *Let G be a perfectly labeled graph with the edges colexicographically. If $H < H'$ and $e = \min E(H') \setminus E(H)$, then the bond induced on $E(H) \cup \{e\}$ is noncrossing.*

Proof. Let G be a graph and let $H \in NC_G$ and suppose that the blocks $B_1, B_2, \cdots, B_k$ are the blocks of $\pi(H)$ which merge to get H', labeled so that $\min B_1 < \min B_2 < \cdots < \min B_k$. An arbitrary subgraph of a perfectly labeled graph need not be perfectly labeled. However, H' is a bond, so all edges within the same block are induced from G, so H' is perfectly labeled. B_1 and B_2 are in the same connected component in H' by assumption, so Lemma 4.3 asserts that there is an increasing path in H' from the smallest vertex of B_1 to the smallest vertex of B_2. Note that Lemma 4.3 only required one vertex r be minimal while the other vertex v is any vertex of G. Here, $\min B_1$ is the smallest vertex in H which is not an isolated vertex. Because this path is increasing, the last edge of this path must be of the form $a \min B_2$ where a is come vertex in B_1. Let a_0 be the smallest vertex in B_1 for which there is an edge $a_0 \min B_2$. By the colexicographic ordering on the edges of G, $a_0 = \min(E(H') \setminus E(H))$. So the bond we obtain by merging B_1 and B_2 is the bond induced on $E(H) \cup \{a_0 \min B_2\}$. And by Lemma 4.4, this bond is noncrossing. This completes the proof. $\square$

Example 4.6. We'll briefly confirm this result with an example. Let G be the graph in Figure 4.2, which is perfectly labeled. Let $H = 12/3/4$ and let $H' = 1234$. Then $B_1 = 12$ and $B_2 = 3$. The path described by Lemma 4.3 is $P = 123$ and we can see that 23 being the last edge has a vertex in B_1 and B_2. Then $a_0 = 1$ so $a_0 \min B_3 = 13$. The colexicographical ordering of the edges gives $12 < 13 < 23 < 24$ (which coincidentally is the regular lexicographic ordering). Notice that $\min(E(H') \setminus E(H)) = \min\{13, 23, 24\} = 13$ which is what we want. The bond induced on $E(H) \cup a_0 \min B_2 = \{12, 13\}$ is the bond 123/4; i.e., the 3-cycle with an isolated vertex 4, clearly noncrossing.

Definition 4.7. Let T be a tree with vertices which are distinct integers. Let r be the smallest vertex of T. We say T is an **increasing tree** if the vertices along any path from r to any other vertex form an increasing sequence. We say a spanning subgraph of a graph G is an **increasing spanning forest** of G if each connected component is an increasing tree.
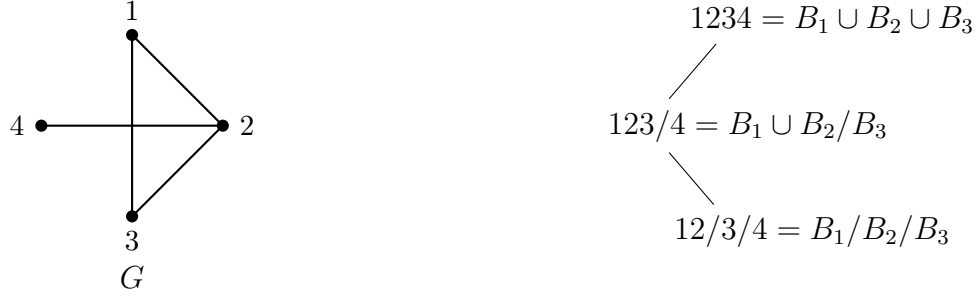
Figure 4.2. Demonstrating the proof of Lemma 4.5

Similar to the notation for NBC sets, let $\mathcal{ISF}(G)$ and $\mathcal{ISF}_k(G)$ denote the set of increasing spanning forests of G and the set of increasing spanning forests of G of size k. Likewise, let $\text{isf}(G)$ and $\text{isf}_k(G)$ denote the number of ISF of G and the number of ISF of G of size k.

Example 4.8. As with NBC sets, we describe an increasing spanning forest as *noncrossing* if none of the edges cross in the graphical representation. Figure 4.3 shows the graph G from Figure 4.1, and three of it's spanning forests F_1, F_2, and F_3. F_3 is not an increasing spanning forest since it contains the sequence 132. F_1 and F_2 are both increasing, though F_2 is crossing whereas F_1 is noncrossing. In this context, crossing edges within the same connected components still earn the spanning forest the title of "crossing" unlike a bond.

In [30] (Theorem 2.4), Hallam et al. showed that when G is a graph on $[n]$ and $E(G)$ is ordered lexicographically, then $\mathcal{ISF}_k(G) = \mathcal{NBC}_k(G)$ when G is perfectly labeled. In [64], Stanley showed that the number of acyclic orientation of an order n graph G is $ao(G) = (-1)^n \text{ch}(G, -1)$, where $\text{ch}(G, -1)$ is the chromatic polynomial of G evaluated at $t = -1$. It's not obvious why this is true, nor is it natural input -1 for t, since t in the context of chromatic polynomials describes the number of colors for the vertices of G. Hence, this is quite an extraordinary discovery! In [30] combine this with Whitney's theorem (Theorem 3.24) for a perfectly ordered graph G on $[n]$ to obtain the following (described with some extra detail):

$$\text{ch}(L_G, -1) = \sum_{k \geq 0} (-1)^k \text{nbc}_k(G)(-1)^{n-k}$$
$$= (-1)^n \sum_{k \geq 0} \text{nbc}_k(G)$$
$$= (-1)^n \text{nbc}(G)$$
$$\implies ao(G) = (-1)^n \cdot (-1)^n \text{nbc}(G)$$
$$= \text{nbc}(G)$$

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The objective of this slight tangent is to demonstrate the usefulness of perfectly labeled graphs. Though, Theorem 2.4 in [30] can be modified to our benefit, even with the colexicographic ordering on $E(G)$. This yields the following lemma.
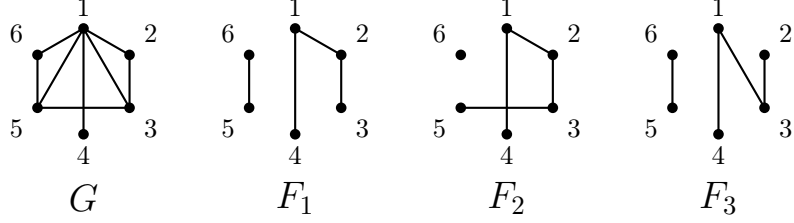
Figure 4.3. Spanning forests of G

Lemma 4.9. *Let G be a perfectly labeled graph with the edges ordered colexicographically. Then for all $k \geq 0$, $\mathrm{ncisf}_k(G) = \mathrm{ncnbc}_k(G)$.*

Theorem 4.10. *Let G be a perfectly labeled graph on $[n]$ such that NC_G has a $\hat{1}$. Then we have the following.*

(a) *NC_G is graded and for $H \in NC_G$, the rank of H is given by $\rho(H) = n - cc(H)$.*

(b) *The minimum labelling with respect to the colexicographic ordering on $E(G)$ is an EL-labelling of NC_G and so NC_G is shellable.*

(c) *For $H \in NC_G$,*

$$\mu(H) = (-1)^{n-cc(H)} \, \mathrm{ncnbc}_{n-cc(H)}(H) = (-1)^{n-cc(H)} \, \mathrm{ncisf}_{n-cc(H)}(H)$$

and

$$\chi(NC_G, t) = \sum_{k \geq 0} (-1)^k \, \mathrm{ncnbc}_k(G) t^{\rho(NC_G)-k} = \sum_{k \geq 0} (-1)^k \, \mathrm{ncisf}(G) t^{\rho(NC_G)-k},$$

where the NBC sets are with respect to the colexicographic ordering on $E(G)$.

Proof. The result follows from Lemma 4.5, Lemma 4.9, and Theorem 3.41. $\qquad \square$

Definition 4.11. A graph is **chordal** if for every cycle of length at least 4 there is an edge between two vertices in the cycle which are not adjacent in the cycle.

Definition 4.12. Let L be a finite lattice. We say that L is **supersolvable** if it possesses a maximal chain $\mathfrak{c}$ such that the sublattice of L generated by $\mathfrak{c}$ and any other chain of L is distributive.

An example of a supersolvable lattice if the lattice of subgroups of a supersolvable group G (ordered by containment).

Definition 4.13 (Björner-Edelman [10]). Let G be a graph on $[n]$ such that NC_G is graded. The **max-min** edge labelling is defined by

$$\lambda(H \lessdot H') = \max\{\min B, \min B'\} - 1$$

where B and B' are the blocks merged when going from H to H'.

Definition 4.14. Let λ be an EL-labelling (Definition 2.22) of a poset P of rank n. Then we say that λ is an $\boldsymbol{S_n}$ **EL-labelling** if every maximal chain of P is labeled by a permutation of $[n]$ (with the natural ordering on $[n]$.
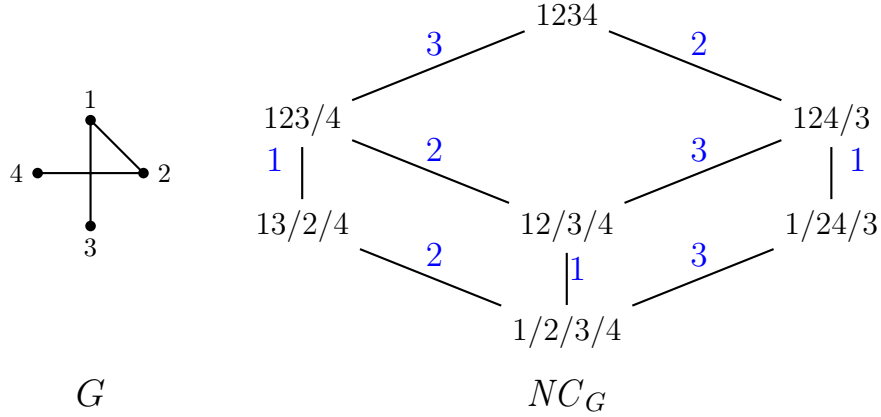
Figure 4.4. A graph and its noncrossing bond poset labeled by the max-min edge labelling.

Proposition 4.15. *Let G be a connected graph on $[n+1]$ such that NC_G is graded. The max-min edge labelling is an S_n EL-labelling of NC_G if and only if G is perfectly labeled.*

Proof. Assume that G is a graph on $[n+1]$ and that NC_G is graded. Then NC_G is a subposet of $NC_{K_{n+1}}$. Since $NC_{K_{n+1}}$ is the noncrossing partition lattice on $[n+1]$, we have that NC_G is a subposet of the noncrossing partition lattice. It follows from the assumption that NC_G is graded with the same rank function as the noncrossing partition lattice (see Proposition 3.16). Once can easily see that the set of maximal chains in NC_G is a subset of the maximal chains of the noncrossing partition lattice. Since the cover relations in NC_G are the same as that in the noncrossing partition

lattice, we also have that the label sequences that appear along the maximal chains in NC_G are the same as those that appear in the noncrossing partition lattice. Since it is known that the max-min edge labelling is an S_n EL-labelling of the noncrossing partition lattice, to finish the proof we can show that each interval of NC_G has an increasing maximal chain if and only if G is perfectly labeled.

By way of contradiction, suppose that G is not perfectly labeled. Then there exists edges ik, jk such that $i < j < k$ and $ij \notin E(G)$. Let H be the bond of G where i, j, k are in the same connected component and every other connected component is a isolated vertex. That is, H cannot contain ij. Now take the interval $[\hat{0}, H]$. Since $ij \notin E(G)$, we obtain the following as we merge blocks:

$$\max\{\min\{i\}, \min\{k\}\} - 1 = k - 1 \qquad \max\{\min\{j\}, \min\{k\}\} - 1 = k - 1$$
$$\max\{\min\{i, k\}, \min\{j\}\} - 1 = j - 1 \qquad \max\{\min\{i\}, \min\{j, k\}\} - 1 = j - 1$$

(see Figure 4.5 for a visual). Hence, this interval has two maximal chains both labeled by $k - 1, j - 1$, both decreasing. Thus the interval has no increasing chain, which is a contradiction.

Next, suppose that G is perfectly labeled. Suppose that $[H, H']$ is an interval in NC_G and suppose that $B_1, B_2, \ldots, B_k$ are the connected components of H that will merge together to get H'. Moreover, assume that $\min B_1 < \min B_2 < \cdots < \min B_k$. It is not hard to see that if there is an increasing maximal chain in $[H, H']$, the first step must be to merge B_1 and B_2. Let H'' be the bond obtained by merging B_1 and B_2 in H. We can apply Lemma 4.4 to see that $H'' \in NC_G$. Now we can use induction in a similar way we've done before. Then $[H'', H']$ has an increasing maximal chain which can be concatenated with the label from H to H'' to give an increasing maximal chain in $[H, H']$. This completes the proof. $\square$
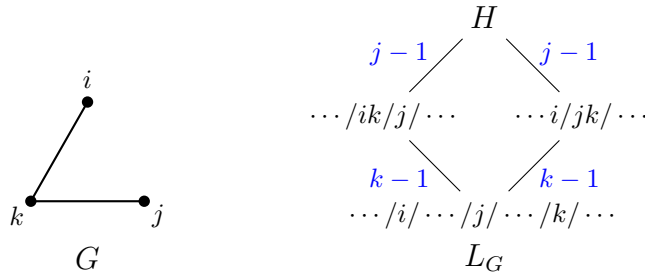
Figure 4.5. Visual aid for Proposition 4.15

Theorem 4.16. *Let G be a perfectly labeled graph. If G is crossing closed, then NC_G is a supersolvable lattice.*

Proof. Suppose that ac and bd cross with $a < b < c < d$. Then in $J(ac, bd)$, there is a path from a to b. Let $P : av_1v_2 \ldots v_k b$ be a path from a and b which is minimal with respect to length. If P is not increasing, then there is a an index i with $v_{i-1}, v_{i+1} < v_i$. But then since G is perfectly labeled, there is an edge $v_{i-1}v_{i+1}$ contradicting the minimality of P. So P must be increasing. Then av_1 is an edge in $E(G)$ and is smaller in colexicographic and lexicographic order than ac and bd. It follows that G is upper crossing closed with respect to colexicographic and lexicographic order. $\qquad\square$

Example 4.17. We mention here that not every perfectly labeled graph is crossing closed (hence the necessity of the crossing closed hypothesis in Theorem 4.16). The graph in Figure 4.6 is perfectly labeled, but not crossing closed. This is because there are two minimal induced connected components containing 16 and 57, namely noncrossing bonds 13567/2/4 and 124567/3.

The reader may be wondering if NC_G being supersolvable implies that G is chordal since this is the case for the bond lattice of a graph. The graph in Figure 3.11 shows this is not true. It is a 4-cycle and thus is not chordal. Nevertheless, its noncrossing bond poset is a supersolvable lattice.
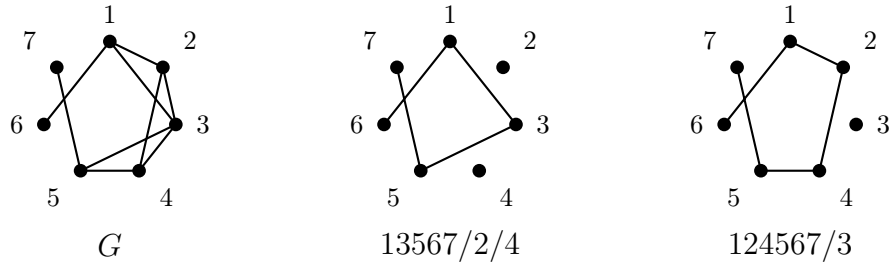
Figure 4.6. A perfectly labeled graph which is not crossing closed

Proposition 4.18. *Let G be a perfectly labeled graph which is crossing closed. Then G is upper crossing closed with respect to the colexicographic and lexicographic order.*

4.2 Tightly Closed graphs

Here, we consider the subset of crossing closed which adhere to the first form presented in Lemma 3.9.

Definition 4.19. Let G be a graph. We say G is **tightly closed** if it is crossing closed and for all edges e and f that cross, $J(e, f)$ is a subgraph of K_4.

Proposition 4.20. *Let G be a complete bipartite graph. Then G is tightly closed.*
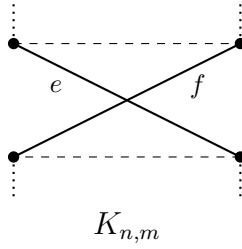
Figure 4.7. Crossing edges in a complete bipartite graph

Proof. Let e and f be crossing edges in $K_{n,m}$ for some $n, m \geq 1$. Since all possible edges with respect to a bipartite graph are present, the crossing edges connect the two parts of the graph; i.e., that two parts of the vertex partition (see Figure 4.7. Hence, they must lie on a (twisted) 4-cycle. Thus, $K_{n,m}$ is tightly closed. $\square$

Proposition 4.21. *If G is 2-connected and crossing closed, then G is tightly closed.*

Proof. By Lemma 3.9, if G was not tightly closed, G would have cut vertices. This is impossible as G is 2-connected. $\square$

It may be tempting to think that 2-connected graphs are automatically crossing closed. This is not true in general. The twisted 6-cycle shown in Figure 4.8 is a graph that is 2-connected but not crossing closed. We demonstrate this by showing two bonds which contain the crossing edges 14 and 36, but these bonds are not comparable and their meet is the crossing bond $14/2/36/5$.
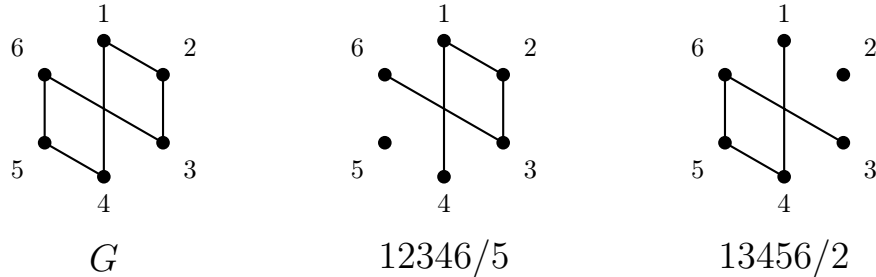
Figure 4.8. A 2-connected graph that is not crossing closed

Theorem 4.22. *If G be a tightly closed graph, then NC_G is graded.*

Proof. Let $H \lessdot H'$. For each edge $f \in E(H') \setminus E(H)$, we will count crossings of f with the edges in $E(H)$. We will call such a crossing *bad* if the edges in the crossing

are in different components of the graph with edge set $E(H) \cup \{f\}$ and vertex set $V(G)$.

We claim that there is an edge in $E(H') \setminus E(H)$ with no bad crossings. To see why, suppose by way of contradiction that this was not the case. So let $e = ac$ be an edge of $E(H') \setminus E(H)$ with a minimum number of bad crossings. The by assumption, e has at least one bad crossing, say with edge $e' = bd$ in H where $a < b < c < d$. Since e and e' are in H' and are crossing and H' is noncrossing, they must lie in the same connected induced component of H'. Thus $J(e, e')$ is a subgraph of this component. Since G is tightly closed, $J(e, e')$ is a subgraph of K_4 and so one of the edges ab, bc, cd, ad must be present in H'. Without loss of generality we may assume that ab is present. Note that ab is not in H as e and e' is assumed to be a bad crossing and e and e' thus lie in different components of the graph with edge set $E(H) \cup \{e\}$.

Since there are no edges in $E(H') \setminus E(H)$ with no bad crossings, ab must have a bad crossing with some edge, say vw. We claim that vw must cross e. If this was not the case, then $a < v < b < w \leq c < d$. This implies that vw crosses $e' = bd$ in H and since H is noncrossing, vw and $e' = bd$ must be in the same component. But then vw and ab do not form a bad crossing. Thus, vw crosses e and so any edge that crosses ab to form a bad crossing will form a bad crossing with e. This means that e has strictly more bad crossings than ab which is impossible as e was chosen to be minimal. Thus, there is an edge of $E(H') \setminus E(H)$ which has no bad crossings.

Let e be an element of $E(H') \setminus E(H)$ which has no bad crossings, and let G' be the graph on $V(G)$ with edge set $E(H) \cup \{e\}$. Since e has no bad crossings, the partition associated to G' is noncrossing. Now let H'' be the bond induced on $E(H) \cup \{e\}$. Then G' and H'' have the same connected components and so correspond to the same partition. It follows that H'' is a noncrossing partition. Since $H < H'' \leq H'$ and $H \lessdot H'$, $H' = H''$. Moreover, by construction there are exactly two components that merge together from H to H' and so by Proposition 3.16, NC_G is graded. $\qquad \square$

The notion of tightly closed may seem odd at first glance. However, there is an order-theoretic way to define tightly closed that is much like the notion of *semimodularity*. We stated previously that that a lattice L is (upper) semimodular if it is graded and for all $x, y \in L$, $\rho(x \vee y) + \rho(x \wedge y) \leq \rho(x) + \rho(y)$. In the case that a_1 and a_2 are distinct atoms of L, semimodularity implies that $\rho(a_1 \vee a_2) = 2$. Tightly closed graphs can be defined by slightly relaxing this idea (despite the ironic choice of words). We so do in the following theorem.

Theorem 4.23. *Let G be a graph which is crossing closed. G is tightly closed if and only if for all distinct atoms $a_1, a_2 \in NC_G$, $\rho(a_1 \vee a_2) = 2$ or $\rho(a_1 \vee a_2) = 3$.*

Proof. We know that all of the atoms of any noncrossing bond poset are the bond which contain each individual edge from G. So let $e, f \in E(G)$ (we are using e and f in place of a_1 and a_2). In the case that e and f do not cross, $\rho(e \vee f) = 2$ because

merging these two edges will induce a noncrossing bond which covers e and f. In the case that e and f do cross, then we get from Proposition 3.12 part (c) that G being crossing closed implies that $J(e, f)$ is the unique nontrivial connected component contained in $e \vee f$ (the component that contains e and f).

If we assume that G is tightly closed, then NC_G is graded and so for any $H \in NC_G$, $\rho(H) = |V(G)| - cc(H)$. This would imply that $\rho(e \vee f) = 3$ if and only if $J(e, f)$ is a connected graph on 4 vertices. Otherwise, $J(e, f)$ would have greater rank. This argument works in the reverse direction, hence the proof is complete. □

Proposition 4.24. *Let G be an upper crossing closed graph which is tightly closed. Then the conclusions of Theorem 3.41 hold. In particular, NC_G is a lattice, graded, shellable, and the Möbius function and characteristic polynomial have a combinatorial interpretation in terms of NCNBC sets.*

Proof. First note that since G is crossing closed, Proposition 3.12 part (b), NC_G is a meet-sublattice of L_G and (e) implies that NC_G has a $\hat{1}$. This gives us that NC_G is a lattice. Now suppose that $H < H'$. Let $e = \min E(H') \setminus E(H)$. Adopting the terminology from the proof of Theorem 4.22, we will show that e has no bad crossings in $H \cup \{e\}$. Suppose this was not the case. Then there is an edge f not in the same connected component of e in $E(H) \cup \{e\}$ which crosses e. Since H' is noncrossing and G is tightly closed, there is an edge, h, connecting an endpoint of e and an endpoint of f. Moreover, we may assume that h precedes e in $\trianglelefteq$ as G is upper crossing closed. Since $e = \min E(H') \setminus E(H)$, this would imply that $h \in E(H)$. So e and f do not form a bad crossing, a contradiction. Since e has no bad crossings, the bond induced on $E(H) \cup \{e\}$ is noncrossing. Applying Theorem 3.41 now completes the proof. □

4.3   Strongly Upper Closed Graphs

Definition 4.25. Let G be a graph with a total ordering, $\trianglelefteq$, on the edge set of G. We say that a graph G is **strongly upper crossed** with respect to $\trianglelefteq$ if whenever ac, bd are crossing edges, there is at least one minimal induced connected component of G containing ac and bd and every edge in each minimal induced connected component of G containing ac and bd precedes ac and bd in the ordering $\trianglelefteq$.

It may be tempting to view this definition and think of it as a "softened" version of crossing closed. Though, we do so while imposing an alternative, yet stronger condition on the ordering of the edges, in contrast to that given for upper crossing closed graphs. Recall the graph from an earlier section, re-posted in Figure 4.9. If we order the edges so that 14 and 35 are the largest, we get that G is strongly upper crossed with respect to that ordering. It's true in general that any graph with only one pair of crossing edges can be strongly upper crossed if we order the crossing edges so that they are the largest.

Notice, though, that in Figure 4.9 is not a chordal graph. Even though the edge 14 graphically passes through the 5-cycle, there are no internal edges within this five cycle. Hence, strongly upper crossed graphs present themselves as a distinct family from chordal graphs. One can also observe that not all upper crossing closed graphs are strongly upper crossed. For example, consider the complete graph K_5. With the lexicographical ordering, K_5 is upper crossing closed. Though, there does not exist an ordering on $E(K_5)$ which makes it strongly upper crossed. To see this, observe that the edges 14 and 25 cross, and 24 is an edge in $J(14, 25)$.

Then 24 needs to be smaller than 14 and 35. Though, 24 and 35 cross and $25 \in J(24, 35)$, meaning that 25 would need to be smaller instead. Hence, there is no way to impose an ordering on $E(K_5)$ which would make it strongly upper crossed. This is not without some irony. It's often the case that when studying graph theory that one would think trivial graphs and complete graphs satisfy all the
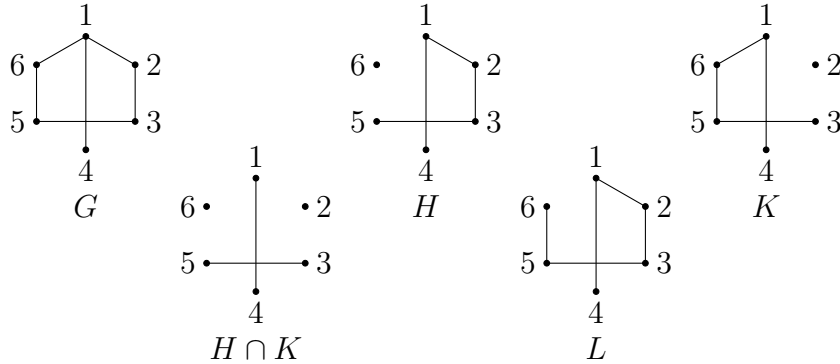
Figure 4.9. A graph and several subgraphs

Lemma 4.26. *Let G be a strongly upper crossed graph. If $H < H'$ and $e = \min E(H') \setminus E(H)$, then the bond induced by $E(H) \cup \{e\}$ is noncrossing.*

Proof. Let H'' be the bond induced by $E(H) \cup \{e\}$ and suppose that H'' is a crossing bond. Let B_1 and B_2 be the blocks that are merged when moving from H to H''. Since H'' is crossing there is some $f \in E(H)$ which crosses an edge between B_1 and B_2 and is not in B_1 and B_2. Thus, f separates B_1 and B_2. Since e connects B_1 and B_2, it too must cross f. Since H' is noncrossing and G is strongly upper crossed, there is a minimal induced connected component containing e and f in H'. Since G is strongly upper crossed, all the edges in this minimal induced connected component are smaller than e and f. Not all these edges can be in H since this would imply f did not cause H'' to be crossing. But this is impossible since since e was the smallest edge. $\qquad\square$

Theorem 4.27. *Let G be a strongly upper crossed graph. Then the conclusions of Theorem 3.41 hold. In particular, NC_G is graded, shellable, and the Möbius function and characteristic polynomial have a combinatorial interpretation in terms of NCNBC sets.*

4.4   A Summary of Results

	Graded	Lattice	NCNBCI	Shellable
Any Graph	Sometimes	Sometimes	Sometimes	Sometimes
Crossing Closed (Definition 3.6)	Sometimes	Always	Sometimes	Sometimes
Upper Crossing Closed (Definition 3.27)	Sometimes	Always	Always	Sometimes
Perfectly Labeled (Definition 4.1)	Always	Sometimes	Always	Always
Tightly Closed (Definition 4.19)	Always	Always	Sometimes	Sometimes
Upper Crossing Closed and Tightly Closed	Always	Always	Always	Always
Strongly Upper Crossed (Definition 4.25)	Always	Sometimes	Always	Always

Table 4.1. Families of graphs and their respective properties

Note that NCNBCI stands for noncrossing non-broken circuit interpretation.

