AN INVESTIGATION ON GRAPH POLYNOMIALS

by

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Table of Contents

List of Tables

List of Figures

Abstract

The chromatic polynomial of a graph G, denoted $\pi(G, x)$, is the polynomial whose evaluations at positive integers x count the number of (proper) x-colourings of G. This polynomial was introduced by Birkhoff in 1912 in an attempt to prove the famous Four Colour Theorem which stood as an unsolved problem for over a century. Since then, the chromatic polynomial has been extensively studied and it has become an important object in enumerative graph theory.

In this thesis, we study the chromatic polynomial and two other related polynomials, namely, the σ-polynomial and the restrained chromatic polynomial. In Chapter 2, we begin with the σ-polynomial. We investigate two central problems on the topic, namely, log-concavity and realness of the σ-roots. In Chapter 3, we focus on bounding the chromatic polynomial and its roots. Chapter 4 is devoted to the restrained chromatic polynomial which generalizes the chromatic polynomial via the restrained colourings. We focus on the problem of determining restraints which permit the largest or smallest number of x-colourings.

List of Abbreviations and Symbols Used

Notation	Description
$V(G)$	The vertex set of a graph G.
$E(G)$	The edge set of a graph G.
$N_G(u)$	The neighbourhood of a vertex u in G.
$N_G[u]$	The closed neighbourhood of a vertex u in G.
$\langle S \rangle_G$	The subgraph induced by S in G.
$\delta(G)$	The minimum degree of a graph G.
$\Delta(G)$	The maximum degree of a graph G.
$\chi(G)$	The chromatic number of a graph G.
$\omega(G)$	The clique number of a graph G.
$\overline{G}$	The complement of a graph G.
$\alpha_o(G)$	The vertex cover number of a graph G.
$\mathcal{G}(H)$	The set of all subgraphs of G which are isomorphic to H.
$\eta_G(H)$	The number of subgraphs of G which are isomorphic to H.
$i_G(H)$	The number of induced subgraphs of G which are isomorphic to H.
$G \odot e$	G weak contraction e.
$G \cdot e$	G contraction e.
$G \vee H$	The join of G and H.
$G \mathbin{\dot\cup} H$	The disjoint union of G and H.
C_n	Cycle graph on n vertices.
K_n	Complete graph on n vertices.
P_n	Path graph on n vertices.
$\Re(z)$	The real part of z.

Notation	**Description**
$\Im(z)$	The imaginary part of z.
$h(G,x)$	The adjoint polynomial of a graph G.
$\sigma(G,x)$	The σ-polynomial of a graph G.
$\pi(G,x)$	The chromatic polynomial of a graph G.
$\pi_r(G,x)$	The restrained chromatic polynomial of a graph G with respect to restraint r.
$\mathbb{C}$	The set of complex numbers.
$\mathbb{R}$	The set of real numbers.
$\mathbb{Q}$	The set of rational numbers.
$\mathbb{Z}$	The set of integers.
$\mathbb{N}$	The set of natural numbers.
$S(n,k)$	The Stirling number of the second kind.
$\mathcal{G}_k(n)$	The family of k-chromatic graphs of order n.
$\mathcal{C}_k(n)$	The family of connected k-chromatic graphs of order n.

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Chapter 1

Introduction

1.1 Background Material

For graph theory terminology, we follow [65] in general. Throughout this thesis, all graphs are finite, simple and undirected.

Given two sets A and B, the union of A and B is denoted by $A \cup B$, their disjoint union is denoted by $A \uplus B$ and their intersection is denoted by $A \cap B$. Let G and H be two graphs. The *union* (respectively *intersection*) of G and H, denoted by $G \cup H$ (respectively $G \cap H$), is the graph whose vertex set is $V(G) \cup V(H)$ (respectively $V(G) \cap V(H)$) and edge set is $E(G) \cup E(H)$ (respectively $E(G) \cap E(H)$). The *disjoint union* of G and H, denoted by $G \uplus H$, is the graph formed by taking the union of vertex disjoint copies of G and H. For positive integer l, the graph lG stands for the disjoint union of l copies of G. Given two distinct vertices u and v of a graph G, the edge containing these two vertices is denoted by uv.

The *join* of vertex disjoint graphs G and H, denoted by $G \vee H$, is the graph whose vertex set is $V(G) \cup V(H)$ and edge set is $E(G) \cup E(H) \cup \{uv|\ u \in V(G) \text{ and } v \in V(H)\}$.

A subset of vertices $S \subseteq V(G)$ is called an *independent set* if $uv \notin E(G)$ for every $u, v \in S$. *The neighbourhood of a vertex u in G*, denoted $N_G(u)$, consists of vertices of G which are adjacent to u. Also, *the closed neighborhood of u in G*, denoted $N_G[u]$, is equal to $N_G(u) \cup \{u\}$.

Given two vertices u and v of a graph G, the *contraction of u* and v in G, denoted $G \cdot uv$, is defined as the graph with vertex set $V(G \cdot uv) = (V(G) \setminus \{u, v\}) \cup \{w\}$

where $w \notin V(G)$ and edge set $E(G \cdot uv) = \{ab \in E(G) \,|\, a, b \notin \{u, v\}\} \cup \{wa \,|\, a \in (N_G(u) \cup N_G(v)) \setminus \{u, v\}\}$. We refer to the vertex w as the vertex obtained by contracting vertices u and v. Also, the *weak contraction of* u and v, denoted by $G \odot e$, is defined as the graph obtained from G by first removing both of the vertices u and v and then introducing a new vertex w and joining this new vertex to only those vertices which are in $N_G(u) \cap N_G(v)$. In Figure 1.1, contraction and weak contraction are illustrated.

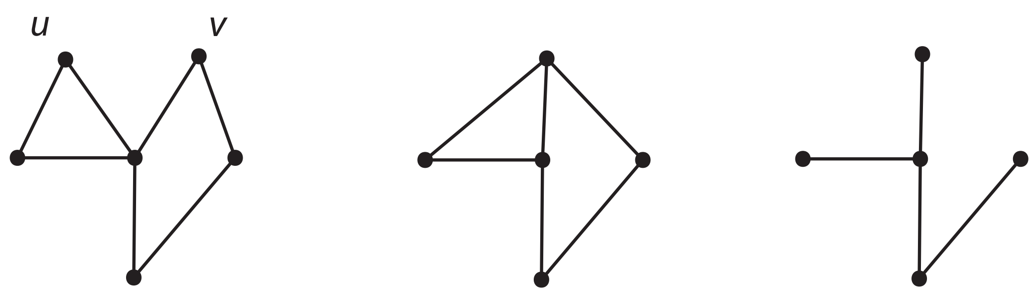

Figure 1.1: From left to right: G, $G \cdot uv$, $G \odot uv$

For an edge $e = uv$ of a graph G, the graph $G - e$ denotes the subgraph of G obtained by deleting the edge e, and $G - \{u, v\}$ denotes the subgraph induced by the vertex set $V(G) - \{u, v\}$. Also, for two non adjacent vertices u and v of G, let $G + uv$ denote the graph obtained from G by adding a new edge uv.

A graph is called *chordal* if it does not contain a cycle of order 4 or more as an induced subgraph. The *comparability graph* of a partially ordered set $(V, \preceq)$ has vertex set V and has an edge uv whenever $u \preceq v$ or $v \preceq u$; a graph is called a *comparability graph* if it is the comparability graph of some partial order.

Given two graphs G and H, we say that G is *H-free* if G does not contain any induced subgraph which is isomorphic to H.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$ (the *order* and *size* of the graph are, respectively, $|V(G)|$ and $|E(G))$. A (proper vertex) *k-colouring* of a graph G is a function $f : V(G) \to \{1, 2, \ldots, k\}$ such that for every edge $e = uv$ of G, $f(u) \neq f(v)$. The *chromatic number* $\chi(G)$ is smallest x for which G has an x-colouring. We say that G is *k-chromatic* if $\chi(G) = k$. The well known *chromatic polynomial* $\pi(G, x)$ of G counts the number of proper colourings of the vertices with x colours, for each $x \in \mathbb{N}$. The fact that $\pi(G, x)$ is a polynomial in x follows from the well-known *edge addition (deletion) - contraction formula*:

Theorem 1.1.1 (Edge addition (deletion) – contraction formula [24]). *Let u and v be two nonadjacent vertices of G. Then*

$$\pi(G, x) = \pi(G + uv, x) + \pi(G \cdot uv, x) \quad \text{if } uv \notin E(G);$$

$$\pi(G, x) = \pi(G - uv, x) - \pi(G \cdot uv, x) \quad \text{if } uv \in E(G).$$

Let $(x)_{\downarrow r} = x(x-1)\ldots(x-r+1)$ be the rth *falling factorial* of x.

Theorem 1.1.2 (Complete Cutset Theorem [24]). *Let G_1 and G_2 be two graphs such that $G_1 \cap G_2 \cong K_r$, then*

$$\pi(G_1 \cup G_2, x) = \frac{\pi(G_1, x)\,\pi(G_2, x)}{(x)_{\downarrow r}}.$$

A graph with only one vertex is called *trivial*. Also, a graph G is *k-connected* if the removal of fewer than k-vertices always leaves a nontrivial connected graph.

Corollary 1.1.3. *[24] If G is a connected graph consisting of blocks $B_1, \ldots, B_t$ then*

$$\pi(G, x) = \frac{1}{x^{t-1}} \prod_{i=1}^{t} \pi(B_i, x).$$

If G consists of the blocks $B_1, \ldots, B_t$ then it is easy to see that

$$\chi(G) = \max\{\chi(B_1), \ldots, \chi(B_t)\}.$$

Also, for $e \notin E(G)$, it is easy to see that

$$\chi(G) = \min\{\chi(G+e)\,,\,\chi(G\cdot e)\}.$$

Let G be a graph of order n. An *i-colour partition* of G is a partition of the vertices of G into i nonempty independent sets. Let $a_i(G)$ denote the number of i-colour partitions of G. The *σ-polynomial* of G (see [4]) is defined as the polynomial

$$\sigma(G,x) = \sum_{i=\chi(G)}^{n} a_i(G)\,x^i.$$

It is easy to see that

$$\pi(G,x) = \sum_{i=\chi(G)}^{n} a_i(G)\,(x)_{\downarrow i}.$$

We refer the reader to [24] for a general discussion of graph colourings and chromatic polynomials.

1.2 An Overview of the Thesis

We investigate the chromatic polynomial and two other related graph polynomials, namely, the σ-polynomial and the restrained chromatic polynomial.

In Chapter 2, we begin with the σ-polynomial. This polynomial arises naturally from a certain expansion of the chromatic polynomial and it has strong connections to several other important polynomials in combinatorics (such as the matching polynomial). The behaviour of the σ-polynomial and its roots is quite different from that of the chromatic polynomial. The roots of the σ-polynomial seem to have a more regular behaviour, as they are more often on the real line. In fact, currently, only finitely many nonreal σ-roots are known. Therefore, one of the main problems in the field has been to have a better understanding of the realness of the σ-roots. Another important problem in the field has been the log-concavity of the σ-polynomial (Read and Tutte [48] conjectured that the σ-polynomial of any graph is strongly log-concave). We investigate these two central problems on the topic, namely, log-concavity and realness of the σ-roots. In particular, we show that graphs of order n with chromatic number at least $n-3$ have all real σ-roots (Theorem 2.3.7), and this proves a conjecture of Brenti [4] from 1992. We also obtain some partial results to these problems in the family of graphs of order n with chromatic number at least $n-4$ (Theorem 2.4.10). Furthermore, we prove the denseness of the real σ-roots in the left real line (Theorem 2.5.3).

In Chapter 3, we study the chromatic polynomial. In the first section of this chapter, we consider two old problems of Tomescu [55, 57, 59] regarding bounding the number of x-colourings of a graph over the family of (connected) graphs of fixed chromatic number and order. We present an improved bound for the number of x-colourings of a graph over the family of graphs of fixed chromatic number and order by using the maximum degree of the graph (Theorem 3.1.5). Then we consider the problem when the connectedness condition is imposed, and all the rest of the results in this section are towards the latter problem. In the second section of Chapter 3, we focus on bounding chromatic roots. We present a new bound on the moduli of the chromatic roots (Theorem 3.2.2) which improves earlier bounds for dense graphs. Also, we study two conjectures proposed by Dong et al. [24] on bounding the real parts of complex chromatic roots. We present counterexamples to one of these conjectures (Theorem 3.2.9) and prove the other one for some graph families which intuitively should include most of the likely candidates to be counterexamples (Theorem 3.2.15 and Theorem 3.2.16).

Chapter 4 is devoted to the restrained chromatic polynomial which generalizes the chromatic polynomial via the restrained colourings, that is colourings where each vertex has a list of forbidden colours attached. We focus on the problem of determining restraints which permit the largest or smallest number of x-colourings. We completely settle the minimization part of this problem for all graphs (Theorem 4.2.4) by showing that constant restraints permit the smallest number of colourings. Also, we give two necessary conditions for a restraint on a general graph to permit the largest number of x-colourings (Theorem 4.2.8). We show that these necessary conditions become sufficient to determine such extremal restraints for complete graphs (Theorem 4.2.6) and bipartite graphs (Theorem 4.2.9). Lastly, we give another necessary condition for a restraint on a (C_3, C_4)-free graph to permit the largest number of x-colourings (Theorem 4.2.12).

Section 2.3 was published in [10]. Also, majority of Sections 3.1 and 3.2 was published in [9] and [8].

Chapter 2

σ-Polynomials

Let G be a graph of order n with chromatic number $\chi(G)$. Recall that the σ-polynomial of G is the polynomial

$$\sigma(G,x) = \sum_{i=\chi(G)}^{n} a_i(G)\, x^i$$

where $a_i(G)$ is the number of i-colour partitions of G.

The coefficients a_i are also known as the *graphical Stirling numbers* [27, 30]. If a graph has no edges then a_i is simply equal to the Stirling number of the second kind $S(n,i)$. So, the σ-polynomials of empty graphs correspond to the generating functions for Stirling numbers and such polynomials were studied by Lieb [40].

These polynomials first arose in the study of chromatic polynomials, since the chromatic polynomial of G is $\pi(G,x) = \sum a_i(G)\,(x)_{\downarrow i}$, where $(x)_{\downarrow i} = x(x-1)\cdots(x-i+1)$ is the *falling factorial of x* (the sequence $\langle a_i \rangle$ has been called the *chromatic vector of G* [32]). The σ-polynomial was first introduced by Korfhage [36] in a slightly different form (he refers to the polynomial $(\sum_{i=\chi(G)}^{n} a_i x^i)/x^{\chi(G)}$ as the σ-polynomial), and σ-polynomials have attracted considerable attention in the literature. Brenti [4] studied the σ-polynomials extensively and investigated both log-concavity and the nature of the roots. Chvátal [18] gave a necessary condition for a subsequence of the chromatic vector to be nondecreasing. Brenti, Royle and Wagner [5] proved that a variety of conditions are sufficient for a σ-polynomial to have only real roots.

The σ-polynomial and its coefficients have strong connections to other graph polynomials and combinatorial structures as well. The partition polynomial of a finite set system studied by Wagner [62] reduces to a σ-polynomial when the finite set system is the independence complex of a graph. The σ-polynomial of the complement of a triangle free graph is just the well known matching polynomial [34] under a simple transformation. Moreover, the widely studied adjoint polynomial (see, for example, [16, 26, 41, 43, 45, 59, 68]) is equal to the σ-polynomial of the complement of the graph. The authors in [32] investigate the rook and chromatic polynomials, and prove that every rook vector is a chromatic vector. In [27] the authors explore relations among the σ-polynomial, chromatic polynomial, and the Tutte polynomial, and implications of these connections. A result on the ordinary Stirling numbers was generalized in [30] by considering the σ-polynomials of some graph families. Moreover, studying σ-polynomials is useful to find chromatically equivalent or chromatically unique graph families [42, 67]. Recently, in [8], the authors obtained upper bounds for the real parts of the roots of chromatic polynomials for graphs with large chromatic number by investigating the σ-polynomials of such graphs.

2.1 Preliminaries

In this section we summarize a number of known results on σ-polynomials that we will make use of in the sequel.

The *matching polynomial* $m(G, x)$ of a graph G is defined as

$$m(G, x) = \sum_{i \geq 0} m_i(G)(-1)^i x^{n-2i},$$

where $m_i(G)$ is the number of matchings of size i in G and $m_0(G) \equiv 1$ by convention (see, for example, [62]). Observe that if G is a triangle-free graph then

$$\sigma(\overline{G}, -x^2) = (-x)^n m(G, x).$$

If $\mathcal{F}$ is a finite set system (that is a collection of finite sets, called *blocks*) then its *partition polynomial* $\rho(\mathcal{F}, x)$ is defined as

$$\rho(\mathcal{F}, x) = \sum_{i \geq 1} a_i(\mathcal{F}) x^i$$

where $a_i(\mathcal{F})$ is the number of ways to partition the vertex set of $\mathcal{F}$ (that is $\cup_{A \in \mathcal{F}} A$) into i nonempty blocks [62]. The *independence complex* of a graph G is the simplicial complex (that is a collection of sets, called *faces*, closed under containment – see [7], for example) on the vertex set of G whose faces correspond to independent sets of the graph. Thus the partition polynomial of the independence complex of a graph is equal to the σ-polynomial of the graph.

Sometimes we will be interested in the σ-polynomial of the complement of a graph rather than the graph itself. Therefore it will be convenient for us to consider the following polynomial. Let $b_i(G)$ be the number of partitions of the vertices of G into i cliques. Then the *adjoint polynomial of* G, denoted by $h(G, x)$, is defined as

$$h(G, x) = \sum b_i(G) x^i.$$

Now, it is clear that for every graph G,

$$\sigma(\overline{G}, x) = h(G, x).$$

We will make use of some useful properties of σ-polynomials under various graph operations.

Let u and v be two nonadjacent vertices of a graph G. The number of partitions of $V(G)$ into i independent sets such that u and v are in different (respectively same) colour classes is equal to $a_i(G + uv)$ (respectively $a_i(G \cdot uv)$). Therefore, it is clear that

$$a_i(G) = a_i(G + uv) + a_i(G \cdot uv).$$

Now, since $a_i(G)$ is the coefficient of x^i in $\sigma(G, x)$, we obtain the following recursive formula to compute the σ-polynomials which is folklore.

Lemma 2.1.1. *[24] Let G be any graph. If e is not an edge of G then*

$$\sigma(G, x) = \sigma(G + e, x) + \sigma(G \cdot e, x)$$

or equivalently, if e is an edge of G then

$$\sigma(G, x) = \sigma(G - e, x) - \sigma(G \cdot e, x).$$

□

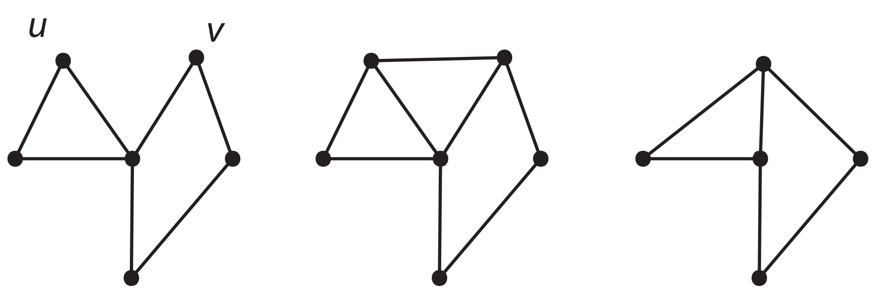

Figure 2.1: From left to right: G, $G + uv$, $G \cdot uv$

The adjoint polynomials also satisfy a similar recursive formula but in this recursion one uses weak contraction instead of contraction. It is known that [24] if e is an edge of G then

$$h(G,x) = h(G-e,x) + h(G \odot e,x) \tag{2.1}$$

or equivalently, if e is not an edge of G then

$$h(G,x) = h(G+e,x) - h(G \odot e,x). \tag{2.2}$$

A consequence of this recursive formula is the following:

Lemma 2.1.2. *Let G be a graph and $e = uv$ be an edge of G such that e is not contained in any triangle of G. Then,*

$$\sigma(\overline{G},x) = \sigma(\overline{G-e},x) + x\sigma(\overline{G-\{u,v\}},x).$$

□

Another well known useful property of the σ-polynomials is that the σ- polynomial of the join of two graphs is equal to the product of the σ-polynomials of these two graphs.

Lemma 2.1.3. *[62, Proposition 2.1.] Let G and H be two graphs then*

$$\sigma(G \vee H,x) = \sigma(G,x)\sigma(H,x)$$

Proof. Every partition of the vertices of $G \vee H$ into i independent sets is obtained by partitioning the vertices of G into k independent sets and the vertices of H into $i-k$ independent sets for some integer $k \geq 1$. Hence,

$$a_i(G \vee H) = \sum_{k \geq 1} a_k(G)a_{i-k}(H)$$

and the result follows. □

Lemma 2.1.4. *[62, Proposition 4.2.] Let G be any graph, then*

$$\sigma(G \cup K_1) = x\left(\sigma(G,x) + \frac{d}{dx}\sigma(G,x)\right).$$

Proof. The number of partitions of the vertex set of $\sigma(G \cup K_1)$ into i nonempty independent sets such that the isolated vertex of K_1 is in a singleton (respectively not in a singleton) is equal to $a_{i-1}(G)$ (respectively $ia_i(G)$). So, $a_i(G \cup K_1) = a_{i-1}(G) + ia_i(G)$ holds. Therefore,

$$\begin{aligned}
\sigma(G \cup K_1, x) &= \sum a_i(G)x^{i+1} + \sum ia_i(G)x^i \\
&= x\sigma(G,x) + x\frac{d}{dx}\sigma(G,x).
\end{aligned}$$

□

Example 2.1.1. Let $u_1, \ldots, u_n$ be the vertices of the path graph P_n such that u_i and u_{i+1} are adjacent. Now, $P_n - u_1u_2 \cong K_1 \cup P_{n-1}$ and $P_n \cdot u_1u_2 \cong P_{n-1}$. So, by applying the edge deletion-contraction formula and then applying Lemma 2.1.4 we get

$$\begin{aligned}
\sigma(P_n, x) &= \sigma(K_1 \cup P_{n-1}, x) - \sigma(P_{n-1}, x) \\
&= x\left(\sigma(P_{n-1}, x) + \frac{d}{dx}\sigma(P_{n-1}, x)\right) - \sigma(P_{n-1}, x) \\
&= (x-1)\sigma(P_{n-1}, x) + x\frac{d}{dx}\sigma(P_{n-1}, x).
\end{aligned}$$

We can indeed generalize Lemma 2.1.4 to the disjoint union of any two graphs. Before doing so, we need to introduce a linear operation that maps the chromatic polynomial of a graph to its σ-polynomial.

Let $S : \mathbb{R}[x] \to \mathbb{R}[x]$ be the linear transformation defined by

$$S : x(x-1)\ldots(x-j+1) \mapsto x^j.$$

It is clear that for any graph G,

$$S(\pi(G,x)) = \sigma(G,x).$$

Also, let us define the $*$-product operation as follows:

$$*\colon \mathbb{R}[x] \times \mathbb{R}[x] \to \mathbb{R}[x] \text{ is given by}$$

$$p(x) * q(x) = \sum_{k\geq 0} \frac{x^k}{k!}\Big(\frac{d^k}{dx}p(x)\Big)\Big(\frac{d^k}{dx}q(x)\Big).$$

For example, if $p(x) = x^3 + x^2$ and $q(x) = x^2 + 2$ then

$$p(x) * q(x) = (x^3 + x^2)(x^2 + 2) + x(3x^2 + 2x)(2x) + \frac{x^2}{2}(6x + 2)(2).$$

Now, we have the following useful result.

Proposition 2.1.5. *[5, Proposition 4.2.] For any $f, g \in \mathbb{R}[x]$ we have*

$$S(fg) = (Sf) * (Sg).$$

□

The following result was proven in [62] for partition polynomials. Here we present a self contained proof by using chromatic polynomials.

Theorem 2.1.6. *[62, Proposition 4.2.] Let G and H be any two graphs then*

$$\sigma(G \cup H, x) = \sigma(G,x) * \sigma(H,x).$$

Proof. The chromatic polynomial satisfies

$$\pi(G \cup H, x) = \pi(G,x)\pi(H,x)$$

so, by applying the S transformation to both sides of the latter equality we obtain

$$\sigma(G \cup H, x) = S(\pi(G,x)\pi(H,x)).$$

By Proposition 2.1.5, $S(\pi(G,x)\pi(H,x)) = S(\pi(G,x)) * S(\pi(H,x))$. Thus, the result is established as $S(\pi(G,x)) = \sigma(G,x)$ and $S(\pi(H,x)) = \sigma(H,x)$.

□

Theorem 2.1.7 (Complete Cutset Theorem for σ-polynomials)**.** *[5, Theorem 4.5.] Let G and H be two graphs such that $G \cap H$ is a complete graph, and $k = |V(G \cap H)|$. Then,*

$$\frac{\sigma(G \cup H, x)}{x^k} = \frac{\sigma(G,x)}{x^k} * \frac{\sigma(H,x)}{x^k}.$$

□

The formulas we have presented in this section have consequences in terms of roots of σ-polynomials that will be presented in the next section.

In the following result we give an inequality which relates two consecutive coefficients of a σ-polynomial. We will make use of this inequality to give an upper bound for the moduli of the roots of σ-polynomials.

Lemma 2.1.8. *Let G be any graph. Then,*

$$b_i(G) \leq m_G b_{i+1}(G)$$

for all $1 \leq i \leq n_G - 1$. Moreover, when the graph has at least one edge the inequalities hold strictly for all $1 \leq i \leq n_G - 2$.

Proof. We proceed by induction on the size of the graph. If G is an empty graph, then $b_i(G) = 0$ for all $1 \leq i \leq n_G - 1$ and hence the equality holds. For the induction step, suppose that G has at least one edge. First, observe that equality holds for $i = n_G - 1$ since $b_{n_G} = 1$ and $b_{n_G - 1} = m_G$. Now, for every $1 \leq i \leq n_G - 2$, we can write

$$\begin{aligned} b_i(G) &= b_i(G-e) + b_i(G \odot e) \\ &\leq m_{G-e} b_{i+1}(G-e) + m_{G\odot e} b_{i+1}(G \odot e) \\ &< m_G b_{i+1}(G-e) + m_G b_{i+1}(G \odot e) \\ &= m_G b_{i+1}(G) \end{aligned}$$

where the first and last equalities follow from the recursive formula for the adjoint polynomial, and the other inequalities hold by the induction hypothesis and the facts that $m_{G-e} < m_G$ and $m_{G\odot e} < m_G$.

□

Note that in the proof of the previous lemma, one needs to handle the case $i = n_G - 1$ separately because the argument $b_i(G \odot e) \leq m_{G\odot e} b_{i+1}(G \odot e)$ does not hold for this case as $n_{G\odot e} = n_G - 1$ and so $b_{i+1}(G \odot e) = 0$.

Since $\binom{n_G}{2} - m_G = m_{\overline{G}}$, the following corollary follows immediately from this lemma.

Corollary 2.1.9. *Let G be any graph. Then,*

$$a_i(G) \leq \left(\binom{n_G}{2} - m_G \right) a_{i+1}(G)$$

for all $1 \leq i \leq n_G - 1$. Moreover, when the graph G is not a complete graph inequalities hold strictly for all $1 \leq i \leq n_G - 2$.

We will use the following classical result on bounding the moduli of roots of real polynomials.

Theorem 2.1.10 (Eneström-Kakeya Theorem)**.** *[46, pg. 255] A polynomial* $f(z) = \sum_{i=0}^{d} c_i z^i$ *with positive coefficients has all its zeros in the annulus*

$$\left\{ z \in \mathbb{C} : \; \min\left\{\frac{c_{i-1}}{c_i}\right\}_{1\leq i\leq d} \leq |z| \leq \max\left\{\frac{c_{i-1}}{c_i}\right\}_{1\leq i\leq d} \right\}$$

Theorem 2.1.11. *Let* G *be a graph of order* n *and size* m*. If* $z \in \mathbb{C}$ *is a root of* $\sigma(G, x)$ *then*

$$|z| \leq \binom{n}{2} - m.$$

Proof. The result follows immediately by Corollary 2.1.9 and the Eneström-Kakeya Theorem. □

A vertex v of a graph G is called a *simplicial vertex* if the neighborhood of v in G induces a complete graph.

Lemma 2.1.12. *Let* v *be a simplicial vertex of a graph* G*. Then,*

$$h(G, x) = x \sum_{S \subseteq N(v)} h(G - (S \cup \{v\}), x).$$

Proof. Since v is a simplicial vertex, every vertex in $N(v)$ can be in the same class with v in a partition of the vertices into cliques. Hence,

$$b_i(G) = \sum_{S \subseteq N(v)} b_{i-1}(G - (S \cup \{v\}))$$

and the proof is complete. □

We now turn to formulas for some coefficients of σ-polynomials.

Let G be a graph whose σ-polynomial is

$$\sigma(G, x) = \sum_{i=\chi(G)}^{n} a_i x^i.$$

For two graphs H and G, we denote by $\eta_G(H)$ the number of subgraphs of G which are isomorphic to H. For example, if $G = K_4$ then we have $\eta_G(K_2) = 6$, $\eta_G(2K_2) = 3$, $\eta_G(K_3) = 4$ and $\eta_G(K_3 \cup K_2) = 0$. Also, for every partition $i = \sum_{j=1}^{k} m_j$ of a positive integer i, we associate a disjoint union of complete graphs $\cup_{j=1}^{k} K_{m_j+1}$, an i^{th} *generation forbidden subgraph* [39] (they are "forbidden" as the complement of any graph with chromatic number $n-k$ cannot contain any $(k+1)^{th}$ generation forbidden graph as a subgraph since otherwise it can be partitioned into $n-k-1$ independent sets).

By the definition of the coefficient a_{n-i}, it is clear that a_{n-i} counts the number of subgraphs of the form $\cup_{j=1}^{n-i} K_{m_j}$ in $\overline{G}$ where $n = \sum_{j=1}^{n-i} m_j$ and $m_j \in \mathbb{N} \setminus \{0\}$. For example,

$$\begin{aligned} a_n &= \eta_{\overline{G}}(nK_1), \\ a_{n-1} &= \eta_{\overline{G}}((n-2)K_1 \cup K_2), \\ a_{n-2} &= \eta_{\overline{G}}((n-3)K_1 \cup K_3) + \eta_{\overline{G}}((n-4)K_1 \cup 2K_2). \end{aligned}$$

Now, by ignoring the singleton cliques in a partition of the n vertices of $\overline{G}$ into $n-i$ nonempty cliques, we see that a_{n-i} counts the number of i^{th} generation forbidden subgraphs. This fact was also observed in [39] and we will use it frequently in the next section.

Observation 2.1.13. *The coefficient a_{n-i} counts the number of subgraphs of the form $\cup_{j=1}^{k} K_{m_j+1}$ in $\overline{G}$, where $i = \sum_{j=1}^{k} m_j$ and $m_j \in \mathbb{N} \setminus \{0\}$.*

Partition of 4	Associated 4^{th} generation forbidden subgraph
4	K_5
$3+1$	$K_4 \cupdot K_2$
$2+2$	$2K_3$
$2+1+1$	$K_3 \cupdot 2K_2$
$1+1+1+1$	$4K_2$

Table 2.1: Fourth generation forbidden subgraphs

From this observation, we find that

$$\begin{aligned}
a_n &= 1, \\
a_{n-1} &= \eta_{\overline{G}}(K_2) = \binom{n}{2} - |E(G)|, \\
a_{n-2} &= \eta_{\overline{G}}(K_3) + \eta_{\overline{G}}(2K_2), \\
a_{n-3} &= \eta_{\overline{G}}(K_4) + \eta_{\overline{G}}(K_3 \cupdot K_2) + \eta_{\overline{G}}(3K_2), \\
a_{n-4} &= \eta_{\overline{G}}(K_5) + \eta_{\overline{G}}(K_4 \cupdot K_2) + \eta_{\overline{G}}(2K_3) + \eta_{\overline{G}}(K_3 \cupdot 2K_2) + \eta_{\overline{G}}(4K_2).
\end{aligned}$$

Proposition 2.1.14. *Let G be a graph of order n and size m. Then*

$$a_{n-2}(G) = S(n, n-2) + \binom{m}{2} - m\binom{n-1}{2} - \eta_G(K_3).$$

Proof. We proceed by induction on the number of edges. If G is an empty graph then $a_{n-2}(G) = S(n, n-2)$ and the formula clearly holds as $m = 0$ and $\eta_G(K_3) = 0$. Now we may assume that G has two vertices u and v such that $e = uv \in E(G)$. Since $G \cdot uv$ has $n-1$ vertices and $m - 1 - |N_G(u) \cap N_G(v)|$ edges, we find that

$$\begin{aligned}
a_{n-2}(G \cdot uv) &= \binom{n_{G\cdot uv}}{2} - m_{G\cdot uv} \\
&= \binom{n-1}{2} - m + 1 + |N_G(u) \cap N_G(v)|.
\end{aligned}$$

The graph $G - uv$ has n vertices and $m - 1$ edges. Also, $\eta_{G-uv}(K_3)$ is equal to $\eta_G(K_3) - |N_G(u) \cap N_G(v)|$. Therefore, by the induction hypothesis on $G - uv$, we obtain that

$$a_{n-2}(G-e) = S(n, n-2) + \binom{m-1}{2} - (m-1)\binom{n-1}{2} - \eta_G(K_3) + |N_G(u) \cap N_G(v)|.$$

Now the result follows since $a_{n-2}(G) = a_{n-2}(G - uv) - a_{n-2}(G \cdot uv)$. $\square$

Remark 2.1.1. Prior to our result, several authors gave false formulas for $a_{n-2}(G)$. Dhurandhar [20, pg. 220] stated and proved incorrectly that

$$a_{n-2}(G) = \tbinom{m}{2} + m\tbinom{n-1}{2} + \tbinom{n}{3}\tfrac{(9n-7)}{4} - \eta_G(K_3).$$

Later, Brenti [4] pointed out the error in Dhurandhar's formula and gave another incorrect statement and proof for $a_{n-2}(G)$ (see Proposition 3.2 on pg. 733), namely that

$$a_{n-2}(G) = \tbinom{m}{2} - m\tbinom{n-1}{2} + \tbinom{n}{3}\tbinom{3n-5}{4} - \eta_G(K_3).$$

It is easy to find many examples for which these formulas do not hold. For example, let G be the leftmost graph in Figure 1.1. Then G has order $n = 6$, size $m = 7$ and exactly one triangle. The σ-polynomial of G is $\sigma(G, x) = x^6 + 8\,x^5 + 15\,x^4 + 6\,x^3$ and therefore the true value of $a_{n-2}(G)$ is 15. However, the first formula yields $a_{n-2}(G) = \tbinom{7}{2} - 7\tbinom{5}{2} + \tbinom{6}{3}\tbinom{13}{4} - 1 = 14250$ and the second formula yields $a_{n-2}(G) = \tbinom{7}{2} + 7\tbinom{5}{2} + \tbinom{6}{3}\tfrac{47}{4} - 1 = 325$.

2.2 Real roots of σ-polynomials

Finding the location of the roots of σ-polynomials (σ-roots) is a difficult problem. Even for empty graphs, it is difficult to determine the location of the roots. As we already mentioned, the σ-polynomial of an empty graph is equal to

$$\sigma(\overline{K}_n, x) = \sum_{i\geq 1} S(n,i)x^i$$

where $S(n,i)$ is the Stirling number of the second kind [24]. Lieb [40] and Harper [33] independently proved that this polynomial has only real roots.

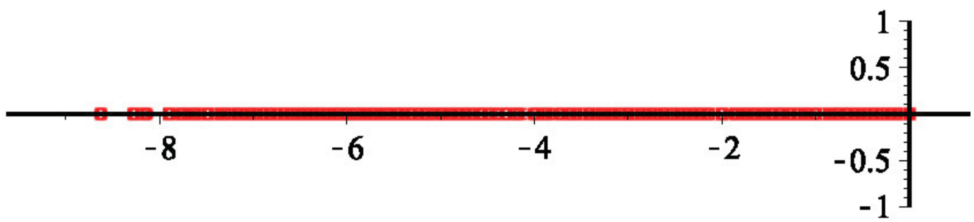

Figure 2.2: The roots of σ-polynomials of all connected 7-vertex graphs.

Computer-aided computations show that σ-polynomials of all graphs of order at most 7 have only real roots. Also, among all $12,346$ many graphs of order 8, there exist only two graphs whose σ-polynomials have nonreal roots and these graphs are depicted in Figure 2.3. In [5], the authors present all connected graphs of order 9 whose σ-polynomials have nonreal roots; there are only 42 out of $274,668$ many such graphs.

In [62] is was shown that the partition polynomial of the independence complex of a chordal graph or the complement of a comparability graph has only real roots. Since the partition polynomial of the independence complex of a graph is equal its σ-polynomial, it follows that σ-polynomials of chordal graphs and of incomparability graphs have only real roots. Moreover, by using this fact about the σ-polynomials

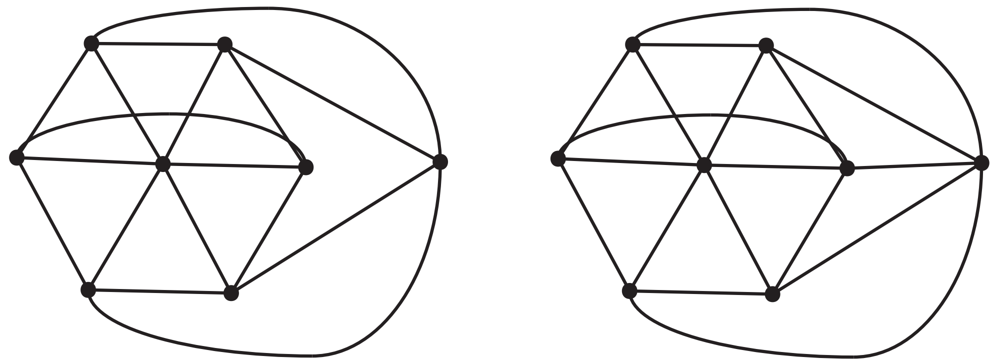

Figure 2.3: The graphs of order 8 whose σ-polynomials have nonreal roots.

of incomparability graphs, Brenti [4] observed that all graphs G with $\chi(G) \geq n-2$ have only real roots.

The matching polynomial of any graph is well known to have only real roots [34]. By the connection between the σ-polynomials and matching polynomials we noted earlier, $\sigma(\overline{G}, x)$ has only real roots for any triangle-free graph G.

In the following theorem we summarize all these results.

Theorem 2.2.1. *[4, 5, 34, 62] If graph G has any of the following properties then $\sigma(G, x)$ has only real roots:*

(i) G has order at most 7.

(ii) G has order n with $\chi(G) \geq n-2$.

(iii) G is chordal.

(iv) $\overline{G}$ is triangle-free.

(v) $\overline{G}$ is a comparability graph.

Remark 2.2.1. σ-polynomials of chordal graphs always have only real roots but unfortunately the same is not true for the complements of such graphs. For example, the graph G in Figure 2.4 is chordal but the σ-polynomial of its complement is

$$\sigma(\overline{G}, x) = x^4(x^5 + 9x^4 + 25x^3 + 26x^2 + 9x + 1)$$

which has real roots at approximately -4.917, -2.183, -1.387, and non-real roots $-0.255 + 0.042i$ and $-0.255 - 0.042i$.

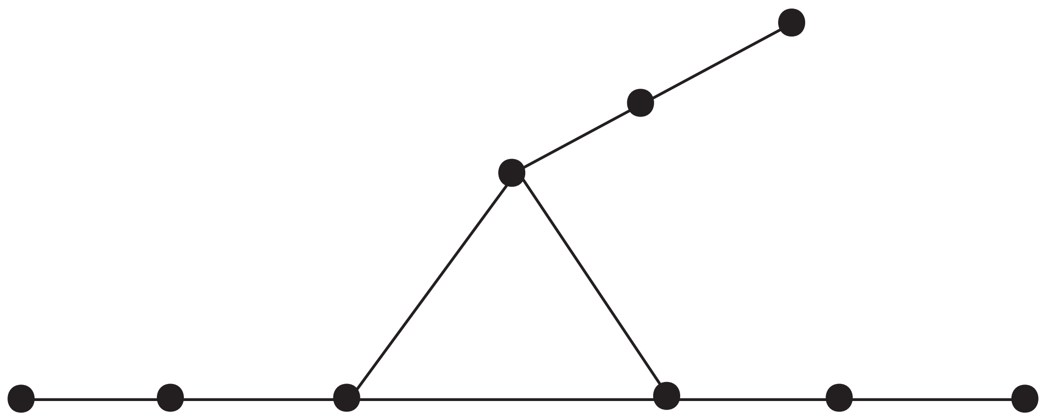

Figure 2.4: A chordal graph G such that $\sigma(\overline{G}, x)$ has non-real roots.

The following result allows us to build larger graphs with all real σ-roots from smaller ones.

Theorem 2.2.2. *[5] Let G and H be two graphs such that both $\sigma(G, x)$ and $\sigma(H, x)$ have only real roots. Then,*

(i) $\sigma(G \vee H, x)$ has only real roots,

(ii) $\sigma(G \mathbin{\dot\cup} H, x)$ has also only real roots,

(iii) If $G \cap H$ is a complete graph, then $\sigma(G \cup H, x)$ has only real roots.

Since a complete bipartite graph is a join of two empty graphs, an immediate consequence of Theorem 2.2.2 (i) is that the σ-polynomial of a complete bipartite has only real roots.

2.3 Graphs G with $\chi(G) \geq n-3$

As we already mentioned, Brenti [4] proved that σ-polynomials of all graphs of order n with chromatic number at least $n-2$ have all real roots, and proposed the following:

Conjecture 2.3.1. [4, Conjecture 7.2. pg. 752] If G is a graph of order n and $\chi(G) \geq n-3$, then $\sigma(G, x)$ has only real roots.

In this section we will prove Brenti's conjecture.

In order to prove the main result of this section, we will use a characterization of the complements of graphs of order n with chromatic number $n-3$, obtained in [39]; specifically, $\chi(G) = n-3$ if and only if $G \cong \overline{H} \vee K_{n-r}$ where $|V(H)| = r \leq n$, and either H is a proper 3-star graph (whose definition will follow shortly), or H is one of the graphs of the families described in Figures 2.5, 2.9 and 2.10.

However, first we need a theorem that determines whether a real polynomial (that is, a polynomial with real coefficients) has all real roots. The *Sturm sequence* of a real polynomial $f(t)$ of positive degree is a sequence of polynomials $f_0, f_1, f_2 \ldots,$ where $f_0 = f$, $f_1 = f'$, and, for $i \geq 2$, $f_i = -\mathrm{rem}(f_{i-2}, f_{i-1})$, where $\mathrm{rem}(h, g)$ is the remainder upon dividing h by g. The sequence is terminated at the last nonzero f_i. The Sturm sequence of f has *gaps in degree* if there exist integers $j \leq k$ such that $\deg f_j < \deg f_{j-1} - 1$. Sturm's well known theorem (see, for example, [12]) is the following:

Theorem 2.3.2 (Sturm's Theorem)**.** *Let $f(t)$ be a real polynomial whose degree and leading coefficient are positive. Then $f(t)$ has all real roots if and only if its Sturm sequence has no gaps in degree and no negative leading coefficients.*

For the next result, we consider the family of graphs F depicted in Figure 2.5. In each of the eight subfamilies, the vertex v is joined to each vertex in an independent set of size m on the right, and to some vertices of a C_5 on the left.