Chapter 5: Open Problems

As we have seen, several of the nice properties of the noncrossing partition lattice and the bond lattice have analogues in the noncrossing bond poset. Given the multitude of nice properties that these lattices enjoy, we encourage the reader to see if their favorite properties have an analogue in the noncrossing bond poset. We collect a few open problems that we have found interesting below. The list is in no way to be considered complete.

Recall that the Whitney numbers of the first kind of a graded poset are the numbers $w_0, w_1, \ldots, w_n$ where w_i is the sum of the Möbius values of elements of P of rank i. In other words, they are the coefficients of the characteristic polynomial. Moreover, recall that a sequence $a_0, a_1, \ldots, a_n$ of real numbers is called *log-concave* if for all $1 \leq i \leq n-1$ we have that $a_{i-1}a_{i+1} \leq a_i^2$. Gian-Carlo Rota conjectured that the Whitney numbers of the first kind for geometric lattices (which include bond lattices) are log-concave. In [37] Huh proved that the Whitney numbers of the first kind for bond lattices are log-concave and further work of Adiprasito, Huh, and Katz [1] proved the more general conjecture concerning the Whitney numbers of the first kind for geometric lattices. Since the noncrossing bond poset is a (relatively) well-behaved subposet of a geometric lattice, it seems natural to ask if the corresponding conjectures hold for the noncrossing bond poset.

Question. *For which graphs are the Whitney numbers of the first kind of NC_G unimodal or log-concave?*

We should note that, unlike the case for the bond lattice, the Whitney numbers of the first kind of the noncrossing bond poset do not need to alternate in sign and can have internal zeros (e.g. the characteristic polynomial of the 5-pointed star in Figure 5.1 has an internal zero). As a result, it is not the case that the absolute values of the Whitney numbers of the first kind are log-concave or unimodal in general. We mention this since, if the sequence did alternate and have no internal zeros, the log-concavity would imply unimodality.

The noncrossing partition lattice is well-known to be rank-symmetric (see, for example [40]). That is, for NC_{n+1}, the number of elements of rank k is the same as the number of elements of rank $n - k$. It seems that it is rare for the noncrossing

G
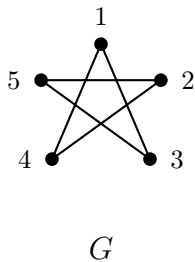
Figure 5.1. 5-pointed star

bond poset to be rank-symmetric. This should not be that surprising as the bond lattice is also rarely rank-symmetric. However, for $n \geq 5$, computations suggest that if we let C_n denote the cycle on n vertices with edges $12, 23, \ldots, n-1n, 1n$, then the complement $\overline{C_n}$ has a noncrossing bond poset which is rank-symmetric. This leads us to a broader question.

Question. *When is NC_G rank-symmetric?*

As we saw in the discussion preceding the previous question, the graph $\overline{C_n}$ seems to have a rank-symmetric noncrossing bond poset. Despite this nice property, it seems that the poset is not shellable. Naturally, this leads us to the following.

Question. *For what graphs is the noncrossing bond poset shellable?*

We note here that $\overline{C_n}$ is tightly closed (but not upper crossing closed). Thus, we know that tightly-closed (and hence crossing closed) does not imply shellability. There is some hope that upper crossing closed graphs produce shellable noncrossing bond posets. However, since they are not always graded, this will require considering non-pure shellings.

Given a graph (or more generally a matroid) one can consider the collection of non-broken circuits. This set forms a simplicial complex called the *broken circuit complex* or NBC complex. It has several nice properties, its f-vector encode the coefficients of the chromatic polynomial of the graph and the complex is known to be shellable. A related complex called the *independence complex* is formed considering all the subsets of the edges sets which form acyclic subgraphs. Since subsets of noncrossing sets are noncrossing, we can also consider the simplicial complex of noncrossing NBC sets and noncrossing independent sets.

Question. *What is the structure of the noncrossing NBC complex and noncrossing independence complex of a graph?*

Part II

Topological Indices of Finite Graphs

Chapter 6: Introduction

We will explore some extremal problems in graph theory related to *topological indices*; functions on finite graphs invariant under isomorphism. The Randić index of a graph G, also known as the *connectivity* or *branching index*, is a widely studied topological index. It is famous for its connection to molecular structures of hydrocarbons, as well as the extremal problems in graph theory it has yielded. Milan Randić is the father of this index, which he describes in [56].

We study the Randić index alongside the the largest eigenvalues of the adjacency, Laplacian, and signless Laplacian matrix of a graph, as well as the graph theoretic radius. Matrices associated to graphs are very powerful tools in graph theory and combinatorics. For instance, the adjacency matrix can be used to count the number of walks of a given length from one vertex of a graph to another, and the Laplacian can be used to count the number of spanning trees of a graph according to Kirchhoff's theorem (see [38]).

Our intention is to find the extremal graphs at which the ratio between the Randić index and one of these other indices is maximized or minimized. We also address an open problem posed in [17], the conjecture that for all connected graphs G except for the even path, the Randić index of G is bounded below by the radius of G (see Conjecture 12.3).

Chapter 7: Preliminaries

Most of the necessary graph theoretic terminology we need for this section was defined in Section 2.3. However, we need several additional definitions and terms which we will define now. We will still only consider finite graphs with vertex set $[n] := \{1, 2, \ldots, n\}$. The *complete graph* or *clique*, denoted by K_n, is the order n graph with all $\binom{n}{2}$ possible edges. The *star*, denoted by S_n, is the graph of order n with one vertex of degree $n-1$ and $n-1$ vertices of degree 1. The *n-cycle*, denoted by C_n, is the order n graph with edge set $\{(i, i+1 \mod n) : i \in [n]\}$. The *n-path*, denoted by P_n, is the order n graph with vertex set $\{(i, i+1) : i \in [n-1]\}$. See Figure 7.1. We will often use the notation $i \sim j$ to denote that $i, j \in V(G)$ and $ij \in E(G)$, and $i \nsim j$ to denote that $i, j \in V(G)$ and $ij \notin E(G)$.

| The Clique K_n | The Star S_n | The Cycle C_n | The Path P_n |
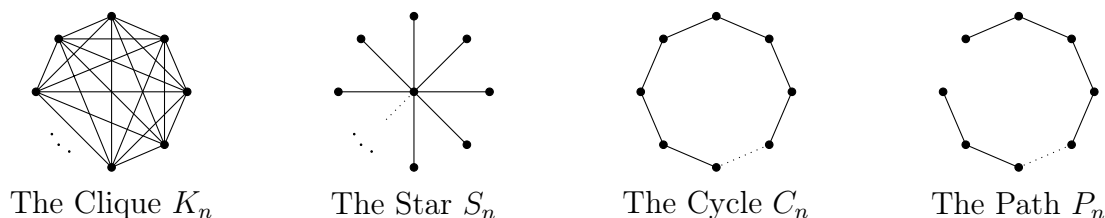
Figure 7.1. Standard order n graphs

We say that G is an *r-regular* graph if for each $v \in E(G)$, $\deg(v) = r$. Hence, K_n is $(n-1)$-regular and C_n is 2-regular. Let $\Delta(G) := \max\{\deg(v) : v \in V(G)\}$ and $\delta(G) := \min\{\deg(v) : v \in V(G)\}$ denote the *maximum degree* and *minimum degree* of G, respectively. We may write Δ and δ when the graph G is clear from context. A graph contains a *cycle* if it contains a walk $W = \{v_1, \ldots, v_k\}$ where $v_1 = v_k$ and no other vertex is repeated. For $v, w \in V(G)$, the *distance* between v and w is the length of the shortest path with v and w as end points, and is denoted by $d(v, w)$.[1]

A *spanning forest* of G if F is an acyclic spanning subgraph of G. We say that T is a *spanning tree* of G if T is a connected spanning forest of G. A *clique* in a graph

---

[1] If v and w are vertices in distinct connected components of G, we say that $d(v, w) = \infty$. However, we only consider connected graphs in this thesis.

G is a complete subgraph of G. The order of the largest clique in G is called its *clique number* and is denoted by $\omega(G)$. An edge e is a *bridge* of a graph G if $G - e$ has more connected components than G. Note that $G - e$ is the graph obtained from G by only deleting the edge e, not the endpoints of e. Note that each edge of P_n or S_n is a bridge.

Definition 7.1. Let G be a finite graph of order n. Then the **adjacency matrix** of G, denoted $A(G)$, is the $n \times n$ matrix such that

$$[A]_{ij} = \begin{cases} 1 & \text{if } ij \in E(G) \\ 0 & \text{if } ij \notin E(G) \end{cases}$$

We may write A instead of $A(G)$, when G is clear from context.

Definition 7.2. Let $\mathcal{G}$ denote the set of all finite simple graphs G. A **topological index** of G is a function $\varphi : \mathcal{G} \to \mathbb{R}$ that is invariant under isomorphism. That is, if $G, H \in \mathcal{G}$ and $G \cong H$, then $\varphi(G) = \varphi(H)$.

Definition 7.3. A **vertex-degree-based topological index** (or VDBTI) φ is a topological index that can be defined as

$$\varphi(G) = \sum_{ij \in E} \varphi_{i,j}$$

where $\varphi_{i,j} = f(\deg(i), \deg(j))$ and $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a symmetric function (i.e. $f(x, y) = f(y, x)$ for all x, y). Note that then $\varphi_{ij} = \varphi_{ji}$ for all $i, j \in V(G)$).

See [29, 53, 54] for more information about general VTBTI's.

Chapter 8: The Randić Index of a Graph

Definition 8.1. If $a \in [-1, 1] - \{0\}$, then $R_a(G)$ is the VDBTI where $\varphi_{i,j} = (\deg(i)\deg(j))^a$, i.e.

$$R_a(G) = \sum_{i \sim j} (\deg(i)\deg(j))^a.$$

We call $R_a(G)$ the **generalized Randić index** of G. The **Randić index** of G is $R(G) = R_{-1/2}(G)$ or

$$R(G) = \sum_{i \sim j} \frac{1}{\sqrt{\deg(i)\deg(j)}}.$$

We will make use of the following basic results on $R(G)$.

Theorem 8.2 ([12])**.** *Let G be a finite simple graph of order n. Then $\sqrt{n-1} \leq R(G)$ with equality if and only if $G = S_n$.*

Theorem 8.3 ([27,50])**.** *Let G be a finite simple graph of order n. Then $R(G) \leq \frac{n}{2}$ with equality if and only if G is a regular graph.*

Theorem 8.4 ([77])**.** *Among trees T of order n, $R(G) \leq \frac{n-3}{2} + \sqrt{2}$ with equality if and only if $T = P_n$.*

Let G be an order n graph and let

$$M = [\deg(1)^\alpha \ \deg(2)^\alpha \ \cdots \deg(n)^\alpha] \ A(G) \begin{bmatrix} \deg(1)^\alpha \\ \deg(2)^\alpha \\ \vdots \\ \deg(n)^\alpha \end{bmatrix} = \sum_{i=1}^{n}\sum_{j=1}^{n}(\deg(i)\deg(j))^\alpha A_{ij}.$$

Note that by the definition of $A(G)$, we have

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\deg(i)\deg(j))^{\alpha}A_{ij} = 2\sum_{i\sim j}(\deg(i)\deg(j))^{\alpha},$$

and therefore

$$R_{\alpha}(G) = \left(\frac{1}{2}\right) \times [\deg(1)^{\alpha}\ \deg(2)^{\alpha}\ \cdots \deg(n)^{\alpha}]\ A(G)\begin{bmatrix}\deg(1)^{\alpha}\\\deg(2)^{\alpha}\\\vdots\\\deg(n)^{\alpha}\end{bmatrix}. \quad (8.1)$$

We will use this result in Subection 8.2 and Sections 10 and 11.

The Randić index assigns a weight of $\frac{1}{\sqrt{\deg(i)\deg(j)}}$ to each $ij \in E(G)$. However, suppose we added some arbitrary edge, say $i'j'$, to a graph G with vertices i' and j'. The weights of the edges incident to i' and j' decrease in value since their degrees will increase by 1. Even though this new edge has positive weight, it is difficult to see in general if adding this edge yields smaller or larger index (or if the index is fixed; see Example 8.7).

Example 8.5. Consider the cycle C_4 and the graph H where $V(H) = V(C_4)$ and $E(H) = E(C_4) \cup \{24\}$ (see Figure 8.1). Then $R(C_4) = 2$ and $R(H) = 1.9663$. Viewed a different way, C_4 is clearly a subgraph of H. So it is not true in general that if H is a spanning subgraph of G, then $R(H) \le R(G)$.
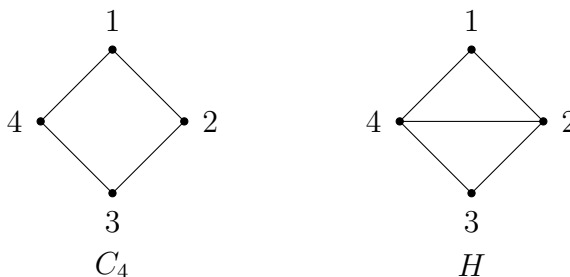
Figure 8.1. Adding edges may decrease the Randić Index

Example 8.6. Consider the graph G in Figure 8.2. Up to isomorphism, there is only one spanning tree of G, which we will call T. It is easy to verify that $R(T) > R(G)$. We will discuss this topic on spanning trees more in Section 12, but our computations show that it is more likely that a spanning tree of a graph G will have smaller Randić index than G itself.
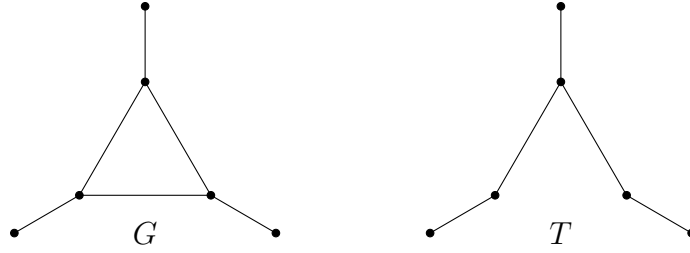
Figure 8.2. A graph with no spanning tree whose Randić index is smaller

Example 8.7. Consider the graphs G and G' as shown in Figure 8.3. We add the edge vw to G to obtain G'. Observe that $R(G) = 2 \cdot \frac{1}{\sqrt{2}} + 1$ and $R(G') = \frac{2}{\sqrt{2}} + 2 \cdot \frac{1}{2}$. This illustrates that it is possible for the Randić index to remain fixed when adding or removing an edge.
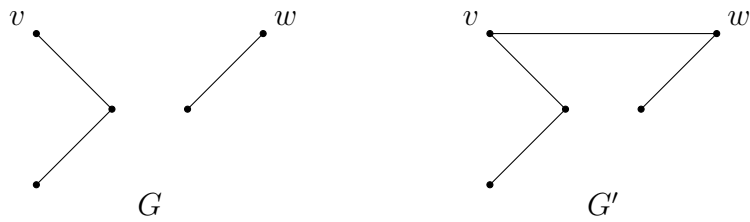
Figure 8.3. Fixed Randić index

Our work on the Randić index is not centered around studying how it is affected by various graph perturbations. However, in the course of our investigations, we discovered some such results and proofs that we could not find in the literature. We give those results here.

The following is a known result but as we could not find a proof in the literature, we present our own.

Proposition 8.8. *Let G be a graph with a vertex v with $\deg(v) \geq 1$ and let G' be some graph obtained by adding a pendant edge to v. Then $R(G) < R(G') + \frac{1}{2\sqrt{n+1}}$.*

Proof. Suppose that $e = vw$ where $v \in V(G)$ and w is the vertex being added to G. Let $\deg(v) = n$, and let $\{v_1, \ldots, v_n\}$ be the set of vertices adjacent to v in G. We have the following picture:
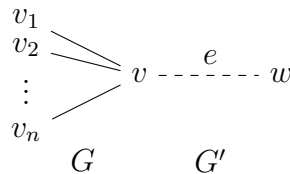
Since e is a pendant edge, we get that

$$R(G') - R(G) = \left(\sum_{i=1}^{n} \frac{1}{\sqrt{(n+1)\deg(v_i)}} + \frac{1}{\sqrt{n+1}} \right) - \left(\sum_{i=1}^{n} \frac{1}{\sqrt{n \cdot \deg(v_i)}} \right)$$

Now, consider the function $f(x) = \sqrt{x}\sqrt{x+1} - x$ on the domain $x \geq 1$. It is easy to check that $f(x)$ is continuous, $f(x) > 0$, $f'(x) > 0$, and $f(x)$ is strictly increasing on $[1, \infty)$. It is also easy to check that $\lim_{x \to \infty} f(x) = 1/2$. This implies that $f(x) < 1/2$ on $[1, \infty)$. For all integers $n \geq 1$, we find that

$$\sqrt{n}\sqrt{n+1} - n = n\left(\frac{\sqrt{n+1}}{\sqrt{n}} - 1 \right) < \frac{1}{2}. \tag{8.2}$$

In G, since $\deg(v_i) \geq 1$ for each $1 \leq i \leq n$,

$$1 \leq \sqrt{\deg(v_i)}$$

$$\implies \frac{1}{\sqrt{\deg(v_i)}} \leq 1$$

$$\implies \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} \leq n$$

$$\implies \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} \left(\frac{\sqrt{n+1}}{\sqrt{n}} - 1 \right) \leq n\left(\frac{\sqrt{n+1}}{\sqrt{n}} - 1 \right) < \frac{1}{2}$$

hence by (8.2) it follows that

$$\sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} \left(\frac{\sqrt{n+1}}{\sqrt{n}} - 1 \right) < \frac{1}{2} \tag{8.3}$$

Distribute the sum on the left hand side of Equation 8.3 to get the following:

$$\frac{\sqrt{n+1}}{\sqrt{n}} \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} - \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} < \frac{1}{2}$$

$$\implies \frac{\sqrt{n+1}}{\sqrt{n}} \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} < \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} + \frac{1}{2}$$

$$\implies \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} < \frac{1}{\sqrt{n+1}} \sum_{i=1}^{n} \frac{1}{\sqrt{\deg(v_i)}} + \frac{1}{2\sqrt{n+1}}$$

$$\implies \sum_{i=1}^{n} \frac{1}{\sqrt{n \cdot \deg(v_i)}} < \sum_{i=1}^{n} \frac{1}{\sqrt{(n+1)\deg(v_i)}} + \frac{1}{2\sqrt{n+1}}$$

Therefore, $R(G) < R(G') + \frac{1}{2\sqrt{n+1}}$. $\qquad\square$

Theorem 8.9. *Let G be the disconnected union of two stars S_n and S_m where $n, m \geq 2$. Let v_n and v_m be the vertices of degrees $n-1$ and $m-1$, in S_n and S_m respectively. If G' is the graph obtained by adding the edge $v_n v_m$ to G, then $R(G) > R(G')$.*
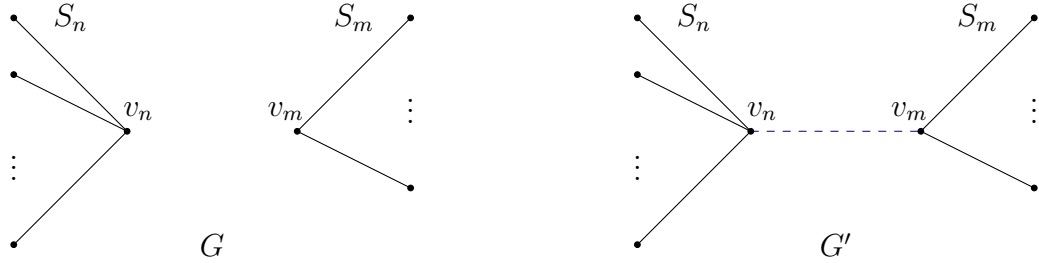
Figure 8.4. A union of stars

Proof. Let $n, m \geq 2$ so that the stars S_n and S_m are not isolated vertices. Let G be the disconnected union of two stars S_n and S_m and let G' be the graph obtained by adding an edge $v_n v_m$ to G, as shown in Figure 8.4. Since $R(S_n) = \sqrt{n-1}$ and $R(S_m) = \sqrt{m-1}$, we obtain the following:

$$R(G') = \sum_{i=1}^{n-1} \frac{1}{\sqrt{n}} + \sum_{i=1}^{m-1} \frac{1}{\sqrt{m}} + \frac{1}{\sqrt{nm}}$$

$$= \frac{n-1}{\sqrt{n}} + \frac{m-1}{\sqrt{m}} + \frac{1}{\sqrt{nm}}$$

$$= \frac{(\sqrt{nm}-1)(\sqrt{n}+\sqrt{m})+1}{\sqrt{nm}}.$$

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We'll show that

$$\sqrt{n-1} + \sqrt{m-1} > \frac{(\sqrt{nm}-1)(\sqrt{n}+\sqrt{m})+1}{\sqrt{nm}},$$

or equivalently, that the function

$$f(n,m) = \sqrt{nm}(\sqrt{n-1}+\sqrt{m-1}) - (\sqrt{nm}-1)(\sqrt{n}+\sqrt{m}) - 1$$

is positive for $n, m \geq 2$.

We'll first consider the one variable function

$$f(n) := f(n,2) = \sqrt{2n}(\sqrt{n-1}+1) - (\sqrt{2n}-1)(\sqrt{n}+\sqrt{2}) - 1$$

It is tedious but straightforward to show that $f(n)$ is increasing for $n \geq 1$ and that $f(2) \approx 0.17$. So for every integer $n \geq 2$, $f(n,2) > 0$. Next we show that for all $m \geq 2$,

$$f(n,m) > f(n,2) \tag{8.4}$$

Since $f(n,m) = f(m,n)$, proving (8.4) implies that $f(n,m) > 0$ for all $n, m \geq 2$. Observe that

$$
\begin{aligned}
f(n,m) &- f(n,2) \\
&= \sqrt{nm(n-1)} + \sqrt{nm(m-1)} - \sqrt{n^2 m} - \sqrt{nm^2} + \sqrt{n} + \sqrt{m} \\
&\quad - \sqrt{2n(n-1)} - \sqrt{2n} + 2\sqrt{n^2} + 2\sqrt{n} + \sqrt{n} + \sqrt{2} \\
&= \sqrt{n(n-1)}(\sqrt{m}-\sqrt{2}) + \sqrt{mn(n-1)} + \sqrt{n}(2-\sqrt{2}) - n(\sqrt{m}-\sqrt{2}) \\
&\quad + (\sqrt{m}-\sqrt{2}) \\
&= \underbrace{\left[\sqrt{n(n-1)} - n + 1\right]}_{\text{define as } h(n)}(\sqrt{m}-\sqrt{2}) + \sqrt{mn(n-1)} + \sqrt{n}(2-\sqrt{2}) \tag{8.5}
\end{aligned}
$$

Except for $h(n) = \sqrt{n(n-1)} - n + 1$, each term in Equation 8.5 is non-negative since $m, n \geq 2$. It also follows from basic calculus that $h(n) > 0$ when $n \geq 2$. Thus, for all $n, m \geq 2$, $f(n,m) \geq f(n,2) \geq f(2,2) > 0$. Hence, $R(G) > R(G')$. $\qquad\square$

Theorem 8.10. *Suppose that G is an order n graph with at least two pendant edges such that vertices adjacent to the leaves have degree at least 2. If G' is obtained by adding an edge between these leaves, then $R(G) < R(G')$.*

Proof. Let G be a graph containing two pendant edges with leaves v and w. The neighbors of v and w will have degrees n and m, respectively, where $n, m \geq 2$. Let G'
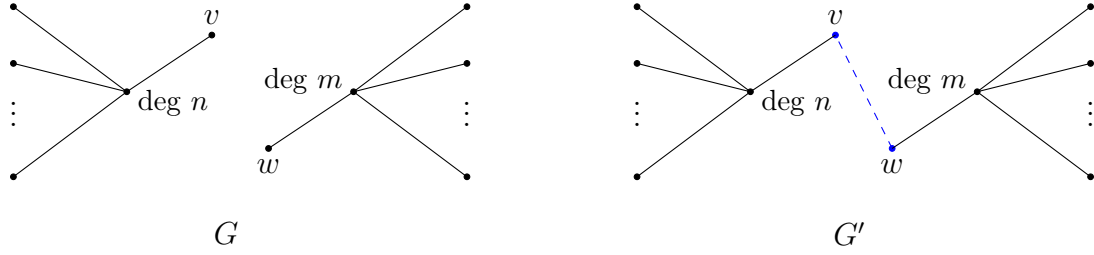
Figure 8.5. Adding an edge between two leaves of a graph

be the graph obtained by adding the edge vw to G, as shown in Figure 8.5. Then by direct computation, we find that

$$
\begin{aligned}
R(G') - R(G) &= \left(\frac{1}{\sqrt{2 \cdot 2}} + \frac{1}{\sqrt{2n}} + \frac{1}{\sqrt{2m}} \right) - \left(\frac{1}{\sqrt{n}} - \frac{1}{\sqrt{m}} \right) \\
&= \frac{\sqrt{nm} + \sqrt{2n} + \sqrt{2m} - 2\sqrt{n} - 2\sqrt{m}}{2\sqrt{nm}} \\
&= \frac{\sqrt{nm} + \sqrt{n}(\sqrt{2} - 2) + \sqrt{m}(\sqrt{2} - 2)}{2\sqrt{nm}}
\end{aligned}
$$

We aim to show that the function

$$
g(n,m) = \sqrt{nm} + \sqrt{n}(\sqrt{2} - 2) + \sqrt{m}(\sqrt{2} - 2)
$$

is positive for all $n, m \geq 2$. When $n = m = 1$, the addition of this edge decreases the Randić index. In the spirit of the previous proof, consider the single variable function g, such that for all $n \geq 2$,

$$
\begin{aligned}
g(n) := g(n,2) &= \sqrt{2n} + \sqrt{n}(\sqrt{2} - 2) + \sqrt{2}(\sqrt{2} - 2) \\
&= (\sqrt{n} - 1)(2\sqrt{2} - 2) \\
&> 0.
\end{aligned}
$$

Further, $g'(n)$ has no real critical points and $g'(2) \approx 0.293$, so $g(n,2)$ is strictly increasing for all $n \geq 2$. Next, we'll show that $g(n,m) \geq g(n,2)$ when $m \geq 2$. Since $g(n,m) = g(m,n)$, this will be enough to show that $g(n,m)$ is positive on the current domain. Observe that since $n, m \geq 2$,

$$g(n,m) - g(n,2) = \sqrt{nm} + \sqrt{n}(\sqrt{2} - 2) + \sqrt{m}(\sqrt{2} - 2) - \sqrt{2n} - \sqrt{n}(\sqrt{2} - 2)$$
$$- \sqrt{2}(\sqrt{2} - 2)$$
$$= (\sqrt{2} - 2)(\sqrt{m} - 2) + \sqrt{n}(\sqrt{m} - \sqrt{2})$$
$$= (\sqrt{m} - 2)(\sqrt{n} + \sqrt{2} - 2)$$
$$\geq 0$$

Therefore, $g(n,m) \geq g(n,2) > 0$ for all $n, m \geq 2$ which implies that $R(G') > R(G)$. $\square$

8.1 Understanding Randić's Discoveries

The Randić index was named after the professor of chemistry Milan Randić of Ruđer Bošković Institute and Drake University. Randić is known for his significant contributions in the fields of computational and mathematical chemistry. He discovered a meaningful connection between the structure of hydrocarbon molecules and graph theory. For the full details of Randić's discovery, see [56].

We will need to discuss some terms and facts from basic chemistry (acquired from [21] and [48]) to provide clear context for Randić's work and how it relates to graph theory. A *covalent bond* is an atomic bond in which an electron is shared between a pair of atoms. A *hydrocarbon* is organic compound that consists only of hydrogen and carbon atoms. We will denote hydrocarbons by C_nH_m where n and m give the number of carbon and hydrogen atoms per molecule, respectively. Hydrogen is univalent, meaning that it is capable of forming at most one covalent bond with another atom. Carbon is tetravalent, meaning that it is capable of forming at most four covalent bonds with other atoms. One may think of carbon atoms as having four "slots" available for electrons; all of which need not be occupied. If one of these slots is vacant, the carbon atom may form a covalent bond with another atom and share the missing electron in order to fill this vacant slot. Since these atoms are sharing one electron, they have what is called a *single bond*. We say a molecule is *saturated* when one substance takes up as much space as possible within another substance and it can take no more molecules; i.e., when a molecule cannot form an additional covalent bond with another atom. To graph a hydrocarbon, we represent atoms as vertices of a graph and draw a single edge between atoms if and only if there is a single covalent bond between them. We will refer to this as the *hydro-chemical graph* of a hydrocarbon. Figure 8.6 gives a graphical illustration of a carbon atom forming a covalent bond with a hydrogen atom, and the corresponding hydro-chemical graph.

As an illustrative example, consider the chemical graph of the hydrocarbon methane (C_1H_4) (see Figure 8.7). With any saturated hydrocarbon, each carbon atom will form
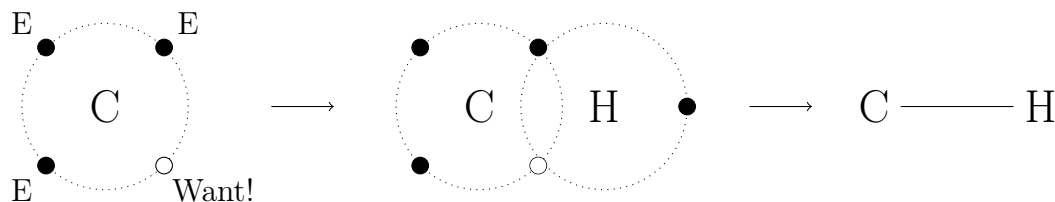
Figure 8.6. Graphical illustration of a single covalent bond

a covalent bond with either another carbon atom or hydrogen atom. Hence, each carbon atom will have a degree of 4 in the hydro-chemical graph. Since hydrogen atoms are univalent, they cannot bond with two atoms simultaneously, so hydrocarbons will always be leaves in a hydro-chemical graph; i.e., vertices of degree 1. Thus, the covalent bonds of carbon atoms with other carbon atoms will uniquely determine the structure of a saturated hydrocarbon. In other words, if we know how the carbon atoms are arranged, we know where the hydrogen atoms must go.

The *chemical graph* of a hydrocarbon is the hydro-chemical graph of a hydrocarbon with all hydrogen atoms removed. It is relatively common in chemistry to disregard hydrogen atoms when studying a chemical compound. In the words of Dr. Michael Dickey[1], "hydrogen atoms are light and cluttery." We obtain a graph displaying the way the carbon atoms are bonded; we call this the *carbon skeleton* of a hydrocarbon. See Figures 8.7 and 8.8 for the chemical graph of methane and propane respectively.

Remark. In the literature, the term chemical graph (or molecular graph) is defined more broadly. Though for our purposes, we are using the terms hydro-chemical graph and chemical graph in reference to hydrocarbons and how they are studied by Randić.

Methane (C_1H_4) is a chemical compound which forms when a carbon atom has zero electrons and forms covalent bonds with four hydrogen atoms, sharing all four of its electrons. The corresponding hydro-chemical graph is the star S_4, but its chemical graph is an isolated vertex. When considering larger chemical compounds we obtain more interesting carbon skeletons. The chemical graphs for the compound propane (C_3H_8) is shown in Figure 8.8 .

Randić observed that hydro-chemical graphs have all vertices of degree 1 or 4, while chemical graphs did not have the same restrictions. This allowed him to study the carbon skeletons of hydrocarbons, which yielded his findings, seen in the famous paper *On Characterization of Molecular Branching* (see [56]). Followers of Randić (including graph theorists) later called this the *Randić* index and generalized it as in Definition 8.1. Randić coined the term "branching index" because he focused primarily

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[1]Professor of chemical engineering at North Carolina State University that we interviewed for this topic.
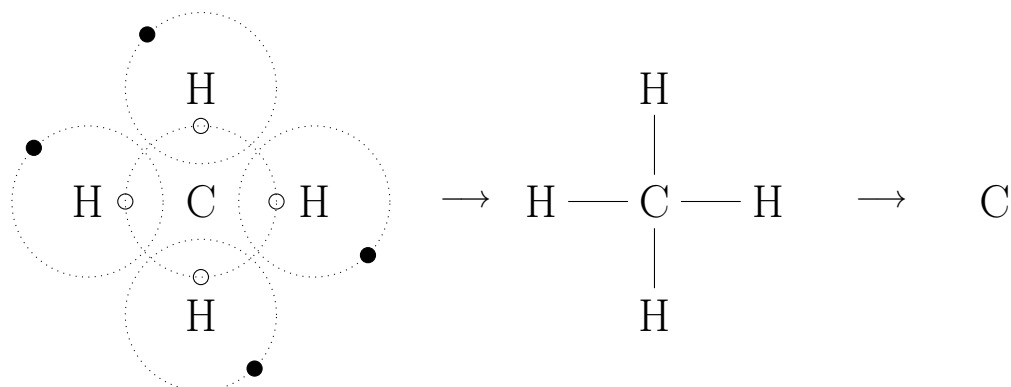
Figure 8.7. Molecular structure and chemical graphs of methane
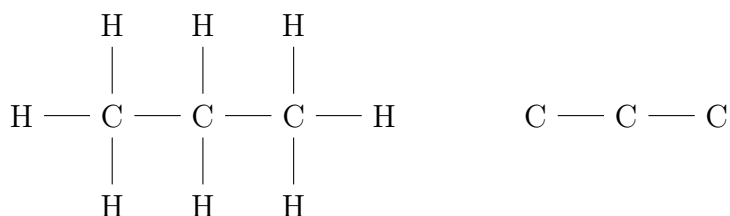
Figure 8.8. Chemical graphs of propane

on hydrocarbons whose chemical graphs were acyclic (i.e., trees). He described hydrocarbons whose chemical graphs had longer internal paths were "branching" less, and hence, more spread out (see Figure 8.9).
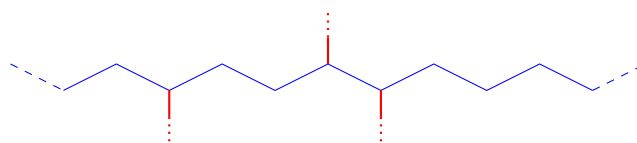
Figure 8.9. Branching of a carbon skeleton

Randić observed that the more a chemical graph resembled the path, the higher the value of the branching index of that hydrocarbon was. Figure 8.10 shows the Randić index of all trees on 6 vertices, and orders them from smallest to greatest, serving as an illustrative description of his choice of terms (we discuss how we performed these computations in Section 8.2 and Appendix B).

Randić's most notable discovery was the following. Let G be the chemical graph of some hydrocarbon H. Randić found that there was a strong correlation between
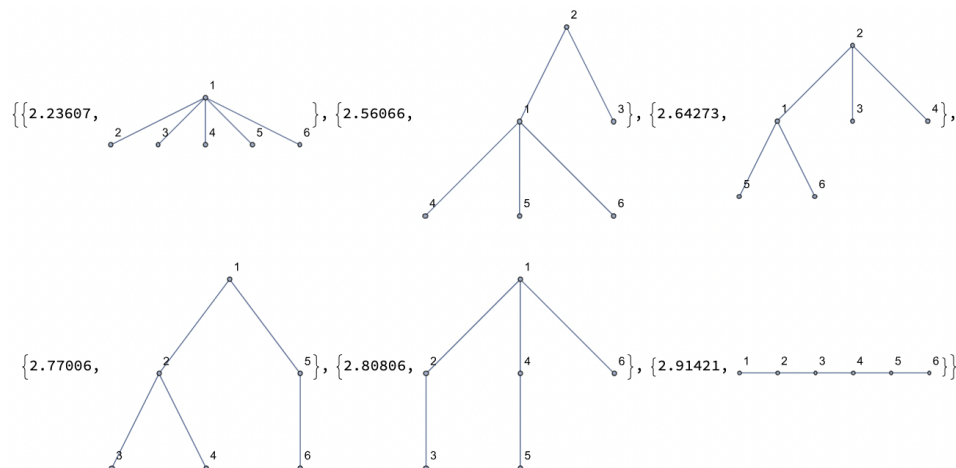
Figure 8.10. Randić index of all trees on 6 vertices

what he called the *branching index*

$$\sum_{i \sim j} \frac{1}{\sqrt{\deg(i) \deg(j)}}$$

and the boiling point of H. It is also a known fact that there is a known correlation between boiling point and the molar mass of a chemical compound. Though, one may consider the following. The five hydrocarbons n-hexane (C_5H_{14}), 3-methylpentane (3-C_6H_{14}), 2-methulpentane (2-C_6H_{14}), 2,3-dimethylbutane (2,3-C_6H_{14}), and 2,2-dimethylbutane (2,2-C_6H_{14}) all have the same molar mass, but different boiling points; see Table 8.1 ([47],[58]) and Figure 8.11 for the corresponding chemical graphs. We see a 19°C difference from n-hexane and 2,2-dimethylbutane which molar mass does not account for. Hence, the Randić index is serving as a stronger predictor for boiling point than molar mass in this example.

	C_5H_{14}	3-C_6H_{14}	2-C_6H_{14}	2,3-C_6H_{14}	2,2-C_6H_{14}
MM	86.18	86.18	86.18	86.18	86.18
BP	69°C	63°C	60°C	57.9°C	50°C
RI	2.914	2.808	2.77	2.6423	2.5607

Table 8.1. Physical chemical properties and Randić indices of five hydrocarbons

Randić's branching index lead to fervent interest in the field of graph theory. It was later given the name of *Randić index*, and generalized as in Definition 8.1; (see [41] for a comprehensive survey). Mathematicians studied the Randić index, as well as indices such as the Harary index ([75]), the Wiener index ([73],[55],[39]), and the
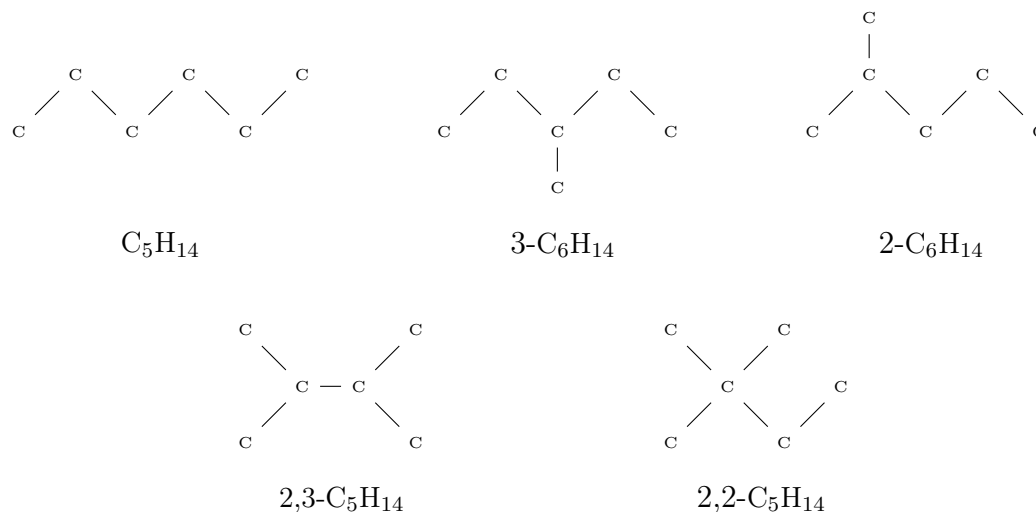
Figure 8.11. Chemical graphs of five hydrocarbons

Hosoya index ([35], [45]). Such indices yield very nice extremal problems in graph theory. That is, given a class of graphs, which graphs are minimal and/or maximal with respect to these indices.

8.2 Computations using Mathematica

We will discuss the computational tools and procedures needed to understand Randić's claims. Also, these computations will be used in Sections 10, 11, and 12 to formulate our own conjectures.

8.2.1 Computations on the Randić Index

Using the websites such as PubChem [47] and ChemSpider [58], we were able to construct a database of over 150 single bonded and multi-bonded hydrocarbons paired with physical chemical properties such as boiling points and melting points. Next, by using Wolfram Mathematica [74], we coded the chemical graphs of each hydrocarbon reflected the carbon skeleton by hand. Mathematica is equipped with functions to allow us to study finite graph theory. Once we code a finite graph, we may use Equation (8.1) to write a function in Mathematica which allows us to compute the generalized Randić index (see Appendix B). Below is an example of four of the chemical graphs we defined, where Figure 8.12 shows the corresponding chemical graphs. Figure 8.10 was generated using our Mathematica code as well.

```
Methylpentane2 = {Range[6], {{1, 2}, {2, 3}, {2, 4}, {4, 5}, {5, 6}}};
```

```
Methylpentane3 = {Range[6], {{1, 2}, {2, 3}, {3, 4}, {3, 5}, {5, 6}}};
Dimethylbutane22 = {Range[6], {{1, 2}, {2, 3}, {2, 4}, {2, 5}, {5, 6}}};
Dimethylbutane23 = {Range[6], {{1, 2}, {2, 3}, {2, 4}, {4, 5}, {4, 6}}};
```
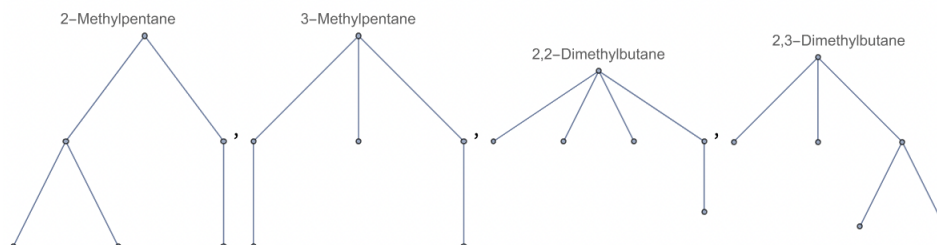

Figure 8.12. Sample of chemical graphs from Mathematica

We computed the Randić index of each single-bonded hydrocarbon that we coded and compared that data to the known boiling points of each hydrocarbon as well. With R, we used methods of simple linear regressions to model our data in the form $\mu\{$Boiling Point | Randić Index$\} = \beta_0 + \beta_1 \times \ln($ Randić Index $)$; the natural log transformation accounts for a slight curve in the original data plot.
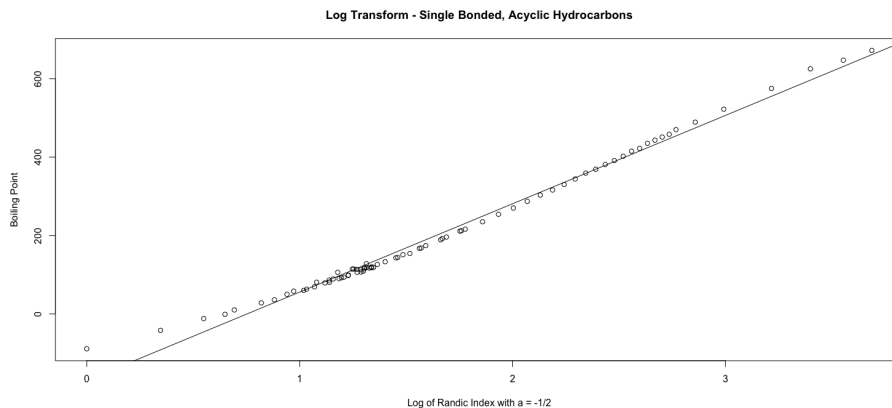
Figure 8.13. Correlation between the Randić index and boiling points of single bonded hydrocarbons

We obtained the following linear model:

$$\mu\{\text{Boiling Point} \mid \text{Randić Index}\} = -169.819 + 225.345 \times \ln(\text{ Randić Index })$$

with an adjusted R^2 value of ≈ 0.97 (see Figure 8.13). While we can observe that there is likely a better fitting model (one which likely includes higher degree polynomial terms), there is no doubt about the claims Randić made regarding the correlation between boiling point and his branching index of the chemical graphs of hydrocarbons.

8.2.2 Generating All Connected Graphs of Order 8 and Below

In this section, we introduce one of our most valuable tools employed in generating ideas and conjectures essential to this project. Specifically, we constructed a Mathematica library which contains all connected graphs of orders ranging from 3 to 8. This repository played a pivotal role in our investigations. Additionally, we defined topological indices alongside the Randić index and computed these indices for all graphs in our collection. This systematic approach enabled us to formulate conjectures. Figure 8.14 shows a portion of our library. For more detail of our methodology, including detailed code and procedures, please refer to Appendix B.

```
(* Graphs on 4 Vertices *)
All4Graphs = {{{1, 2, 3, 4}, {1↔2, 1↔3, 1↔4}}, {{1, 2, 3, 4}, {1↔4, 2↔3, 3↔4}}, {{1, 2, 3, 4}, {1↔2, 1↔3, 1↔4, 2↔3}},
    {{1, 2, 3, 4}, {1↔3, 1↔4, 2↔3, 2↔4}}, {{1, 2, 3, 4}, {1↔2, 1↔3, 1↔4, 2↔3, 2↔4}}, {{1, 2, 3, 4}, {1↔2, 1↔3, 1↔4, 2↔3, 2↔4, 3↔4}}};

(* Graphs on 5 Vertices *)
All5Graphs = {{{1, 2, 3, 4, 5}, {1↔2, 1↔3, 1↔4, 1↔5}}, {{1, 2, 3, 4, 5}, {1↔5, 2↔5, 3↔4, 4↔5}}, {{1, 2, 3, 4, 5}, {1↔5, 2↔4, 3↔4, 3↔5}},
    {{1, 2, 3, 4, 5}, {1↔2, 1↔3, 1↔4, 1↔5, 2↔3}}, {{1, 2, 3, 4, 5}, {1↔5, 2↔4, 3↔4, 3↔5, 4↔5}}, {{1, 2, 3, 4, 5}, {1↔5, 2↔4, 2↔5, 3↔4, 3↔5}},
    {{1, 2, 3, 4, 5}, {1↔5, 2↔3, 2↔4, 3↔4, 4↔5}}, {{1, 2, 3, 4, 5}, {1↔4, 1↔5, 2↔3, 2↔5, 3↔4}}, {{1, 2, 3, 4, 5}, {1↔2, 1↔3, 1↔4, 1↔5, 2↔3, 2↔4}},
    {{1, 2, 3, 4, 5}, {1↔5, 2↔3, 2↔4, 3↔4, 3↔5, 4↔5}}, {{1, 2, 3, 4, 5}, {1↔4, 1↔5, 2↔4, 2↔5, 3↔4, 3↔5}},
    {{1, 2, 3, 4, 5}, {1↔4, 1↔5, 2↔3, 2↔5, 3↔4, 4↔5}}, {{1, 2, 3, 4, 5}, {1↔4, 1↔5, 2↔3, 2↔5, 3↔4, 3↔5, 4↔5}},
    {{1, 2, 3, 4, 5}, {1↔4, 1↔5, 2↔3, 2↔4, 2↔5, 3↔4, 3↔5}}, {{1, 2, 3, 4, 5}, {1↔4, 1↔5, 2↔3, 2↔4, 2↔5, 3↔4, 3↔5}},
    {{1, 2, 3, 4, 5}, {1↔2, 1↔3, 1↔4, 1↔5, 2↔3, 2↔4, 2↔5, 3↔4}}, {{1, 2, 3, 4, 5}, {1↔3, 1↔4, 1↔5, 2↔3, 2↔4, 2↔5, 3↔5, 4↔5}},
    {{1, 2, 3, 4, 5}, {1↔2, 1↔3, 1↔4, 1↔5, 2↔3, 2↔4, 2↔5, 3↔4, 3↔5}}, {{1, 2, 3, 4, 5}, {1↔2, 1↔3, 1↔4, 1↔5, 2↔3, 2↔4, 2↔5, 3↔4, 3↔5, 4↔5}}};
```

Figure 8.14. Sample of our graph library

In Sections 10, 11, and 12, we use out library to compute various ratios involving the Randić index, as well as maximum eigenvalues from matrices of finite graphs.

Chapter 9: Spectral Radii of Graphs

In this section, we discuss the topological index of a graph known as the *spectral radius*. We present some expository results on this topic, and also present proofs of results in the literature whose proofs contained errors or lacked sufficient detail. We end this section with the result that inspired Theorems 10.25 and 11.9.

For a graph G, we defined the adjacency matrix $A(G)$ in Definition 7.1. It is well known that if G and H are isomorphic graphs, then $A(G)$ and $A(H)$ are similar matrices, which, in particular, implies that they will have the same eigenvalues. Since the adjacency matrix is a symmetric matrix, all of its eigenvalues will be real. Thus the maximum eigenvalue of $A(G)$ is invariant under isomorphisms of G and is hence a topological index.

Definition 9.1. Let M be any matrix of $F^{n \times n}$ for some field F. The **spectrum** of M is the set of all eigenvalues of M, denoted by $\mathrm{spec}(M)$.

Definition 9.2. The **spectral radius** of a graph G is the largest eigenvalue of the adjacency matrix, denoted by
$$a(G) := \max\{\mathrm{spec}(A(G))\}.$$

Definition 9.3. A matrix A is called **irreducible** if it is not similar via a permutation matrix to a block upper triangular matrix, i.e., there is no permutation matrix matrix P such that $PAP^{-1} = \begin{pmatrix} E & F \\ 0 & G \end{pmatrix}$.

It is well known that if a graph G is connected, then $A(G)$ is irreducible.

Theorem 9.4 (The Perron-Frobenius Theorem for Irreducible Non-negative Matrices). *Let A be an irreducible non-negative $n \times n$ matrix with spectral radius r. Then the following statements hold.*

1. *The number r is a positive real number, often called the Perron-Frobenius eigenvalue.*

2. *The eigenvalue r is simile; i.e., it is a root of the characteristic polynomial of A with multiplicity 1.*

3. *The matrix A has both right and left eigenvectors with the eigenvalue r whose components are all positive.*

Hence, we know that $a(G)$ will be a positive, simple eigenvalue whenever G is connected.

This section will give brief exposition on the spectral radius of a graph. This will include some results that regard how spectral radii are affected by graph perturbations.

9.1 Known Bounds on the Spectral Radius of a Graph

The following are some known results and bounds regarding the spectral radii of finite graphs.

Proposition 9.5 ([42]). *Let G be any finite connected graph. Then $a(G) \leq \Delta(G)$.*

The following is a widely known result in spectral graph theory, stating that amongst all connected graphs G of order n, the spectral radius $a(G)$ is minimized by the path P_n and maximized by the complete graph K_n.

Proposition 9.6 ([18]). *If G is a connected graph of order n, then*

$$2 \cos \left(\frac{\pi}{n+1} \right) = a(P_n) \leq a(G) \leq a(K_n) = n - 1.$$

The lower bound occurs only when G is the path P_n and the upper bound occurs only when G is the complete graph K_n.

A proof sketch of the first inequality of Proposition 9.6 goes as follows. By Proposition 9.5, we know that graphs of smaller maximum degree will yield smaller spectral radii than graphs of higher maximum degree. For graphs of degree 4 or lower, the result can be shown by brute force. It is easy to see that if G is an order n, connected graph, then $\Delta(G) = 2$ implies that G is either the path P_n or the cycle C_n. Any connected graph G that is not P_n or C_n will have a maximum degree of at least 3. It is given in [18] and in [34] that

$$a(P_n) = 2 \cos \left(\frac{\pi}{n+1} \right) \leq 2 \quad \text{and} \quad a(C_n) = 2 \cos \left(\frac{2\pi(0)}{n} \right) = 2.$$

The result follows immediately.

There are also some nice bounds on the spectral radius of a graph which depend on graph properties which are easy to compute; i.e., order and number of edges of a graph.

Proposition 9.7 ([24]). *For any connected graph G of order n and spectral radius $a(G)$,*

$$a(G) \geq \sqrt{\frac{1}{n} \sum_{i \in V(G)} \deg(i)^2}.$$

Proposition 9.8 ([34]). *For any connected graph G of order n, spectral radius $a(G)$, and m edges, $a(G) \leq \sqrt{2m - n + 1}$ with equality if and only if G is either K_n or S_n.*

Proposition 9.9 ([24]). *For any order n, connected graph G with spectral radius $a(G)$ ad m edges,*

$$a(G) \geq \frac{m}{R(G)}.$$

9.2   Exposition on Characteristic Polynomials

Before we present the following results, we will need to standardize some notation due to some inconsistencies in the literature. Cvetković, Rowlinson, and Simić authored a textbook entitled *Eigenspaces of Graphs* [19]. This book focuses on topics in spectral graph theory, and serves as a great exposition on this topic. Though, we found that some proofs in Chapter 6 of this book included errors (e.g. abuse of and incorrect notation) and/or lacked sufficient detail. Thus, in this section we present accurate proofs for Lemma 9.12 and Theorem 9.13.

Let G be a graph and let uv some edge of G. For nonnegative integers k and ℓ, let $G_u(k, \ell)$ denote the graph obtained by adding pendant paths of length k and ℓ to u, and let $G_{uv}(k, \ell)$ be the graph obtained by adding a pendant path of length k to u and one of length ℓ to v. Also, let G_i and $G - i$ denote the graphs obtained by adding a pendant edge to G at a vertex i and deleting the vertex i respectively. See Figure 9.1 for a reference of all four notations.

Remark. We describe two notions of adding paths to one vertex u or two vertices u and v above, as both are needed for the proofs of Lemma 9.12 and Theorem 9.13. However, in [19], they use the notation "$G(k, \ell)$" for both $G_u(k, \ell)$ and $G_{uv}(k, \ell)$ interchangeably, making the proofs erroneous. Further, in the proof provided for Theorem 9.13 in [19], there is the issue of attaching paths of negative lengths to vertices, which is impossible. Hence, we offer correct proofs of these results.

Let G be a graph. The *characteristic polynomial of $A(G)$* is defined as $P_{A(G)}(x) = \det(xI_n - A(G))$. When the matrix and variable are clear from context, we will simply denote this polynomial by P_G.