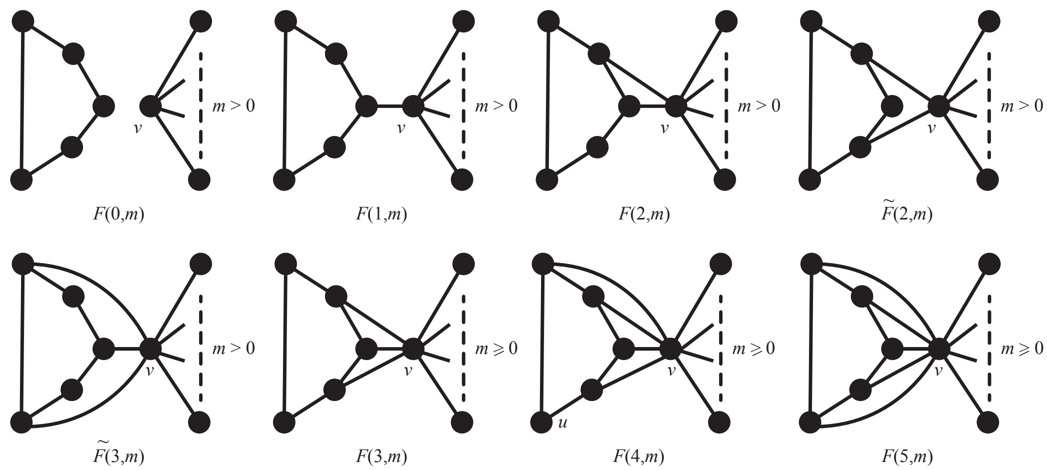

Figure 2.5: The F family

Lemma 2.3.3. *Let G be a graph whose complement $\overline{G}$ is in the F family (see Figure 2.5). Then $\sigma(G,x)$ has only real roots.*

Proof. It is clear that if $\overline{G}$ is equal to $F(0,m)$, $F(1,m)$, $\tilde{F}(2,m)$ or $\tilde{F}(3,m)$ then it is triangle-free, hence $\sigma(G,x)$ has only real roots by Theorem 2.2.1 (iv).

If $\overline{G} = F(2,m)$ then we find that $\eta_{\overline{G}}(K_2) = m+7$, $\eta_{\overline{G}}(K_3) = 1$, $\eta_{\overline{G}}(2K_2) = 5m+11$, $\eta_{\overline{G}}(K_4) = 0$, $\eta_{\overline{G}}(K_3 \cup K_2) = 2$ and $\eta_{\overline{G}}(3K_2) = 5m+2$. Therefore, by Observation 2.1.13 we obtain that

$$\sigma(G,x)/x^{m+3} = x^3 + (m+7)x^2 + (5m+12)x + (5m+4).$$

Calculations show that the leading coefficients of this polynomial's Sturm sequence are

$$1, 3, \frac{2}{9}(m^2 - m + 13) \text{ and } \frac{9(5m^4 - 16m^3 + 88m^2 - 92m + 272)}{4\left(m^2 - m + 13\right)^2},$$

all of which are strictly positive and that there are no gaps in degree. Hence, we get the result by Theorem 2.3.2.

Also, if $\overline{G} = F(3,m)$ then we find that $\eta_{\overline{G}}(K_2) = m+8$, $\eta_{\overline{G}}(K_3) = 2$, $\eta_{\overline{G}}(2K_2) = 5m+14$, $\eta_{\overline{G}}(K_4) = 0$, $\eta_{\overline{G}}(K_3 \cup K_2) = 4$ and $\eta_{\overline{G}}(3K_2) = 5m+3$. Again by Observation 2.1.13, we get

$$\sigma(G,x)/x^{m+3} = x^3 + (m+8)x^2 + (5m+16)x + (5m+7).$$

The leading coefficients of this polynomial's Sturm sequence turn out to be

$$1, 3, \frac{2}{9}(m^2+m+16) \text{ and } \frac{9(5m^4+2m^3+99m^2+46m+469)}{4\left(m^2+m+16\right)^2},$$

all of which are obviously strictly positive for $m \geq 0$ and there are no gaps in degree. Hence, we conclude as above.

Now let $\overline{G} = F(4,m)$ and v be the vertex of $\overline{G}$ which is adjacent to m leaves in $\overline{G}$ and u be the vertex which is not adjacent to v in $\overline{G}$. Let H be the edge induced by u and v in G. Now, $G = (C_5 \vee K_m) \cup H$, and the intersection of $C_5 \vee K_m$ and H is equal to $\{u\}$ in G. Note that $\sigma(C_5, x)$ has only real roots by Theorem 2.2.1 (i). Also, $\sigma(C_5 \vee K_m, x) = x^m \sigma(C_5, x)$ holds by Theorem 2.2.2 (i), so the polynomial $\sigma(C_5 \vee K_m, x)$ has only real roots. Hence, the result follows from Theorem 2.2.2 (iii).

Lastly, suppose that $\overline{G} = F(5,m)$, then $G = (C_5 \vee K_m) \cup K_1$. Now, we obtain the result from Theorem 2.2.2 (ii), since both $\sigma(C_5 \vee K_m, x)$ and $\sigma(K_1, x) = x$ have only real roots.

□

The proof of the realness of the roots of the σ-polynomials of the other classes of graphs will require a more subtle argument than just Sturm sequences, and we rely on an approach taken by Chudnovsky and Seymour [17] in their proof for the realness of the roots of independence polynomials of claw-free graphs. Following [17], we say that polynomials $f_1, \ldots f_k$ in $\mathbb{R}[x]$ are *compatible* if for all $c_1, \ldots, c_k \geq 0$, all the roots of the linear combination $\sum_{i=1}^{k} c_i f_i(x)$ are real, and the polynomials are called *pairwise compatible* if for all i, j in $\{1, \dots, k\}$, the polynomials $f_i(x)$ and $f_j(x)$ are compatible. The following observation will be utilized later.

Observation 2.3.4. *Suppose that $f(x), g(x) \in \mathbb{R}[x]$ are two polynomials with positive leading coefficients and all roots real. Then, f and g are compatible if and only if for all $c > 0$, the polynomial $cf(x) + g(x)$ has all real roots.*

We need a few more definitions. Let $a_1 \geq \cdots \geq a_m$ and $b_1 \geq \cdots \geq b_n$ be two sequences of real numbers. We say that the first *interleaves* the second if $n \leq m \leq n+1$ and

$$a_1 \geq b_1 \geq a_2 \geq b_2 \geq \cdots .$$

Let f be a polynomial of degree d with only real roots. Suppose that $r_1, \dots, r_d$ are the roots of f such that $r_1 \geq \cdots \geq r_d$. Then the sequence $(r_1, \dots, r_d)$ is called the *root sequence* of f. Let $f_1, \dots, f_k$ be polynomials with positive leading coefficients and all roots real. A *common interleaver* for $f_1, \dots, f_k$ is a sequence that interleaves the root sequence of each f_i.

The key analytic result we need from [17] is the following:

Theorem 2.3.5. *[17] Let $f_1, \dots f_k$ be polynomials with positive leading coefficients and all roots real. Then the following statements are equivalent:*

(i) *$f_1, \dots, f_k$ are pairwise compatible,*

(ii) *for all s, t such that $1 \leq s < t \leq k$, the polynomials f_s and f_t have a common interleaver,*

(iii) *$f_1, \dots, f_k$ have a common interleaver,*

(iv) *$f_1, \dots, f_k$ are compatible.*

We now return to proving the realness of the roots of the σ-polynomials for the remaining classes of graphs with $\chi(G) = n - 3$. We say that a subset of vertices S of a graph G is a *vertex cover* of G if every edge of G contains at least one vertex of S. The *vertex cover number*, $\alpha_o(G)$, is the cardinality of a minimum vertex cover. Note that S is a vertex cover of G if and only if $V(G) - S$ induces an independent set, and that if $\alpha_o(\overline{G}) = k$ then G contains a complete subgraph of order $n - k$, and hence $\chi(G) \geq n - k$. A graph G is called a *proper k-star* [39] if $\alpha_o(G) = k$ and G contains at least one k^{th} generation forbidden subgraph. In the following proof, n_G and n_H denotes the number of vertices of the graph G and subgraph H, respectively.

Theorem 2.3.6. *Let G be a graph such that $\alpha_o(\overline{G}) \leq 3$. Then $\sigma(G, x)$ has only real roots.*

Proof. We may assume that $\alpha_o(\overline{G}) = 3$ and $\chi(G) = n_G - 3$, since otherwise $\chi(G) \geq n_G - 2$ and the result holds by Theorem 2.2.1 (ii). Also, we may assume that $\overline{G}$ has no isolated vertices by Theorem 2.2.2(i). Let $S = \{u_1, u_2, u_3\}$ be a vertex cover of $\overline{G}$, so that $V(G) - S$ is an independent set of $\overline{G}$. We set $V = V(G) = V(\overline{G})$. There are four cases we need to consider: S induces either an independent set, K_3, P_3, or $K_2 \cup K_1$ in $\overline{G}$.

Case 1: S induces an independent set in $\overline{G}$.

In this case $\overline{G}$ is a triangle-free graph and we are done by Theorem 2.2.1 (iv).

Case 2: The subgraph of $\overline{G}$ induced by S is isomorphic to K_3.

Here G can be partitioned into a clique and independent set, so one can check that G is, in fact, chordal and hence the result follows from Theorem 2.2.1(iii).

Case 3: S induces in $\overline{G}$ a P_3.

Without loss of generality, we may assume that u_2 is adjacent to both u_1 and u_3 in $\overline{G}$. Let H_1 (respectively H_2) be the subgraph induced by $V - \{u_1, u_3\}$ (respectively $V - \{u_2\}$) in G (see Figure 2.6). Clearly, $H_1 \cap H_2$ is a complete graph in G and

$H_1 \cup H_2 = G$. Also, $\sigma(H_1, x)$ and $\sigma(H_2, x)$ have only real roots by Theorem 2.2.1(ii) because $\chi(H_1) \geq n_{H_1} - 2$ and $\chi(H_2) \geq n_{H_2} - 2$. Therefore, we obtain the result by Theorem 2.2.2(iii).

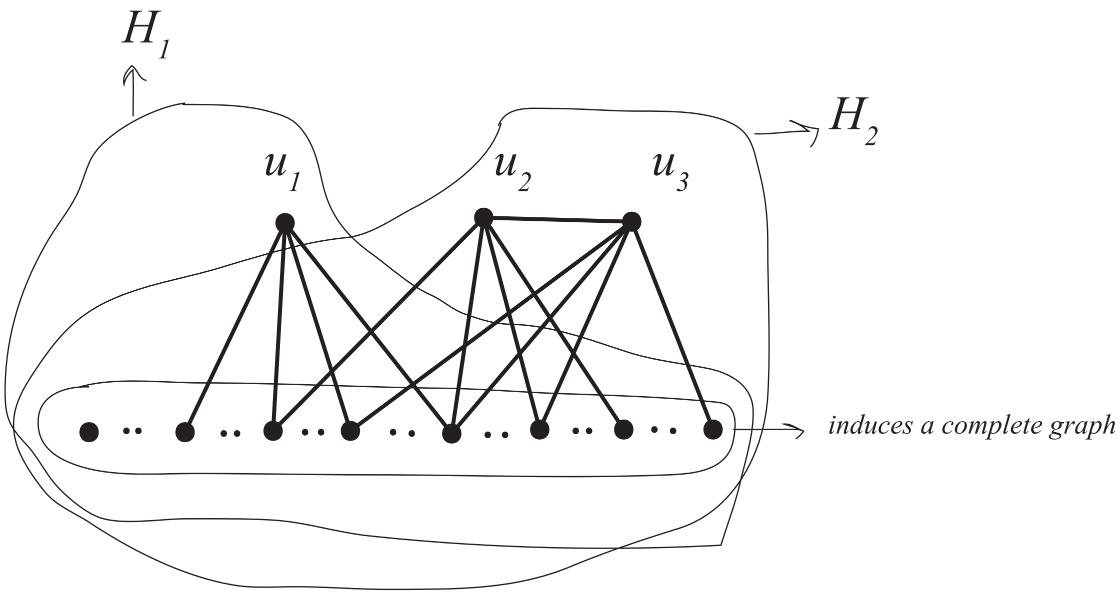

Figure 2.6: The graph G in Case 3. (S induces in $\overline{G}$ a P_3, hence S induces in G a $K_1 \,\dot{\cup}\, K_2$.)

Case 4: The subgraph induced by S in $\overline{G}$ is isomorphic to $K_2 \,\dot{\cup}\, K_1$.

Without loss, let u_1 and u_2 be adjacent to each other in $\overline{G}$; we will partition the remaining vertices into sets by their neighbourhood in S (see Figure 2.7). Let P be the set of vertices which are adjacent to all vertices of S in $\overline{G}$. By Theorem 2.2.2(iii), it suffices to prove the result when $P = \emptyset$ (because the intersection of the graphs $\langle V(G) - S \rangle_G$ and $\langle V(G) - P \rangle_G$ is a complete graph and their union gives the graph G). Let M_i be the set of all leaves which are adjacent to u_i in $\overline{G}$, and $m_i = |M_i|$. Also, let R be the set of all common neighbours of u_1 and u_2 in $\overline{G}$. Similarly, let J (respectively, K) be the set of all common neighbours of u_2 and u_3 (u_1 and u_3, respectively) in $\overline{G}$. Recall that $V(G) - S$ is an independent set of $\overline{G}$ since S is a vertex cover of $\overline{G}$. Let $r = |R|$, $j = |J|$ and $k = |K|$. If $j = 0$ or $k = 0$, then $\overline{G}$

is a comparability graph (see Figure 2.8 for $k = 0$) and we obtain the result from Theorem 2.2.1(v). Hence, we may assume that $j, k \geq 1$. Now, let H be the subgraph of $\overline{G}$ induced by $V - (M_3 \cup \{u_3\})$. Let also H_J (respectively H_K) be any subgraph of $\overline{G}$ induced by $V - (M_3 \cup \{u_3, v_J\})$ (respectively $V - (M_3 \cup \{u_3, v_K\})$) where v_J (respectively v_K) is a vertex of J (respectively K). None of the edges incident to u_3 are contained in a triangle in $\overline{G}$. We now apply the recursive formula in Lemma 2.1.2 to all edges incident to u_3 successively. We set G_i be an induced subgraph of $\overline{G}$ which is obtained from $\overline{G}$ by deleting i vertices of M_3. Beginning with the edges between M_3 and u_3, we find from Lemma 2.1.2 (and the fact from Theorem 2.2.2(i) that any isolated vertex in the complement of a graph adds a factor of x to the σ-polynomial) that

$$\begin{aligned}
\sigma(G, x) &= \sigma(G_0, x) \\
&= x\sigma(G_1, x) + x \cdot x^{m_3-1}\sigma(\overline{H}, x) \\
&= x\sigma(G_1, x) + x^{m_3}\sigma(\overline{H}, x) \\
&= x\left(x\sigma(G_2, x) + x^{m_3-1}\sigma(\overline{H}, x)\right) + x^{m_3}\sigma(\overline{H}, x) \\
&= x^2\sigma(G_2, x) + 2x^{m_3}\sigma(\overline{H}, x) \\
&= \cdots \\
&= x^{m_3}\sigma(G_{m_3}, x) + m_3x^{m_3}\sigma(\overline{H}, x).
\end{aligned}$$

We then continue to successively remove the other edges incident to u_3 in G_{m_3}, and using a similar argument, we find that $\sigma(G_{m_3}, x) = jx\sigma(\overline{H_J}, x) + kx\sigma(\overline{H_K}, x) + x\sigma(\overline{H}, x)$, so that

$$\sigma(G, x) = x^{m_3}\left(x\sigma(\overline{H}, x) + jx\sigma(\overline{H_J}, x) + kx\sigma(\overline{H_K}, x) + m_3\sigma(\overline{H}, x)\right).$$

None of the graphs H, H_J or H_K contain a third generation forbidden subgraph. So, the chromatic number of each of the graphs $\overline{H}, \overline{H_J}$ and $\overline{H_K}$ is at least the order of the graph minus 2 and hence σ-polynomials of these graphs have only real roots by Theorem 2.2.1(ii).

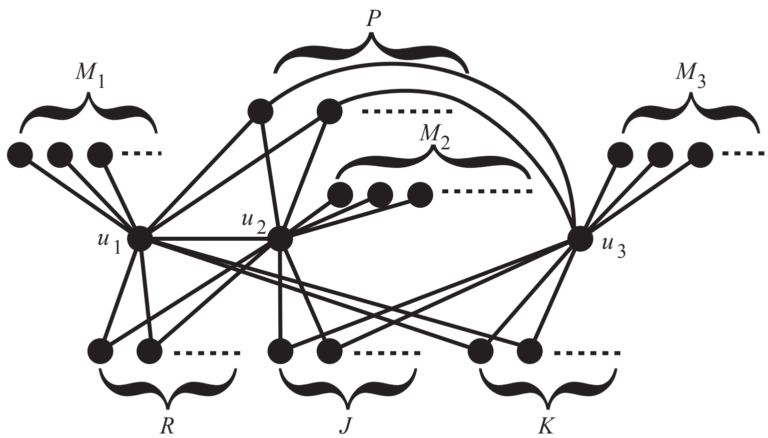

Figure 2.7: The graph $\overline{G}$ with vertex cover $\{u_1, u_2, u_3\}$

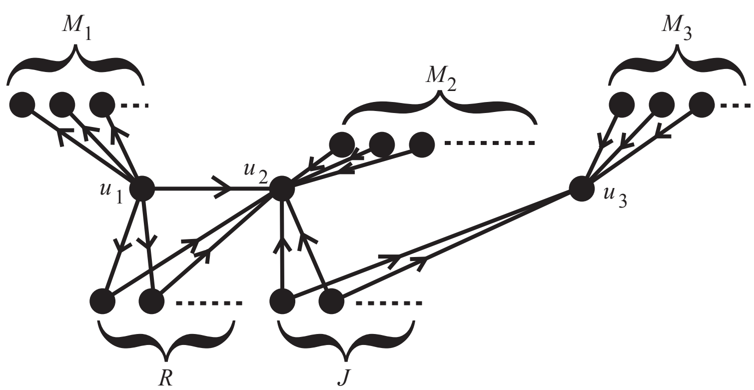

Figure 2.8: A comparability graph of a subclass of graphs from Figure 2.7.

Now, by Theorem 2.3.5, it suffices to show that the polynomials

$$\sigma(\overline{H}, x),\ x\sigma(\overline{H}, x),\ x\sigma(\overline{H_J}, x),\ \text{and}\ x\sigma(\overline{H_K}, x)$$

are pairwise compatible. Let $\alpha = m_2 + j + r$ and $\beta = m_1 + k + r$. Now the number of K_2's, K_3's and $2K_2$'s in $\overline{H}$ are, respectively, $\alpha + \beta + 1$, r and $\alpha\beta - r$, and hence

$$\sigma(\overline{H}, x) \quad = \quad x^{n_H - 2}\left(x^2 + (\alpha + \beta + 1)x + \alpha\beta\right).$$

Moreover, as $\overline{H_J}$ and $\overline{H_K}$ are graphs of the same form as H with j replaced by $j-1$ and k replaced by $k-1$ respectively (and hence α and β decreased by 1, respectively), we see that

$$\begin{aligned} x\sigma(\overline{H_J}, x) &= x^{n_H - 2}\left(x^2 + (\alpha + \beta)x + (\alpha - 1)\beta\right), \text{ and} \\ x\sigma(\overline{H_K}, x) &= x^{n_H - 2}\left(x^2 + (\alpha + \beta)x + \alpha(\beta - 1)\right). \end{aligned}$$

Let r_1, r_2, and r_3 be the roots of $x^3 + (\alpha + \beta + 1)x^2 + \alpha\beta x$, and t_1 and t_2 be the roots of $x^2 + (\alpha + \beta)x + (\alpha - 1)\beta$, so $r_1 = 0$,

$$\begin{aligned} r_2 &= \frac{-(\alpha + \beta + 1) + \sqrt{(\alpha + \beta + 1)^2 - 4\alpha\beta}}{2}, \\ r_3 &= \frac{-(\alpha + \beta + 1) - \sqrt{(\alpha + \beta + 1)^2 - 4\alpha\beta}}{2}, \\ t_1 &= \frac{-(\alpha + \beta) + \sqrt{(\alpha + \beta)^2 - 4(\alpha - 1)\beta}}{2}, \text{ and} \\ t_2 &= \frac{-(\alpha + \beta) - \sqrt{(\alpha + \beta)^2 - 4(\alpha - 1)\beta}}{2}. \end{aligned}$$

All these roots are real, as we already mentioned that the σ-polynomials of the graphs $\overline{H}, \overline{H_J}$ and $\overline{H_K}$ have only real roots. Now we shall prove that

$$0 = r_1 > t_1 > r_2 > t_2 > r_3.$$

It is clear that $0 = r_1 > t_1$ because the nonzero real roots of σ-polynomials are always negative. To prove the inequality $r_2 < t_1$, it suffices to verify the following list of equivalent inequalities:

$-(\alpha+\beta+1)+\sqrt{(\alpha+\beta+1)^2-4\alpha\beta} < -(\alpha+\beta)+\sqrt{(\alpha+\beta)^2-4(\alpha-1)\beta}$,

$-1+\sqrt{(\alpha+\beta+1)^2-4\alpha\beta} < \sqrt{(\alpha+\beta)^2-4(\alpha-1)\beta}$,

$1+(\alpha+\beta+1)^2-4\alpha\beta-2\sqrt{(\alpha+\beta+1)^2-4\alpha\beta} < (\alpha+\beta)^2-4(\alpha-1)\beta$,

$2+2(\alpha+\beta)-4\beta < 2\sqrt{(\alpha+\beta+1)^2-4\alpha\beta}$,

$1+\alpha-\beta < \sqrt{(\alpha+\beta+1)^2-4\alpha\beta}$,

$1+\alpha-\beta < \sqrt{(\alpha-\beta)^2+2(\alpha+\beta)+1}$.