Lemma 9.10 ([19]). *For any connected graph G, $P_{G_i} = xP_G - P_{G-i}$.*

Lemma 9.11 ([19]). *If H is a spanning subgraph of some graph G, then $P_G(x) \leq P_H(x)$ for all $x \geq a(G)$. If further $a(H) < a(G)$, then the inequality is strict.*

Figure 9.2 provides a visual reference of Lemma 9.11.
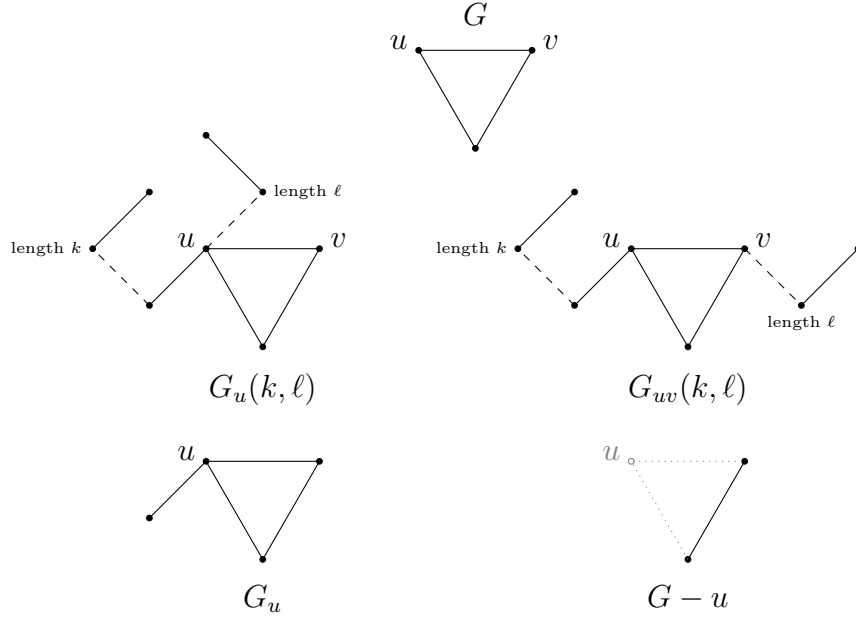
Figure 9.1. Adding pendants and pendant paths to a graph G
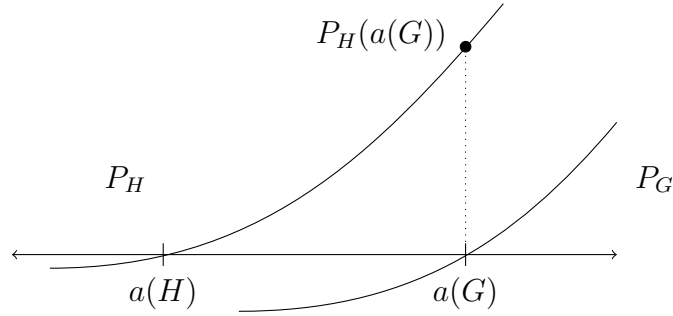
Figure 9.2. Characteristic polynomial of a spanning subgraph H of G.

Lemma 9.12 ([19]). *Let G be a graph. If $1 \leq \ell \leq k$, then $a(G_u(k, \ell)) > a(G_u(k+1, \ell-1))$.*

Proof. By Lemma 9.10, $P_{G_i}(x) = xP_G(x) - P_{G-i}(x)$. Applying this fact gives us the following:

$$P_{G_u(k,\ell)}(x) = xP_{G_u(k,\ell-1)}(x) - P_{G_u(k,\ell-2)}(x)$$
$$P_{G_u(k+1,\ell-1)}(x) = xP_{G_u(k,\ell-1)}(x) - P_{G_u(k-1,\ell-1)}(x)$$
$$\implies P_{G_u(k,\ell)}(x) - P_{G_u(k+1,\ell-1)}(x) = P_{G_u(k-1,\ell-1)}(x) - P_{G_u(k,\ell-2)}(x)$$

By repeating this process, we obtain the following:

$$P_{G_u(k,\ell)}(x) - P_{G_u(k+1,\ell-1)}(x) = P_{G_u(k-\ell+1,1)}(x) - P_{G_u(k-\ell+2,0)}(x)$$

We aim to show that this difference of characteristic polynomials is positive for certain values of x. To avoid having negative arguments for $G_u(*, *)$, define the graph $H = G_u(k-\ell+1, 0) - u$. Then H isomorphic to a proper spanning subgraph of $G_u(k-\ell, 0)$ where all edges incident to u are deleted except for the edge along the added pendant path of length $k-\ell$. Then observe the following.

$$P_{G_u(k-\ell+1,1)}(x) = xP_{G_u(k-\ell+1,0)}(x) - P_{G_u(k-\ell,0)}(x), \text{ and}$$
$$P_{G_u(k-\ell+2,0)}(x) = xP_{G_u(k-\ell+1,0)}(x) - P_H(x)$$

By Lemma 9.11, $P_H(x) > P_{G_u(k-\ell,0)}(x)$ for $x \geq a(G_u(k-\ell,0))$ since H is a proper spanning subgraph of $G(k-\ell, 0)$. Notice that $G_u(k-\ell, 0)$ is a proper subgraph of $G_u(k, \ell)$ which implies that $a(G_u(k,\ell)) > a(G_u(k-\ell,0))$.

$$P_{G_u(k,\ell)}(x) - P_{G_u(k+1,\ell-1)}(x) = P_{G_u(k-\ell,0)}(x) - P_H(X) < 0 \text{ for } x \geq a(G_u(k,\ell))$$

and

$$P_{G_u(k,\ell)}(x) - P_{G_u(k+1,\ell-1)}(x) < 0 \text{ for } x \geq a(G_u(k,\ell)).$$

When evaluated at $a(G_u(k,\ell))$, this quantity becomes negative, which implies that $P_{G_u(k+1,\ell-1)}(x)$ is positive at this eigenvalue. Therefore, we may assert that

$$a(G_u(k,\ell)) > a(G_u(k+1,\ell-1)).$$

$\square$

Theorem 9.13 ([19]). *Let G be a graph with $uv \in E(G)$. If $1 \geq \ell \geq k$, then $a(G_{uv}(k,\ell)) > a(G_{uv}(k+1,\ell-1))$.*

Proof. We will again utilize the fact that $P_{G_i}(x) = xP_G(x) - P_{G-i}(x)$ to find that

$$P_{G_{uv}(k,\ell)}(x) = xP_{G_{uv}(k,\ell-1)}(x) - P_{G_{uv}(k,\ell-2)}(x)$$
$$P_{G_{uv}(k+1,\ell-1)}(x) = xP_{G_{uv}(k,\ell-1)}(x) - P_{G_{uv}(k-1,\ell-1)}(x)$$
$$\implies P_{G_{uv}(k,\ell)}(x) - P_{G_{uv}(k+1,\ell-1)}(x) = P_{G_{uv}(k-1,\ell-1)}(x) - P_{G_{uv}(k,\ell-2)}(x)$$

which, by repeating this process, implies that

$$P_{G_{uv}(k,\ell)}(x) - P_{G_{uv}(k+1,\ell-1)}(x) = P_{G_{uv}(k-\ell+1,1)}(x) - P_{G_{uv}(k-\ell+2,0)}(x).$$

Define the graph H so that $H \cong G_{uv}(k-\ell+1) - v$ (shown in Figure 9.3). Observe that

$$P_{G_{uv}(k-\ell+1,1)}(x) = xP_{G_{uv}(k-\ell+1,0)}(x) - P_{G_{uv}(k-\ell,0)}(x), \text{ and}$$
$$P_{G_{uv}(k-\ell+2,0)}(x) = xP_{G_{uv}(k-\ell+1,0)}(x) - P_H(x)$$

Next, let M be the graph obtained by removing all edges incident to v (except for uv) from $G_{uv}(k-\ell,0)$ (see Figure 9.3). Then M is a proper spanning subgraph of $G_{uv}(k-\ell,0)$, which implies that $a(G_{uv}(k-\ell,0)) > a(M)$. Since v is a leaf in M, $a(M) > a(H)$ by Lemma 9.12, thus $a(G_{uv}(k-\ell,0)) > a(H)$ as desired.

It remains to be shown that $P_H \geq P_{G_{uv}(k-\ell,0)}(x)$ for $x \geq a(G_{uv}(k-\ell,0))$. Since M is a proper spanning subgraph of $G_{uv}(k-\ell,0)$, $P_M \geq P_{G_{uv}(k-\ell,0)}(x)$ when $x \geq a(G(k-\ell,0))$, and by the proof of Lemma 9.12, we know that $P_H(x) \geq P_M(x)$ when $x \geq a(M)$. Since $a(G_{uv}(k-\ell,0)) > a(M) > a(H)$, we find that $P_H \geq P_{G_{uv}(k-\ell,0)}$ for $x \geq a(G_{uv}(k-\ell,0))$. Further, since $G(k-\ell,0)$ is a proper subgraph of $G(k,\ell)$, $a(G_{uv}(k,\ell)) > a(G_{uv}(k-\ell,0))$ so

$$P_{G_{uv}(k,\ell)}(x) - P_{G_{uv}(k+1,\ell-1)}(x) = P_{G_{uv}(k-\ell,0)}(x) - P_H(x) < 0 \text{ for } x \geq a(G_{uv}(k,\ell))$$

This implies that $P_{G_{uv}(k,\ell)}(x) - P_{G_{uv}(k+1,\ell-1)}(x) < 0$ when evaluated at $x = a(G_{uv}(k,\ell))$ which implies that $P_{G_{uv}(k+1,\ell-1)}(x)$ would then be positive. Therefore, we find that

$$a(G_{uv}(k,\ell) > a(G_{uv}(k+1,\ell-1)).$$

$\square$
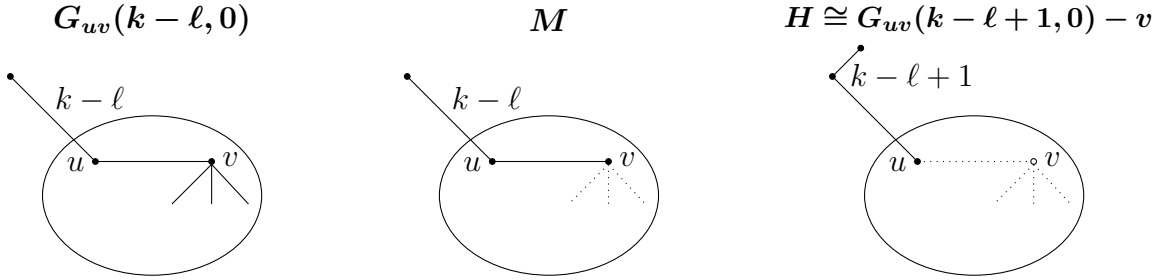
Figure 9.3. An illustration of the proof of Theorem 9.13

Suppose that S and T are graphs where $v \in V(S)$ and $w \in V(T)$. Then let $SvwT$ denote the graph obtained by connecting S and T by the new edge vw.

Lemma 9.14 ([19]). *Suppose that S and T are graphs where $v \in V(S)$ and $w \in V(T)$. Then $P_{SvwT}(x) = P_S(x)P_T(x) - P_{S-v}(x)P_{T-w}(x)$.*

The above results are used in a paper by Stevanović and Hansen entitled *The Minimum Spectral Radius of Graphs with a Given Clique Number* [69]. Proposition 9.6 states that amongst all connected graphs G of order n, the spectral radius is minimized by P_n. Stevanović

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and Hansen explore an extremal problem of similar nature. Namely, what graph amongst all connected order n graphs G with a given clique number minimizes $a(G)$? We present their argument for the sake of expository study, and a more clear proof of their main result Theorem 9.17.

Lemma 9.15 ([69])**.** *Let S and T be finite graphs where u and v are vertices of S. If $P_{S_v}(x) < P_{S_u}(x)$ for $x \geq a(S_v)$, then $a(SuwT) < a(SvwT)$ for any vertex w of T.*

Proof. By Proposition 9.14 it known that $P_{SvwT}(x) = P_S(x)P_T(x) - P_{S-v}(x)_{T-w}P(x)$. We also have that $P_{G_u}(x) = xP_G(x) - P_{G-u}(x)$, so we get that

$$P_{SvwT}(x) = P_S(x)P_T(x) - P_{S-v}(x)_{T-w}P(x)$$
$$= P_S(x)P_T(x) - P_{T-w}(xP_S(x) - P_{S_v})$$

Repeating this for $P_{SuwT}(x)$, we get that

$$P_{SvwT}(x) - P_{SuwT}(x) = P_{T-w}(P_{S_v}(x) - P_{S_u}(x))$$

It's clear that $T - w$ is a subgraph of $SuwT$, so $a(T - w) < a(SuwT)$. This implies that if $x > a(SuwT)$, then $x > a(T - w)$. This implies that $P_{T-w}(x) > 0$ when $x > a(SuwT)$. By assumption, $x > a(P_{S_u})$ as well, so $x > \min\{a(P_{S_u}), a(SuwT)\}$. This implies that $P_{S_v}(x) - P_{S_u}(x) < 0$ for such values of x. This implies that $P_{SvwT}(x) - P_{SuwT}(x) < 0$ when $x > \min\{a(P_{S_u}), a(SuwT)\}$ which implies that $a(SuwT) > a(SvwT)$ as desired. $\square$

For a graph G, suppose that $x, y, z \in V(G)$. If $xy \in E(G)$, then let $G - xy$ denote the graph obtained by removing the edge xy. Likewise, if $yz \notin E(G)$, let $G + yz$ denote the graph obtained by adding the edge yz to G.

Lemma 9.16 ([69])**.** *Let G be a connected graph with a bridge vw and suppose there is a path of length $k \geq 1$, attached to v, with u being the other end vertex of this path. Then $a(G - vw + uw) \leq a(G)$, with equality if and only if $\deg(v) = 2$.*

Proof. We will consider G as the graph with connected components S and T with $v \in V(S)$ and $w \in V(T)$. Further, let $v' \in V(S)$, with $\deg(v') = 2$, be adjacent to v and along the k-length path connecting v and u, while the rest of this path is not apart of S.
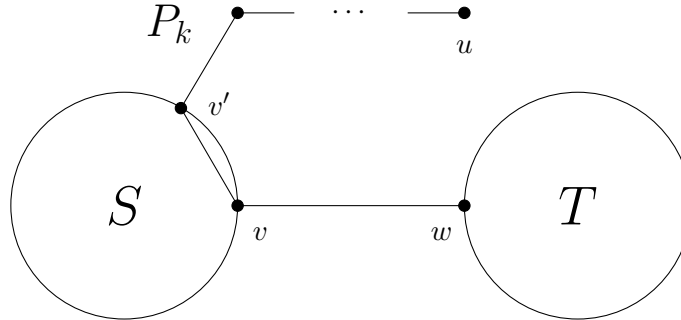
If $\deg(v) = 2$, then $S = \{\{v, v'\}, \{vv'\}\}$ and hence, $G - vw + uw \cong G$, so the result clearly holds. Now, suppose that $\deg(v) \geq 3$, so that S is more than the graph consisting of one edge. Next, let S' be the subgraph of G formed by S and the path from u to v. Obverse that

$$S'_u = S_{vv'}(k+1, 0) \qquad\qquad S'_v = S_{vv'}(k, 1)$$

Thus, we know that $a(S'_u) < a(S'_v)$ by Lemma 9.12, which implies that for all $x > a(S'_v)$, $P_{S'_u}(x) > P_{S'_v}(x)$. Further, notice that $G - vw + uw = S'uwT$ and $S'vwT = G$. With this, we may use Lemma 9.16 to assert that

$$a(G - vw + uw) = a(S'uwT) < a(S'vwT) = a(G)$$

which is the desired result. $\qquad\square$

With these lemmas, we are now able to prove the following result. For $n \geq \omega \geq 2$, let $\mathcal{G}_{n,\omega}$ denote the set of all connected graphs of order n with a maximum clique size ω. Further, the *kite graph*, denoted by $PK_{m,w}$ is a graph on $m + w$ vertices obtained from the path P_m and the complete graph K_w by adding an edge between an end vertex of P_m and a vertex of K_ω.

Theorem 9.17 ([69]). *If $G \in \mathcal{G}_{n,\omega}$ with $n \geq \omega \geq 2$, then $a(G) \geq a(PK_{n-\omega,\omega})$ with equality if and only if G is isomorphic to $PK_{n-\omega,\omega}$.*

Proof. In the case that $n = \omega$, then $\mathcal{G}_{n\omega} = \{K_n\}$, so the proof is trivial. When $\omega = 2$, then by Proposition 9.6, P_n minimizes the spectral radius amongst all connected graphs of order n. It's easily seen that $\mathcal{G}_{n,2} = \{P_n\}$.

Now suppose that $n > \omega \geq 3$, and let $G \in \mathcal{G}_{n,\omega}$ be arbitrary. Then G must contain a clique K of size ω. In this proof, we will preform perturbations on G so that we obtain $PK_{n-\omega,\omega}$ where each perturbation will decrease the spectral radius. We know from the proof of the Perron-Frobenius Theorem (see [26, 51]) that the deletion of an edge of a connected graph will strictly decrease the graph's spectral radius.

For our first set of perturbations, we will remove edges from G so that the resultant graph remains within $G_{n,\omega}$. So let G_1 be the graph obtained by removing all edges from G which are not apart of K and which are contained in a cycle. Then G_1 is a spanning subgraph of G where G_1 is the clique K with a number of rooted trees attached to vertices of K.

G_1
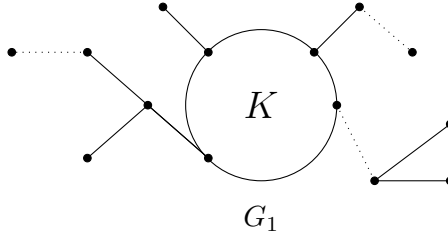
We get that $a(G_1) \leq a(G)$ with equality if and only if $G = G_1$; i.e., if no edge was removed in this first step.

The second set of perturbations will result in a "flattening out" of the rooted trees by transforming them into paths. Let T be one of the rooted trees and label by u a leaf of T which is farthest from K. Then let v be a vertex of T of degree at least 3 that is closest to u. In the case that T is not already a path, there is a neighbor w of v which is not on the path from v to u. So we will replace T with $T - vw + uw$.
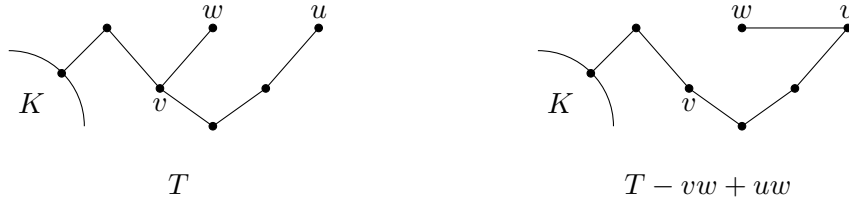
Notice that in this tree, the distance from K to the farthest leaf of this tree increases. We also know from Lemma 9.16 that this perturbation will decrease the spectral radius. Then we may repeat this process with every rooted tree of G_1 until each tree is transformed into a path. So we obtain the graph G_2 where $a(G_1) \geq a(G_2)$ with equality if and only if each tree was a path in G_1.

G_2
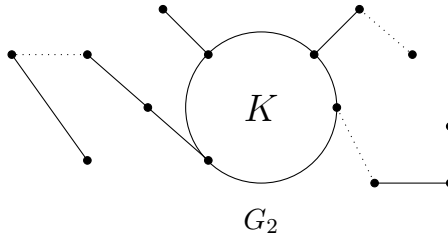
Finally, since G_2 is composed of a clique K of size ω with rooted paths attached to the vertices of K of varying length. Call these paths $P_{k_1}, P_{k_2}, \cdots, P_{k_m}$, with $k_1 \geq k_2 \geq \cdots \geq k_m$ which are attached to m distinct vertices of K. Note that the second set of perturbations implies this distinction. Since K is a clique, each of the paths are connected by an edge of K. Hence, we may use Lemma 9.12 for the last set of perturbations. Namely, for any two paths P_{k_i} and P_{k_j} with $i \geq j$, we may remove the pendant edge from P_{k_j} and attached that edge to the end of P_{k_i} and decrease the spectral radius in the process. We will then repeat this action until there is only one path attached to a vertex of K. This will result in the kite graph $PK_{n-\omega,\omega}$. As desired, the spectral radius will have decreased over each perturbation, which implies that $a(G) \geq a(PK_{n-\omega,\omega})$ and this completes the proof. □

9.3 Motivation for New Problems

As we referenced above, there is a survey paper on the Randić index which includes several bounds and problems regarding this index. The following extremal result piqued our interest.

Theorem 9.18. *[41] Let G be any connected, order n graph. Then*

$$\frac{n}{2n-2} \leq \frac{R(G)}{a(G)} \leq \begin{cases} \dfrac{n}{4} & \text{if } 4 \leq n \leq 26 \\[2ex] \dfrac{\frac{n-3}{2} + \sqrt{2}}{2\cos\left(\frac{\pi}{n+1}\right)} & \text{if } n \geq 27 \end{cases}$$

with equality on the left if and only if $G = K_n$, and with equality on the right if and only if $G = P_n$ and $G = C_n$ respectively.

This theorem poses an extremal problem in graph theory and resolves it by presenting which graphs minimize and maximize the ratio $R(G)/a(G)$.

Chapter 10: Laplacian Spectral Radii

Definition 10.1. Let G be a finite simple graph of order n. Then the **degree matrix** of G, denoted $D(G)$, is the $n \times n$ real matrix such that $[D]_{ii} = \deg(i)$ and $[D]_{ij} = 0$ for $i \neq j$. We use D when G is clear from context.

Definition 10.2. Let G be a finite simple graph of order n. Then the **Laplacian matrix** of G, denoted $L(G)$, is defined as $L(G) = D(G) - A(G)$.

Definition 10.3. The **Laplacian spectral radius** of G is defined as

$$\ell(G) := \max\{\text{spec}(L(G))\}.$$

The Laplacian matrix of a graph is a widely considered matrix in graph theory. Its eigenvalues are bounded by graph characteristics which are easily computed (e.g., maximum degree), and yield nice quadratic forms (see Lemma 10.6). One highly notable consequence of the Laplacian matrix was discovered by Kirchhoff in his original paper written in 1847, which was translated by J.B. O'Toole in 1958 in [38].

Theorem 10.4 (Kirchhoff's Theorem). *Let G be a connected, order n graph and let $L(G)$ be the Laplacian matrix of G. Let $L(G)^*$ be the matrix obtained by removing the i-th row and column of $L(G)$ for any $1 \leq i \leq n$. Then $\det(L(G)^*)$ is the number of spanning trees of G.*

Example 10.5. Let G be the graph in Figure 10.1. One can compute, by hand, the number of non-isomorphic spanning trees of G, and find exactly 8.

Then, observe the following computations, which verify Theorem 10.4.

$$L(G) = \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -2 \\ 0 & -1 & -1 & 2 \end{pmatrix} \qquad L(G)^* = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 2 \end{pmatrix} \qquad \det(L(G)^*) = 8.$$

See $[2, 28, 44, 63]$ for more information in the Laplacian matrix of a graph.

Propositions 10.8 and 10.7 present known results, though we were unable to find a sufficient proof in the literature so we provide our own.

First, we may use the Rayleigh quotient to express this spectral radius as

$$\ell(G) = \max_{||\boldsymbol{x}||=1} \boldsymbol{x}^T L(G) \boldsymbol{x}.$$
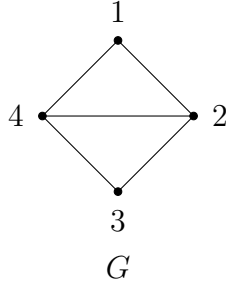
Figure 10.1. A graph with 8 spanning trees

A notable observation is the following. Let $\boldsymbol{x}(i)$ be the unit vector with 1 as the i-th entry and zeros everywhere else. Then it is easy to see that $\boldsymbol{x}(i)^T L(G)\boldsymbol{x}(i) = \deg(i)$, so $\ell(G) \geq \Delta(G)$ since the Laplacian spectral radius is a maximal eigenvalue by definition. We will discuss situations where products such as $\boldsymbol{x}^T L(G)\boldsymbol{x}$ become particularly useful.

Lemma 10.6. *Let G be a graph of order n, and let $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$. Then $\boldsymbol{x}^T L(G)\boldsymbol{x} = \sum_{i \sim j}(x_i - x_j)^2$. Furthermore, for every graph G there is a unit vector $\boldsymbol{v}$ in $\mathbb{R}^n$ such that $\ell(G) = \boldsymbol{v}^T L(G)\boldsymbol{v} = \sum_{i \sim j}(v_i - v_j)^2$.*

Proof. Let G be any graph of order n and let $\boldsymbol{x} = (x_1 \ x_2 \ \ldots \ x_n)$ be an arbitrary vector of $\mathbb{R}^n$. Enumerate the edges of G as $e_1, \ldots, e_m$ and define the $n \times n$ *edge matrix* E_k of $e_k = ij$ where $[E_k]_{ii} = [E_k]_{jj} = 1$, $[E_k]_{ij} = [E_k]_{ji} = -1$, and all remaining entries are 0. Then we get that

$$\boldsymbol{x}^t E_k \boldsymbol{x} = x_i^2 - 2x_i x_j + x_j^2 = (x_i - x_j)^2$$

Since $L(G) = \sum_{k=1}^m E_k$, we obtain the following:

$$\boldsymbol{x}^T L(G)\boldsymbol{x} = \boldsymbol{x}^T \left(\sum_{i=1}^m E_k \right) \boldsymbol{x} = \sum_{k=1}^m \boldsymbol{x}^T E_k \boldsymbol{x} = \sum_{i \sim j}(x_i - x_j)^2$$

Since $\ell(G) = \max_{||\boldsymbol{x}||=1} \boldsymbol{x}^T L(G)\boldsymbol{x}$ and the set of all vectors $\boldsymbol{x}$ in $\mathbb{R}^n$ with $||\boldsymbol{x}|| = 1$ is a compact set, there is some vector $\boldsymbol{v}$ in $\mathbb{R}^n$ with $||v|| = 1$, such that $\ell(G) = \boldsymbol{v}^T L(G)\boldsymbol{v} = \sum_{i \sim j}(v_i - v_j)^2$. $\qquad \square$

Proposition 10.7. *Let G be a connected graph. If H is a spanning subgraph of G, then $\ell(H) \leq \ell(G)$.*

Proof. By Lemma 10.6 we have a unit vector $\boldsymbol{y}$ such that $\ell(H) = \boldsymbol{y}^T L(H)\boldsymbol{y}$. It also follows

from Proposition 10.6 that

$$\begin{aligned}
\ell(G) &= \max_{||\boldsymbol{x}||=1} \boldsymbol{x}^T L(G)\boldsymbol{x} \\
&\geq \boldsymbol{y}^T L(G)\boldsymbol{y} \\
&= \sum_{i \sim j \text{ in } G} (y_i - y_j)^2 \\
&\geq \sum_{i \sim j \text{ in } H} (y_i - y_j)^2 \\
&= \boldsymbol{y}^T L(H)\boldsymbol{y} \\
&= \ell(H)
\end{aligned}$$

which completes the proof. $\square$

A quick corollary of this lemma is:

Proposition 10.8. *Amongst all connected graphs G on n vertices, $\ell(G)$ is maximized by K_n.*

Now that we have an upper bound on the Laplacian spectral radius of a graph, we present the lower bound.

Theorem 10.9. *Amongst all connected graphs G of order n,*

1. *$\ell(P_n) = \ell(C_n) \leq \ell(G)$ if n is odd and*

2. *$\ell(P_n) < \ell(C_n) \leq \ell(G)$ if n is even.*

We will need several lemmas and results before we can prove Theorem 10.9. While the upper and lower bounds for the spectral radius of a graph was resolved by Proposition 9.6, the lower bound result for the Laplacian spectral radius was not found in the literature. So we will resolve it in this thesis, as it is crucial to the proof of Theorem 10.25. Note that we are not claiming that this is a new result, since there are known bounds on $a(G)$ and $s\ell(G)$ (see Theorem 11.9).

The outline for the framework of Theorem 10.9 goes as follows. First, we need two results from the literature, Lemmas 10.10 and 10.11, accompanied by one of our own; Lemma 10.12. Next, the results in Subsections 10.1 and 10.2 provide the spectrum of $L(P_n)$ and $L(C_n)$; i.e., the set of eigenvalues of these Laplacian matrices, given later in 10.1 and 10.2. These results were presented by Spielman in his survey (see [63]), though, the proofs were lacking in detail. Hence, we provide thorough justification in Subsections 10.1 and 10.2.

Lemma 10.10. *[2, 44] Let G be a simple graph with at least one edge. Then*

$$\ell(G) \leq \max\{\deg(i) + \deg(j) : ij \in E(G)\}.$$

Lemma 10.11. *[28, 78] Let G be a connected simple graph with at least one edge. The*

$$\ell(G) \geq \Delta(G) + 1.$$

First, we will state and prove a result regarding the function $\varphi(G) := \max\{\deg(i) + \deg(j) : ij \in E(G)\}$. It follows from the definition that if G is a graph with $E(G) \geq 1$, then $\varphi(G) \geq 2$.

Lemma 10.12. *Let G be a connected graph of order n. The the following is true about $\varphi(G)$:*

1. *if $n \geq 4$, then $\varphi(G) \geq 4$;*

2. *if $n \geq 5$, then $\varphi(G) = 4$ if and only if $G = P_n$ or $G = C_n$.*

Proof. (1) Assume by way of contradiction that G is a connected graph of order at least 4 such that $\varphi(G) < 4$. If $\varphi(G) = 2$, then every vertex of G has degree 1, which would make G disconnected. If $\varphi(G) = 3$, then there is an edge $ij \in E(G)$ with $\deg(i) = 2$ and $\deg(j) = 1$. Let v be the other neighbor of i, which also has degree 1; otherwise, G would contain an edge with two incident vertices of degree 2 which contradicts the maximality of $\varphi(G)$. So $\deg(v) = \deg(j) = 1$ and $\deg(i) = 2$. Since $n \geq 4$, G at least one more vertex, say w. Observe that $N(i) \cup N(j) \cup N(v) = \{i, j, v\}$, which makes it impossible for there to be a path in G which contains w and any i (the same can be said about j and v). This contradicts the assumption that G is connected. This proves (1).

(2) Suppose that $n \geq 5$. The converse is clear. So assume that $\varphi(G) = 4$. If ij is an edge such that $\deg(i) + \deg(j) = \varphi(G)$, we will call ij a maximal edge. Suppose there is a maximal edge ij where $\deg(i) = 3$ and $\deg(j) = 1$. Then i has three neighbors, but G is a graph of order at least 5. Hence, there is some vertex v for which no path of G contains i and w; a contradiction. So any maximal edge ij of G must have the property that $\deg(i) = \deg(j) = 2$. Therefore, G must either be the path P_n or the cycle C_n. □

Remark. Part (2) of Lemma 10.12 specified that $n \geq 5$ and not 4. We required $n \geq 5$ so that we could arrive at the contradiction in our proof. If n was allowed to be 4, then $\varphi(G) = 4$ if and only if $G = P_n$ or $G = C_n$ or $G = S_n$. For our purposes, we must avoid consideration of the star in this Lemma.

10.1   Spectrum of the Laplacian Matrix of the Cycle

As we stated above, the results from this and the following subsections are stated in [63], but the corresponding proofs omit critical details that cannot be overlooked. The original statement of the result for the spectrum of $L(C_n)$ goes as follows.

Proposition 10.13. *[63] The Laplacian of C_n has eigenvectors*

$$\boldsymbol{x}_k(a) = \cos(2\pi ka/n), \quad and$$
$$\boldsymbol{y}_k(a) = \sin(2\pi ka/n),$$

for $0 \leq k \leq n/2$, ignoring $\boldsymbol{y_0}$ which is the all zero's vector, and for even n ignoring $\boldsymbol{y}_{n/2}$ for the same reason. Eigenvectors $\boldsymbol{x}_k$ and $\boldsymbol{y}_k$ have eigenvalue $2 - 2\cos(2\pi k/n)$.

Our recipe for correcting the errors in [63] is to present Lemmas 10.14, 10.15, 10.16, and 10.17 with new proofs; all of which will verify an identical result as Proposition 10.13.

Lemma 10.14. *Let $v_k \in \mathbb{R}^{\{0,\dots,n-1\}}$ be defined by $v_k(a) = e^{2\pi i k a/n}$ for $0 \le k \le n-1$. Then $\mathcal{B} = (v_k)_{k=0}^{n-1}$ is an orthogonal basis of $\mathbb{C}^n$ consisting of eigenvectors of L. More specifically, $Lv_k = \lambda_k v_k$ where $\lambda_k = 2 - 2\cos(2k\pi/n)$.*

Proof. Let $C_n = \{\{a, (a-1) \bmod (n)\} : 0 \le a \le n\}$ be the n cycle for $n \ge 4$ and let $L = L(C_n) \in \mathbb{R}^{\{0,\dots,n-1\} \times \{0,\dots,n-1\}}$ be the Laplacian matrix of C_n. Then

$$L = \begin{cases} 2 & i = j \\ -1 & \begin{aligned}j &= i+1 \bmod n \text{ or}\\ j &= i-1 \bmod n\end{aligned} \\ 0 & \text{otherwise} \end{cases}$$

Now let $v_k \in \mathbb{R}^{\{0,\dots,n-1\}}$ be defined by $v_k(a) = e^{2\pi i k a/n}$, where $i^2 = -1$, for $0 \le k \le n-1$. We aim to show that $\mathcal{B} = (v_k)_{k=0}^{n-1}$ is an orthogonal basis for $\mathbb{C}^n$ which consists of eigenvectors of L. Let $0 \le a, b, k, \ell \le n-1$. Then it easy to show that

$$v_k(a)v_k(b) = v_k(a+b) \qquad v_k(a)v_\ell(a) = \underbrace{v_{k+\ell}(a)}_{\text{taken mod } n} \qquad v_k(-a) = \overline{v_k(a)}$$

and

$$\begin{aligned} |v_k(a)| &= \left| e^{2\pi i k a/n} \right| \\ &= \left| \cos\left(\frac{2\pi i k a}{n}\right) + i \sin\left(\frac{2\pi i k a}{n}\right) \right| \\ &= \sqrt{\cos^2\left(\frac{2\pi i k a}{n}\right) + \sin^2\left(\frac{2\pi i k a}{n}\right)} \\ &= 1. \end{aligned}$$

Further, if $0 \le k, \ell \le n-1$ with $k \ne \ell$, then $1 \le |k-\ell| \le n-1$, so $v_{k-\ell}(1) = e^{2i(k-\ell)\pi/n} \ne 1$. Now, $v, w \in \mathbb{C}^{\{0,\dots,n-1\}}$ let $\langle v, w \rangle = \sum_{a=0}^{n-1} \overline{v_a} w_a$ be the complex inner product. Then we get that

$$\begin{aligned} \langle v_k, v_k \rangle &= \sum_{a=0}^{n-1} \overline{v_k(a)} v_k(a) \\ &= \sum_{a=0}^{n-1} |v_k(a)|^2 \\ &= \sum_{a=0}^{n-1} 1 \\ &= n \end{aligned}$$

Next, observe that if $k \neq \ell$, then

$$\langle v_k, v_\ell \rangle = \sum_{a=0}^{n-1} \overline{v_k(a)} v_\ell(a)$$

$$= \sum_{a=0}^{n-1} v_k(-a) v_\ell(a)$$

$$= \sum_{a=0}^{n-1} e^{\frac{2i(k-\ell)a\pi}{n}}$$

$$= \sum_{a=0}^{n-1} v_{k-\ell}(a)$$

Next, we will cyclically shift the vector components to obtain the following:

$$\sum_{a=0}^{n-1} v_{k-\ell}(a) = \sum_{a=0}^{n-1} v_{k-\ell}(a+1)$$

$$= \sum_{a=0}^{n-1} v_{k-\ell}(a) v_{k-\ell}(1)$$

$$= v_{k-\ell}(1) \sum_{a=0}^{n-1} v_{k-\ell}(a)$$

$$= v_{k-\ell} \langle v_k, v_\ell \rangle$$

Thus, we've shown that $\langle v_k, v_\ell \rangle = v_{k-\ell}(1) \langle v_k, v_\ell \rangle$, and since $v_{k-\ell}(1) \neq 0$, it must be the case that $\langle v_k, v_\ell \rangle = 0$; i.e., if $k \neq \ell$, then v_k and v_ℓ are orthogonal complex vectors. In summary,

$$\langle v_k, v_\ell \rangle = \begin{cases} n & k = \ell \\ 0 & k \neq \ell \end{cases}$$

Since orthogonal sets are linearly independent, we find that $\mathcal{B}$ is an orthogonal basis of $\mathbb{C}^n$.

Next, we will show that $L\, v_k = \lambda_k v_k$ where $\lambda_k = 2\left(1 - \cos\left(\frac{2\pi k}{n}\right)\right)$ (as defined in the lemma statement) by showing that $(L\, v_k)(a) = \lambda_k v_k(a)$ for each $0 \leq a \leq n-1$. First, observe that

$$v_k(1) = e^{2ik\pi/n} \qquad\qquad v_k(-1) = \overline{v_k(1)}$$

$$= \cos\left(\frac{2k\pi}{n}\right) + i\sin\left(\frac{2k\pi}{n}\right) \qquad\qquad = \cos\left(\frac{2k\pi}{n}\right) - i\sin\left(\frac{2k\pi}{n}\right)$$

so

$$v_k(1) + v_k(-1) = v_k(1) + \overline{v_k(1)}$$

$$= \cos\left(\frac{2k\pi}{n}\right) + i\sin\left(\frac{2k\pi}{n}\right) + \cos\left(\frac{2k\pi}{n}\right) - i\sin\left(\frac{2k\pi}{n}\right)$$

$$= 2\cos\left(\frac{2k\pi}{n}\right)$$

and thus

$$\lambda_k = 2 - 2\cos\left(\frac{2k\pi}{n}\right)$$

$$= 2 - v_k(1) - \overline{v_k(1)}.$$

We also have that for all $0 \leq a \leq n - 1$

$$(L\,v_k)(a) = \left(\left(\begin{pmatrix} 2 & -1 & 0 & \cdots & -1 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ -1 & \cdots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} v_k(0) \\ v_k(1) \\ \vdots \\ v_k(n-1) \end{pmatrix}\right)\right)(a)$$

$$= 2v_k(a) - v_k(a+1) - v_k(a-1)$$

$$= v_k(a)\,(2 - v_k(1) - v_k(-1))$$

$$= v_k(a)\left(2 - v_k(1) - \overline{v_k(1)}\right)$$

$$= \lambda_k v_k(a)$$

Therefore, $L\,v_k = \lambda_k v_k$ as desired. This demonstrates that $\mathcal{B} = (v_k)_{k=0}^{n-1}$ consists of eigenvectors of L which completes the proof. $\qquad\square$

Lemma 10.15. *Let $m \geq 1$. If $n = 2m$, then the eigenspaces of $\mathbb{C}^n$ with respect to L are as follows:*

1. *$\mathcal{E}_0$ with basis $\{v_0\}$ with eigenvalue $\lambda_0 = 0$;*

2. *$\mathcal{E}_k$ with basis $\{v_k, v_{n-k}\}$ for $1 \leq k \leq m - 1$ with eigenvalues $0 \leq \lambda_k = \lambda_{n-k} = 2(1 - \cos(2k\pi/n)) < 4$;*

3. *$\mathcal{E}_m$ with basis $\{v_m\}$ with eigenvalue $\lambda_m = 4$.*

These eigenspaces are orthogonal to each other.

Proof. We have that

$$\lambda_{n-k} = 2(1 - \cos((n-k)2\pi/n))$$

$$= 2(1 - \cos(2\pi - 2k\pi/n))$$

$$= 2(1 - \cos(-2k\pi/n))$$

$$= 2(1 - \cos(2k\pi/n))$$

$$= \lambda_k$$

It's easy to see that $\lambda_0 < \lambda_1 < \cdots < \lambda_{m-1} < \lambda_m = 4$ so we get that the eigenspaces $\mathcal{E}_0, \cdots, \mathcal{E}_m$ are all distinct. Further, these bases form a partition of $\mathcal{B}$ from the previous Lemma. Hence, the eigenspaces $\mathcal{E}_0, \cdots, \mathcal{E}_m$ are orthogonal and together span $\mathbb{C}^n$. $\qquad\square$

Lemma 10.16. *Let $m \geq 1$ and let $n = 2m + 1$. The eigenspaces of $\mathbb{C}^n$ with respect to L are as follows:*

1. *$\mathcal{E}_0$ with basis $\{v_0\}$ with eigenvalue $\lambda_0 = 0$;*

2. *$\mathcal{E}_k$ with basis $\{v_k, v_{n-k}\}$ for $1 \leq k \leq m - 1$ with eigenvalues $0 \leq \lambda_k = \lambda_{n-k} = 2(1 - \cos(2k\pi/n)) < 4$.*

These eigenspaces are orthogonal.

Proof. The proof is the same as that of the previous lemma. $\qquad\qquad\square$

When $0 \leq k \leq n - 1$, it's important to consider the following relation.

$$
\begin{aligned}
v_{n-k}(a) &= e^{\frac{2\pi i(n-k)a}{n}} \\
&= e^{2\pi i a - \frac{2\pi i k a}{n}} \\
&= e^{i(2\pi a - \frac{2\pi k a}{n})} \\
&= \cos\left(2\pi \cdot a - \frac{2\pi k a}{n}\right) + i\sin\left(2\pi \cdot a - \frac{2\pi k a}{n}\right) \\
&= \cos\left(\frac{2\pi k a}{n}\right) - i\sin\left(\frac{2\pi k a}{n}\right) \\
&= \overline{\cos\left(\frac{2\pi i k a}{n}\right) + i\sin\left(\frac{2\pi i k a}{n}\right)} \\
&= \overline{e^{\frac{2\pi i k a}{n}}} \\
&= \overline{v_k(a)}.
\end{aligned}
$$

This fact will be useful in some of the following proofs.

Before we state the next result, let $0 \leq k \leq n/2$ and define $x_k := v_k + v_{n-k}$. Then

$$
\begin{aligned}
x_k &= v_k + \overline{v_k} \\
&= 2 \cdot \mathrm{Re}(v_k) \\
&= \left(2\cos\left(\frac{2\pi k a}{n}\right)\right)_{a=0}^{n-1}
\end{aligned}
$$

Likewise, when we define $y_k := v_k - v_{n-k}$ we obtain the following:

$$
\begin{aligned}
y_k &= v_k - \overline{v_k} \\
&= 2 \cdot \mathrm{Im}(v_k) \\
&= \left(2\sin\left(\frac{2\pi k a}{n}\right)\right)_{a=0}^{n-1}
\end{aligned}
$$

Then $x_k, y_k \in \mathbb{R}^n$. Further, for any $v, w \in \mathbb{R}^n$, define

$$v \cdot w = \sum_{a=0}^{n-1} v_a w_a$$

$$= \sum_{a=0}^{n-1} \overline{v_a} w_a$$

$$= \langle v, w \rangle.$$

where $\overline{v_a} = v_a$ since v_a is a real valued vector. This brings us to the following result.

Lemma 10.17. *Let $m \geq 1$. If $n = 2m$, then $\mathcal{B}_{2m} = \{x_0, \ldots, x_m\} \cup \{y_1, \ldots, y_{m-1}\}$ is an orthogonal basis of eigenvectors of L in $\mathbb{R}^n$ and the eigenspaces are:*

1. *$\mathcal{E}_0$ with basis $\{x_0\}$ and eigenvalue $\lambda_0 = 0$;*

2. *$\mathcal{E}_k$ with basis $\{x_k, y_k\}$ and eigenvalues $\lambda_k = 2 - 2\cos\left(\frac{2\pi k}{n}\right)$ for $1 \leq k \leq m-1$, so $0 < \lambda_k < 4$;*

3. *$\mathcal{E}_m$ with basis $\{x_m\}$ and eigenvalue $\lambda_m = 4$.*

If $n = 2m + 1$, then $\mathcal{C}_{2m+1} = \{x_0, \ldots, x_m\} \cup \{y_1, \ldots, y_m\}$ is an orthogonal basis of eigenvectors of L in $\mathbb{R}^n$ and the eigenspaces are:

1. *$\mathcal{E}_0$ with basis $\{x_0\}$ and eigenvalue $\lambda_0 = 0$;*

2. *$\mathcal{E}_k$ with basis $\{x_k, y_k\}$ and eigenvalues $\lambda_k = 2 - 2\cos\left(\frac{2\pi k}{n}\right)$ for $1 \leq k \leq m-1$, so $0 < \lambda_k < 4$.*

Proof. The $n = 2m$ case will be considered first. We get automatically that

$$x_0 = v_0 + \overline{v_0} = 2\mathrm{Re}(v_0) = 2v_0 \in \mathbb{R}^n \text{ a basis for } \mathcal{E}_0$$
$$x_m = v_m + \overline{v_m} = 2\mathrm{Re}(v_m) = 2v_m \in \mathbb{R}^n \text{ a basis for } \mathcal{E}_m$$

and for $1 \leq k \leq m - 1$,

$$x_k = v_k + \overline{v_k} \qquad\qquad y_k = v_k - \overline{v_k}$$
$$= v_k + v_{n-k} \qquad\qquad\qquad = v_k - v_{n-k}$$

both are real vectors in $\mathcal{E}_k$. Observe that from a previous Lemma,

$$x_k \cdot x_k = \langle x_k, x_k \rangle$$
$$= \langle v_k + v_{n-k}, v_k + v_{n-k} \rangle$$
$$= \langle v_k, v_k \rangle + \langle v_k, v_{n-k} \rangle + \langle v_{n-k}, v_k \rangle + \langle v_{n-k}, v_{n-k} \rangle$$
$$= n + 0 + 0 + n$$
$$= 2n$$

which is non-zero. By a similar argument, $y_k \cdot y_k \neq 0$. Thus,

$$
\begin{aligned}
x_k \cdot y_k &= \langle x_k, y_k \rangle \\
&= \langle v_k + v_{n-k}, v_k - v_{n-k} \rangle \\
&= \langle v_k, v_k \rangle - \langle v_k, v_{n-k} \rangle + \langle v_{n-k}, v_k \rangle - \langle v_{n-k}, v_{n-k} \rangle \\
&= n - 0 + 0 - n \\
&= 0
\end{aligned}
$$

which shows that x_k and y_k are orthogonal, meaning $\{x_k, y_k\}$ is an orthogonal basis of $\mathcal{E}_k$. Previous results show that $\mathcal{E}_0, \cdots, \mathcal{E}_m$ are orthogonal eigenspaces, hence B_{2m} is a basis of orthogonal vectors. The proof for $n = 2m + 1$ is similar. $\qquad\square$

10.2 Spectrum of the Laplacian Matrix of the Path

In the same spirit as in Subsection 10.1, we will state the original result from Spielman, and offer our own result statements and more thorough proofs.

Proposition 10.18. *[63] Let $P_n = (V, E)$ where $V = \{1, \ldots, n\}$ and $E = \{(a, a+1) : 1 \leq a < n\}$. The Laplacian of P_n has the same eigenvalues as C_{2n}, excluding 2. That is, P_n has eigenvalues namely $2(1 - \cos(\pi k/n))$, and eigenvectors*

$$
v_k(a) = \cos(\pi k a/n - \pi k/2n)
$$

for $0 \leq k < n$.

We will show an identical result by way of Definition 10.19 and Lemma 10.21. Then Corollary 10.22 will display the spectra of both $L(C_n)$ and $L(P_c)$.

Definition 10.19. Let $\pi \in S_n$ where $\pi : [n] \to [n]$ is a bijection. Then define the **permutation matrix** of π as $P_\pi \in \mathbb{R}^{n \times n}$ where

$$
[P_\pi]_{i,j} = \begin{cases} 1 & \text{if } \pi(j) = i \\ 0 & \text{otherwise} \end{cases}
$$

Note that if π is the identity map, then $P_\pi(i, j) = 1$ if and only if $i = j$, so $P_\pi = I_n$. Suppose that $\pi_1 = \pi_2$. Then for each $j \in [n]$, $\pi_1(j) = \pi_2(j)$, so P_π is well defined and unique. Moreover, P_π is the unique matrix such that

$$
P_\pi e_i = e_{\pi(i)}
$$

where e_i is the standard basis vector of $\mathbb{R}^n$.

Example 10.20. Let $\pi = (1432)$ and $\sigma = (1234) = \pi^{-1}$ be permutations in S_4. Then

$$
P_\pi = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad\qquad P_\sigma = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}
$$

It follows that if $\pi, \sigma \in S_n$, then for each $i \in [n]$,

$$P_\sigma P_\pi e_i = e_{\sigma(\pi(i))} = e_{(\sigma \circ \pi)(i)} = P_{\sigma \circ \pi} e_i$$

which implies that $P_\sigma P_\pi = P_{\sigma \pi}$. If $\sigma = \pi^{-1}$, then

$$P_\sigma P_\pi = P_{\pi^{-1}} P_\pi = P_{\pi^{-1} \pi} = P_{id} = I_n$$

Hence, $(P_\pi)^{-1} = P_{\pi^{-1}}$. Now observe that

$$\begin{aligned}
P_\pi^T(i,j) &= P_\pi(j,i) \\
&= \begin{cases} 1 & \text{if } \pi(i) = j \\ 0 & \text{otherwise} \end{cases} \\
&= \begin{cases} 1 & \text{if } \pi^{-1}(j) = i \\ 0 & \text{otherwise} \end{cases} \\
&= P_{\pi^{-1}}(i,j)
\end{aligned}$$

so $P_{\pi^{-1}} = P_\pi^T$.

Let G be some graph with $V(G) = [n]$ and suppose that $M_G : R^{V(G) \times V(G)} \to \mathbb{R}$ is any matrix which is invariant under isomorphism. That is, for any isomorphism $\pi : H \to G$, $M_H(i,j) = M_G(\pi(i), \pi(j))$. Clearly,

$$M_H(i,j) = e_i^T M_H e_j$$

so it follows that

$$\begin{aligned}
M_G(\pi(i), \pi(j)) &= e_{\pi(i)}^T M_G e_{\pi(j)} \\
&= (P_\pi e_i)^T M_G P_\pi e_j \\
&= e_i^T \left(P_\pi^T M_G P_\pi \right) e_j
\end{aligned}$$

This shows that $M_H = P_\pi^T M_G P_\pi$ when $\pi : H \to G$ is an isomorphism.

Continue to assume that $\pi : H \to G$ is an isomorphism. Now suppose that $\{(v_i, \lambda_i)\}_{i=1}^n$ are eigenpairs for M_G, and let $w_i = P_{\pi^{-1}} v_i$. Observe that

$$\begin{aligned}
M_H w_i &= P_{\pi^{-1}} M_G P_\pi P_{\pi^{-1}} v_i \\
&= P_{\pi^{-1}} M_G v_i \\
&= P_{\pi^{-1}} \lambda_i v_i \\
&= \lambda_i w_i
\end{aligned}$$

This shows that $\{(w_i, \lambda_i)\}_{i=1}^n$ are eigenpairs for M_H.

The Laplacian matrix of a graph is an example of this. Suppose that $G \cong H$ is a finite simple graph without loops. If $\pi : H \to G$, the following holds:

$$
L_H(i,j) = \begin{cases} d_H(i) = d_H(j) & \text{if } i = j \\ -1 & \text{if } i \sim_H j \\ 0 & \text{if } i \nsim_H j \end{cases}
$$

$$
= \begin{cases} d_G(\pi(i)) = d_G(\pi(j)) & \text{if } i = j \\ -1 & \text{if } \pi(i) \sim_G \pi(j) \\ 0 & \text{if } \pi(i) \nsim_G \pi(j) \end{cases}
$$

$$
= L_G(\pi(i), \pi(j))
$$

Lemma 10.21. *Let*

$$
v_k = \left\{ \cos\left(\frac{2\pi k a}{2m} - \frac{1}{2} \frac{2\pi k}{2m} \right) \right\}_{a=1}^{m}
$$

$$
= \left\{ \cos\left(\frac{\pi k a}{m} - \frac{\pi k}{2m} \right) \right\}_{a=1}^{m}
$$

for $k = 0, \ldots, m-1$ is an orthonormal eigenbasis for $L(P_m)$ with eigenvalues

$$
\lambda_k = 2 - 2\cos\left(\frac{k\pi}{m} \right)
$$

Proof. Let $\vec{1}$ denote the all 1's vector with dimension dependant on the context in which it is being used. Consider the cycle C_{2m} on $\{0, 1, \ldots, 2m-1\}$, let $0 \le a \le 2m-1$, and let $L = L(C_{2m})$. We have the following eigenspaces:

1. $\mathcal{E}_0$ with eigenbasis $v_0 = \vec{1}$ and eigenvalue $\lambda_0 = 0$;

2. $\mathcal{E}_k$ with eigenbasis $\{v_k, v_{2m-k}\}_{a=1}^{2m}$ where $v_k = e^{\frac{2\pi i k a}{2m}} = e^{\frac{\pi i k a}{m}}$ and eigenvalues $\lambda_k = 2 - 2\cos\left(\frac{k\pi}{m} \right)$;

3. $\mathcal{E}_m$ with eigenbasis $v_m = ((-1)^a)_{a=0}^{2m-1}$ and eigenvalue $\lambda_m = 4$.

   Consider also C_{2m} on $\{0, 1, \ldots, 2m-1\}$ with $1 \le a \le 2m$ (index shift) where we have:

1. $\mathcal{E}_0$ with eigenbasis $v_0 = \vec{1}$ and eigenvalue $\lambda_0 = 0$;

2. $\mathcal{E}_k$ with eigenbasis $\{v'_k, v'_{2m-k}\}_{a=1}^{2m}$ where $v'_k = e^{\frac{\pi i k (a-1)}{m}}$ and $v'_{2m-k} = e^{\frac{-\pi i k (a-1)}{m}} = \overline{v'_k}$ having eigenvalues $\lambda_k, \lambda_{2m-k}$;

3. $\mathcal{E}_m$ with eigenbasis $v'_m = ((-1)^{(a-1)})_{a=0}^{2m-1}$ and eigenvalue λ_m.

   From what we've described above, we know that C_{2m} and L are both invariant under cyclic rotations. So we may rotate all the coordinates on the eigenvectors formed and set up the following:

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1. $\mathcal{E}_0$ with eigenbasis $v_0 = \vec{1}$ and eigenvalue $\lambda_0 = 0$;

2. for $1 \le k \le m-1$, $\mathcal{E}_k$ with eigenbasis $\{v_k'', v_{2m-k}''\}_{a=1}^{2m}$ where $v_k'' = e^{\frac{\pi i k a}{m}}$ and $v_{2m-k}'' = e^{\frac{-\pi i k a}{m}} = \overline{v_k''}$ having eigenvalues $\lambda_k, \lambda_{2m-k}$;

3. $\mathcal{E}_m$ with eigenbasis $v_m'' = ((-1)^a)_{a=1}^{2m}$ and eigenvalue λ_m.

Since the v_i'''s have been defined for $1 \le k \le 2m$, we can scale them in the following way. Let

$$\alpha_k = e^{\frac{-2\pi i k}{m} \cdot \frac{1}{2}} = e^{\frac{-\pi i k}{m}} \ne 0.$$

Then we will define the following:

1. for $1 \le k \le m-1$, $v_k''' = \alpha_k v_k''$ and $v_{2m-k}''' = \overline{\alpha_k v_{2m-k}''} = \overline{v_k'' \alpha_k}$;

2. $v_m''' = \alpha_m v_m''$.