The last inequality is clear because

$$\sqrt{(\alpha-\beta)^2+2(\alpha+\beta)+1} > \sqrt{(\alpha-\beta)^2+2(\alpha-\beta)+1} = \sqrt{(\alpha-\beta+1)^2}.$$

To see that $r_2 > t_2$ holds, it is enough to check that

$$\begin{aligned}
-\sqrt{(\alpha+\beta)^2-4(\alpha-1)\beta} &< 0 \\
&< -1+\sqrt{1+(\alpha-\beta)^2+2(\alpha+\beta)} \\
&= -1+\sqrt{(\alpha+\beta+1)^2-4\alpha\beta}.
\end{aligned}$$

Lastly, to prove that $t_2 > r_3$ holds, it is enough the verify the following sequence of equivalent inequalities where the last inequality clearly holds:

$$\begin{aligned}
1+\sqrt{(\alpha+\beta+1)^2-4\alpha\beta} &> \sqrt{(\alpha+\beta)^2-4(\alpha-1)\beta} \\
1+2\sqrt{(\alpha+\beta+1)^2-4\alpha\beta}+(\alpha+\beta+1)^2-4\alpha\beta &> (\alpha+\beta)^2-4(\alpha-1)\beta \\
\sqrt{(\alpha+\beta+1)^2-4\alpha\beta} &> \beta-\alpha-1 \\
\sqrt{(\beta-\alpha)^2+2(\alpha+\beta)+1} &> \beta-\alpha-1.
\end{aligned}$$

Now, $0 = r_1 > t_1 > r_2 > t_2 > r_3$ implies that $\sigma(\overline{H}, x)$, $x\sigma(\overline{H}, x)$, and $x\sigma(\overline{H_J}, x)$ have a common interleaver. Since j and k play symmetric roles, it is also clear that the same argument works to prove that $\sigma(\overline{H}, x)$, $x\sigma(\overline{H}, x)$, and $x\sigma(\overline{H_K}, x)$ also have a common interleaver.

Finally, we need to show that $\sigma(\overline{H_J}, x)$ and $\sigma(\overline{H_K}, x)$ are compatible. So, we shall prove that $x^2+(\alpha+\beta)x+(\alpha-1)\beta$ and $x^2+(\alpha+\beta)x+\alpha(\beta-1)$ are compatible. We use Remark 2.3.4, and show that $c(x^2+(\alpha+\beta)x+(\alpha-1)\beta)+x^2+(\alpha+\beta)x+\alpha(\beta-1)$ has all real roots for all $c > 0$.

Let $c > 0$. Then $(c+1)(\alpha-\beta)^2 > -4(c\beta+\alpha)$ which is equivalent to $(c+1)(\alpha+\beta)^2 > 4(c+1)\alpha\beta-4c\beta-4\alpha$ or $(c+1)^2(\alpha+\beta)^2 > 4(c+1)(c(\alpha-1)\beta+\alpha(\beta-1))$. This implies that the discriminant of the quadratic $(c+1)x^2+(c+1)(\alpha+\beta)x+c(\alpha-1)\beta+\alpha(\beta-1)$ is nonnegative, and hence $x^2+(\alpha+\beta)x+(\alpha-1)\beta$ and $x^2+(\alpha+\beta)x+\alpha(\beta-1)$ are compatible. This completes the proof. $\square$

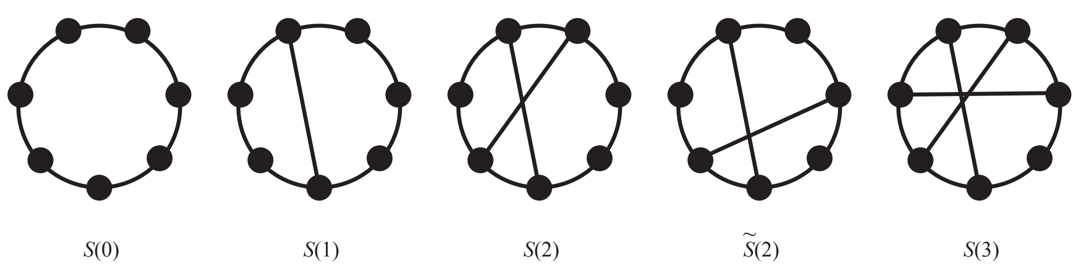

Figure 2.9: The S family

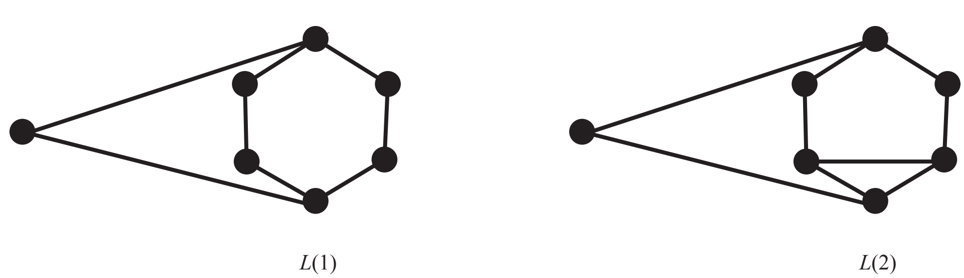

Figure 2.10: The L family

We are ready to tie everything all together in a proof of Brenti's conjecture.

Theorem 2.3.7. *Let G be a graph on n vertices. If $\chi(G) = n - 3$, then $\sigma(G, x)$ has only real roots.*

Proof. In [39], it was shown that for a graph G with n vertices, $\chi(G) = n - 3$ if and only if G is isomorphic to $H \vee K_{n-r}$ where $|V(H)| = r \leq n$ and $\overline{H}$ is a proper 3-star graph or $\overline{H}$ is one of the graphs of the F, S and L families. So, by Theorem 2.2.2(i), it suffices to show that $\sigma(H, x)$ has only real roots. As we already noted earlier, the σ-polynomials of all graphs of order at most 7 have all real roots. Hence, the result is clear if $\overline{H}$ is a graph in one of the S or L families (see Figures 2.9 and 2.10). Also, if $\overline{H}$ is in the F family, we get the desired result by Lemma 2.3.3. Finally, if $\overline{H}$ is a proper 3-star, then the result is established by Theorem 2.3.6. □

Finally, a well known result due to Newton (see [19, pp. 270–271]) states that if a real polynomial $\sum_{i=0}^{d} a_i x^i$ has only real roots then the sequence $a_0, a_1, \ldots, a_d$ is *log-concave*, that is, $a_i^2 \geq a_{i-1}a_{i+1}$ for $i = 1, \ldots, d-1$ (if a log concave sequence has no internal zeros, then it is unimodal in absolute value). Brenti [4] posed the question of whether the coefficients of σ-polynomials of all graphs are log-concave. Indeed, Read and Tutte mention the following conjecture in [48] :

Conjecture 2.3.8. [48] The σ-polynomial of any graph G is strongly log-concave.

As a corollary of Theorem 2.3.7, we show that Conjecture 2.3.8 holds for graphs with $\chi(G) \geq n - 3$.

Corollary 2.3.9. *The σ-polynomials of all graphs with $\chi(G) \geq n-3$ are log-concave.*

2.4 Graphs G with $\chi(G) \geq n - 4$

As the σ-polynomials of graphs of order n with chromatic number at least $n - 3$ have all real roots, the question remains how far down can the chromatic number go before nonreal roots arise? For chromatic number $n-5$ there are indeed such graphs. Figure 2.3 shows the two smallest examples (known as *Royle graphs* [49, pg. 265]), of order 8. Moreover, by taking the join of such a graph with a complete graph, we see that there are graphs of all order $n \geq 8$ with chromatic number $n-5$ whose σ-polynomials have a nonreal root.

So the question remains – are there any graphs of order n with chromatic number $n-4$ whose σ-polynomials have nonreal roots? In this section, we are going to study the roots of σ-polynomials of such graphs.

In [5] all graphs of order $n \leq 9$ whose σ-polynomials have a nonreal root are listed, and none of these have chromatic number $n-4$. By using Gordon Royle's database for graphs, we have verified as well that all of the σ-polynomials of the 113,272 graphs of order 10 and chromatic number 6 have all real roots, so that if there is a graph with chromatic number $n-4$ whose σ-polynomial has a nonreal root, then it has order at least 11.

In [39] Li gives a characterization of all graphs of order n such that $\chi(G) = n-4$ and we will use this characterization to prove our results. This characterization is too complicated to include here so will not present it. However we will mention a consequence of this characterization which is as follows:

Theorem 2.4.1. *[39] Let G be a graph of order n such that $\chi(G) = n-4$. Then,*

$$G \cong H \vee K_{n-r}$$

where $|V(H)| = r \leq n$ and $\overline{H}$ is either

(i) a graph of order at most 10*,*

(ii) a proper 4*-star, or*

(iii) isomorphic to one of the graphs in the M_1 or M_2 families which are depicted in Figures 2.11 and 2.12 respectively.

We begin studying the σ-polynomials of graphs G having $\chi(G) \geq n-4$ with two elementary results, the first result is obtained by simple computations.

Lemma 2.4.2. *For any graph G of order at most 8, $\sigma(G,x)$ is strongly log-concave.*

Lemma 2.4.3. *Let C_n be a cycle and u be a vertex which is not in C_n. Let G be the graph obtained from C_n and u by adding i edges between u and any i vertices of C_n. Then G contains at most i triangles.*

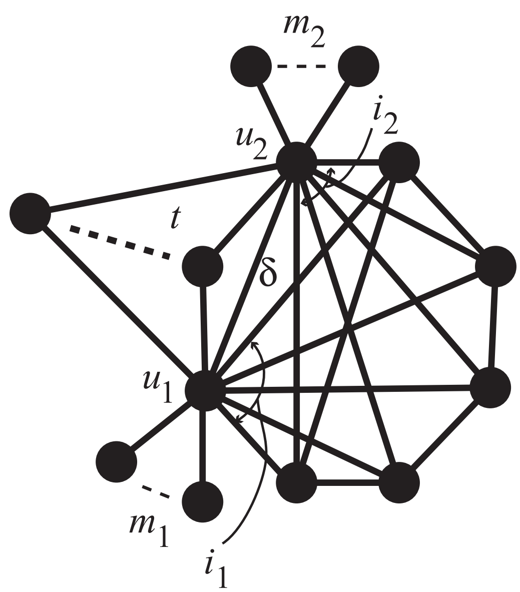

Figure 2.11: The M_1 family

Definition 2.4.1. A graph G is in the M_1 family (see Figure 2.11) if and only if G consists of a cycle C_5 and a proper 2-star graph consisting of two stars: $K_{1,m_1+i_1+t+\delta}$ and $K_{1,m_2+i_2+t+\delta}$ where $\delta = 0$ or 1 (if the universal vertices of these two stars are adjacent then $\delta = 1$; otherwise $\delta = 0$) such that these two stars have $t \geq 0$ vertices in common, and C_5 and $K_{1,m_j+i_j+t+\delta}$ have i_j $(0 \leq i_j \leq 5)$ vertices in common, and when the i_j common vertices are contained in a minimum vertex cover of C_5, $m_j+t+\delta > 0$, and otherwise, $m_j + t + \delta \geq 0$, where $j = 1, 2$.

Theorem 2.4.4. *Let G be a graph of order N in the M_1 family, then $\sigma(\overline{G}, x)$ is strongly log-concave. Moreover, if $\sigma(\overline{G}, x) = \sum b_i x^i$, then $b_{N-3} > b_{N-4}$.*

Proof. Let u_k be the stem of the star $K_{1,m_k+i_k+t+\delta}$ for $k = \{1, 2\}$. Let H be the subgraph induced by the cycle C_5 and the vertices u_1 and u_2. Suppose that $\sigma(\overline{H}, x) = \sum a_k x^k$ and $\sigma(\overline{G}, x) = \sum b_k x^k$, and $|V(H)| = n$ and $|V(G)| = N$. Note that $\sigma(\overline{H}, x)$ is logconcave by Lemma 2.4.2. Define $\alpha_k = b_{N-k} - a_{n-k}$ for $1 \leq k \leq 4$ and let x_k be the number of edges of the cycle C_5 whose both endpoints are adjacent to u_k. Then we get, by counting the subgraphs,

$$
\begin{aligned}
\alpha_1 &= m_1 + m_2 + 2t, \\
\alpha_2 &= \delta t + m_2(5 + i_1) + m_1(5 + i_2) + t(10 + i_1 + i_2) + t(m_1 + m_2) + m_1 m_2, \\
\alpha_3 &= 5\delta t + x_1(m_2 + t) + x_2(m_1 + t) + 5(m_1 m_2 + m_1 + m_2) + 5t(m_1 + m_2) \\
&\quad +3(m_2 i_1 + m_1 i_2) + t(10 + 3i_1 + 3i_2) \\
\alpha_4 &= 5\delta t + 2t(x_1 + x_2) + 2(x_2 m_1 + x_1 m_2) + i_1(m_2 + t) + i_2(m_1 + t) \\
&\quad +5(m_1 m_2 + t m_2 + t m_1).
\end{aligned}
$$

It is clear that $a_{n-1} = \delta + 5 + i_1 + i_2$ and $\alpha_1^2 + 2a_{n-1}\alpha_1 \geq \alpha_2$. Also, $a_{n-1}^2 > a_{n-2}$ holds by the strong log-concavity of $\sigma(\overline{H}, x)$. Hence, we obtain

$$b_{N-1}^2 = a_{n-1}^2 + \alpha_1^2 + 2a_{n-1}\alpha_1 > a_{n-2} + \alpha_2 = b_{N-2} b_N$$

since $b_N = 1$. Now, in order to find formulas for the other coefficients, we need to introduce some other parameters which are in terms of the number of certain kinds of subgraphs. Let y_2 be the number of $2K_2$'s in H such that one of the edges contains u_1 and a vertex from C_5, and the other edge contains u_2 and another vertex from C_5. Suppose that u_1 and u_2 have j common neighbors in C_5. So, we have

$$a_{n-2} = \delta j + x_1 + x_2 + 5(1+\delta) + 3(i_1+i_2) + y_2.$$

Let $w_3 = \eta_H(K_4)$ and y_3 be the number of $K_3 \cup K_2$'s in H such that both K_3 and K_2 contain at least one the vertices u_1 and u_2. Also, let z_3 be the number of matchings of size 3 in H which contain both u_1 and u_2, and u_1 and u_2 are nonadjacent to each other.

Then, we have

$$a_{n-3} = w_3 + 3\delta j + 2x_1 + 2x_2 + y_3 + 5\delta + i_1 + i_2 + z_3.$$

Now, with the aid of Maple we find that $b_{N-2}^2 - b_{N-1}b_{N-3}$ is equal to

$5(5-w_3) + 5\delta(5-j) + 5(2y_2 - z_3) + m_2(20m_2 - w_3) + m_1(20m_1 - w_3) + (i_1 + i_2)(25 - w_3) + 16i_1i_2 - 5y_3 + m_2i_2(3i_1 - x_1) + m_1i_1(3i_2 - x_2) + m_1t(2m_1i_2 - x_2) + m_2t(2m_2i_1 - x_1) + (7i_2 - x_2)(m_1^2 + 2t^2 + m_1\delta) + (7i_1 - x_1)(m_2^2 + 2t^2 + m_2\delta) + (i_1 + i_2)(4x_1 + 4x_2 - y_3) + \delta(20\delta - w_3) + m_2(24i_2 - y_3) + m_1(24i_1 - y_3) + (10y_2 - z_3)(\delta + m_2 + m_1 + 2t) + (6y_2 - z_3)(i_1 + i_2) + \delta(24i_1 - y_3) + 2t(40t - w_3 - y_3) + P(i_k, m_k, t, j, \delta, x_k, y_3, w_3)$

where $P(i_k, m_k, t, j, \delta, x_k, y_3, w_3)$ is a polynomial with nonnegative coefficients.

It is clear that j and w_3 can be at most 5. By Lemma 2.4.3, $i_k \geq x_k$ for $k = 1, 2$. Removal of any two vertices of C_5 leaves a graph with at most two edges and therefore $2y_2 \geq z_3$ holds. Now, we shall show that

$$y_3 \leq \min\{3x_1, x_1i_2, 3i_2\} + \min\{3x_2, x_2i_1, 3i_1\}. \tag{2.3}$$

Let y_3' (resp. y_3'') be the number of $K_3 \cup K_2$'s in H such that K_3 contains the vertex u_1 (resp. u_2) and K_2 contains the vertex u_2 (resp. u_1). Since K_3 and K_2 are disjoint, we have $y_3 = y_3' + y_3''$. So, to prove the inequality (2.3), it suffices to show that $y_3' \leq \min\{3x_1, x_1i_2, 3i_2\}$ and $y_3'' \leq \min\{3x_2, x_2i_1, 3i_1\}$. First, let us show that $y_3' \leq \min\{3x_1, x_1i_2, 3i_2\}$. Observe that $y_3' \leq 3x_1$ because we have x_1 choices to pick a triangle (such triangle contains u_1 and two vertices of C_5) and once we choose the triangle we have at most three choices to pick the edge (such edge contains u_2 and a vertex of C_5). Similarly, we obtain $y_3' \leq x_1i_2$. Furthermore, we can consider first picking an edge (we would have i_2 choices) and then picking a triangle (we would have at most three choices for the triangle). So, we get $y_3' \leq 3i_2$. Thus, we obtain $y_3' \leq \min\{3x_1, x_1i_2, 3i_2\}$. The proof for $y_3'' \leq \min\{3x_2, x_2i_1, 3i_1\}$ is similar.

The inequality (2.3) immediately implies that $y_3 \leq 3(x_1 + x_2) \leq 30$. Moreover, since $x_k \leq i_k$ we get $y_3 \leq 2i_1i_2$. Lastly, observe that y_3 is zero whenever i_1 or i_2 is zero, hence we also obtain $y_3 \leq 18i_k$ for $k = 1, 2$. Now, all these together yields $b_{N-2}^2 > b_{N-1}b_{N-3}$.

Let $y_4 = \eta_{\overline{H}}(K_4 \uplus K_2)$, $z_4 = \eta_{\overline{H}}(2K_3)$ and w_4 be the number of $K_3 \cup 2K_2$ in H such that K_3 contains exactly one vertices of u_1 and u_2, and one K_2 is an edge of the cycle C_5, and the other K_2 contains exactly one vertices of u_1 and u_2 and a vertex of C_5. So, we have

$$a_{n-4} = y_4 + z_4 + w_4 + j.$$

Now,

$$\alpha_3 - \alpha_4 = (2i_1 - x_1)(m_2 + t) + (2i_2 - x_2)(m_1 + t) + 5(m_1 + m2) + 10t.$$

Hence, $\alpha_3 \geq \alpha_4$ because $i_k \geq x_k$. Moreover, one can check that $j \leq \min\{i_1, i_2\}$, $w_4 \leq y_3$, $y_4 \leq z_3$ and $z_4 \leq \min\{2x_1, 2x_2\}$. So, $a_{n-3} \geq a_{n-4}$ holds. If $m_1 + m_2 + t > 0$ then the strict inequality $\alpha_3 > \alpha_4$ holds and we get $b_{N-3} > b_{N-4}$. Now suppose that $m_1 + m_2 + t = 0$. In this case $i_1 + i_2 > 0$ must hold because otherwise $G \cong K_2 \uplus C_5$ and $G \cong K_2 \uplus C_5$ do not belong to M_1 family. So, $i_1 + i_2 > j$ and we get the strict inequality $a_{n-3} > a_{n-4}$. Thus, we obtain again that $b_{N-3} > b_{N-4}$.

Lastly, let us prove that $b_{N-3}^2 > b_{N-2}b_{N-4}$. First of all, $a_{n-3}^2 > a_{n-2}a_{n-4}$ holds by the strong log-concavity of $\sigma(\overline{H}, x)$. Moreover, $\alpha_3 a_{n-3} \geq \alpha_2 a_{n-4}$ because $a_{n-3} \geq a_{n-4}$ and $\alpha_3 \geq \alpha_2$. Hence, it suffices to prove that $\alpha_3^2 + \alpha_3 a_{n-3} \geq \alpha_2\alpha_4 + \alpha_4 a_{n-2}$. Now, with the aid of Maple, we find that $\alpha_3^2 + \alpha_3 a_{n-3} - \alpha_2\alpha_4 - \alpha_4 a_{n-2}$ is equal to

$$5m_1(5m_1i_2 - x_2i_1) + 5m_2(5m_2i_1 - x_1i_2) + 5m_1(5m_1 - \delta x_2) + 5m_2(5m_2 - \delta x_1) + (3z_3 - y_2)(m_2i_1 + m_1i_2) + 5t(20t - \delta y_2) + 2t(8ti_1i_2 - x_1y_2 - x_2y_2) + 2m_2(4m_2i_1^2 - x_1y_2) + 2m_1(4m_1i_2^2 - x_2y_2) + t(50t - y_2)(i_1 + i_2) + m_1m_2(24m_2i_1 - 5y_2) + tm_1(24ti_2 - 5y_2) + tm_2(24ti_1 - 5y_2) + Q(\delta, t, j, m_k, i_k, x_k, y_2, y_3, z_3, w_3)$$

where $Q(\delta, t, j, m_k, i_k, x_k, y_2, y_3, z_3, w_3)$ is a polynomial with nonnegative coefficients.

Now, one can easily check that $y_2 \leq z_3$ and $y_2 \leq \min\{4i_1, 4i_2\} \leq 20$. Also, as we already noted earlier, $x_k \leq i_k \leq 5$ holds. Therefore, the result is established.

$\square$

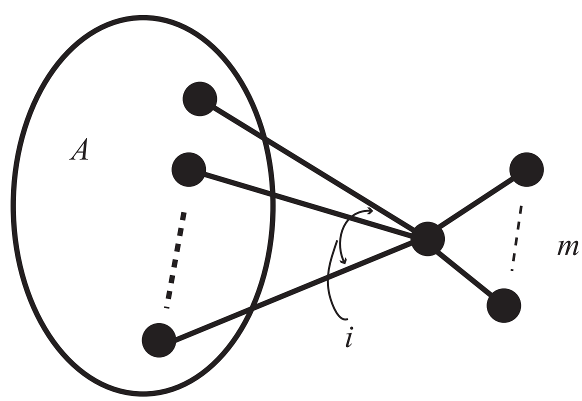

Figure 2.12: M_2 family

Definition 2.4.2. A graph G is in the M_2 family (see Figure 2.12) if and only if it consists of a star $K_{1,i+m}$ and a graph A which belongs to the L or S families such that

$K_{1,i+m}$ and A have i $(0 \leq i \leq |V(A)|)$ vertices in common, and when the i common vertices are contained in a minimum vertex cover of A, $m > 0$; otherwise, $m \geq 0$.

The following two results are obtained by computer aid.

Lemma 2.4.5. *Let A be a graph belonging to S or L families which are depicted in Figure 2.9 and Figure 2.10 respectively. Let H be graph of order 8 which contains a vertex v such that $H - v \cong A$. If $\sigma(\overline{H}, x) = \sum a_j x^j$ then $a_5 > a_4$.*

Lemma 2.4.6. *Let A be graph such that either A belongs to the S family or A is equal to $L(1)$. Then $\eta_A(2K_2) > \eta_A(3K_2)$.*

For a vertex u of a graph G, *the edge neighbourhood of* u, denoted by $EN_G(u)$, is defined as the set of all edges of G which contain the vertex u.

Theorem 2.4.7. *Let G be a graph of order N in M_2 family, then $\sigma(\overline{G}, x)$ has only real roots. Moreover, if $\sigma(\overline{G}, x) = \sum b_i x^i$, then $b_{N-3} > b_{N-4}$.*

Proof. Let v be the vertex of G which is adjacent to m leaves and i vertices of A. Let H be the subgraph induced by A and v. First, let us show that $\sigma(\overline{G}, x)$ has only real roots. By applying the recursive formula (Lemma 2.1.1) for σ-polynomials on the pendant edges of G, we obtain

$$\sigma(\overline{G}, x) = x^m(\sigma(\overline{H}, x) + m\sigma(\overline{A}, x)).$$

Let $u_1, \ldots, u_i$ be the vertices of A such that vu_j is an edge of G for $j = 1, \ldots, i$. Also, we apply the recursive formula on the edges vu_j for $j = 1, \ldots, i$ and we find that

$$\sigma(\overline{H}, x) = x\sigma(\overline{A}, x) + \sum_{j=1}^{i} \sigma(\overline{A_j}, x)$$

where A_j is a subgraph obtained from A by deleting some of the edges in $EN_G(u_j)$, that is, $A_j = A - S_j$ for some $S_j \subseteq EN_G(u_j)$. So,

$$\sigma(\overline{G}, x) = x^m \left((x+m)\sigma(\overline{A}, x) + \sum_{j=1}^{i} \sigma(\overline{A_j}, x) \right).$$

Let us define a family of graphs $\mathcal{G}$ as follows:

$$\mathcal{G} := \{A - S_j : \ A \in L \cup S \,\text{and}\, S_j \subseteq EN_G(u_j) \,\text{for some vertex}\, u_j \,\text{of}\, A\}.$$

Given a graph G, let $r_1(G) \leq r_2(G) \leq \ldots$ be the root sequence of $\sigma(G, x)$. Now let

$$R_i(\mathcal{G}) := \{r_i(G) : \ G \in \mathcal{G}\}.$$

With the aid of Maple, we find that $R_6(\mathcal{G}) = R_7(\mathcal{G}) = \{0\}$ and approximately

$$\begin{aligned}
-10 < \min R_1(\mathcal{G}) &\approx -9.063 \quad \text{and} \quad \max R_1(\mathcal{G}) \approx -6.274 < -5;\\
-5 < \min R_2(\mathcal{G}) &\approx -4.475 \quad \text{and} \quad \max R_2(\mathcal{G}) \approx -3.149 < -2;\\
-2 < \min R_3(\mathcal{G}) &\approx -1.880 \quad \text{and} \quad \max R_3(\mathcal{G}) \approx -1.142 < -1;\\
-1 < \min R_4(\mathcal{G}) &\approx -0.530 \quad \text{and} \quad \max R_4(\mathcal{G}) \approx -0.195 < -0.15;\\
-0.15 < \min R_5(\mathcal{G}) &\approx -0.134 \quad \text{and} \quad \max R_5(\mathcal{G}) = 0.
\end{aligned}$$

(Note that $\max R_5(\mathcal{G})$ is precisely zero because σ-polynomials always have nonpositive roots and R_5 must contain at least one zero, as the graphs in $S \cup L$ have chromatic number 4 and hence their σ-polynomials have exactly three non-zero roots. However, for our purposes, it will not matter whether it is precisely zero).

Thus, the polynomials

$$(x+m)\sigma(\overline{A}, x) \ \text{ and } \ \sigma(\overline{A_1}, x), \ldots, \sigma(\overline{A_i}, x)$$

are compatible for $m \geq 10$ because the sequence

$$0 = 0 = 0 > -0.15 > -1 > -2 > -5 > -10$$

interleaves the root sequences of all those polynomials. Therefore, $\sigma(\overline{G}, x)$ has only real roots by Theorem 2.3.5. If $m \leq 9$ there are only finitely many cases and those cases are verified by computer aided computations.

Now we shall show that $b_{N-3} > b_{N-4}$. Let $\sigma(\overline{H}, x) = \sum a_j x^j$ and $n = |V(H)| = 8$. We consider two cases:

Case 1: $A = L(2)$.

The matching polynomial of A is $m(A, x) = 1 + 9x + 21x^2 + 10x^3$. Note that $\eta_G(K_4)$ is equal to $\eta_H(K_4)$. Since $L(2)$ has exactly one triangle, we have $\eta_G(K_3 \cup K_2) = \eta_H(K_3 \cup K_2) + m$. Also, $\eta_G(3K_2) = \eta_H(3K_2) + m\eta_A(K_2) = \eta_H(3K_2) + 21m$. Therefore,

$$b_{N-3} = a_{n-3} + 22m.$$

G does not contain any subgraph which is isomorphic to $K_5, K_4 \cup K_2$ or $2K_3$ (and neither does H). Also,

$$\eta_G(K_3 \cup 2K_2) = \eta_H(K_3 \cup 2K_2) + m\eta_A(K_3 \cup K_2) = \eta_H(K_3 \cup 2K_2) + 3m$$

and

$$\eta_G(4K_2) = \eta_H(4K_2) + m\eta_A(3K_2) = \eta_H(4K_2) + 10m.$$

Thus,

$$b_{N-4} = a_{n-4} + 13m.$$

By Lemma 2.4.5, we know that $a_{n-3} > a_{n-4}$. Now, since m is a nonnegative integer we obtain that $b_{N-3} > b_{N-4}$.

Case 2: $A = L(1)$ or $A \in S$.

First note that $\eta_G(K_4) = \eta_H(K_4) = 0$. Also, $\eta_G(K_3 \,\dot\cup\, K_2) = \eta_H(K_3 \,\dot\cup\, K_2)$ and $\eta_G(3K_2) = \eta_H(3K_2) + m\eta_A(2K_2)$. Therefore,

$$b_{N-3} = a_{n-3} + m\eta_A(2K_2).$$

Now, G does not contain any subgraph isomorphic to K_5, $K_4 \dot\cup K_2$ or $2K_3$ (and neither does H). Also, $\eta_G(K_3 \,\dot\cup\, 2K_2) = \eta_H(K_3 \,\dot\cup\, 2K_2)$ and $\eta_G(4K_2) = \eta_H(4K_2) + m\eta_A(3K_2)$. Hence,

$$b_{N-4} = a_{n-4} + m\eta_A(3K_2).$$

By Lemma 2.4.5, we know that $a_{n-3} > a_{n-4}$. Furthermore, by Lemma 2.4.6, $\eta_A(2K_2) > \eta_A(3K_2)$. Thus, the result follows.

□

Lemma 2.4.8. *Let G be a graph with $\alpha_0(G) = 4$ and a minimum vertex cover S. If $\langle S \rangle_G$ is not isomorphic to one of the graphs*

$$P_4,\ K_3 \,\dot\cup\, K_1,\ 2K_2,\ P_3 \,\dot\cup\, K_1,\ \textit{or}\ K_2 \,\dot\cup\, 2K_1$$

then, $\sigma(\overline{G}, x)$ has all real roots.

Proof. We consider three cases.

Case 1: The maximum degree of $\langle S \rangle_G$ is 3.

In this case there is a vertex v of S such that v is not adjacent to any vertex of $S - \{v\}$ in $\overline{G}$. Let $H = \langle V(G) - \{S - \{v\}\} \rangle_{\overline{G}}$ and $\tilde{H} = \langle V(G) - \{v\} \rangle_{\overline{G}}$, then we have $\overline{G} = H \cup \tilde{H}$. Now, by Theorem 2.3.7, both $\sigma(H, x)$ and $\sigma(\tilde{H}, x)$ have all real roots because $\chi(H) \geq |V(H)| - 1$ and $\chi(\tilde{H}) \geq |V(\tilde{H})| - 3$. Moreover, $H \cap \tilde{H}$ is a complete graph in $\overline{G}$. Thus, $\sigma(\overline{G}, x)$ has all real roots by the Complete Cut-set Theorem.

Case 2: The maximum degree of $\langle S \rangle_G$ is at most 2.

This means that $\langle S\rangle_G$ is a disjoint union of cycles and paths. So $\langle S\rangle_G$ is isomorphic to $P_4,\ K_3 \cup K_1,\ 2K_2,\ P_3 \cup K_1,\ K_2 \cup 2K_1,\ 4K_1$ or C_4. By the assumption, the first five of these cases are excluded. So we need to consider the cases $4K_1$ and C_4.

Subcase 1: S induces an independent set in G.

Then G is a triangle-free graph and we are done by Theorem 2.2.1(iv).

Subcase 2: $\langle S\rangle_G \cong C_4$.

Then $\langle S\rangle_{\overline{G}} \cong 2K_2$. Let $S = \{u_1, u_2, v_1, v_2\}$ and u_1u_2 and v_1v_2 be edges of $\overline{G}$. Let $H = \langle V(G) - \{v_1, v_2\}\rangle_{\overline{G}}$ and $\tilde{H} = \langle V(G) - \{u_1, u_2\}\rangle_{\overline{G}}$, then $\overline{G} = H \cup \tilde{H}$. Notice that $\chi(H) \geq |V(H)| - 2$ and $\chi(\tilde{H}) \geq |V(\tilde{H})| - 2$, so by Theorem 2.3.7, the σ-polynomials of H and $\tilde{H}$ have all real roots. Thus, the result follows again from the Complete Cut-set Theorem. □

The following result is folklore.

Theorem 2.4.9. *A product of log-concave polynomials with nonnegative coefficients and no internal zero coefficients is again log-concave.* □

The results proven in this section yield the following.

Theorem 2.4.10. *If $G \cong H \vee K_{n-r}$ is a graph of order n with $\chi(G) \geq n - 4$ where $\overline{H}$ is not equal to one of the graphs which are excluded in Lemma 2.4.8, then $\sigma(G, x)$ is log-concave.* □

2.5 Density of the real roots of σ-polynomials in $(-\infty, 0)$

We have seen that most of the σ-roots of small graphs are real, and Figure 2.2 suggests that the real roots may fill up to the negative real axis. In this section, we show that this is indeed the case, by considering related polynomials as well.

For a sequence $\{f_n(x)\}$ of polynomials, z is called a *limit of roots* of $\{f_n(x)\}$ if there is a sequence $\{z_n\}$ such that $f_n(z_n) = 0$ and z_n converges to z. Let $P_0(x), P_1(x), \ldots$

be a sequence of polynomials in $\mathbb{C}[x]$ which satisfy the recursion of degree k

$$P_{n+k}(x) = -\sum_{j=1}^{k} f_j(x) P_{n+k-j}(x) \tag{2.4}$$

where the f_j are polynomials. The *characteristic equation* of this recursion is

$$\lambda^k + \sum_{j=1}^{k} f_j(x)\lambda^{k-j} = 0. \tag{2.5}$$

Let $\lambda_1(x), \ldots, \lambda_k(x)$ be the roots of the characteristic equation. If the $\lambda_j(x)$ are distinct for a particular x, then it is well known that the solution of the recursion in (2.4) has the form

$$P_n(x) = \sum_{j=1}^{k} \alpha_j(x)\lambda_j(x)^n. \tag{2.6}$$

If there are repeated roots values at x, (2.6) is modified in the usual way, (e.g., if the root λ has multiplicity t then the term $\alpha_1\lambda^n + \alpha_2\lambda^n + \cdots + \alpha_t\lambda^n$ is replaced by a term $\alpha_1\lambda^n + n\alpha_2\lambda^n + \cdots + n^{t-1}\alpha_t\lambda^n$). The $\alpha_j(x)$ are determined in any event by solving the k linear equations in the $\alpha_j(x)$ obtained by letting $n = 0, 1, \ldots, k-1$ in (2.6) or its variant.

We define the *nondegeneracy conditions* on the recursive family of polynomials in (2.4) as follows

(i) $\{P_n\}$ does not satisfy a recursion of order less than k.

(ii) For no pair $i \neq j$ is $\lambda_i(x) \equiv \omega\lambda_j(x)$ for some $\omega \in \mathbb{C}$ of unit modulus.

The following result is due to Beraha, Kahane and Weiss [3] (see also [13] for how it can be applied to functions of the form given in Equation (2.6)).

Theorem 2.5.1 (Beraha-Kahane-Weiss Theorem, [3])**.** *Suppose that* $\{P_n(x)\}$ *is a sequence of polynomials which satisfies* (2.4) *and the nondegeneracy requirements. Then* z *is a limit of roots of* $\{P_n\}$ *if and only if one of the following holds in* (2.6)*:*

(i) two or more of the $\lambda_i(z)$ *are of equal modulus and strictly greater in modulus than the others (if any).*

(ii) for some j, $\lambda_j(z)$ *has modulus strictly greater than all the other* $\lambda_i(z)$ *have and* $\alpha_j(z) = 0$.

Theorem 2.5.2. *Let* G *be any graph with an identified vertex* v*. We define a family of graphs,* $\mathfrak{F}(G, v)$*, which consists of* $G_0, G_1, G_2, \ldots$ *where* $G_0 = G$*,* G_1 *is obtained from* G *by attaching a leaf vertex* v_1 *to* v*, and for* $i \geq 1$*,* G_{i+1} *is obtained from* G_i *by attaching a new leaf vertex* v_{i+1} *to* v_i*. Then the roots of adjoint polynomials of graphs in* $\mathfrak{F}(G, v)$ *are dense in* $(-4, 0)$*.*

Proof. First note that by the edge deletion-contraction formula we have

$$\begin{aligned} h(G_n, x) &= h(G_n - v_{n-1}v_n, x) + h(G_n \odot v_{n-1}v_n, x) \\ &= h(G_{n-1} \cup K_1, x) + h(G_{n-2} \cup K_1, x) \\ &= xh(G_{n-1}, x) + xh(G_{n-2}, x). \end{aligned}$$

For simplicity, let $f_n(x) = h(G_n, x)$. Now we have a sequence of polynomials $f_1(x), f_2(x), \ldots$ satisfying a recursion of degree 2. So the characteristic equation of this recursion is

$$\lambda^2 - x\lambda - x = 0.$$

The roots of this characteristic equation are

$$\lambda_1(x) = \frac{x + \sqrt{x^2 + 4x}}{2} \quad \text{and} \quad \lambda_2(x) = \frac{x - \sqrt{x^2 + 4x}}{2}.$$

It is easy to check that the nondegeneracy conditions are satisfied. Therefore, by Beraha-Kahane-Weiss Theorem, every $x \in \mathbb{C}$ satisfying

$$\left|\frac{x+\sqrt{x^2+4x}}{2}\right| = \left|\frac{x-\sqrt{x^2+4x}}{2}\right| \tag{2.7}$$

is a limit of the roots of the sequence $\{f_n(z)\}_{n=1}^{\infty}$. Observe that $x \in \mathbb{C}$ satisfies (2.7) if and only if

$$\left|x+\sqrt{x^2+4x}\right| = \left|x-\sqrt{x^2+4x}\right|$$

or equivalently,

$$\left|1+\frac{\sqrt{x^2+4x}}{x}\right| = \left|1-\frac{\sqrt{x^2+4x}}{x}\right| \tag{2.8}$$

when $x \neq 0$. Now, $x \in \mathbb{C}$ is a solution of (2.8) if and only if $\frac{\sqrt{x^2+4x}}{x}$ is equidistant from 1 and -1, that is, $\frac{\sqrt{x^2+4x}}{x}$ is on the imaginary axis. For $a \in \mathbb{R}$,

$$\frac{\sqrt{x^2+4x}}{x} = ai \quad \Longleftrightarrow \quad \frac{x^2+4x}{x^2} = -a^2 \quad \Longleftrightarrow \quad x = -\frac{4}{1+a^2}.$$

Thus, $x = -\frac{4}{1+a^2}$ is a limit of the roots of $\{f_n(z)\}_{n=1,2,\ldots}$ for every real number a. Therefore, the roots of $\{f_n(z)\}_{n=1,2,\ldots}$ are dense in $(-4, 0)$. $\square$

Given a graph G of order n, the *adjacency matrix of* G, $A(G)$, is the $n \times n$ matrix with ij-entry equal to 1 if the i-th vertex of G is adjacent to the j-th, and equal to 0 otherwise. The *characteristic polynomial* $\phi(G, x)$ of G is defined by

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

It is known that (see, for example, [31, pg. 2]) if G is a forest then $\phi(G, x) = m(G, x)$.

A tree T is called a *balanced rooted tree with a root* w [35] if T has a vertex w and there exist integers $n_1, n_2, \ldots, n_k$ such that $V(T) \setminus \{w\}$ can be partitioned into k

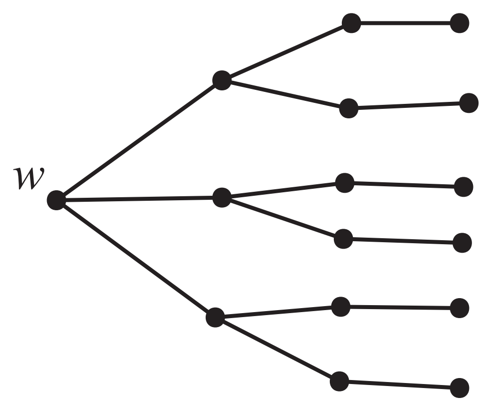

Figure 2.13: A balanced rooted tree $T(3, 2, 1)$ with a root w.

subsets $A_1, A_2, \ldots, A_k$, where w has exactly n_k neighbours in A_k and each vertex in A_i has exactly n_{i-1} neighbours in A_{i-1} for $2 \leq i \leq k$, see, for example, Figure 2.13. We will denote T by $T(n_k, n_{k-1}, \ldots, n_1)$. Note that if $n_i = n$ for every i with $1 \leq i \leq k$ then $T(n_k, n_{k-1}, \ldots, n_1)$ is a complete n-ary tree on $\frac{n^{k+1}-1}{n-1}$ vertices and we denote it by T_n^k. The *front divisor of* $T(n_k, n_{k-1}, \ldots n_1)$ is a directed graph $D(n_k, n_{k-1}, \ldots n_1)$ with vertices $v_0, v_1, \ldots v_k$; a vertex v_i is joined by n_{k-i} parallel arcs to v_{i+1} and v_{i+1} is joined by one arc to v_i, for $0 \leq i \leq k-1$. In [35] it was shown that for $k \geq 2$

$$\phi(D(n_k, n_{k-1} \ldots n_1), x) = x\, \phi(D(n_{k-1}, n_{k-2} \ldots n_1), x) - n_k\, \phi(D(n_{k-2}, n_{k-1} \ldots n_1), x).$$

Since the characteristic polynomial of $D(n_k, n_{k-1}, \ldots n_1)$ divides the characteristic polynomial of $T(n_k, n_{k-1}, \ldots n_1)$ (see [35]), it follows that the roots of the characteristic polynomial of $T(n_k, n_{k-1}, \ldots n_1)$ include the roots of the following recursively defined polynomial $P_k(x)$:

$$P_j(x) = x\, P_{j-1}(x) - n_j\, P_{j-2}(x) \tag{2.9}$$

where $j = 2, \ldots, k$.

Theorem 2.5.3. *The roots of σ-polynomials are dense in* $(-\infty, 0)$.