These vectors will span the same eigenspace and are now orthonormal. That is;

$$v_k''' = \left(\exp\left(i \left(\frac{\pi k}{m} - \frac{\pi k}{2m} \right) \right) \right)_{a=1}^{2m} \qquad v_{2m-k}''' = \left(\exp\left(-i \left(\frac{\pi k}{m} - \frac{\pi k}{2m} \right) \right) \right)_{a=1}^{2m}$$

This provides us with a new orthonormal basis for $\mathcal{E}_k$. We can so construct $\mathcal{E}_k$ with the following vectors:

$$x_k' = \frac{v_k'' + \overline{v_k''}}{2} \qquad\qquad y_k' = \frac{v_k'' - \overline{v_k''}}{2}$$

$$= \left(\cos\left(\frac{k\pi a}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m} \qquad\qquad = \left(\sin\left(\frac{k\pi a}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

Then observe the following:

$$x_k'(2m+1-a) = \left(\cos\left(\frac{k\pi(2m+1-a)}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

$$= \left(\cos\left(2\pi k + \frac{\pi k}{m} - \frac{\pi k a}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

$$= \left(\cos\left(\frac{\pi k}{m} - \frac{\pi k a}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

$$= \left(\cos\left(-\frac{\pi k a}{m} + \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

$$= \left(\cos\left(\frac{\pi k a}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

$$= x_k'(a)$$

Hence, $x_0', x_1', \ldots, x_{m-1}'$ are orthogonal vectors for $L(C_{2m})$ on $\{1, 2, \ldots, 2m\}$ where $x_k'(a) = x_k'(2m+1-a)$.

Let $G = C_{2m}$ be the cycle drawn below.
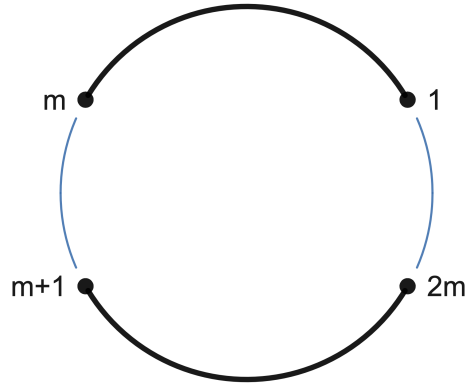
For this, we've got the following eigenbasis:

$$x_k = \left(\cos \left(\frac{\pi k a}{m} - \frac{k\pi}{2m} \right) \right)_{a=1}^{2m}$$

for $0 \le k \le m - 1$ with eigenvalues λ_k with respect to L_G where $x_k(a) = x_k(2m + 1 - a)$.

Next, let $H = C'_{2m}$ be the cycle drawn below:
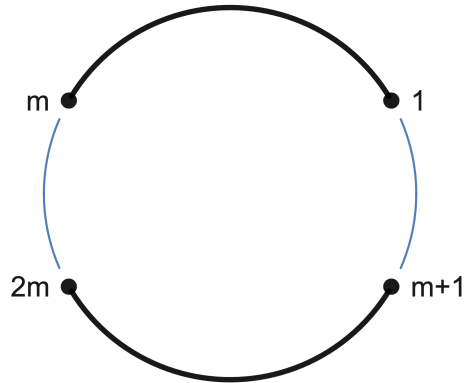
This yields the following isomorphism. Let $\pi : H \to G$ be defined as follows:

$$\pi(i) = \begin{cases} m + 1 \mapsto 2m \\ \quad \vdots \\ 2m \mapsto m + 1 \\ x \mapsto 3m + 1 - x \end{cases}$$

Thus, we have an eigenbasis of vectors for L_H. From what we've shown above, we get that

$$x'_k = P_\pi^{-1} x_k$$
$$\implies x'_k(a) = x_k(\pi(a))$$
$$\implies x'_k(a + m) = x_k(\pi(a + m))$$
$$= x_k(3m + 1 - (a + m))$$
$$= x_k(2m + 1 - a)$$
$$= x_k(a)$$
$$= x_k(\pi(a))$$
$$= x'_k(a)$$

Now, consider the Laplacian matrix $L_H = L(H)$ for the cycle above. Then

$$L_H = \left[\begin{array}{ccccc|ccccc} 2 & -1 & 0 & \cdots & 0 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & & \ddots & & \vdots & \vdots & & \ddots & & \vdots \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & -1 & 2 & 0 & 0 & \cdots 0 & 0 & -1 \\ \hline -1 & 0 & 0 & \cdots & 0 & 2 & -1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & & \vdots & \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 0 & 0 & 0 & -1 & 2 \end{array} \right]$$

From here, we can see that

$$[I_m \mid I_m] L_H \begin{bmatrix} I_m \\ I_m \end{bmatrix} = 2L(P_n)$$

Let $v_k(a) = x_k(\pi(a))$ for $1 \leq a \leq,$. Then

$$\begin{bmatrix} I_m \\ I_m \end{bmatrix} v_k = x'_k$$
$$\implies L_H \begin{bmatrix} I_m \\ I_m \end{bmatrix} v_k = L_H x_k = \lambda_k x_k$$
$$\implies [I_m \mid I_m] L_H \begin{bmatrix} I_m \\ I_m \end{bmatrix} v_k = \lambda_k [I_m \mid I_m] x'_k = 2\lambda_k v_k$$

That is,

$$2L(P_n)v_k = 2\lambda_k v_k$$
$$\implies L(P_n)v_k = \lambda_k v_k$$

Hence, we obtain the following:

$$
\begin{aligned}
x'_k \cdot x'_\ell &= \sum_{a=1}^{2m} x'_k(a)x'_\ell(a) \\
&= \sum_{a=1}^{2m} \left(x'_k(a)x'_\ell(a) + x'_k(a+m)x'_\ell(a+m) \right) \\
&= 2\sum_{a=1}^{2m} x'_k(a)x'_\ell(a) \\
&= 2\sum_{a=1}^{2m} v_k(a)v_\ell(a) \\
&= 2v_k \cdot v_\ell
\end{aligned}
$$

Therefore, we have the orthonormal basis of $L(P_m)$, namely,

$$
v_k = \left\{ \cos\left(\frac{\pi k a}{m} - \frac{\pi k}{2m} \right) \right\}_{a=1}^m
$$

with eigenvalues

$$
\lambda_k = 2 - 2\cos\left(\frac{k\pi}{m} \right).
$$

This completes the proof. $\qquad\square$

Corollary 10.22. *The spectrum of $L(P_n)$ and $L(C_n)$ are as follows:*

$$
spec(L(P_n)) = \left\{ 2 - 2\cos\left(\frac{\pi k}{n} \right) : 0 \le k \le n-1 \right\} \quad and \tag{10.1}
$$

$$
spec(L(C_n)) = \left\{ 2 - 2\cos\left(\frac{2\pi k}{n} \right) : 0 \le k \le n-1 \right\}. \tag{10.2}
$$

10.3 Graphs with Minimal Laplacian Spectral Radii

We now have all necessary results to prove Theorem 10.9; showing that amongst all connected graphs of order n, that $\ell(G)$ is minimized by P_n when n is even and both P_n and C_n when n odd.

Proof of Theorem 10.9. Let G be any connected graph of order n and let $\varphi(G) = \max\{\deg(i) + \deg(j) : ij \in E(G)\}$. If $n \le 4$, the result can be shown by brute force, since the number of connected graphs of order 4 and lower is less than 10. So assume that $n \ge 5$. By Lemmas 10.11 and 10.10,

$$
\Delta(G) + 1 \le \ell(G) \le \max\{\deg(i) + \deg(j) : ij \in E(G)\}.
$$

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Now consider the graph P_n and C_n. Both have maximum degree of 2, and $\varphi(P_n) = \varphi(C_n) = 4$. If G were is a connected graph not equal to P_n or C_n, then $\Delta(G) \geq 3$ and $\varphi(G) \geq 5$ (by Lemma 10.12) which would imply that $4 \leq \ell(G)$. However, if G is equal to P_n or C_n, then $3 \leq \ell(G) \leq 4$ so the Laplacian spectral radius must be minimized by either P_n or C_n.

By Corollary 10.22, we have the spectrum of $L(P_n)$ and $L(C_n)$, so we will determine $\max\{\text{spec}(L(P_n))\}$ and $\max\{\text{spec}(L(C_n))\}$, and compare them analytically.

Case 1: Assume that n is odd. Define the functions which represent the spectra of the path and cycle respectively:

$$p(x) = 2 - 2\cos\left(\frac{\pi x}{n}\right) \quad \text{and} \quad c(x) = 2 - 2\cos\left(\frac{2\pi x}{n}\right). \tag{10.3}$$

where $x \in \mathbb{R}_{\geq 0}$. Then

$$p'(x) = \frac{2\pi}{n}\sin\left(\frac{\pi x}{n}\right) \quad \text{and} \quad c'(x) = \frac{4\pi}{n}\sin\left(\frac{2\pi x}{n}\right) \tag{10.4}$$

It follows that $p(x)$ has a local maximum at $x = n$ and $c(x)$ has a local maximum at $x = n/2$. First, by Equation 10.1, we may only consider $0 \leq x \leq n - 1$ when we take x to be an integer. Hence, $p(x)$ will be maximized at $x = n - 1$ by the symmetry of $p(x)$. Second, n is an odd integer, so $c(n/2) \notin \text{spec}(L(C_n))$; i.e., $\ell(C_n) \neq 2$. Thus, by the symmetry of $c(x)$, $c(x)$ is maximized at $x = (n - 1)/2$ when we take $0 \leq x \leq n - 1$ to be an integer (see Equation 10.2). Then we obtain the following:

$$\max\{\text{spec}(L(P_n))\} = p(n - 1) \qquad\qquad \max\{\text{spec}(L(C_n))\} = c\left(\frac{n - 1}{2}\right)$$

$$= 2 - 2\cos\left(\frac{\pi(n - 1)}{n}\right) \qquad\qquad = 2 - 2\cos\left(\frac{2\pi\left(\frac{n-1}{2}\right)}{n}\right)$$

$$= 2 - 2\cos\left(\frac{\pi(n - 1)}{n}\right).$$

Therefore, $\ell(P_n) = \ell(C_n) \leq \ell(G)$ when n is odd.

Case 2: Assume that n is even. The local maximums of $p(x)$ and $c(x)$ are still analytically the same. Though, since n is even, $n/2$ is an integer, so $c(x)$ is maximized when $x = n/2$ ($p(x)$ is still maximized by $n - 1$). Hence,

$$c\left(\frac{n}{2}\right) = 2 - 2\cos\left(\frac{\pi\left(\frac{n}{2}\right)}{n}\right) = 4.$$

It is clear that $p(n - 1) = 2 - 2\cos\left(\frac{\pi(n-1)}{n}\right) < 4$, so we may conclude that $\ell(P_n) < \ell(C_n) = 4 \leq \ell(G)$ when n is even. This completes the proof. $\square$

10.4 Main Theorem for the Ratio of the Randić Index and the Laplacian Spectral Radius

We are now ready to address our main result which find the maximal graph amongst all connected, order n graphs of the ratio $R(G)/\ell(G)$.

Lemma 10.23. *If H is a connected graph such that $R(H) > R(P_n)$, then $R(H)/\ell(H) \leq R(C_n)/\ell(C_n)$.*

Proof. Suppose to the contrary that $R(H)/\ell(H) > R(C_n)/\ell(C_n)$, which means $H \neq C_n$. This implies that

$$R(H)\ell(C_n) > R(C_n)\ell(H)$$

Then $\ell(H) > \ell(C_n)$ so we get that $R(C_n)\ell(H) > R(C_n)\ell(H)$ and thus

$$R(H)\ell(C_n) > R(C_n)\ell(C_n)$$
$$\implies R(H) > R(C_n) = \frac{n}{2}$$

which is a contradiction since $R(G)$ is bounded above by $n/2$ by Theorem 8.2. This completes the proof. $\qquad\square$

Lemma 10.24. *There exists a unique $x \geq 4$ such that $\cos(\pi/x) = \frac{4\sqrt{2}-6}{x} + 1$*

Proof. Suppose that $x \geq 4$ and let $g(x) = \cos(\pi/x)$ and $h(x) = \frac{4\sqrt{2}-6}{x} + 1$, then let $f(x) = g(x) - h(x)$. First, observe that as $x \to \infty$, $\cos(\pi/x) \to 1$, then $0 \leq g(x) < 1$ One can easily verify that $f(x)$ has a root on the interval $[4, 15]$; namely $x_1 \approx 14.323$. We aim to show that no other root greater than x_1 exists. Observe that

$$f'(x) = \frac{4\sqrt{2} - 6 + \pi \sin(\pi/x)}{x^2}$$

Since $x \geq 4$, the function $k(x) = 4\sqrt{2}-6+\pi \sin(\pi/x)$ has a unique root; namely, $x_2 \approx 28.7047$. This implies that $f(x)$ has exactly one critical point on $[4,\infty)$, hence it will not oscillate for any $x > x_2$. So $f(x)$ decreases on (x_2, ∞). Since $\lim_{x\to\infty} f(x) = 0$, we may conclude that $f(x)$ will have no root on $[4, \infty)$ other than x_1. $\qquad\square$

Theorem 10.25. *Amongst all connected graphs of order n, the ratio $R(G)/\ell(G)$ has the following properties:*

1. *if n is odd, then $R(G)/\ell(G)$ is maximized by C_n;*

2. *if n is even, then $R(G)/\ell(G)$ is maximized by*

    i *P_n for $4 \leq n \leq 14$;*

ii C_n for $n \geq 16$.

Proof. Let G be a connected graph of order n, and let $n \geq 4$.

   Case 1. Let n be even. The for any graph $G \neq C_n, \ell(P_n) < \ell(C_n) < \ell(G)$ by Theorem 10.9. Since

$$R(C_n) = \frac{n}{2} \qquad\qquad R(P_n) = \frac{n-3}{2} + \sqrt{2},$$

and

$$\frac{R(C_n)}{\ell(C_n)} = \frac{n/2}{4} \quad \text{and} \quad \frac{R(P_n)}{\ell(P_n)} = \frac{\frac{n-3}{2} + \sqrt{2}}{2 - 2\cos\left(\frac{\pi(n-1)}{n}\right)},$$

we define

$$c(x) = \frac{x}{8} \qquad\qquad p(x) = \frac{x + 2\sqrt{2} - 3}{4 + 4\cos(\pi/x)}.$$

Then $c(x) = p(x)$ is equivalent to $\cos(\pi/x) = \frac{4\sqrt{2}-6}{x} + 1$. We know from Lemma 10.24 that if $x \geq 4$, then $x \approx 14.3235$ is the unique solution to this equation. This implies that $R(C_n)/\ell(C_n) < R(P_n)/\ell(P_n)$ for $4 \leq n \leq 14$ and $R(P_n)/\ell(P_n) < R(C_n)/\ell(C_n)$ for $n \geq 16$. It remains to be shown that for all even n, P_n and C_n are the maximal graphs of $R(G)/\ell(G)$ when $4 \leq n \leq 14$ and $n \geq 16$ respectively.

   First, consider the case where $4 \leq n \leq 14$. Assume to the contrary that there exists a graph H such that $R(H)/\ell(H) > R(P_n)/\ell(P_n)$, implying that $H \neq P_n$. We know $H \neq C_n$ from what we've shown above, so $\ell(H) \geq \ell(C_n) > \ell(P_n)$ by Theorem 10.9 and the parity of n. Obverse that since $R(H)/\ell(H) > R(P_n)/\ell(P_n)$,

$$R(H)\ell(P_n) > R(P_n)\ell(H) > R(P_n)\ell(P_n)$$
$$\implies R(H) > R(P_n).$$

More specifically, $n/2 \geq R(H) > R(P_n)$. Therefore, Lemma 10.23 implies that $R(H)/\ell(H) \leq R(C_n)/\ell(C_n)$. This contradicts what we've shown above, and this proves that there does not exist such an H. Thus, $R(G)/\ell(G)$ is maximized by P_n for even values of $4 \leq n \leq 14$.

   Second, consider the case where $n \geq 16$. Then $R(C_n)/\ell(C_n) > R(P_n)/\ell(P_n)$. Again, suppose to the contrary that there exists some graph H such that $R(H)/\ell(H) > R(C_n)/\ell(C_n)$; clearly $H \neq C_n$. Then $\ell(H) > \ell(C_n) > \ell(P_n)$ by Theorem 10.9. It follows that

$$R(H)\ell(C_n) > R(C_n)\ell(H) > R(C_n)\ell(C_n)$$
$$\implies R(H) > R(C_n).$$

We've arrived at the same contradiction as before, proving no such H exists. Therefore $R(G)/\ell(G)$ is maximized by C_n for even values of $n \geq 16$ which concludes the case where n is even.

Case 2. Let n be odd. We know that amongst all connected, order n graphs G, $R(G)$ is maximized by any regular graph by Theorem 8.2. So $R(C_n) \geq R(G)$. Likewise, we know that $\ell(G) \geq \ell(C_n) = \ell(P_n)$ when n is odd; i.e., $1/\ell(C_n) \geq 1/\ell(G)$. Then we obtain the following:

$$R(C_n) - \ell(C_n) \geq R(G) - \ell(G)$$
$$\implies \frac{R(C_n) - \ell(C_n)}{\ell(G)} \geq \frac{R(G) - \ell(G)}{\ell(G)}$$
$$\implies \frac{R(C_n) - \ell(C_n)}{\ell(C_n)} \geq \frac{R(G) - \ell(G)}{\ell(G)}$$
$$\implies \frac{R(C_n)}{\ell(C_n)} - 1 \geq \frac{R(G)}{\ell(G)} - 1$$
$$\implies \frac{R(C_n)}{\ell(C_n)} \geq \frac{R(G)}{\ell(G)}.$$

This completes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Chapter 11: Signless Laplacian Spectral Radii

Definition 11.1. Let G be a finite simple graph of order n. The **signless Laplacian matrix** of G, denoted $SL(G)$, is defined as $SL(G) = D(G) + A(G)$.

Definition 11.2. The **signless Laplacian spectral radius** of G is defined as defined as

$$sl(G) := \max\{\text{spec}(SL(G))\}.$$

The signless ratio Randic result [20]

The extremal graphs for the signless Laplacian spectral radius are known, so we present the following theorem.

Theorem 11.3. *[76] Let G be a connected graph of order n. Then $2\cos(\pi/n) \leq sl(G) \leq 2n-4$ where the lower bound is sharp if $G = P_n$ and the upper bound is sharp when $G = K_n$.*

The results in this following subsection were not given in [63]. While the spectra of $SL(P_n)$ and $SL(C_n)$ are likely known, we were not able to locate explicit statements in the literature. So we present the spectra of $SL(P_n)$ and $SL(C_n)$ in Equation 11.1 and Lemma 11.8.

11.1 Spectrum of the Signless Laplacian Matrix of the Cycle

Lemma 11.4. *Let $v_k \in \mathbb{R}^{\{0,\cdots,n-1\}}$ be defined by $v_k(a) = e^{2\pi ika/n}$ for $0 \leq k \leq n-1$.. Then $\mathcal{B} = (v_k)_{k=0}^{n-1}$ is an orthogonal basis of $\mathbb{C}^n$ consisting of eigenvectors of L. More specifically, $SL\ v_k = \mu_k v_k$ where $\mu_k = 2 + 2\cos(2k\pi/n)$.*

Proof. In a similar spirit of a previous Lemma, let $C_n = \{\{a, (a_1) \bmod (n)\} : 0 \leq a \leq n\}$ be the n cycle for $n \geq 4$ and let $SL = SL(C_n) \in \mathbb{R}^{\{0,...,n-1\}\times\{0,...,n-1\}}$ be the signless Laplacian matrix of C_n. Then

$$SL = \begin{cases} 2 & i = j \\ 1 & j = i+1 \bmod n \text{ or} \\ & j = i-1 \bmod n \\ 0 & \text{otherwise} \end{cases}$$

Now let $v_k \in \mathbb{R}^{\{0,\cdots,n-1\}}$ be defined by $v_k(a) = e^{2\pi i k a/n}$, where $i^2 = -1$, for $0 \leq k \leq n-1$. The argument for showing that $\mathcal{B} = (v_k)_{k=0}^{n-1}$ is an orthogonal basis for $\mathbb{C}^n$ is the same as the previous lemma. We still know $v_k(1) + \overline{v_k(1)} = 2\cos\left(\frac{2\pi}{n}\right)$. So for all $0 \leq a \leq n-1$, we obtain the following:

$$(SL\ v_k)(a) = \left(\begin{pmatrix} 2 & 1 & 0 & \cdots & 1 \\ 1 & 2 & 1 & \cdots & 0 \\ & \vdots & & \ddots & & \vdots \\ 0 & \cdots & 1 & 2 & 1 \\ 1 & \cdots & 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} v_k(0) \\ v_k(1) \\ \vdots \\ v_k(n-1) \end{pmatrix}\right)(a)$$

$$= 2v_k(a) + v_k(a+1) + v_k(a-1)$$

$$= v_k(a)\left(2 + v_k(1) + v_k(-1)\right)$$

$$= v_k(a)\left(2 + v_k(1) + \overline{v_k(1)}\right)$$

$$= \mu_k v_k(a)$$

Hence, the vectors v_k are orthogonal eigenvectors of SL with eigenvalues $\mu_k = 2 + 2\cos\left(\frac{2\pi k}{n}\right)$, and this completes the proof. □

Now that we've got the eigenvalues of $SL(C_n)$, $\mu_k = 2 + 2\cos\left(\frac{2\pi k}{n}\right)$ for $0 \leq k \leq n-1$, it's easy to see that $\max_{0 \leq k \leq n-1} \mu_k = SL(C_n) = 4$. Once can deduce that 0 is an eigenvalue of $SL(C_n)$ if and only if n is even.

Lemma 11.5. *Let $m \geq 1$. If $n = 2m$, then the eigenspaces of $\mathbb{C}^n$ with respect to $SL(C_n)$ are as follows:*

1. *$\mathcal{E}_0$ with basis $\{v_0\}$ with eigenvalue $\mu_0 = 4$;*

2. *$\mathcal{E}_k$ with basis $\{v_k, v_{n-k}\}$ for $1 \leq k \leq m-1$ with eigenvalues $0 \leq \mu_k = \lambda_{n-k} = 2 + 2\cos(2k\pi/n)) < 4$;*

3. *$\mathcal{E}_m$ with basis $\{v_m\}$ with eigenvalue $\mu_m = 0$.*

These eigenspaces are orthogonal to each other. If $n = 2m + 1$, then the eigenspaces of $\mathbb{C}^n$ with respect to $SL(C_n)$ are as follows:

1. *$\mathcal{E}_0$ with basis $\{x_0\}$ and eigenvalue $\mu_0 = 4$;*

2. *$\mathcal{E}_k$ with basis $\{x_k, y_k\}$ and eigenvalues $\mu_k = 2 + 2\cos\left(\frac{2\pi k}{n}\right)$ for $1 \leq k \leq m-1$, so $0 < \mu_k < 4$.*

These eigenspaces are orthogonal.

The proofs for both are similar to those regarding the Laplacian.

Lemma 11.6. *Let $m \geq 1$. If $n = 2m$, then $\mathcal{B}_{2m} = \{x_0, \ldots, x_m\} \cup \{y_1, \ldots, y_{m-1}\}$ is an orthogonal basis of eigenvectors of L in $\mathbb{R}^n$ and the eigenspaces are:*

1. $\mathcal{E}_0$ with basis $\{x_0\}$ and eigenvalue $\lambda_0 = 0$;

2. $\mathcal{E}_k$ with basis $\{x_k, y_k\}$ and eigenvalues $\lambda_k = 2 - 2\cos\left(\frac{2\pi k}{n}\right)$ for $1 \leq k \leq m-1$, so $0 < \lambda_k < 4$;

3. $\mathcal{E}_m$ with basis $\{x_m\}$ and eigenvalue $\lambda_m = 4$.

If $n = 2m+1$, then $\mathcal{C}_{2m+1} = \{x_0, \ldots, x_m\} \cup \{y_1, \ldots, y_m\}$ is an orthogonal basis of eigenvectors of L in $\mathbb{R}^n$ and the eigenspaces are:

1. $\mathcal{E}_0$ with basis $\{x_0\}$ and eigenvalue $\lambda_0 = 0$;

2. $\mathcal{E}_k$ with basis $\{x_k, y_k\}$ and eigenvalues $\lambda_k = 2 + 2\cos\left(\frac{2\pi k}{n}\right)$ for $1 \leq k \leq m-1$, so $0 < \lambda_k < 4$.

Proof. The $n = 2m$ case will be considered first. We get automatically that

$$x_0 = v_0 + \overline{v_0} = 2\mathrm{Re}(v_0) = 2v_0 \in \mathbb{R}^n \text{ a basis for } \mathcal{E}_0$$
$$x_m = v_m + \overline{v_m} = 2\mathrm{Re}(v_m) = 2v_m \in \mathbb{R}^n \text{ a basis for } \mathcal{E}_m$$

and for $1 \leq k \leq m-1$,

$$\begin{array}{ll} x_k = v_k + \overline{v_k} & y_k = v_k - \overline{v_k} \\ \quad = v_k + v_{n-k} & \quad = v_k - v_{n-k} \end{array}$$

both are real vectors in $\mathcal{E}_k$. Observe that from a previous Lemma,

$$\begin{aligned} x_k \cdot x_k &= \langle x_k, x_k \rangle \\ &= \langle v_k + v_{n-k}, v_k + v_{n-k} \rangle \\ &= \langle v_k, v_k \rangle + \langle v_k, v_{n-k} \rangle + \langle v_{n-k}, v_k \rangle + \langle v_{n-k}, v_{n-k} \rangle \\ &= n + 0 + 0 + n \\ &= 2n \end{aligned}$$

which is non-zero. By similar argument, $y_k \cdot y_k \neq 0$. Thus,

$$\begin{aligned} x_k \cdot y_k &= \langle x_k, y_k \rangle \\ &= \langle v_k + v_{n-k}, v_k - v_{n-k} \rangle \\ &= \langle v_k, v_k \rangle - \langle v_k, v_{n-k} \rangle + \langle v_{n-k}, v_k \rangle - \langle v_{n-k}, v_{n-k} \rangle \\ &= n - 0 + 0 - n \\ &= 0 \end{aligned}$$

which shows that x_k and y_k are orthogonal, meaning $\{x_k, y_k\}$ is an orthogonal basis of $\mathcal{E}_k$. Previous Lemmas show that $\mathcal{E}_0, \cdots, \mathcal{E}_m$ are orthogonal eigenspaces, hence B_{2m} is a basis of orthogonal vectors. The proof for $n = 2m+1$ is similar. $\qquad\square$

Corollary 11.7. *The spectrum of $SL(C_n)$ is as follows:*

$$spec(SL(C_n)) = \left\{ 2 + 2\cos\left(\frac{2\pi k}{n}\right) : 0 \leq k \leq n-1 \right\}. \tag{11.1}$$

11.2 Spectrum of the Signless Laplacian Matrix of the Path

Lemma 11.8. *For $n \geq 1$, the matrices $L(P_n)$ and $SL(P_n)$ have the same eigenvalues.*

Proof. We will prove this result by demonstrating that $L(P_n)$ and $SL(P_n)$ are similar matrices. Define the matrix D so that $D_{ij} = 0$ if and only if $i \neq j$ and $D_{ii} = (-1)^{i+1}$; this matrix is Hermitian. Further, it's easy to see that $D^{-1} = D^T = D$, so $D^T L(P_n)D = DL(P_n)D$. Let $M = D^T L(P_n)$, then

$$M_{ij} = \sum_{k=1}^{m} D_{ik} L(P_n)_{kj}$$
$$= (-1)^{i+1} L(P_n)_{ij}$$

so

$$(MD)_{ij} = \sum_{k=1}^{m} M_{ik} D_{kj}$$
$$= M_{ij} D_{jj}$$
$$= (-1)^{i+1} L(P_n)_{ij} (-1)^{j+1}$$
$$= L(P_n)_{ij} (-1)^{i+j+2}$$
$$= L(P_n)_{ij} (-1)^{i+j}$$
$$= \begin{cases} 1(-1)^{2i} & \text{if } i = j = 1 \text{ or } i = j = n \\ 2(-1)^{2i} & \text{if } i = j \text{ and } 1 < i, j < n \\ (-1)(-1)^{i+(i\pm1)} & \text{if } j = i \pm 1 \\ 0 & \text{otherwise} \end{cases}$$
$$= \begin{cases} 2 & \text{if } i = j > 1 \\ 1 & \text{if } j = i \pm 1 \\ & \text{or } i = j = 1 \\ & \text{or } i = j = n \\ 0 & \text{otherwise} \end{cases}$$
$$= SL(P_n)_{ij}$$

Hence, $DL(P_n)D = SL(P_n)$. Therefore, $\operatorname{spec}(L(P_n)) = \operatorname{spec}(SL(P_n))$ $\qquad \square$

Suppose that (v, λ) is some eigenpair for $L = L(P_n)$. Observe that

$$SL(P_n) \cdot Dv = DLD \cdot Dv$$
$$= DLv$$
$$= D\lambda v$$
$$= \lambda Dv$$

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This shows that for each eigenpair (v, λ) if $L(P_n)$, (Dv, λ) is an eigenpair of $SL(P_n)$. Specifically, if we pick some eigenvector v of $L(P_n)$, then the $Dv's$ have the following form:

$$Dv = \begin{pmatrix} v_0 \\ -v_1 \\ \vdots \\ (-1)^n v_{n-1} \end{pmatrix}$$

Further, we know that D is orthogonal, and since $x \cdot y = x^T y$, we get that

$$\begin{aligned} Dx \cdot Dy &= (Dx)^T Dy \\ &= x^T D^T Dy \\ &= x^T y \\ &= x \cdot y. \end{aligned}$$

Since we've already shown that the set of eigenvectors for $L(P_n)$ are orthogonal, this implies that the set of eigenvectors $\{Dv : v$ is an eigenvector of $L(P_n)\}$ is orthogonal.