Proof. Since every triangle-free graph G satisfies $\sigma(\overline{G}, -x^2) = (-x)^n\, m(G, x)$, it suffices to show that the roots of matching polynomials of triangle-free graphs are dense in $(0, \infty)$. Obviously, trees are triangle-free graphs. Also, as we already mentioned, the matching polynomials of trees are equal to their characteristic polynomials [31]. So it suffices to show that the roots of characteristic polynomials of complete n-ary trees are dense in $(0, \infty)$. Let n be a fixed positive integer. By the formula given in (2.9), the roots of the characteristic polynomial of T_n^k include the roots of the polynomial $P_k(x)$ which is defined recursively as follows:

$$P_k(x) = x\, P_{k-1}(x) - n\, P_{k-2}(x)$$

for $k \geq 2$. Now we have a sequence of polynomials $P_2(x), P_3(x), \ldots$ satisfying a recursion of degree 2. So the characteristic equation of this recursion is

$$\lambda^2 - x\lambda + n = 0.$$

The roots of this characteristic equation are

$$\lambda_1(x) = \frac{x + \sqrt{x^2 - 4n}}{2} \quad \text{and} \quad \lambda_2(x) = \frac{x - \sqrt{x^2 - 4n}}{2}.$$

It is easy to check that the nondegeneracy conditions are satisfied. Therefore, by Beraha-Kahane-Weiss Theorem, every $x \in \mathbb{C}$ satisfying

$$\left| \frac{x + \sqrt{x^2 - 4n}}{2} \right| = \left| \frac{x - \sqrt{x^2 - 4n}}{2} \right| \tag{2.10}$$

is a limit of the roots of the sequence $\{P_k(z)\}_{k=2}^{\infty}$. Observe that $x \in \mathbb{C}$ satisfies (2.10) if and only if

$$\left|x + \sqrt{x^2 - 4n}\right| = \left|x - \sqrt{x^2 - 4n}\right|$$

or equivalently,

$$\left|1 + \frac{\sqrt{x^2 - 4n}}{x}\right| = \left|1 - \frac{\sqrt{x^2 - 4n}}{x}\right| \tag{2.11}$$

Now, $x \in \mathbb{C}$ is a solution of (2.11) if and only if $\frac{\sqrt{x^2-4n}}{x}$ is equidistant from 1 and -1, that is, $\frac{\sqrt{x^2-4n}}{x}$ is on the imaginary axis. For $a \in \mathbb{R}$,

$$\frac{\sqrt{x^2 - 4n}}{x} = ai \quad \Longleftrightarrow \quad \frac{x^2 - 4n}{x^2} = -a^2 \quad \Longleftrightarrow \quad x = \pm 2\sqrt{\frac{n}{1 + a^2}}.$$

Thus, $x = \pm 2\sqrt{\frac{n}{1+a^2}}$ is a limit of the roots of $\{P_k(z)\}_{k=2}^{\infty}$ for every real number a. Therefore, the roots of $\{P_k(z)\}_{k=2}^{\infty}$ are dense in $(-2\sqrt{n}, 2\sqrt{n})$. Now, letting $n \to \infty$, we obtain that the roots of the characteristic polynomials of complete k-ary trees are dense in $\mathbb{R}$. $\square$

Chapter 3

Chromatic Polynomials

In this chapter we will present new bounds for chromatic polynomials and their roots.

3.1 New Bounds for the Chromatic Polynomial

Let $\mathcal{G}_k(n)$ be the family of all k-chromatic graphs of order n. Given a natural number $x \geq k$, it is natural to inquire about the maximum number of x-colourings among k-chromatic graphs of order n, that is, among graphs in $\mathcal{G}_k(n)$. Tomescu [57] studied this problem and showed the following:

Theorem 3.1.1. *[57, pg. 239] Let G be a graph in $\mathcal{G}_k(n)$. Then for every $x \in \mathbb{N}$,*

$$\pi(G, x) \leq (x)_{\downarrow k}\, x^{n-k}.$$

Moreover, when $x \geq k$, the equality is achieved if and only if $G \cong K_k \cup (n-k)K_1$ (the graph consisting of a k-clique plus $n-k$ isolated vertices).

The next natural problem is to maximize the number of x-colourings of a graph over the family of *connected* k-chromatic graphs of order n (we denote this family by $\mathcal{C}_k(n)$). Interestingly, the problem becomes much more complicated when the connectedness condition is imposed. The answer is trivial when $x = k = 2$, as any 2-chromatic connected graph has precisely two 2-colourings. It is well known that (see, for example, [24]) if G is a connected graph of order n then $\pi(G, x) \leq x(x-1)^{n-1}$ for every $x \in \mathbb{N}$ and furthermore, when $x \geq 3$ the equality is achieved if and only if

G is a tree. Therefore, for $k = 2$ and $x \geq 3$, the maximum number of x-colourings of a graph in $\mathcal{C}_2(n)$ is equal to $x(x-1)^{n-1}$ and extremal graphs are trees.

Tomescu settled the problem for $x = k = 3$ in [56] and later extended it for $x \geq k = 3$ in [59] by showing that if G is a graph in $\mathcal{C}_3(n)$ then

$$\pi(G, x) \leq (x-1)^n - (x-1) \quad \text{for odd } n$$

and

$$\pi(G, x) \leq (x-1)^n - (x-1)^2 \quad \text{for even } n$$

for every integer $x \geq 3$ and furthermore the extremal graph is the odd cycle C_n when n is odd and an odd cycle with a vertex of degree 1 attached to the cycle (denoted C_{n-1}^1) when n is even.

One might subsequently think that maximizing the number of x-colourings of a graph in $\mathcal{C}_k(n)$ should depend on the value of k. Let $\mathcal{C}_k^*(n)$ be the set of all graphs in $\mathcal{C}_k(n)$ which have size $\binom{k}{2} + n - k$ and clique number k (that is, $\mathcal{C}_k^*(n)$ consists of graphs which are obtained from a k-clique by recursively attaching leaves). In [55] Tomescu considered the problem for $x = k \geq 4$ and conjectured the following (see also [58, 59]):

Conjecture 3.1.2. [55] Let G be a graph in $\mathcal{C}_k(n)$ where $k \geq 4$. Then

$$\pi(G, k) \leq k!\,(k-1)^{n-k},$$

or, equivalently, $a_k(G) \leq (k-1)^{n-k}$, with the extremal graphs belong to $\mathcal{C}_k^*(n)$.

The authors in [24] mention the following conjecture which broadly extends Conjecture 3.1.2 to all nonnegative integers x:

Conjecture 3.1.3. [24, pg. 315] Let G be a graph in $\mathcal{C}_k(n)$ where $k \geq 4$. Then for every $x \in \mathbb{N}$,

$$\pi(G,x) \leq (x)_{\downarrow k}(x-1)^{n-k}.$$

Moreover, for $x \geq k$, the equality holds if and only if G belongs to $\mathcal{C}_k^*(n)$.

It is not hard to see that Conjecture 3.1.3 implies Theorem 3.1.1 because the chromatic polynomial of a graph is equal to the product of chromatic polynomials of its connected components. However, the problem of maximizing the number of colourings appears more difficult when graphs are connected, since the answer to this problem depends on the value of k (the structure of extremal graphs seem to be different for $k = 2$ and 3). As Tomescu points out [57], the difficulty may lie in the lack of a good characterization of k-*critical* graphs (those minimal with respect to k-chromaticity) when $k \geq 4$.

If $G \in \mathcal{C}_k^*(n)$ then $\pi(G,x) = (x)_{\downarrow k}\,(x-1)^{n-k}$, as one can first colour the clique of order k and then recursively colour the remaining vertices (which have only one coloured neighbour). On the other hand, one can see that if $\pi(G,x) = (x)_{\downarrow k}\,(x-1)^{n-k}$ then $G \in \mathcal{C}_k^*(n)$ because the multiplicity of the root 1 of the chromatic polynomial of a graph G is equal to the number of blocks of G [24, pg. 35]. Therefore, in Conjecture 3.1.3, the extremal graphs are automatically determined if one can show that $\pi(G,x) \leq (x)_{\downarrow k}\,(x-1)^{n-k}$.

In this section, we first improve Tomescu's general upper bound (Theorem 3.1.1), and show that if $G \in \mathcal{G}_k(n)$, then

$$\pi(G,x) \leq (x)_{\downarrow k}(x-1)^{\Delta(G)-k+1}x^{n-1-\Delta(G)}$$

for every $x \in \mathbb{N}$ (Theorem 3.1.5). Secondly, we discuss Conjecture 3.1.3 and show that if $G \in \mathcal{C}_k(n)$ where $k \geq 4$ then $\pi(G,x)$ is at most $(x)_{\downarrow k}(x-1)^{n-k}$ for every real $x \geq n-2+\left(\binom{n}{2}-\binom{k}{2}-n+k\right)^2$ (Theorem 3.1.8).

3.1.1 An improved upper bound for the number of x-colourings

Our goal is to improve Theorem 3.1.1 by finding an upper bound that is dependent on the maximum degree in the graph. We start by considering the case where there is a *universal vertex*, that is one with degree $n-1$.

Lemma 3.1.4. *Let G be a graph in $\mathcal{G}_k(n)$ having $\Delta(G) = n-1$. Then for every $x \in \mathbb{N}$,*

$$\pi(G,x) \;\leq\; (x)_{\downarrow k}\,(x-1)^{n-k}.$$

Moreover for $x \geq k$, the equality holds if and only if $G \in \mathcal{C}_k^*(n)$.

Proof. Let u be a vertex of G with maximum degree. Since u is a universal vertex, it cannot be in the same colour class with any other vertex. Therefore, $\chi(G-u) = k-1$ and $\pi(G,x) = x \cdot \pi(G-u, x-1)$. Now, by Theorem 3.1.1,

$$\pi(G-u,x) \leq (x)_{\downarrow k-1}\, x^{(n-1)-(k-1)}$$

for every $x \in \mathbb{N}$ and equality holds for $x \geq k-1$ if and only if $G-u \cong K_{k-1} \,\dot\cup\, (n-k)K_1$. Replacing x with $x-1$ in the latter inequality yields

$$\pi(G-u,x-1) \leq (x-1)_{\downarrow k-1}\,(x-1)^{n-k}$$

for every integer $x \geq 1$ and equality holds for $x \geq k$ if and only if $G-u \cong K_{k-1} \,\dot\cup\, (n-k)K_1$. Hence, the result follows as $\pi(G,x) = x \cdot \pi(G-u, x-1)$ and $(x)_{\downarrow k} = x\,(x-1)_{\downarrow k-1}$.

$\square$

Theorem 3.1.5. *Let G be a graph in $\mathcal{G}_k(n)$. Then for every natural number x,*

$$\pi(G,x) \;\leq\; (x)_{\downarrow k}\,(x-1)^{\Delta(G)-(k-1)}\,x^{n-1-\Delta(G)}.$$

Proof. We proceed by induction on the number of vertices. For the basis step, $n = k$ and G is a complete graph, so $\pi(G,x) = (x)_{\downarrow k}$. Now the result is clear as $\Delta(K_k) = k-1$.

Now we may assume that G is a k-chromatic graph of order $n \geq k+1$. If $\Delta(G) = n-1$ then the result follows by Lemma 3.1.4. So let us assume that $\Delta(G) < n-1$. Let u be a vertex of maximum degree. Set $t = n-1-\Delta(G)$ and let $\{v_1, \ldots, v_t\}$ be the set of non-neighbours of u in G, (that is, $\{v_1, \ldots, v_t\} = V(G) \setminus N_G[u]$). We set $G_0 = G$ and

$$G_i = G_{i-1} + uv_i$$

$$H_i = G_i \cdot uv_i$$

for $i = 1, \ldots, t$. By repeated use of the edge addition-contraction formula,

$$\pi(G,x) = \pi(G_t,x) + \sum_{i=1}^{t} \pi(H_i,x).$$

It is clear that $k \leq \chi(G_t), \chi(H_i) \leq k+1$ for $i = 1, 2, \ldots, t$. Also, observe that G_t is a graph of order n having $\Delta(G_t) = n-1$ and each H_i is a graph of order $n-1$ having $\Delta(H_i) \geq \Delta(G) + i - 1$, and hence

$$\Delta(H_i) - \Delta(G) - i + 1 \geq 0.$$

<u>Claim 1:</u> $\pi(G_t,x) \leq (x)_{\downarrow k}\,(x-1)^{n-k}$ for every $x \in \mathbb{N}$.

Proof of Claim 1: Since $\Delta(G_t) = n-1$, we obtain by Lemma 3.1.4 that

$$\pi(G_t, x) \;\leq\; (x)_{\downarrow\chi(G_t)}\,(x-1)^{n-\chi(G_t)}.$$

Also, $(x)_{\downarrow\chi(G_t)}\,(x-1)^{n-\chi(G_t)} \;\leq\; (x)_{\downarrow k}\,(x-1)^{n-k}$ as $\chi(G_t) \geq k$ and $(x)_{\downarrow k+1}\,(x-1)^{n-(k+1)} \leq (x)_{\downarrow k}\,(x-1)^{n-k}$ for $x \geq k$). Hence Claim 1 follows.

<u>Claim 2:</u> $\pi(H_i, x) \leq (x)_{\downarrow k}\,(x-1)^{\Delta(G)+i-k}\,x^{n-i-\Delta(G)-1}$ for every $x \in \mathbb{N}$.

Proof of Claim 2: By the induction hypothesis on H_i, if $\chi(H_i) = k$ then

$$\pi(H_i, x) \;\;\leq\;\; (x)_{\downarrow k}\,(x-1)^{\Delta(H_i)-k+1}x^{n-2-\Delta(H_i)}$$

and if $\chi(H_i) = k+1$ then

$$\begin{aligned}
\pi(H_i, x) \;&\leq\; (x)_{\downarrow k+1}\,(x-1)^{\Delta(H_i)-(k+1)+1}\,x^{(n-1)-1-\Delta(H_i)} \\
&=\; (x)_{\downarrow k+1}(x-1)^{\Delta(H_i)-k}x^{n-2-\Delta(H_i)} \\
&\leq\; (x)_{\downarrow k}(x-1)^{\Delta(H_i)-(k-1)}x^{n-2-\Delta(H_i)}
\end{aligned}$$

for every $x \in \mathbb{N}$.

Since $\Delta(H_i) - \Delta(G) - i + 1 \geq 0$, we find that

$$(x-1)^{\Delta(H_i)-\Delta(G)-i+1} \leq x^{\Delta(H_i)-\Delta(G)-i+1},$$

which is equivalent to

$$(x-1)^{\Delta(H_i)-k+1}x^{n-2-\Delta(H_i)} \leq (x-1)^{\Delta(G)+i-k}x^{n-i-\Delta(G)-1}.$$

This completes the proof of Claim 2.

The inequality proven in Claim 2 yields

$$\begin{aligned}\sum_{i=1}^{t}\pi(H_i,x) &\leq \sum_{i=1}^{t}(x)_{\downarrow k}\,(x-1)^{\Delta(G)+i-k}\,x^{n-i-\Delta(G)-1}\\ &= (x)_{\downarrow k}(x-1)^{\Delta(G)-k}x^{n-\Delta(G)-1}\sum_{i=1}^{t}\left(\frac{x-1}{x}\right)^{i}\end{aligned}$$

Summing the geometric series, we find

$$\sum_{i=1}^{t}\left(\frac{x-1}{x}\right)^{i} = \frac{1-\left(\frac{x-1}{x}\right)^{t+1}}{1-\left(\frac{x-1}{x}\right)} - 1.$$

Now, simplifying the expression on the right hand side of the latter equality and then substituting $t = n-1-\Delta(G)$ we get

$$\sum_{i=1}^{t}\left(\frac{x-1}{x}\right)^{i} = (x-1) - \frac{(x-1)^{n-\Delta(G)}}{x^{n-1-\Delta(G)}}.$$

Therefore,

$$\begin{aligned}\sum_{i=1}^{t}\pi(H_i,x) &\leq (x)_{\downarrow k}(x-1)^{\Delta(G)-k}x^{n-\Delta(G)-1}\left((x-1) - \frac{(x-1)^{n-\Delta(G)}}{x^{n-1-\Delta(G)}}\right)\\ &= (x)_{\downarrow k}\left((x-1)^{\Delta(G)-k+1}x^{n-\Delta(G)-1} - (x-1)^{n-k}\right).\end{aligned}$$

Furthermore, recall that $\pi(G_t,x) \leq (x)_{\downarrow k}\,(x-1)^{n-k}$ by the inequality proven in Claim 1, so

$$\begin{aligned}\pi(G,x) &= \pi(G_t,x) + \sum_{i=1}^{t}\pi(H_i,x)\\ &\leq (x)_{\downarrow k}\,(x-1)^{n-k} + (x)_{\downarrow k}\left((x-1)^{\Delta(G)-k+1}x^{n-\Delta(G)-1} - (x-1)^{n-k}\right)\\ &= (x)_{\downarrow k}\,(x-1)^{\Delta(G)-k+1}\,x^{n-\Delta(G)-1}\end{aligned}$$

and we are done. $\square$

3.1.2 Maximizing the number of colourings for connected graphs of fixed order and chromatic number

Conjecture 3.1.3 is true for many graph families. For example, Tomescu [59] proved it for $k = 4$ under the additional restriction of G being also planar. Also, it is easy to see that if the clique number of graph G in $\mathcal{C}_k(n)$ is equal to k then G contains a spanning subgraph which is isomorphic to a graph in $\mathcal{C}_k^*(n)$. Therefore, Conjecture 3.1.3 holds for every graph G in $\mathcal{C}_k(n)$ having $\omega(G) = k$ (such graphs include all *perfect* graphs [65]).

It is known that (see, for example, [55, 65]) the minimum number of edges of a graph in $\mathcal{C}_k(n)$ is equal to $\binom{k}{2}+n-k$. Furthermore, when $k = 3$, the extremal graphs are unicyclic graphs with an odd cycle, and when $k \neq 3$, extremal graphs belong to $\mathcal{C}_k^*(n)$. As the chromatic polynomial of a graph of order n with m edges has the form $\pi(G, x) = x^n - m\,x^{n-1} + \cdots$ it is not difficult to see that Conjecture 3.1.3 holds for all sufficiently large x. However it becomes quite difficult to find the smallest such value of x.

We begin with a lemma which gives an upper bound for the number of colour partitions of a graph. We will need this result in the sequel to bound the chromatic polynomial and its roots.

Lemma 3.1.6. *Let G be a graph of order n and size m. Then for $1 \leq i \leq n-1$,*

$$a_i(G) \leq \frac{1}{(n-i)!}\left(\binom{n}{2} - m\right)^{n-i}.$$

Proof. We proceed by induction on $\binom{n}{2}-m$, the number of non-edges of the graph. For the basis step, suppose that G is a complete graph. Then, $a_i(G) = 0$ for $1 \leq i \leq n-1$ and $a_n(G) = 1$. Hence the result is clear. Now we may assume that G has at least one pair of nonadjacent vertices, say u and v. The graph $G+uv$ has order n and size $m+1$. Also, the graph $G \cdot uv$ has order $n-1$ and size $m - |N_G(u) \cap N_G(v)|$. Thus the number of non-edges of $G+uv$ and $G \cdot uv$ are strictly less than the number of non-edges of G. Note that if $i = n-1$ then the result is clear since $a_{n-1}(G) = \binom{n}{2} - m$, so we may assume that $1 \leq i \leq n-2$. Set $\beta = \binom{n}{2} - m$. Then by the induction hypothesis,

$$a_i(G+uv) \leq \frac{1}{(n-i)!}(\beta - 1)^{n-i}$$

and

$$a_i(G \cdot uv) \leq \frac{1}{(n-1-i)!}(\beta - 1)^{n-1-i}.$$

By the edge addition-contraction formula,

$$a_i(G) = a_i(G+uv) + a_i(G \cdot uv).$$

Therefore,

$$\begin{aligned}
a_i(G) &\leq \frac{1}{(n-i)!}(\beta-1)^{n-i} + \frac{1}{(n-1-i)!}(\beta-1)^{n-1-i} \\
&= \frac{1}{(n-i)!}\left((\beta-1)^{n-i} + (n-i)(\beta-1)^{n-1-i}\right) \\
&\leq \frac{1}{(n-i)!}\sum_{j=0}^{n-i}\binom{n-i}{j}(\beta-1)^{n-i-j} \\
&= \frac{1}{(n-i)!}\beta^{n-i}
\end{aligned}$$

where the last inequality holds since

$$\sum_{j=0}^{n-i}\binom{n-i}{j}(\beta-1)^{n-i-j} = (\beta-1)^{n-i} + (n-i)(\beta-1)^{n-1-i} + \binom{n-i}{2}(\beta-1)^{n-2-i} + \cdots.$$

Thus, the proof is complete. □

Let $f(z) = \sum_{i=0}^{d} c_i z^i$ be a real polynomial of degree $d \geq 1$. Then the *Cauchy bound of* f (see, for example, [46, pg. 243]), denoted by $\rho(f)$, is defined as the unique positive root of the equation

$$|c_0| + |c_1|x + \cdots + |c_{d-1}|x^{d-1} = |c_d|x^d$$

when f is not a monomial, and zero otherwise (the fact that f has a unique positive real root follows from the Intermediate Value Theorem and Descartes' rule of signs). It is known that the maximum of the moduli of the roots of f is bounded by $\rho(f)$, and the Cauchy bound satisfies (see [46, pg. 247])

$$\rho(f) \leq 2 \max \left\{ \left| \frac{c_i}{c_d} \right|^{1/(d-i)} \right\}_{0 \leq i \leq d-1}. \tag{3.1}$$

Let $\xi_1, \xi_2, \ldots$ be a sequence of real numbers. Then the polynomials

$$P_0(z) := 1, \qquad P_d(z) := \prod_{j=1}^{d} (z - \xi_j) \qquad (d = 1, 2, \ldots)$$

are called the *Newton bases with respect to the nodes* $\xi_1, \xi_2, \ldots$; they form a basis for the vector space of all real polynomials [46, pg. 256].

Theorem 3.1.7. *[46, pg. 266] Let $f(z) = \sum_{j=0}^{d} c_j P_j(z)$ be a polynomial of degree d where P_j's are the Newton bases with respect to the nodes $\xi_1, \ldots \xi_d$. Then f has all its roots in the union of the discs*

$$\mathcal{D}_j := \{z \in \mathbb{C} : |z - \xi_j| \leq \rho\} \qquad (j = 1, \ldots, d)$$

where ρ is the Cauchy bound of $\sum_{j=0}^{d} c_j z^j$.

Theorem 3.1.8. *Let G be a graph in $\mathcal{C}_k(n) \setminus \mathcal{C}_k^*(n)$ where $k \geq 4$. Then*

$$\frac{1}{(x)_{\downarrow k}} \pi(G, x) < (x-1)^{n-k}$$

for every real number x where $x > n - 2 + \left(\binom{n}{2} - \binom{k}{2} - n + k\right)^2$.

Proof. Let G^* be a graph in $\mathcal{C}_k^*(n)$. Then $\pi(G^*, x) = (x)_{\downarrow k}(x-1)^{n-k}$. Let

$$\begin{aligned} f(x) &= \frac{1}{(x)_{\downarrow k}} \left(\pi(G^*, x) - \pi(G, x)\right) \\ &= \frac{1}{(x)_{\downarrow k}} \sum_{r=k}^{n} \left(a_r(G^*) - a_r(G)\right)(x)_{\downarrow r}. \end{aligned}$$

Now, $a_n(G) = a_n(G^*) = 1$. Also, $a_{n-1}(G^*) = \binom{n}{2} - \binom{k}{2} - (n-k)$ and $a_{n-1}(G) = \binom{n}{2} - m$. Since $m > \binom{k}{2} + (n-k)$ we have $a_{n-1}(G^*) > a_{n-1}(G)$. Therefore, $f(x)$ is a polynomial of degree $n-k-1$ with the leading coefficient $a_{n-1}(G^*) - a_{n-1}(G) > 0$. As the leading coefficient of the polynomial f is positive, it suffices to show that the largest real root of f is at most $n - 2 + \left(\binom{n}{2} - \binom{k}{2} - n + k\right)^2$. Indeed, we shall prove a stronger statement, namely that if $z \in \mathbb{C}$ is a root of f then $\Re(z) \leq n - 2 + \left(\binom{n}{2} - \binom{k}{2} - n + k\right)^2$.

Set $\alpha_r = a_r(G^*) - a_r(G)$. Thus $\alpha_{n-1} = a_{n-1}(G^*) - a_{n-1}(G) > 0$ and all α_r's are integers, and

$$f(x) = \alpha_k + \alpha_{k+1}(x-k) + \alpha_{k+2}(x-k)(x-k-1) + \cdots + \alpha_{n-1}(x-k)\cdots(x-n+2)$$

that is,

$$f(x) = \sum_{j=0}^{n-1-k} \alpha_{k+j} \, P_j(x)$$

where $P_j(x)$'s are Newton bases with respect to nodes $k,\ k+1, \ldots,\ n-2$.

By Theorem 3.1.7, f has all its roots in the union of the discs centered at

$$k,\ k+1, \ldots, n-3,\ n-2$$

each of radius ρ where ρ is the Cauchy bound of

$$g = \alpha_{n-1}z^{n-k-1} + \alpha_{n-2}z^{n-k-2} + \alpha_{n-3}z^{n-k-3} + \cdots + \alpha_k.$$

By the inequality given in (3.1), the Cauchy bound of g satisfies

$$\rho \leq 2\max\left\{\left|\frac{\alpha_{n-r}}{\alpha_{n-1}}\right|^{1/(r-1)}\right\}_{2\leq r\leq n-k}.$$

Note that as all of the α_r's are integers with $\alpha_{n-1} > 0$,

$$\left|\frac{\alpha_{n-r}}{\alpha_{n-1}}\right| \leq |\alpha_{n-r}| \leq \max\{a_{n-r}(G), a_{n-r}(G^*)\}.$$

Moreover, by Lemma 3.1.6,

$$a_{n-r}(G) \leq \frac{\left(\binom{n}{2} - m\right)^r}{r!} \quad \text{and} \quad a_{n-r}(G^*) \leq \frac{\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^r}{r!}.$$

Now, since $m > \binom{k}{2} + n - k$ we obtain that

$$\max\{a_{n-r}(G), a_{n-r}(G^*)\} \leq \frac{\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^r}{r!}.$$

So,

$$\left|\frac{\alpha_{n-r}}{\alpha_{n-1}}\right|^{1/(r-1)} \leq \left(\frac{\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^r}{r!}\right)^{1/(r-1)} = \frac{\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^{r/(r-1)}}{(r!)^{1/(r-1)}}.$$

As r increases, $\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^{r/(r-1)}$ decreases. Also, we have the following list of equivalent inequalities

$$\begin{aligned}
((r+1)!)^{1/r} &\geq (r!)^{1/r-1} \\
((r+1)!)^{r-1} &\geq (r!)^{r} \\
((r+1)!)^{r-1} &\geq (r!)^{r-1} r! \\
(r+1)^{r-1} &\geq r!
\end{aligned}$$

where the last inequality is clear. So, $(r!)^{1/(r-1)}$ increases as r increases. Hence

$$\left\{ \frac{\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^{r/(r-1)}}{(r!)^{1/(r-1)}} \right\}_{2 \leq r \leq n-k}$$

is a decreasing sequence and therefore,

$$\max \left\{ \left| \frac{\alpha_{n-r}}{\alpha_{n-1}} \right|^{1/(r-1)} \right\}_{2 \leq r \leq n-k} \leq \frac{\left(\binom{n}{2} - \binom{k}{2} - n + k\right)^{2}}{2}.$$

Thus, we obtain that $\rho \leq \left(\binom{n}{2} - \binom{k}{2} - n + k\right)^{2}$ and the result follows. $\square$

If G is a connected graph of order n and size m with $\pi(G, x) = \sum_{i=1}^{n} (-1)^{n-i} h_i\, x^i$ then it is easy to see that

$$\binom{n-1}{i} \leq h_{n-i} \leq \binom{m}{i} \tag{3.2}$$

from the Broken Cycle Theorem.

The *Turán graph* $T_{n,k}$ is the complete k-partite graph of order n whose partite sets differ in size by at most 1. So, this means that each partite set has size $\lfloor n/k \rfloor$ or $\lceil n/k \rceil$. In the next theorem, we will use the fact that among all k-colourable graphs with n vertices, $T_{n,k}$ is the unique graph with the most edges (see, for example, [65, pg. 207]).

Theorem 3.1.9. *Let G be a graph in $\mathcal{C}_k(n) \setminus \mathcal{C}_k^*(n)$ where $k \geq 4$. Then*

$$\pi(G, x) < (x)_{\downarrow k}(x-1)^{n-k}$$

for every real number x where $x > 2\binom{|E(T_{n,k})|}{2}$.

Proof. Let G^* be in $\mathcal{C}_k^*(n)$, then $\pi(G^*, x) = (x)_{\downarrow k}(x-1)^{n-k}$. Let

$$\begin{aligned} f(x) &= \pi(G^*, x) - \pi(G, x) \\ &= \sum_{i=1}^{n-1}(-1)^{n-i}(h_{n-i}(G^*) - h_{n-i}(G))x^i \\ &= \sum_{i=1}^{n-1} \alpha_i\, x^i. \end{aligned}$$

So, f is a polynomial of degree $n-1$ with a positive leading coefficient $\alpha_{n-1} = m_G - m_{G^*} > 0$. Now it suffices to show that the largest real root of f is at most $2\binom{|E(T_{n,k})|}{2}$. In fact we shall show that if $z \in \mathbb{C}$ is a root of f then $|z| \leq 2\binom{|E(T_{n,k})|}{2}$. Let $z \in \mathbb{C}$ be a root of f and $\rho(f)$ be the Cauchy bound of f, then by (3.1), we know that

$$|z| \leq \rho(f) \leq 2 \max\left\{\left|\frac{\alpha_i}{\alpha_{n-1}}\right|^{1/n-1-i}\right\}_{1\leq i\leq n-2}.$$

Moreover,

$$\left|\frac{\alpha_i}{\alpha_{n-1}}\right| \leq |\alpha_i| = |h_{n-i}(G^*) - h_{n-i}(G)| \leq \max\{h_{n-i}(G^*), h_{n-i}(G)\}.$$

By the inequality given in 3.2, we have

$$h_{n-i}(G^*) \leq \binom{m_{G^*}}{i} \quad \text{and} \quad h_{n-i}(G) \leq \binom{m_G}{i}.$$

Let $M = |E(T_{n,k})|$. Since $M \geq m_G > m_{G^*}$ we obtain that

$$\max\{h_{n-i}(G^*), h_{n-i}(G)\} \leq \binom{M}{i}.$$

Now it is easy to see that

$$\binom{M}{2} \geq \binom{M}{i+1}^{1/i}$$

for every i with $1 \leq i \leq n-2$ because

$$\frac{M^i(M-1)^i}{2^i} \geq \frac{M(M-1)(M-2)\cdots(M-i)}{(i+1)!}.$$

Thus, $\rho(f) \leq 2\binom{M}{2}$ and the result follows. □

In [24] it was shown that if G is a connected graph of order n, then for every $x \in \mathbb{N}$,

$$\pi(G, x) \;\leq\; x(x-1)^{n-1}$$

where equality holds for $x \geq 3$ if and only if G is a tree. From this we can prove that to prove Conjecture 3.1.3, it is sufficient to prove it for 2-connected graphs.

Lemma 3.1.10. *Let G be a graph in $\mathcal{G}_k(n)$ consisting of t blocks $B_1, \ldots, B_t$ and n_i be the order of B_i. Let also x be a natural number. Suppose that for some block B_i with $\chi(B_i) = k$, the inequality $\pi(B_i, x) \leq (x)_{\downarrow k}\,(x-1)^{n_i-k}$ holds. Then,*

$$\pi(G, x) \;\leq\; (x)_{\downarrow k}\,(x-1)^{n-k}.$$

Moreover, for $x \geq k$ the equality $\pi(G, x) = (x)_{\downarrow k}\,(x-1)^{n-k}$ holds if and only if G has exactly one k-chromatic block, say B_i, and for this block the equality $\pi(B_i, x) = (x)_{\downarrow k}\,(x-1)^{n_i-k}$ holds, and all the rest of the blocks are K_2's.

Proof. Clearly $n_1 + n_2 + \cdots n_t = n + t - 1$. Let B_1 be a block of G such that $\chi(B_1) = k$ and $\pi(B_1, x) \le (x)_{\downarrow k}\,(x-1)^{n_1-k}$. Since B_i is a connected graph, $\pi(B_i, x) \le x(x-1)^{n_i-k}$ for each $i \ge 2$, as noted earlier. Also, by the corollary of the Complete Cutset Theorem, we obtain that

$$
\begin{aligned}
\pi(G, x) &= \pi(B_1, x)\,\frac{\pi(B_2, x)}{x}\cdots\frac{\pi(B_t, x)}{x} \\
&\le (x)_{\downarrow k}\,(x-1)^{n_1-k}(x-1)^{n_2-1}\cdots(x-1)^{n_t-1} \\
&= (x)_{\downarrow k}\,(x-1)^{n_1+n_2+\cdots n_t-k-(t-1)} \\
&= (x)_{\downarrow k}\,(x-1)^{n+t-1-k-(t-1)} \\
&= (x)_{\downarrow k}\,(x-1)^{n-k}.
\end{aligned}
$$

Now, $\pi(G, x) = (x)_{\downarrow k}\,(x-1)^{n-k}$ if and only if $\pi(B_1, x) = (x)_{\downarrow k}\,(x-1)^{n_1-k}$ and $\pi(B_i, x) = x(x-1)^{n_i-1}$ for $i \ge 2$. The latter equality holds if and only if B_i is a tree. But since B_i is a block this means that B_i is equal to a K_2. □

In fact, we can show that to prove Conjecture 3.1.3 it is sufficient to prove it in a subclass of 2-connected graphs, namely k-critical graphs. A graph G with no isolated vertices is called *k-critical* if $\chi(G) = k$ and $\chi(G-e) = k-1$ for every edge $e \in E(G)$. Also, it it is not difficult to see that if G is k-critical then $\delta(G) \ge k-1$ and G is 2-connected.

Lemma 3.1.11. *Suppose that for every k-critical graph of order n with $k \ge 4$ and for every $x \in \mathbb{N}$ with $x \ge k$, the inequality $\pi(G, x) < (x)_{\downarrow k}(x-1)^{n-k}$ holds. Then, for every graph $G \in \mathcal{C}_k(n)$ and for every $x \in \mathbb{N}$, the inequality $\pi(G, x) < (x)_{\downarrow k}(x-1)^{n-k}$ holds. Furthermore, in this case, when $x \ge k$ the equality is achieved if and only if $G \in \mathcal{C}_k^*(n)$.*

Proof. We proceed by induction on the number of edges of G. If G has the minimum number of edges among all connected k-chromatic graphs of order n then $G \in \mathcal{C}_k^*(n)$ and therefore $\pi(G, x) = (x)_{\downarrow k}(x-1)^{n-k}$ for every x. By the assumption, we may assume that G is not a k-critical graph. Also, the result is trivial when $x < k$, so we assume that $x \geq k$. Now we will consider two cases:

Case 1: G is a 2-connected graph.

Since G is not k-critical, there exist an edge $e \in E(G)$ such that $\chi(G - e) = k$. Also, $G - e$ is a connected graph, as G is 2-connected. So, $G - e \in \mathcal{C}_k(n)$.

If $G - e \notin \mathcal{C}_k^*(n)$ then by the induction hypothesis on $G - e$ we have $\pi(G, x) < (x)_{\downarrow k}(x-1)^{n-k}$. Thus, we obtain that

$$\pi(G, x) = \pi(G - e, x) - \pi(G \cdot e, x) < (x)_{\downarrow k}(x-1)^{n-k}.$$

Now suppose that $G - e \in \mathcal{C}_k^*(n)$. Then $\chi(G \cdot e) = k$ since G is 2-connected, and therefore $\pi(G \cdot e, x) > 0$. Again we obtain that $\pi(G, x) = \pi(G - e, x) - \pi(G \cdot e, x) < (x)_{\downarrow k}(x-1)^{n-k}$ as $\pi(G \cdot e, x) > 0$.

Case 2: G is not a 2-connected graph.

Let $B_1, \ldots, B_t$ be the blocks of G and $t \geq 2$. Since the chromatic number of G is equal to the maximum of the chromatic numbers of its blocks, there is a block, say B_1, such that $\chi(B_1) = k$. By the induction hypothesis on B_1, we have $\pi(B_1, x) < (x)_{\downarrow k}(x-1)^{n_{B_1}-k}$. Thus, the result follows from Lemma 3.1.10. $\square$

In Lemma 3.1.10, we showed that to prove Conjecture 3.1.3, it is sufficient to prove it for 2-connected graphs. Therefore, one might want to determine the maximum number of x-colourings of a 2-connected k-chromatic graph of order n. In [60], the maximum number of x-colourings of a 2-connected 3-chromatic graph of order n was determined. For $k \geq 4$, from some computations on small graphs, we have noted that the following strengthening of Conjecture 3.1.3 might hold.

Conjecture 3.1.12. Let G be a 2-connected k-chromatic graph of order $n > k \geq 4$. Then for all $x \geq k$,

$$\pi(G, x) \leq \frac{(x)_{\downarrow k}\pi(C_{n-k+2}, x)}{x(x-1)},$$

with equality holding if G arises by attaching an ear to K_k (an *ear* is a new path or cycle that overlaps an existing graph only in its two endpoints).

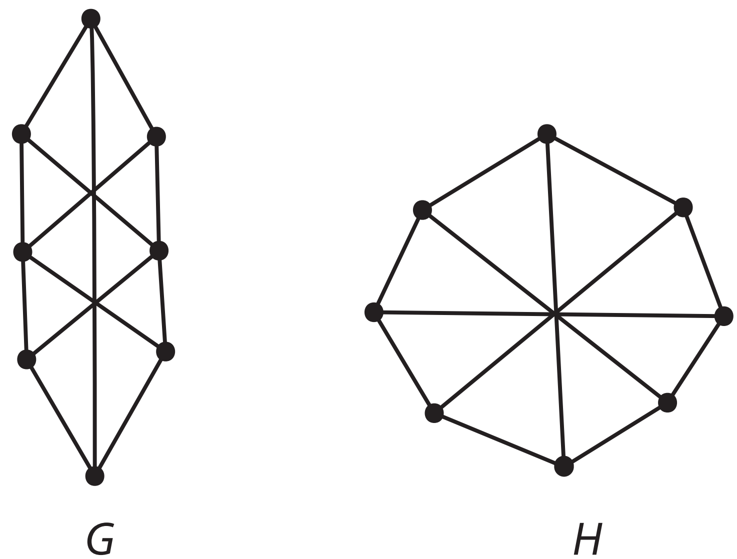

Figure 3.1: Among all 3-connected 3-chromatic graphs of order 8, the graph G has the largest number of 3-colourings whereas the graph H has the largest number of 4-colourings.

What about for even higher connectivity? We have found that among all 3-connected 3-chromatic graphs of order 8, the graph G shown at the left of Figure 3.1 is the unique 3-connected 3-chromatic graph of order 8 with the largest number of 3-colourings (66), but the graph H on the right (which happens to be a circulant graph) has the most 4-colourings, 2140 (compared to G's 2060 4-colourings). Of course, for any positive integers l and k, there is always an l-connected k-chromatic graph of order n with the most x-colourings, provided x is large enough, but our example shows that for some classes, we cannot start necessarily at $x = k$.

3.1.3 Maximizing the number of i-colour partitions

It is straightforward to see that if some graph in a subclass of k-chromatic graphs has the largest number of i-colour partitions for every i among all such graphs, it necessarily has the largest number of x-colourings in the subclass. It seems reasonable that the extremal graphs in $\mathcal{C}_k^*(n)$ have the largest number of i-colour partitions, and likewise for the graphs in Conjecture 3.1.12. In [59], this was proposed as a conjecture.

Conjecture 3.1.13. [59] Let $k \geq 4$ and $k \leq i \leq n-1$. If a graph G achieves the maximum number of i-colour partitions over the family of connected k-chromatic graphs of order n then $G \in \mathcal{C}_k^*(n)$.

It is not difficult to see that the chromatic polynomials of two graphs are the same if and only if their σ-polynomials are the same. All graphs in $\mathcal{C}_k^*(n)$ have the same chromatic polynomial, namely $(x)_{\downarrow k}(x-1)^{n-k}$. Therefore, if G and and H are two graphs in $\mathcal{C}_k^*(n)$ then $a_i(G) = a_i(H)$ for every i.

Let $\mathrm{ext}_i(n,k)$ denote the number of i-colour partitions of a graph in $\mathcal{C}_k^*(n)$. Also, let $Q_{n,k} \cong K_1 \vee (K_{k-1} \cup (n-k)K_1)$. That is, $Q_{n,k}$ is the graph obtained from a k-clique by attaching $n-k$ leaves to a single vertex of the k-clique.

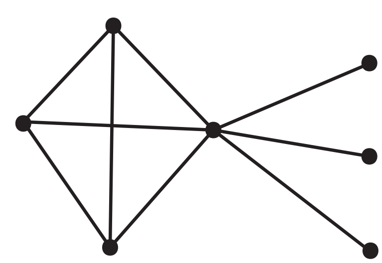

Figure 3.2: The graph $Q_{7,4}$

It is known that [57] (see Theorem 3.1.14) $K_k \cup (n-k)K_1$ is the unique graph which maximizes the number of i-colour partitions of a k-chromatic graph of order n for $k \leq i \leq n-1$. By using this, we can show that Conjecture 3.1.13 holds for graphs which have a universal vertex.

Theorem 3.1.14. *[57] Let $k \leq i \leq n-1$. If a graph G achieves the maximum number of i-colour partitions over the family of k-chromatic graphs of order n then $G \cong K_k \cup (n-k)K_1$.*

Proposition 3.1.15. *Let $G \in \mathcal{C}_k(n)$ be a graph such that $\Delta(G) = n-1$. Then for every i with $k \leq i \leq n-1$,*

$$a_i(G) \leq \text{ext}_i(n,k)$$

where the equality is achieved if and only if $G \cong Q_{n,k}$.

Proof. Let u be a universal vertex of G. So, $a_i(G) = a_{i-1}(G-u)$. Since $G-u$ is a $(k-1)$-chromatic graph of order $n-1$, by Theorem 3.1.14 we find that

$$a_{i-1}(G-u) \leq a_{i-1}(K_{k-1} \cup (n-k)K_1)$$

where the equality is achieved for $n-1 \geq i-1 \geq k-1$ if and only if $G-u \cong K_{k-1} \cup (n-k)K_1$. Let v be the universal vertex of $Q_{n,k}$. Since $Q_{n,k}-v \cong K_{k-1} \cup (n-k)K_1$ we find that $a_i(Q_{n,k}) = a_{i-1}(Q_{n,k}-v) = a_{i-1}(K_{k-1} \cup (n-k)K_1)$. Therefore, $a_i(G) \leq \text{ext}_i(n,k)$ for $k \leq i \leq n-1$ where the equality is achieved if and only if $G \cong Q_{n,k}$. $\square$

Now we shall prove some recursive formulas for $\text{ext}_i(n,k)$.

Proposition 3.1.16. *Let $n > i \geq k$. Then*

(i) $\text{ext}_i(n,k) = \text{ext}_{i-1}(n-1,k) + (i-1)\,\text{ext}_i(n-1,k)$;

(ii) $\text{ext}_i(n,k) = \text{ext}_i(n,k+1) + (k-1)\,\text{ext}_i(n-1,k)$;

(ii) $\text{ext}_i(n,k) = \text{ext}_{i-1}(n-1,k-1) + (i-k+1)\,\text{ext}_i(n-1,k-1)$.