11.3 Main Theorem for the Ratio of the Randić Index and the Signless Laplacian Spectral Radius

Theorem 11.9. *Amongst all connected graphs of order $4 \leq n$, the ratio $R(G)/sl(G)$ is maximized by:*

1. *P_n for $4 \leq n \leq 14$;*

2. *C_n for $n \geq 15$.*

Remark. The graphs which maximize $R(G)/sl(G)$ do not alternate according to the parity n as the ratio did for Theorem 10.25.

Proof. By Theorem 11.3, $s\ell(P_n) < s\ell(C_n) \leq s\ell(G)$ for any connected order n graph G. Then, by Theorem 10.25, Corollary 11.7, and Lemma 11.5, the proof is the same as the even case of 10.25. $\square$

Chapter 12: Graph Theoretic Radius

In this final section, we will address a conjecture on Randić index and the *radius* of a graph that was first introduced in 2000 in [17]. While we are not able to completely resolve this conjecture, we will propose a new conjecture which, if true, would prove the main conjecture.

Definition 12.1. Let G be a graph. The **eccentricity** of a vertex v in G is

$$\text{ecc}_G(v) := \max\{d(u,v) : u \in V(G)\}.$$

If the graph is clear from context, we will denote eccentricity of a vertex v by $\text{ecc}(v)$. Then the **radius** and **diameter** of G are defined as

$$r(G) := \min\{\text{ecc}_G(v) : v \in V(G)\} \quad \text{and} \quad D(G) := \max\{\text{ecc}_G(v) : v \in V(G)\},$$

respectively.

Remark. While we only consider connected graphs in this section, Definition 12.1 does not require G to be a connected graph.

The *center* of a graph is the set of all vertices of G whose eccentricities are equal to $r(G)$, denoted by $\text{cen}(G)$. Note that $\#(\text{cen}(G))$ is not necessarily equal to 1. Figure 12.1 shows a graph where $\text{ecc}(1) = 3, \text{ecc}(4) = 2, r(G) = 2, D(G) = 4$, and $\text{cen}(G) = \{4\}$. For instance, the cycle C_4 has the property that $\text{cen}(C_4) = V(C_4)$ definition. For the second, suppose that $u, v, w \in G$ such that $d(u,v) = D(G)$, and $\text{ecc}(w) = r(G)$. Then by the triangle inequality,

$$d(u,v) = d(u,w) + d(w,v) \leq r(G) + r(G) = 2r(G).$$
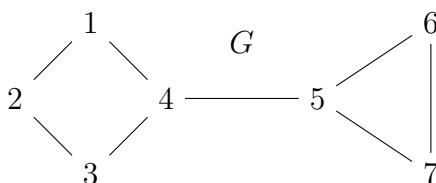
Figure 12.1. An illustrative example of graph radius

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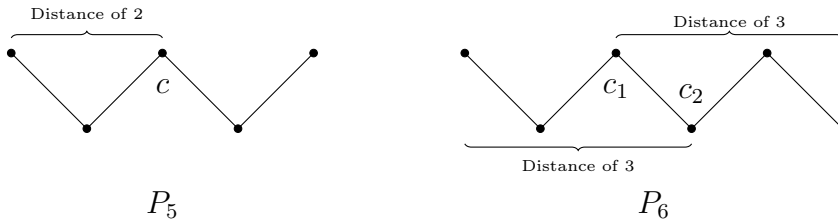
Figure 12.2. Centers for P_5 and P_6

Example 12.2. The graph G in Figure 12.1 has diameter equal to twice its radius. Though, an example of a graph where the second inequality for $r(G) \leq D(G) \leq 2r(G)$ is strict is the graph P_6 with a radius is 3 and diameter is 5. On the other hand, C_4 is a graph with a radius and diameter of 2.

We are ready to introduce main conjecture for this chapter.

Conjecture 12.3. *[17] Let G be a graph such that $G \neq P_n$ for even values of $n \geq 4$. Then $R(G) \geq r(G)$.*

Conjecture 12.3 was originally proposed in [17] by Caporossi and Hansen, though it was motivated by a conjecture which appears in [22] stating that for all graphs G, $R(G) \geq r(G)-1$. This conjecture also remains unresolved, and will be considered in our future work. Carparossi and Hansen used what is known as the AutoGraphiX System, described in [31]. It is a data analysis system designed and used for the purposes of suggesting and refuting conjectures about finite graphs with focuses on graph invariants and extremal graphs.

Example 12.4. Observe that $R(P_2) = 1 = r(P_2)$. Though if $G = P_n$ for any even $n \geq 3$, then

$$R(P_n) = \frac{n-3}{2} + \sqrt{2} < \frac{n}{2} = r(P_n)$$

by simple algebra.

There are some known results regarding the radius and diameter of trees which will also be useful for us.

Proposition 12.5. *[32] Every tree has a center consisting of either one point or two adjacent points.*

This proposition makes it easy to see that odd ordered paths have one central point while even ordered paths have two central points, illustrated by Figure 12.2. We will use this fact to help prove Lemma 12.14.

The following proposition is known, but without an explicit reference in the literature, we present our own proof.

Proposition 12.6. *If T is a tree with diameter $D(T)$, then $r(T) = \lceil D(T)/2 \rceil$.*

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Proof. Let $D = D(T)$ and $r = r(T)$. We'll first show that $r \leq \lceil D/2 \rceil$ for all trees.

Assume the case that $D = 2k$. Let P be a path of length D with endpoints x and y, and let v be a center of T; i.e., $\operatorname{ecc}(v) = r$. Then $d(x, v) = d(v, y) = k$. Suppose by way of contradiction that there exists some $w \in V(T)$ with $d(v, w) = r > k$. Clearly, w is not a vertex in P so there is w' in P which connects w to P, as shown in Figure 12.3. It is possible that $w' = v$. Then $k + 1 \geq d(v, w)$. Since T is a tree, there is exactly one path between every pair of vertices, so $d(x, w) = d(x, v) + d(v, w) \geq k + k + 1 = 2k + 1$, which contradicts P being of maximal length in T. Hence, $r \leq k$.

In the case that $D = 2k + 1$, and let P be a path witnessing this length with end points x and y. Then will have at least two distinct centers since a longest path of length $2k + 1$ will be an even ordered path. Suppose that v and v' are centers of T. Then $d(x, v) = d(v', y) = k + 1$. Suppose by way of contradiction that there is some w_1 and w' such that $d(v, w_1) > k + 1$ where the path witnessing this length passes through v'. Then $d(x, w_1) = d(x, v) + d(v, v') + d(v', w') \geq k + 1 + (k + 1) = 2k + 2$, which contradicts our assumption of P being of maximal length. If we assume next that there is some w_2 and w'' such that $d(v', w_2) > k + 1$ where the path witnessing this length passes through v, we'd arrive at the same contradiction. Hence, $r \leq k + 1$ in this case. Thus, $r \leq \lceil \frac{D}{2} \rceil$.

Next, we'll show that $r \geq \lceil \frac{D}{2} \rceil$. Let v be a center of T and let P be a path of length D. It is known that for all graphs, $r \geq D/2$, so if $D = 2k$, then we're done. If $D = 2k + 1$, then $\lceil \frac{D}{2} \rceil = k + 1$. If P be a path of length D, then P has $2k + 2$ vertices which implies that T has distinct centers v and v'. Let P have end points x and y so that $d(x, v') = d(v, y) = r$. Then there exists a unique path from x to y, so

$$
\begin{aligned}
2k + 1 = d(x, y) &= d(x, v) + d(v, v') + d(v', y) \\
&\leq (r - 1) + 1 + (r - 1) \\
&= 2r - 1 \\
\implies 2r + 1 &\geq 2k + 1 \\
\implies r &\geq k + 1
\end{aligned}
$$

as desired.

Therefore, if T is a tree, then $r = \lceil \frac{D}{2} \rceil$. $\qquad \square$

Corollary 12.7. *Let T be a tree and suppose that P is a path of length equal to the diameter of T. Then $r(T) = r(P)$.*

Proof. Since $D(T) = D(P)$, the result follows by Proposition 12.6. $\qquad \square$

Remark. If we take an graph G and some spanning tree T of G, then $r(G) \leq r(T)$. To see this, consider any two vertices u and v in T. There is exactly one path between u and v in T, though there could be multiple uv-paths in G shorter than the uv-path in T. In other words, if one were to take a tree and start adding edges between the existing vertices, then the distance between vertices can either be fixed or can become shorter.
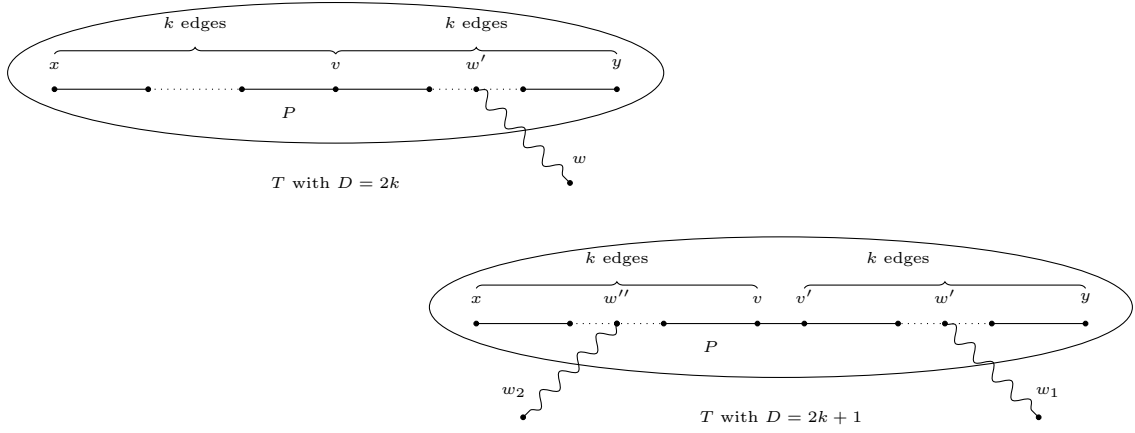
Figure 12.3. Showing $r(T) = \lceil \frac{D(T)}{2} \rceil$

Caporossi and Hansen present a proof in [17] showing that Conjecture 12.3 is resolved for all trees. However, this proof omits non-trivial details, so we present a more accurate proof below.

Lemma 12.8. *[17] For all trees T, $R(T) - r(T) \geq \sqrt{2} - \frac{3}{2} \approx -0.087$.*

Proof. Let T be some and let $D(T)$ denote the diameter of this tree. If T is of order 2 or 3, T can only be a path. Since $R(P_2) = r(P_2) = 1$ and $R(P_3) = \sqrt{2} > 1 = r(P_3)$, the result follows immediately for these cases. So we'll assume that $n \geq 4$. Suppose that x and y the vertices of T with $d(x,y) = D(T)$ and for ease of notation, set $n = D(T) + 1$. Next, let $T_0 = T$ and ℓ_1 be any leaf of T not equal to x or y. Then let $T_1 = T_0 - \ell_1$. Recursively repeat these steps until $T_k = P_n$ By Proposition 8.8, we have that $R(T_i) \geq R(T_j)$ for each $0 \leq i \leq j \leq k$. Since T_0 is a tree, Corollary 12.7 gives $r(T_0) = r(T_k)$.

Observe that

$$R(T_k) - r(T_k) = R(P_n) - r(P_n)$$
$$= \frac{n-3}{2} + \sqrt{2} - \left\lfloor \frac{n}{2} \right\rfloor$$
$$\geq \frac{n-3}{2} + \sqrt{2} - \frac{n}{2}$$
$$= \frac{n}{2} - \frac{3}{2} + \sqrt{2} - \frac{n}{2}$$
$$= \sqrt{2} - \frac{3}{2}$$

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Then, we get that

$$\begin{aligned}
R(T) - r(T) = R(T_0) - r(T_k) \\
\geq R(T_k) - r(T_k) \\
= \sqrt{2} - \frac{3}{2}
\end{aligned}$$

and we're done. □

Before we state and prove the next theorem, observe that when let $n \geq 3$:

1. when n is odd, then $R(P_n) > r(P_n)$;

2. when n is even, then $R(P_n) < r(P_n)$.

It's easy to verify the above formulas numerically. Since $\sqrt{2} - 3/2 \approx -0.086$, we obtain the following for n odd on the left and n even on the right:

$$\frac{n}{2} + \sqrt{2} - \frac{3}{2} - \left\lfloor \frac{n}{2} \right\rfloor = 0.5 - 0.086 > 0, \qquad \frac{n}{2} + \sqrt{2} - \frac{3}{2} - \left\lfloor \frac{n}{2} \right\rfloor = -0.086 < 0$$

We'll refer to paths with even order as *even paths* from now on; likewise, paths with odd order will be called *odd paths*. Conjecture 12.3 has been shown in [17] to be true for all trees not equal to the even path. However, the proof provided leaves out crucial details which do not automatically follow from their given statements and assumptions. Hence, we write our own proof and provide the necessary analysis and details.

Theorem 12.9. *[17] Let T be a tree of order n. If T is not an even path, then $R(T) \geq r(T)$.*

Proof. Suppose that T is a tree which is not an even path. We'll assume that $n \geq 3$, since as shown in the proof of Lemma 12.8, this case is immediate. Then define T' as we defined T_k in the proof of Lemma 12.8 (i.e., T_k is a path) and let $n = D(T) + 1$. Now let T'' be any tree we obtain by adding an edge to T' from $T \backslash T'$. There are two cases: the edge is attached to a vertex which is adjacent to a leaf, or the edge is added to a vertex which is adjacent to two vertices both having degree of 2. Since T' has the same diameter of T, the additional edge cannot be attached to a leaf. In both of the following cases, we aim to show that $R(T'') > r(T)$.

Case 1: In this case, T'' is the graph obtained by adding an edge to T' from $E(T) \backslash E(T')$ such that this edge is added to a vertex of degree 2 incident to an pendant edge.

T' $\qquad\qquad$ T''
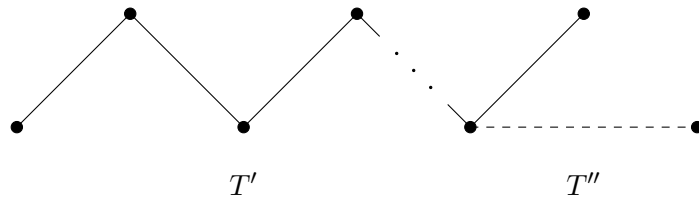
Denote $T' = P_n$, observe the following:

$$R(T'') - R(T') = \left[\frac{n-4}{\sqrt{2 \cdot 2}} + \frac{1}{\sqrt{2 \cdot 1}} + \frac{1}{\sqrt{2 \cdot 3}} + \frac{2}{\sqrt{3 \cdot 1}}\right] - \left[\frac{n-3}{2} + \sqrt{2}\right]$$

$$= \frac{n-4}{2} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} - \frac{n-3}{2} - \sqrt{2}$$

$$= \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} - \frac{1}{2} - \frac{1}{\sqrt{2}}$$

$$\approx 0.356$$

Suppose it is the case that T' is an odd path; that is, n is odd. Then we know that

$$r(T') < R(T')$$
$$\implies r(T') - R(T'') < R(T') - R(T'')$$
$$\implies R(T'') - r(T') > R(T'') - R(T')$$

We've shown that $R(T'') - R(T') > 0$ directly, we get that $R(T'') - r(T') > 0$ as well. Since $r(T') = r(T)$, we also get that $R(T'') - r(T) > 0$. Finally, by the incremental lemma, we know that $R(T) \geq R(T'')$, so we find that $R(T) \geq r(T)$ as desired.

Now suppose that T' is an even path, so $r(T') > R(T')$. Suppose by way of contradiction that $r(T') \geq R(T'')$. Now, $R(T'')$ is not an integer unless T' is the tree on two vertices, so we assume that $r(T') > R(T'')$. The number-line below helps us visualize the relations:
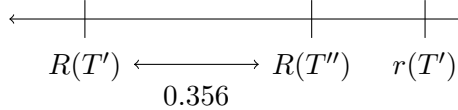
It's still the case that $R(T'') - R(T') = 0.356$, so it must be the case that $r(T') - R(T') > 0.356$. Though, from Lemma 12.8 that since T' is a tree that

$$R(T') - r(T') \geq -0.086$$
$$\implies r(T') - R(T') \leq 0.086$$

which gives us a contradiction. Therefore, it must be the case that $R(T'') > r(T')$

Case 2: Now suppose that T'' is the graph obtained by adding an edge to T' from $E(T) \backslash E(T')$ such that the edge is added to a vertex which is adjacent to two vertices both having degree of 2; observe the following picture:
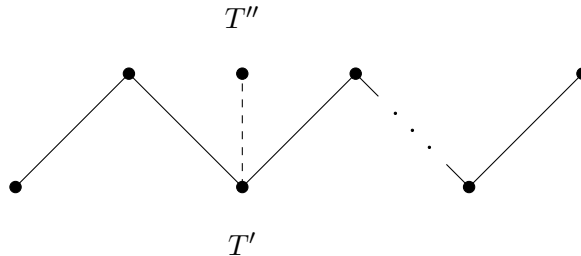
Now consider the following:

$$R(T'') - R(T') = \left[\frac{(n-1)-4}{\sqrt{2\cdot 2}} + \frac{2}{\sqrt{2\cdot 1}} + \frac{2}{\sqrt{2\cdot 3}} + \frac{1}{\sqrt{3\cdot 1}}\right] - \left[\frac{n-3}{2} + \sqrt{2}\right]$$
$$= \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - 1$$
$$\approx 0.394$$

In the case that T' is an odd path, then we get that $R(T'') > R(T') > r(T')$ instantly. In the case that T'' is an even path, we assume by way of contradiction that $r(T') > R(T'')$; the inequality is strict by similar reason as in Case 1.

$$R(T') \xleftrightarrow{\quad 0.394 \quad} R(T'') \quad r(T')$$
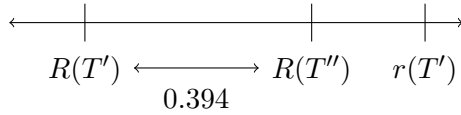
It must then be the case that $r(T') - R(T') > 0.394$. Again, from Lemma 12.8 that

$$R(T') - r(T') \geq -0.086$$
$$\implies r(T') - R(T') \leq 0.086$$

which gives us a contradiction. Therefore, it must be the case that $R(T'') > r(T')$.

Hence, in both Case 1 and in Case 2, we find that $R(T'') > r(T') = r(T)$. Then by Proposition 8.8, $R(T) \geq R(T'')$ so we may conclude that $R(T) \geq r(T)$ for all trees T which are not even paths. $\square$

It should be noted that trees are well behaved graphs whose radii are very predictable. When trying to approach Conjecture 12.3, it may be natural to consider whether or not a graph G contains a spanning tree T whose radius is the same as G but whose Randić index is smaller.

Example 12.10. Consider again the graphs G and T from Example 8.6. It is easy to verify the following:

$$R(G) < R(T) \qquad\qquad r(G) = r(T) \qquad\qquad D(G) < D(T)$$

Hence, it's possible to remove edges from arbitrary graphs which don't disconnect the graph and still increase some invariant. Further, notice that G' is a spanning subgraph of G with larger Randić index than G. That is, it's not true in general that if T is a spanning subtree of G that $R(G) \geq R(T)$.
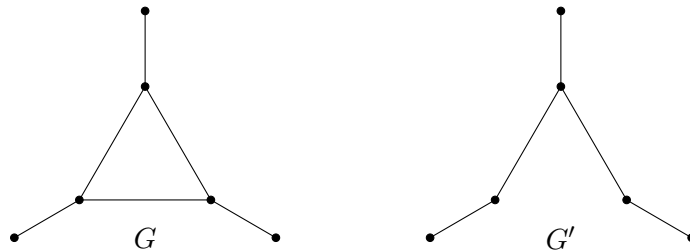
This is meant to briefly demonstrate that resolving Conjecture 12.3 becomes difficult when discussing arbitrary graphs.

From now on, we will assume that $G \ncong P_{2m}$ for $m \geq 1$. We will approach this conjecture by asking the following question: **Among all graphs with fixed radius, which graph has the smallest Randić index?** If we knew the answer to this question, we would be able to present a sharp lower bound for $R(G)/r(G)$. This will guide the direction for the remainder of this section. To begin, we will need the following family of trees.

Definition 12.11. Denote by $P_{n,m}$ the tree obtained by by identifying the center of S_{n+1} with a vertex of degree 1 of P_m, as shown in Figure 12.4. This tree is called a **comet**. We call $P_{m,n}$ a **proper comet** if $P_{n,m}$ is not isomorphic to a star or path.
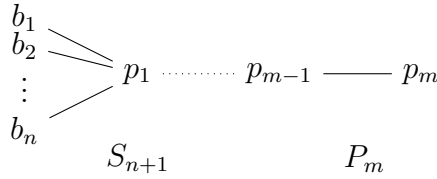
Figure 12.4. General comet graph $P_{n,m}$

It has already been shown in the literature that amongst all trees with fixed diameter D, the comet $P_{n-D,D}$ is the unique minimizer with respect to the Randić index. This is given by the following theorem from Zhoa and Li.

Theorem 12.12. [79] Let T be a tree of order n with diameter $D \geq 3$. Then we have that

$$R(T) \geq \frac{n-D}{n-D+1} + \frac{1}{\sqrt{2(n-D+1)}} + \frac{D-3}{2} + \frac{\sqrt{2}}{2},$$

where equality holds if and only if $T \cong P_{n-D,D}$.

Notice that Theorem 12.12 applies to graphs of diameters 1 and 2. It is easy to see that if T is a tree with diameter 1, then $G = P_2$ so the result follows immediately. If T is a tree of diameter 2, then T must be the star, since any other tree would contain a path of length at least 3 which again yields the desired result.

We will show that this theorem may be directly applied to our situation. To rephrase, if $D(T)$ is even, $D(T) = 2 \cdot r(T)$ and if $D(T)$ is odd, then $D(T) = 2 \cdot r(T) - 1$. It follows immediately that either

$$P_{n-2r+1,2r-1} \text{ or } P_{n-2r,2r}$$

will be the unique minimizer amongst all trees of $R(T)$. We will show in Lemma 12.15 that $P_{n-2r+1,2r-1}$ has the smaller Randić index. Before we present a proof, we need to consider two cases which relate the order of a graph to its radius. The relevant propositions to this first case are the following.

Proposition 12.13. *[36] Every connected graph G of radius $r(G)$ has an induced path of order $2r(G) - 1$.*

We will see that Lemma 12.15 examines tree graphs and depends on two main cases regarding graph order and it's relation to it's radius. That is, if T is a tree of order n and radius $r(T)$, we will consider the case where $n \geq 2r(T) + 1$ and when $n \geq 2r(T) + 2$; the latter case being relevant to Lemma 12.15. Note that it is a known fact that $n \geq 2r(T)$ for all graphs G. The lemma is a relatively simple result, though it was not found in the literature, so we'll state and prove it here.

Lemma 12.14. *Let G be a connected graph of order n and radius $r(G)$. Then $n = 2r(G)$ if and only if G is the even path or the even cycle.*

Proof. The proof of the converse is trivial. So, suppose by way of contradiction that $n = 2r(G)$ and that G is not equal to P_n nor C_n. Then by Proposition 12.13, there is an induced, order $n - 1 = 2(G) - 1$) path $P = \{p_1, \ldots, p_{n-1}\}$. Since n is even, P is an odd path with $D(P) = n - 2$. Further, G must have a vertex, say v, not contain in P; say that $vp_i \in E(G)$ for some $2 \leq i \leq n - 2$. Let T be the spanning tree of G obtained by removing all edges from G except for vp_i and all edges in the induced path P. It follows from Proposition 12.6 that since $G \neq P_n, C_n$, that $D(T) = n - 2$. Then $r(G) \leq r(T) = \frac{n-2}{2} = \frac{2r(G)-2}{2} = r(G) - 1$; a contradiction. This completes the proof. $\square$

As we proceed, we will assume that all graphs G of order n and radius $r(G)$ satisfy $n \geq 2r(G) + 1$. In this case, we yield some promising results.

We use our library of all finite graphs of order 8 and below to determine which graph minimizes the Randić index. Table 12.1 showed our findings.

$n \backslash r$	2	3	4
4	$P_{1,3}$	–	–
5	$P_{2,3}$	–	–
6	$P_{3,3}$	$P_{1,5}$	–
7	$P_{4,3}$	$P_{2,5}$	–
8	$P_{5,3}$	$P_{3,5}$	$P_{1,7}$

Table 12.1. Graphs of fixed radius with minimal Randić index

Lemma 12.15 makes a statement about proper comets, since it is possible to have n, m such that $P_{n,m} \cong S_\ell$ or $P_{n,m} \cong P_\ell$ for the appropriate ℓ. In the former case, we have a radius one graph which is already minimal with respect to Randić, by Theorems 8.2 and 8.3. In the latter case, we have the path P_m, whose radius is $\lfloor m/2 \rfloor$. Since we don't consider the even path, the radius of P_m is $\frac{m-1}{2}$.

Lemma 12.15. *Assume n and r are integers such $P_{n-2r+1,2r-1}$ is a proper comet and $P_{n-2r,2r}$ is a proper comet or the odd path. If n denotes the number of vertices and r denotes the radius of these graphs, then*

$$R(P_{n-2r,2r}) \geq R(P_{n-2r+1,2r-1})$$

when $P_{n-2r+1,2r-1} \not\cong P_m$ for some m.

Proof. It's easy to see that $P_{n-2r,2r}$ and $P_{n-2r+1,2r-1}$ are graphs of order n and radius r. Since $P_{n-2r,2r}$ has a path longest of length $2r = D(P_{n-2r,2r})$. Likewise, $P_{n-2r+1,2r-1}$ has a longest path of length $2r - 1 = D(P_{n-2r+1,2r-1})$ (see Figure 12.4). Now, observe the following;

$$
\begin{aligned}
R(P_{n-2r,2r}) &- R(P_{n-2r+1,2r-1}) \\
&= \left(\frac{n-2r}{\sqrt{n-2r+1}} + \frac{1}{\sqrt{2(n-2r+1)}} + \frac{2r-3}{2} + \frac{\sqrt{2}}{2} \right) \\
&\quad - \left(\frac{n-2r+1}{\sqrt{n-2r+2}} + \frac{1}{\sqrt{2(n-2r+2)}} + \frac{2r-4}{2} + \frac{\sqrt{2}}{2} \right) \quad (12.1)
\end{aligned}
$$

In the case that $n = 2r + 1$. Then

$$
\begin{aligned}
R(P_{n-2r,2r}) - R(P_{n-2r+1,2r-1}) &= R(P_{1,2r}) - R(P_{2,2r-1}) \\
&= 1 + \frac{1}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} \\
&\approx 0.144158 \\
&> 0
\end{aligned}
$$

which proves the lemma for this case. Now, assume that $n \geq 2r + 2$. We will proceed by

simplifying 12.1 and isolating terms which will be nonnegative. Observe,

$$R(P_{n-2r,2r}) - R(P_{n-2r+1,2r-1})$$

$$= (n-2r)\left(\frac{1}{\sqrt{n-2r+1}} - \frac{1}{\sqrt{n-2r+2}}\right)$$

$$+ \left(\frac{1}{\sqrt{2(n-2r+1)}} - \frac{1}{\sqrt{2(n-2r+2)}}\right)$$

$$+ r - \frac{3}{2} - r + 2 - \frac{1}{\sqrt{n-2r+2}}$$

$$= (n-2r)\underbrace{\left(\frac{1}{\sqrt{n-2r+1}} - \frac{1}{\sqrt{n-2r+2}}\right)}_{>0}$$

$$+ \underbrace{\left(\frac{1}{\sqrt{2(n-2r+1)}} - \frac{1}{\sqrt{2(n-2r+2)}}\right)}_{>0}$$

$$+ \frac{1}{2} - \frac{1}{\sqrt{n-2r+2}}.$$

Since $n \geq 2r+2$, it's easily shown with algebra that $\frac{1}{2} - \frac{1}{\sqrt{n-2r+2}} \geq 0$. This completes the proof. $\qquad\square$

Lemma 12.16. *Let T be a tree of order n with radius $r \geq 1$. Then we have that*

$$R(T) \geq \frac{n-2r+1}{\sqrt{n-2r+2}} + \frac{1}{\sqrt{2(n-2r+2)}} + \frac{2r-4}{2} + \frac{1}{\sqrt{2}},$$

where equality holds if and only if $T \cong P_{n-2r+1,2r-1}$.

Proof. The proof follows from Theorem 12.12 and Lemma 12.15. $\qquad\square$

Now, we presents new conjecture which generalizes to all connected graphs.

Conjecture 12.17. *Amongst all connected G graphs with order n and radius $r = r(G)$, $R(G) \geq R(P_{n-2r+1,2r-1})$.*

We believe there is strong evidence to support this conjecture. First, we've been able to test all graphs of order 8 or less by brute force. Though, we also known from Erdös that amongst all order n graphs, $R(G) \geq R(S_n) = \sqrt{n-1}$. While comets are not always stars, they are "star like." T

Now, we are able to consider the ratio $R(G)/r(G)$, but we will do so by supposed that $r(G)$ is fixed; i.e., we'll regard $r(G) = 1, 2, \cdots, \lfloor n/2 \rfloor$. So, if we can show that for all $G \neq P_{2m}$ that

$$\frac{R(G)}{r(G)} \geq 1,$$

then we will have a route towards proving Conjecture 12.3.

Corollary 12.18. *For all graphs G except the even path, $R(G) \geq r(G)$.*

Proof. Let $r = r(G)$. If Conjecture 12.17 is true, then $R(G) \geq R(P_{n-2r+1,2r-1})$ for all connected graphs G of order n and fixed radius r. Hence, if we consider all graphs G with fixed radius $r(G) = r \geq 1$, then

$$\frac{R(G)}{r} \geq \frac{R(P_{n-2r+1,2r-1})}{r}.$$

Thus, we desire to show that $\frac{R(P_{n-2r+1,2r-1})}{r} \geq 1$, so we'll show that

$$\frac{n-2r+1}{\sqrt{n-2r+2}} + \frac{1}{\sqrt{2(n-2r+2)}} + \frac{2r-4}{2} + \frac{1}{\sqrt{2}} \geq r$$

or equivalently,

$$f(n,r) := \frac{n-2r+1}{\sqrt{n-2r+2}} + \frac{1}{\sqrt{2(n-2r+2)}} + -2 + \frac{1}{\sqrt{2}} \geq 0.$$

Observe that

$$\frac{\partial}{\partial n}\left[f(n,r)\right] = \frac{6 - \sqrt{2} + 2n - 4r}{4(n-2r+2)^{3/2}}$$

Clearly, the numerator is nonnegative since $n \geq 2r$ in general. Further, it's easy to check that the two variable function $6 - \sqrt{2} + 2n - 4r$ has exactly one non-integral root, namely $n_0 = \frac{1}{2}(-6 + \sqrt{2} + 4r)$. Since

$$-6 + \sqrt{2} < 0$$
$$\implies -6 + \sqrt{2} + 4r < 4r$$
$$\implies n_0 = \frac{1}{2}(-6 + \sqrt{2} + 4r) < 2r$$

Now, if $n = 2r$, then $\frac{\partial}{\partial n}\left[f(n,r)\right]$ will be negative, but we are not considering this case since the only graph which has order equal to twice the radius is the even path. Hence, if $n > 2r$, then $\frac{\partial}{\partial n}\left[f(n,r)\right]$ is positive for all $r \geq 1$. So $f(n,r)$ is an increasing function on this interval. One can easily verify that $f(3,1) > 0$, and this completes the proof. $\square$

Chapter 13: Future Direction

The most immediate goal is to resolve Conjecture 12.17.

We discussed how there exists graphs G for which there is no spanning tree T of G whose Randić index is smaller. We believe that answering this question will aid us in resolving Conjecture 12.17.

Question. *For which connected, order n graphs G have no spanning tree T such that $R(G) > R(T)$?*

We aim to continue studying the Randić and other topological indices, in search of new extremal problems. As in Definition 8.1, the Randić index generalizes. Hence, we intend to explore the consequences of using parameters $\alpha \in [-1, 0) \cup (0, 1]$ other than $\alpha = -1/2$.

Question. *If we consider $R_\alpha(G)$ where $\alpha \in [-1, 0)$, which of our results still hold?*

We also intend to explore indices such as the Harary and the Wiener index.

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Chapter A: Appendix: Algorithms

In this appendix, we give two important algorithms on NC_G, Algorithms A.1 and A.6. We also give a forbidden subgraph characterization of upper crossing closed graphs in Theorem A.4.

Algorithm A.1 decides if NC_G is a lattice in time on the order of n^7 where n the number of vertices of the graph G. This is proved in Theorem A.2. Note that a brute-force algorithm to test if NC_G is a lattice can take time super-exponential in n. For example, an algorithm that checks if every pair of elements in NC_G has a meet and a join, could take time at least on the order of the number of elements of NC_G. For an n vertex graph, that may be as large as the Bell number B_n of the number of set partitions of $[n]$ and $B_n > (n/e \log(n))^n$ [6]. Note that we call Algorithm A.1 the "crossing-closed" algorithm as it is actually checking if G is crossing closed. Of course, NC_G being a lattice is equivalent to G being crossing closed, see Theorem 3.11.

Algorithm A.6 determines if a graph G is an upper crossing closed graph. Recall that if G is upper crossing closed then the Möbius function and characteristic polynomial of NC_G have nice interpretations in terms of noncrossing NBC sets, see Theorem 3.28. When given a graph G, Algorithm A.6 will either produce a specific upper crossing closed ordering of $E(G)$ or will produce what we term an obstruction (see Definition A.3), a specific subgraph of G that clearly shows there can be no such ordering. This also gives a forbidden subgraph characterization of upper crossing closed graphs, Theorem A.4.

In Theorem A.7, we prove that the Algorithm A.6 will run in time on the order of n^8 where again n is the number of vertices of G. Note that a brute force algorithm could again take time super-exponential in n, if it is forced to test some positive fraction of the $\binom{n}{2}!$ possible orderings on the edges of G.

We first present our algorithm that decides if G is crossing closed, i.e. if NC_G is a lattice.

Algorithm A.1. Crossing Closed Algorithm
Input: *A graph G on $[n]$.*
Output: *A yes/no decision as to whether G is crossing closed, or, equivalently, whether NC_G is a lattice.*
Method: *For each pair of crossing edges e and f find a shortest path $P(e, f) = x_0 x_1 \ldots x_k$ with $e = x_0 x_1$ and $f = x_{k-1} x_k$ and $k \geq 3$. If for some crossing pair e and f, $P(e, f)$ fails to exist or has $k \geq 4$ and has some vertex x_i with $2 \leq i \leq k - 2$ such that x_i does not separate e and f then return "No, G is not crossing closed." Otherwise return "Yes, G is crossing closed."*

Theorem A.2. *Algorithm A.1 is a correct algorithm that runs in time $O(n^7)$ where n is the number of vertices of G.*

Proof. First, we will compute the complexity of the algorithm. The Floyd-Warshall algorithm gives a shortest path between all pairs of vertices in $O(n^3)$ time [25]. With that pre-processing done, there are at most $\binom{n}{4}$ pairs of crossing edges to check. For each pair e and f of crossing edges, there are at most n vertices on the shortest path connecting them to check. Checking that one of those vertices separates e and f can be done by breadth-first search in $O(n^2)$ time so this algorithm will run in $O(n^7)$ time.

Next, we show that the algorithm always gives the correct output. Suppose G is crossing closed. We will show that the algorithm will return a "yes". For every pair of crossing edges e and f, $J(e, f)$ exists. If there is an edge incident to e and f (where incident means having a common vertex), then $P(e, f)$ will be a path (e, g, f) for some edge g connecting e and f and the algorithm will not give a "no" answer based on this pair. If there is no edge incident to both e and f, then by Lemma 3.9, $J(e, f)$ will be a dumbbell graph, see Figure 3.5, a graph induced by e, f and a path Q with one end adjacent to e and the other end adjacent to f with all vertices in Q separating e and f. Thus the vertices $\{x_2, \ldots, x_{k-2}\}$ on $P(e, f)$ must be the vertices of Q. The algorithm will not give a "no" answer based on this pair either. Thus the algorithm will return a "yes".

Suppose now that the algorithm returns a "yes". We will show that G is crossing closed. Let e and f be a pair of crossing edges. Since the algorithm returned a "yes", a shortest path $P(e, f)$ must exist. If the path has 3 vertices, i.e. there is an edge connecting e and f, then $J(e, f) = G[e \cup f]$ exists. Suppose now that the path contains at least 4 vertices. Let M be the subgraph of G induced on the vertices of $P(e, f)$. We claim that M is contained in every connected, induced subgraph of G that contains e and f and so $J(e, f) = M$. Let x be any vertex in $P(e, f)$ that is not in e or f and let H be an connected induced subgraph of G containing e and f. If x is not in H then it cannot separate e and f. Since the algorithm returned "yes", x must separate e and f and so x must be in H. Thus every vertex of M is in H and since they are both induced, M is in H. $\square$

Now we turn our attention to the problem of deciding whether a graph is upper crossing closed. First, let us note that not all crossing closed graphs are upper crossing closed. As an example, consider the 5-pointed star, drawn again below. It is not hard to verify that if e and f cross in the 5-pointed star, $J(e, f)$ is a subgraph of K_4 and so is crossing closed. However, every edge of the graph is crossed and so it is impossible to have an ordering that is upper crossing closed as the smallest edge must be noncrossing. As it turns out, this kind of issue is the only obstacle to a crossing closed graph being upper crossing closed.
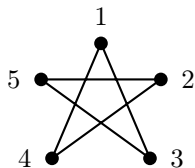
G : The five pointed star

Definition A.3. Let G be a crossing closed graph. We say a subgraph H of G is an *obstruction* to G being upper crossing closed if for every edge e in H there is an edge f in H which crosses e such that $J(e, f) \subseteq H$.

Theorem A.7 proves that Algorithm A.6 below will, when given a graph G, either produce an upper crossing closed ordering on $E(G)$ or an obstruction. It also proves that an obstruction demonstrates no such ordering is possible. Thus we get the following structural characterization of upper crossing closed graphs.

Theorem A.4. *A graph G is upper crossing closed if and only if it contains no obstruction as a subgraph.*

Note also that if every edge e in G crosses some other edge of G, then G itself is an obstruction of G. Thus we also have the following.

Corollary A.5. *If G is a graph with every edge crossing some other edge, then G is not upper crossing closed.*

Note that Corollary A.5 shows that the graph G of Figure 3.14 and the 5-pointed star of Figure 5.1 are not upper crossing closed.

Algorithm A.6. Upper Crossing Closed Algorithm
Input: *A graph G on $[n]$.*
Output: *A yes/no decision on whether G is crossing closed. Then if G is crossing closed, a yes/no decision on whether G is upper crossing closed. If G is upper crossing closed, an upper crossing closed ordering is produced, and if G is crossing closed but not upper crossing closed, an obstruction is produced.*
Method:

1. *Run the crossing closed algorithm on G, Algorithm A.1. If the answer is no, return "No. G is not crossing closed and hence not upper crossing closed." and terminate. If the answer is yes, return "Yes. G is crossing closed." and continue.*

2. *Let $L = \emptyset$ and let $\sigma = \emptyset$. (Throughout the algorithm, L will be a subset of $E(G)$ and σ will be an ordering on L.)*

3. *Let L' be the set of edges e in $E(G) \setminus L$ such that for every edge $f \in E(G) \setminus L$ that crosses e, $E(J(e, f)) \cap L \neq \emptyset$.*

4. If $L' \neq \emptyset$ update L to be $L \cup L'$ and update σ to be the ordering on $L \cup L'$ that orders L according to σ and then puts all the edges of L' after the edges of L. The ordering within L' can be arbitrary. Go back to step 3.

5. If $L' = \emptyset$, decide on the output of the algorithm. If $L = E(G)$, return "Yes, G is upper crossing closed, and σ is an upper crossing closed ordering on $E(G)$." If $L \neq E(G)$, return "No. G is not upper crossing closed, and the spanning subgraph of G with edge set $E(G) \setminus L$ is an obstruction."

We will now show how the algorithm runs on two graphs, one upper crossing closed and the other not. First, let G be the twisted 4-cycle in Figure 3.11. As we have already seen, G is crossing closed and upper crossing closed with respect to the lexicographic order on its edges. The algorithm will thus correctly conclude that G is crossing closed in step 1 and will set $L = \emptyset$ and $\sigma = \emptyset$ in step 2. Next, it will go to step 3. Since L is empty, L' is the set of edges which cross no other edges. So $L' = \{12, 34\}$. Then the algorithm passes to step 4 where L is set to be $\{12, 34\}$ and σ is set to be some total ordering of $\{12, 34\}$. Now we return to step 3. Now, $E(G) \setminus L = \{13, 24\}$. Since 13 and 24 form the only crossing in G and $J(13, 24) = G$ intersects L, the algorithm sets $L' = \{13, 24\}$. Next, we go to step 4, where L is set to be $\{12, 34, 13, 24\}$ and σ is some total ordering where the first two elements are 12 and 34 and the last two elements are 13 and 24. Then we return to step 3, where L' is set to be empty. Finally, we go to step 5 and since $L = E(G)$, the algorithm returns that G is upper crossing closed with respect to the ordering σ, which indeed it is. The reader may have noticed that the ordering the algorithm produces is not the lexicographic ordering. This is because the algorithm always puts edges with no crossing before any edge with a crossing. Thus the algorithm is not always capable of producing all possible upper crossing closed orderings.

Now we give an example of how the algorithm runs on a graph G that is not upper crossing closed. Let G be the 5-pointed star in Figure 5.1. Since G is crossing closed, the algorithm will pass to step 2 and set $L = \emptyset$ and $\sigma = \emptyset$. Then it moves to step 3. Since all the edges in G cross some other edge and L is empty, L' is empty too. As a result, the algorithm moves to step 5. Since $L \neq E(G)$, the algorithm returns that G is not upper crossing closed and correctly provides G as an obstruction. We should note that for any graph in which every edge crosses another edge, the algorithm will terminate with $L' = L = \emptyset$ and thus will correctly conclude that the spanning subgraph with edge set $E(G) \setminus L = E(G)$, i.e. G itself, is an obstruction.

We now prove that Algorithm A.6 is correct and runs in polynomial time.

Theorem A.7. *Let G be a graph. Then we have the following.*

(a) *Algorithm A.6 runs in time $O(n^8)$ where n is the number of vertices of G.*

(b) *If Algorithm A.6 concludes by giving a purported obstruction H, then H is indeed an obstruction.*

(c) *If Algorithm A.6 produces an obstruction, then G is not upper crossing closed.*

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(d) If Algorithm A.6 does not produce an obstruction, then G is upper crossing closed and the order σ it produces is an upper crossing closed ordering.

(e) Algorithm A.6 is correct.

Proof. First, we show (a). The crossing closed algorithm runs in $O(n^7)$ time as a subroutine in step 1. During the course of that run, shortest paths $P(e, f)$ connecting all pairs of crossing edges e and f are created. By the proof of Theorem A.2, these paths determine $J(e, f)$ for each such pair of edges. When running step 3, there are at most n^2 edges $e \in E(G) \setminus L$ to check and then for each such e there are at most n^2 edges f that cross e to check. Since the $J(e, f)$ are already calculated it takes n^2 comparisons to calculate $J(e, f) \cap L$, so step 3 takes $O(n^6)$ time each time it is run. It is run at most n^2 times so the algorithm takes $O(n^8)$ time.

Now we verify (b). If the algorithm terminates with $L' = \emptyset$ and $L \neq E(G)$, then the output of the algorithm is the spanning subgraph H with edge set $E(G) \setminus L$. Since $L' = \emptyset$, every edge $e \in E(G) \setminus L$ must cross another edge $f \in E(G) \setminus L$ such that $E(J(e, f)) \subseteq E(G) \setminus L$. Thus H is indeed an obstruction. Now we verify (c). Let H be an obstruction. Then for every ordering $\trianglelefteq$ of $E(G)$, the first edge e of H will cross some other edge f of H with $J(e, f) \subseteq H$. But since $J(e, f) \subseteq H$ and e is the minimum edge of H, no edge $g \in J(e, f)$ will satisfy $g \triangleleft e, f$. It follows that G is not upper crossing closed with respect to any ordering.

Next, we prove (d). Suppose no obstruction is found. We claim that the ordering σ on $E(G)$ that is produced is an upper crossing closed ordering. Let e and f be a pair of crossing edges in G. Consider the first point in time during the run of the algorithm in which $e, f \notin L$ and e or f or both are in L'. Say $e \in L'$. Then $J(e, f) \cap L \neq \emptyset$ otherwise e would not be in L'. So there will be an edge $g \in J(e, f) \cap L$. In the ordering σ, all the edges in L are less than all the edges not in L so g will be less than e and f. This shows that G is upper crossing closed with respect to σ.

Finally, let us show (e). Suppose that G is not upper crossing closed. Then the algorithm must find an obstruction. If it did not, by part (d), σ would be an upper crossing closed ordering. By part (b), what the algorithm produces is really an obstruction and by part (c) this obstruction demonstrates that G is not upper crossing closed. Thus the algorithm will return an obstruction and correctly returns that G is not upper crossing closed.

Now suppose that G is upper crossing closed. Then by the contrapositive of part (c) and by part (b) the algorithm produces no purported obstruction. So then by part (d), it returns an upper crossing closed ordering. It will then correctly return that the graph is upper crossing closed. $\qquad\square$

Chapter B: Appendix: Mathematica Package

Below are functions that we defined and used for computing topological indices and generating large libraries of connected graphs.

Code Snippet 1.

```
(* Indices *)
Randic[G_, a_] :=
    (1/2) {Map[(#)^a &,
        VertexDegree[Graph[G[[1]], G[[2]]]]]} . (AdjacencyMatrix[
        Graph[G[[1]], G[[2]]]] // Normal) .
      Transpose[{Map[(#)^a &,
        VertexDegree[Graph[G[[1]], G[[2]]]]]}])[[1]][[1]]
(* Matrices *)
DegreeMatrix[G_] :=
    Map[#*VertexDegree[Graph[G[[1]], G[[2]]]] &,
    IdentityMatrix[Length[G[[1]]]]]
LaplacianMatrix[G_]
    := DegreeMatrix[G] - AdjacencyMatrix[Graph[G[[1]], G[[2]]]]
SignlessLaplacianMatrix[G_]
    := DegreeMatrix[G] + AdjacencyMatrix[Graph[G[[1]], G[[2]]]] // Normal
RandicMatrix[G_, a_] :=
    Table[
        Table[
            If[MemberQ[G[[2]], {IndexI, IndexJ}] ||
            MemberQ[G[[2]], {IndexJ, IndexI}] == True,
                (VertexDegree[Graph[G[[1]], G[[2]]]][[IndexI]]*
                VertexDegree[Graph[G[[1]], G[[2]]]][[IndexJ]])^a, 0],
                {IndexJ, 1, Length[G[[1]]]}
            ],
        {IndexI, 1, Length[G[[1]]]}
        ]
(* Radii *)
```

```
SpectralRadius[g_] :=
    Max[Eigenvalues[AdjacencyMatrix[Graph[g[[1]], g[[2]]]]]]
LaplacianSpectralRadius[g_] :=
    Max[Eigenvalues[LaplacianMatrix[g]]]
SignlessLaplacianSpectralRadius[g_] :=
    Max[Eigenvalues[SignlessLaplacianMatrix[g]]]
```

To generate all graphs, we used an old Mathematica package called Combinatorica. This package is no longer in use, though we were able to call it and utilize its functions to build all connected graphs. Our code, in concert with the Combinatorica function `ListGraphs[n,m]` (returns all graphs of order n with m edges) is as follows:

Code Snippet 2.

```
(* Generate All Connected Graphs of Orders 4 to 8 *)
<< Utilities`CleanSlate`
<< Combinatorica`
CleanSlate["Combinatorica`"]
AdjMat[x_] :=
    Block[{e, n, m},
    e = Flatten[x[[1]], 1];
    n = Length[x[[2]]];
    m = Table[
            Table[
                If[MemberQ[e, {Min[i, j], Max[i, j]}], 1, 0], {i, 1, n}
                ],
            {j, 1, n}
            ];
    Return[m]]
ConnQ[x_] :=
    ConnectedGraphQ[AdjacencyGraph[AdjMat[x]]]
ConnGraphs[n_, m_] :=
    Select[ListGraphs[n, m], ConnQ[#] &]
```

The raw output of `ListGraphs[n,m]` provides Cartesian coordinates for vertices and the edges of the graph in the form `{i,j}`. For example, the following code gives all trees of order 4:

Code Snippet 3.

```
In[1] := ListGraphs[4, 3]
Out[1] := {
    Combinatorica`Graph[{
        {{1, 2}}, {{1, 3}}, {{1, 4}}},
        {{{0, 1.}}, {{-1., 0}}, {{0, -1.}}, {{1., 0}}}],
```

```
Combinatorica'Graph[{
    {{2, 3}}, {{2, 4}}, {{3, 4}}},
    {{{0, 1.}}, {{-1., 0}}, {{0, -1.}}, {{1., 0}}}],
Combinatorica'Graph[{
    {{1, 4}}, {{2, 3}}, {{3, 4}}},
    {{{0, 1.}}, {{-1., 0}}, {{0, -1.}}, {{1., 0}}}]}
```

This raw output was not compatible with our functions and procedures. Hence, we defined a special adjacency matrix function designed for this output. With this, we were able to convert the raw Combinatorica output into the same format we used to define our chemical graphs by hand. The following code helped us achieve our goal. Note that `Out[%]` allows the user to call the most recent Mathematica output.

Code Snippet 4.

```
A = Map[AdjMat[#] &, Out[%%]];
Table[
    {VertexList[AdjacencyGraph[A[[i]]]],
    EdgeList[AdjacencyGraph[A[[i]]]]}, {i, 1, Length[Out[%%]]}]
```

By letting the procedure from Code Snippet 4 act on the output from Code Snippet 3, we obtain the following:

Code Snippet 5.

```
{{{1, 2, 3, 4}, {1 - 2, 1 - 3, 1 - 4}},
 {{1, 2, 3, 4}, {2 - 3, 2 - 4, 3 - 4}},
 {{1, 2, 3, 4}, {1 - 4, 2 - 3, 3 - 4}}}
```

We ran the procedure

```
Apply[Join, Table[ConnGraphs[n, i], {i, n-1, Binomial[n, 2]}]]
```

for $4 \leq n \leq 8$, capturing all connected graphs of order n with $n - 1 \leq m \leq \binom{n}{2}$ edges. An order n graph with $n - 1$ edges is a tree, and an order n graph with $\binom{n}{2}$ edges is K_n. Figure B.1 displays a preview of the large output from generating all connected graphs of order 8.[1] We did not posses the computing power nor time to generate all connected graphs of order 9. Though, we had sufficient data to formulate the conjectures and results of this thesis.

---

[1]This process took approximately 100 hours to finish.

```
In[•]:= Apply[Join, Table[ConnGraphs[8, i], {i, 7, Binomial[8, 2]}]]
```

```
Out[•]= {- Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-,
         - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-,
         - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-,
         - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-,
         - Graph:< 7,8,Undirected >-, - Graph:< 7,8,Undirected >-, - Graph:< 8,8,Undirected >-,
         - Graph:< 8,8,Undirected >-, - Graph:< 8,8,Undirected >-, ⋯ 11065 ⋯ , - Graph:< 23,8,Undirected >-, - Graph:< 23,8,Undirected >-,
         - Graph:< 23,8,Undirected >-, - Graph:< 23,8,Undirected >-, - Graph:< 23,8,Undirected >-, - Graph:< 23,8,Undirected >-,
         - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-,
         - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-,
         - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-, - Graph:< 24,8,Undirected >-, - Graph:< 25,8,Undirected >-,
         - Graph:< 25,8,Undirected >-, - Graph:< 25,8,Undirected >-, - Graph:< 25,8,Undirected >-, - Graph:< 25,8,Undirected >-,
         - Graph:< 26,8,Undirected >-, - Graph:< 26,8,Undirected >-, - Graph:< 27,8,Undirected >-, - Graph:< 28,8,Undirected >-}
```

large output   show less   show more   show all   set size limit...

```
In[•]:= A = Map[AdjMat[#] &,
         Out[13]];
       Table[{VertexList[AdjacencyGraph[A[[i]]]],
         EdgeList[AdjacencyGraph[A[[i]]]]}, {i, 1, 11117}]
```

```
In[•]:= {{{1, 2, 3, 4, 5, 6, 7, 8}, {1↔2, 1↔3, 1↔4, 1↔5, 1↔6, 1↔7, 1↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔8, 5↔8, 6↔7, 7↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔8, 5↔7, 6↔7, 7↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔8, 5↔7, 6↔7, 6↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔7, 5↔7, 6↔7, 7↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔7, 5↔7, 6↔7, 6↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔7, 5↔6, 6↔8, 7↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔7, 5↔6, 6↔7, 7↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔8, 4↔7, 5↔6, 5↔8, 6↔7}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔7, 4↔7, 5↔6, 5↔8, 6↔7}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔7, 4↔7, 5↔6, 6↔7, 6↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔7, 4↔7, 4↔8, 5↔6, 6↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔7, 4↔7, 4↔7, 4↔8, 5↔6, 6↔7}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔7, 4↔6, 5↔6, 5↔7, 5↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔8, 3↔7, 4↔6, 4↔8, 5↔6, 5↔7}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔7, 3↔7, 3↔8, 4↔6, 5↔6, 5↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔7, 3↔6, 4↔5, 5↔8, 6↔8, 7↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔7, 3↔6, 4↔5, 5↔8, 6↔7, 7↔8}},
        {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔7, 3↔6, 4↔5, 4↔8, 5↔7, 6↔8}}, {{1, 2, 3, 4, 5, 6, 7, 8}, {1↔8, 2↔7, 3↔6, 4↔5, 4↔8, 5↔6, 5↔7}},
```

Figure B.1. Mathematica screenshot of the output for all graphs of order 8

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