Proof. By the definition, $\text{ext}_i(n,k) = a_i(Q_{n,k})$. Let $V(Q_{n,k}) = A \cup B$ where A induces a k-clique and B consists of the $n-k$ leaves. Also let $u \in A$ be the universal vertex of $Q_{n,k}$ and $A \setminus \{u\} = \{u_1, \ldots, u_{k-1}\}$.

(i) Let $v \in B$. Then by the edge deletion-contraction formula,

$$a_i(Q_{n,k}) = a_i(Q_{n,k} - uv) - a_i(Q_{n,k} \cdot uv).$$

Observe that

$$Q_{n,k} - uv \cong K_1 \cup Q_{n-1,k} \quad \text{and} \quad Q(n,k) \cdot uv \cong Q_{n-1,k}.$$

Also, recall that $a_i(G \cup K_1) = a_{i-1}(G) + ia_i(G)$ for any graph G. Therefore,

$$\begin{aligned}
a_i(Q_{n,k}) &= a_i(Q_{n,k} - uv) - a_i(Q_{n,k} \cdot uv) \\
&= a_i(K_1 \cup Q_{n-1,k}) - a_i(Q_{n-1,k}) \\
&= a_{i-1}(Q_{n-1,k}) + ia_i(Q_{n-1,k}) - a_i(Q_{n-1,k}) \\
&= a_{i-1}(Q_{n-1,k}) + (i-1)a_i(Q_{n-1,k}) \\
&= \operatorname{ext}_{i-1}(n-1,k) + (i-1)\operatorname{ext}_i(n-1,k).
\end{aligned}$$

(ii) By adding and contracting the edges $vu_1, vu_2, \ldots vu_{k-1}$ successively, one can verify that

$$a_i(Q_{n,k}) = a_i(Q_{n,k+1}) + (k-1)a_i(Q_{n-1,k}).$$

(iii) By deleting and contracting the edges $u_1u, u_1u_2, \ldots, u_1u_{k-1}$ successively one can verify that

$$a_i(Q_{n,k}) = a_{i-1}(Q_{n-1,k-1}) + (i-k+1)a_i(Q_{n-1,k-1}).$$

□

In the next result we show that to prove Conjecture 3.1.13 it suffices to prove it for critical graphs.

Theorem 3.1.17. *Suppose that for every k-critical graph of order n with $k \geq 4$ and for every i with $k \leq i \leq n-1$ the strict inequality $a_i(G) < \operatorname{ext}_i(n,k)$ holds. Then, for every graph $G \in \mathcal{C}_k(n)$ and for every i with $k \leq i \leq n-1$ the inequality $a_i(G) \leq \operatorname{ext}_i(n,k)$ holds. Furthermore, the equality is achieved if and only if $G \in \mathcal{C}_k^*(n)$.*

Proof. We proceed by induction on the number of edges of G. If G has the minimum number of edges among all connected k-chromatic graphs of order n then $G \in \mathcal{C}_k^*(n)$ and therefore $a_i(G) = \mathrm{ext}_i(n, k)$ for every i. By the assumption, we may assume that G is not a k-critical graph. Now we will consider two cases:

Case 1: G is a 2-connected graph.

Since G is not k-critical, there exist an edge $e \in E(G)$ such that $\chi(G - e) = k$. Also, $G - e$ is a connected graph, as G is 2-connected. So, $G - e \in \mathcal{C}_k(n)$.

If $G - e \notin \mathcal{C}_k^*(n)$ then by the induction hypothesis on $G - e$ we obtain that $a_i(G - e) < \mathrm{ext}_i(n, k)$. Thus, we get $a_i(G) = a_i(G - e) - a_i(G \cdot e) < \mathrm{ext}_i(n, k)$ as $a_i(G - e) < \mathrm{ext}_i(n, k)$.

Now suppose that $G - e \in \mathcal{C}_k^*(n)$. Then $\chi(G \cdot e) = k$ and therefore $a_i(G \cdot e) > 0$. Again we obtain that $a_i(G) = a_i(G - e) - a_i(G \cdot e) < \mathrm{ext}_i(n, k)$ as $a_i(G \cdot e) > 0$.

Case 2: G is not a 2-connected graph.

Let $B_1, \ldots, B_t$ be the blocks of G and $t \geq 2$. Since the chromatic number of G is equal to maximum of the chromatic numbers of its blocks, there is a block, say B_1, such that $\chi(B_1) = k$.

Subcase i: There is a block B_i with $i \geq 2$ such that B_i is not isomorphic to K_2.

We pick an edge $e \in E(B_i)$. Now it is clear that $G - e \in \mathcal{C}_k(n)$. So, by the induction hypothesis on $G - e$, we have $a_i(G - e) \leq \mathrm{ext}_i(n, k)$.

If $\chi(G \cdot e) \leq k$ then $a_i(G \cdot e) > 0$. Therefore, $a_i(G) = a_i(G - e) - a_i(G \cdot e) < \mathrm{ext}_i(n, k)$ as $a_i(G \cdot e) > 0$.

On the other hand, if $\chi(G \cdot e) = k + 1$ then $G - e \notin \mathcal{C}_k^*(n)$. Therefore, by the induction hypothesis on $G - e$, we have $a_i(G - e) < \mathrm{ext}_i(n, k)$. Now again we obtain that $a_i(G) = a_i(G - e) - a_i(G \cdot e) < \mathrm{ext}_i(n, k)$ since $a_i(G - e) < \mathrm{ext}_i(n, k)$ and $a_i(G \cdot e) \geq 0$.

Subcase ii: For every $i \geq 2$, the block B_i is isomorphic to K_2.

Let u be a leaf of G and v be the neighbour of u in G. By the edge deletion-contraction formula, we have $a_i(G) = a_i(G - uv) - a_i(G \cdot uv)$. Also, let $G' = G - u$. It is clear that $G' \in \mathcal{C}_k(n-1)$. Now, $G - uv \cong K_1 \cup G'$ and $G \cdot uv \cong G'$. So,

$$a_i(G - uv) = a_i(K_1 \cup G') = a_{i-1}(G') + ia_i(G').$$

Hence, we obtain that

$$a_i(G) = a_{i-1}(G') + (i-1)a_i(G').$$

Note that $G' \in \mathcal{C}_k^*(n-1)$ if and only if $G \in \mathcal{C}_k^*(n)$. So, we may assume that $G' \notin \mathcal{C}_k^*(n-1)$. It is clear that $a_{k-1}(G') = 0$. Furthermore, by the induction hypothesis on G',

$$a_{i-1}(G') < \mathrm{ext}_{i-1}(n-1,k) \quad \text{ for } i > k.$$

Since by Prposition 3.1.16 (i) $\mathrm{ext}_i(n,k) = \mathrm{ext}_{i-1}(n-1,k) + (i-1)\,\mathrm{ext}_i(n-1,k)$, it follows that $a_i(G) < \mathrm{ext}_i(n,k)$. Thus, the proof is complete. $\square$

As we already mentioned, Conjecture 3.1.14 is true for $i = n-1$, as the problem of maximizing the number of $(n-1)$-colour partitions of a graph is equivalent to the problem of minimizing the number of edges. The next natural direction for us is to study this conjecture for $i = n-2$. In the sequel, we will show that Conjecture 3.1.13 holds when $i = n-2$ and G is a k-critical graph of order n where $k \geq 5$ and n is sufficiently large compared to k. We begin with giving an explicit formula for the number of $(n-2)$-colour partitions of a graph in $\mathcal{C}_k^*(n)$.

Lemma 3.1.18. *Let G be a graph in $\mathcal{C}_k^*(n)$ then*

$$a_{n-2}(G) = (3k-2)\binom{n-k}{3} + \binom{n-k}{2}(k-1) + 3\binom{n-k}{4}.$$

Proof. We may assume that G is $Q(n,k)$ since all graphs in $\mathcal{C}_k^*(n)$ have the same number of $(n-2)$-colour partitions. Let $V(Q(n,k)) = A \cup B$ where A induces a

k-clique and B consists of the $n-k$ leaves. Let $u \in A$ be the universal vertex of $Q(n,k)$. Since $a_{n-2}(G) = \eta_G(\overline{K_3}) + \eta_G(2\overline{K_2})$, we shall find $\eta_G(\overline{K_3})$ and $\eta_G(2\overline{K_2})$.

First, let us find the number of independent sets of size 3. One can choose all three vertices from the set B (there are $\binom{n-k}{3}$ ways to do so) or one can choose two vertices from the set B and one vertex from the set $A \setminus \{u\}$ (there are $\binom{n-k}{2}(k-1)$ ways to do so). Therefore,

$$\eta_G(\overline{K_3}) = \binom{n-k}{3} + \binom{n-k}{2}(k-1).$$

Now, let us find the number of subgraphs which are isomorphic to $2\overline{K_2}$, that is, the number of two unordered independent sets of size 2. One can choose both of the independent sets from the set B (there are $\frac{1}{2}\binom{n-k}{2}\binom{n-k-2}{2}$ ways to do so), or one can choose one of the independent sets from B and pick one of the vertices of the other independent set from $A \setminus \{u\}$ (there are $\binom{n-k}{2}(k-1)(n-k-2)$ ways to do so). Therefore,

$$\eta_G(2\overline{K_2}) = \frac{1}{2}\binom{n-k}{2}\binom{n-k-2}{2} + \binom{n-k}{2}(k-1)(n-k-2).$$

Thus, the result follows as $a_{n-2}(G) = \eta_G(\overline{K_3}) + \eta_G(2\overline{K_2})$. $\square$

Lemma 3.1.19. *Let G be a k-critical graph of order n. Then*

$$a_{n-2}(G) \leq \frac{n(n-k)(n-k-1)}{6} + \frac{n(n-k)^2(n-2)}{8}.$$

Proof. First let us show that the number of ordered triples of pairwise nonadjacent vertices is at most $n(n-k)(n-k-1)$. Let (u_1, u_2, u_3) be a such triple. There are n ways to pick the first vertex u_1. Since G is k-critical, $\delta(G) \geq k-1$. Therefore, there are at most $n-k$ choices to choose u_2 and at most $n-k-1$ choices for u_3. Thus,

$$\eta_G(\overline{K_3}) \leq \frac{n(n-k)(n-k-1)}{6}.$$

Similarly, it is not difficult to see that

$$\eta_G(2\overline{K_2}) \leq \frac{n(n-k)^2(n-2)}{8}.$$

Hence, the result follows as $a_{n-2}(G) = \eta_G(\overline{K_3}) + \eta_G(2\overline{K_2})$. $\square$

Theorem 3.1.20. *Let $k \geq 5$ and $n \geq 8k^2 - 24k$. If G is a k-critical graph of order n and $G^* \in \mathcal{C}_k^*(n)$ then*

$$a_{n-2}(G) < a_{n-2}(G^*).$$

Proof. Let $p_k(n)$ be equal to

$$(3k-2)\binom{n-k}{3} + \binom{n-k}{2}(k-1) + 3\binom{n-k}{4} - \frac{n(n-k)(n-k-1)}{6} - \frac{n(n-k)^2(n-2)}{8}.$$

By Lemma 3.1.18 and Lemma 3.1.19, we know that $a_{n-2}(G^*) - a_{n-2}(G) \geq p_k(n)$. Now we consider $p_k(n)$ as a polynomial function of n with coefficients being polynomial functions of k. More precisely, we rewrite $p_k(n)$ as follows:

$$\begin{aligned} p_k(n) &= \left(-1 + \frac{1}{4}k\right)n^3 + \left(\frac{25}{12}k + \frac{49}{24} - \frac{7}{8}k^2\right)n^2 + \left(k^3 - \frac{11}{12} - \frac{41}{12}k - \frac{7}{6}k^2\right)n \\ &\quad + \frac{3}{8}k^4 + \frac{1}{12}k^3 + \frac{11}{12}k + \frac{11}{8}k^2 \\ &= c_0(k)\,n^3 + c_1(k)\,n^2 + c_2(k)\,n + c_3(k). \end{aligned}$$

Note that $c_0(k) = \frac{1}{4}k - 1 \geq \frac{1}{4} > 0$ when $k \geq 5$. So $p_k(n)$ has a positive leading coefficient when $k \geq 5$ and therefore it suffices to show that the largest real root of $p_k(n)$ is less than $2k^2 - 6k$. Now, by computer, one can verify that

$$|c_i(k)| < (k^2 - 3k)^i \quad \text{for } i = 1, 2, 3.$$

Hence, the Cauchy bound of $p_k(n)$ is at most

$$2 \max \left\{ \left| \frac{c_i(k)}{c_0(k)} \right|^{1/i} \right\}_{1 \le i \le 3} < 8(k^2 - 3k).$$

Thus, the result follows as the moduli of the roots of a polynomial is bounded by its Cauchy bound. □

If one can show that the graphs in $\mathcal{C}_k^*(n)$ maximize the number of $(n-2)$-colour partitions, then in Theorem 3.1.8 the bound on x can be improved from a quartic to a cubic function of n.

Theorem 3.1.21. *Let $k \ge 5$ and $n \ge 2k^2 - 6k$. If G is a k-critical graph of order n then*

$$\frac{1}{(x)_{\downarrow k}} \pi(G, x) < (x-1)^{n-k}$$

for every real number x where $x \ge n - 2 + \frac{2}{\sqrt{6}} \left(\binom{n}{2} - \binom{k}{2} - n + k \right)^{3/2}$.

Proof. One can apply a similar argument as in the proof of Theorem 3.1.8. The result then follows by Theorem 3.1.20 and Theorem 3.2.1. □

As we already mentioned, if $a_j(H) \le a_j(G)$ for all j, then $\pi(H, x) \le \pi(G, x)$ for all $x \ge \chi(H)$. Thus if some graph in a subclass of k-chromatic graphs has the largest a_j sequence (term-wise) among all such graphs, it necessarily has the largest number of x-colourings in the subclass. If we try to determine such extremal graphs in the family of 3-connected graphs of fixed chromatic number and order, then there are not necessarily graphs which achieve the maximum number of i colour-partitions for every i. As we mentioned earlier, the graph G shown at the left of Figure 3.1 is the unique 3-connected 3-chromatic graph of order 8 with the largest number of 3-colourings among all 3-connected 3-chromatic graphs of order 8, and its a_j sequence,

$\langle 11, 74, 124, 71, 15, 1\rangle$, is thus the only candidate for a largest such sequence, but the graph H on the right has sequence $\langle 8, 82, 144, 60, 16, 1\rangle$, so no optimal sequence exists.

3.2 Roots of Chromatic Polynomials

A *chromatic root* is a root of the chromatic polynomial of a graph. If $z \in \mathbb{C}$ satisfies $\pi(G, z) = 0$, then z is called a *chromatic root* of G (the chromatic roots of graphs of order 7 are shown in Figure 3.3.

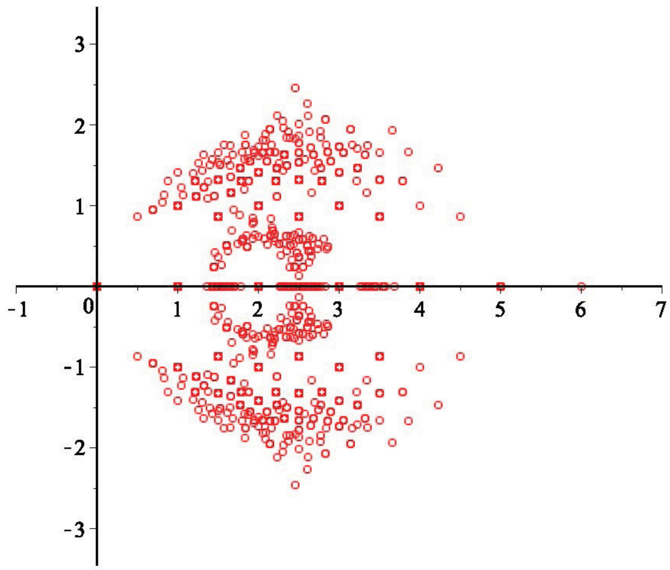

Figure 3.3: Chromatic roots of all graphs of order at most 7.

A trivial observation is that all of $0, 1, \ldots, \chi(G) - 1$ are chromatic roots – the chromatic number is merely the first positive integer that is *not* a chromatic root. The Four Colour Theorem is equivalent to the fact that 4 is never a chromatic root of a planar graph, and interest in chromatic roots began precisely from this connection. The roots of chromatic polynomials have subsequently received a considerable amount of attention in the literature. Chromatic polynomials also have strong connections to the Potts model partition function studied in theoretical physics, and the complex roots play an important role in statistical mechanics (see, for example, [50]).

3.2.1 A new bound for the moduli of the chromatic roots of all graphs

A central problem in the study of chromatic roots has been to bound the moduli of the chromatic roots in terms of graph parameters. There has been considerable interest in chromatic roots, particularly on bounding the moduli of the roots (see, for example, [24, Ch. 14]). In this section, we will give a new bound (which is incomparable to the existing ones) for the moduli of chromatic roots of all graphs. This bound is sharp and the equality is obtained when the graph is a complete graph. Furthermore, this bound gives better estimates than earlier bounds for dense graphs. Let us begin with summarizing some of the earlier results regarding bounding chromatic roots.

Sokal [50] showed that for every graph G, there exists a function $\omega : V(G) \to \mathbb{C}$ which assigns complex weights to the vertices of the graph such that the chromatic polynomial of G can be expressed as

$$\pi(G, x) = x^{|V(G)|} \sum_{I \in \mathcal{I}(G)} \prod_{v \in I} \omega(v)$$

where $\mathcal{I}(G)$ is the family of all independent sets of G. By making use of this expression, Sokal applied Dobrushin's Theorem (which is known to be equivalent to the Lovász Local Lemma) to show that the complex roots of $\pi(G, x)$ lie in the disc $|z| \leq 7.963907\Delta(G)$. This bound was later improved in the constant to 6.908 in [29] by Fernandez and Procacci . We shall note that these bounds are not sharp.

Brown [6] used another approach to bound chromatic roots. If G is a connected graph of order n then one can express

$$\pi(G, x) = (-1)^{n-1} x \sum_{i=1}^{n-1} t_i (1 - x)^i$$

where t_i is the number of spanning trees with "external activity" 0 and "internal activity" i, and this is known as the *tree expansion* of the chromatic polynomial. By using the tree expansion, Brown [6] applied the Enestrom-Kakeya Theorem to show that the chromatic roots of a graph G of order n and size m lie in $|z-1| \leq m-n+1$. This bound is sharp, with equality obtained when the graph is a tree or a cycle, and is good for graphs of bounded corank.

Our approach will be to make use of the complete graph expansion of the chromatic polynomial. We will use the upper bound given in Lemma 2.1.9 on the number of colour partitions of a graph. Also, we will need the following theorem that locates the roots of a polynomial expressed in terms of Newton bases.

Theorem 3.2.1. *[46, pg. 267] Let $f(z) = \sum_{i=0}^{d} c_i P_i(z)$ be a polynomial of degree d where $P_i(z)$'s are Newton bases with respect to the nodes $\xi_1, \ldots, \xi_d$. Denote by ρ the Cauchy bound of $c_d z^d + \sum_{i=0}^{d-2} c_i z^i$. Then f has all its roots in the union $\mathcal{U}$ of the discs centered at $\xi_1, \ldots \xi_{d-1}, \xi_d - \frac{c_{d-1}}{c_d}$, each of radius ρ.* $\square$

We are ready to prove our new bound on chromatic roots.

Theorem 3.2.2. *Let G be a k-chromatic graph of order n and size m. Then $\pi(G, z)$ has all its roots in $\{0, 1, \ldots, k-1\} \cup \mathcal{U}$ where $\mathcal{U}$ is the union of the discs centered at*

$$k,\ k+1, \ldots, n-2,\ n-1-\binom{n}{2}+m,$$

each of radius $\sqrt{2}\left(\binom{n}{2}-m\right)$. Thus the modulus of a chromatic root of a graph of order n with m edges is bounded above by $n-1+\sqrt{2}\left(\binom{n}{2}-m\right)$.

Proof. First recall that $\pi(G, z) = \displaystyle\sum_{i=k}^{n} a_i(G)\,(z)_{\downarrow i}$ and let $\pi(G, z) = (z)_{\downarrow k}\, f(z)$. The roots of $\pi(G, z)$ are precisely $\{0, 1, \ldots, k-1\}$ union the roots of $f(z)$. Hence, it suffices to show that the roots of $f(z)$ lie in $\mathcal{U}$. Now,

$$\begin{aligned} f(z) &= a_k \frac{(z)_{\downarrow k}}{(z)_{\downarrow k}} + a_{k+1} \frac{(z)_{\downarrow k+1}}{(z)_{\downarrow k}} + \cdots + a_n \frac{(z)_{\downarrow n}}{(z)_{\downarrow k}} \\ &= a_k + a_{k+1}(z-k) + \cdots + a_n(z-k)\cdots(z-n+1). \end{aligned}$$

Hence,

$$f(z) = \sum_{j=0}^{n-k} a_{k+j} P_j(z)$$

where $P_j(z)$'s are Newton bases with respect to the nodes $k, k+1, \ldots, n-1$. Therefore, by Theorem 3.2.1, $f(z)$ has all its roots in the union of the discs centered at

$$k,\ k+1, \ldots, n-2,\ n-1-\binom{n}{2}+m$$

each of radius ρ where ρ is the Cauchy bound of the polynomial

$$g = a_n z^{n-k} + a_{n-2} z^{n-k-2} + \cdots + a_{k+1} z + a_k.$$

(Note that $n-1-\binom{n}{2}+m$ may not be the largest of the numbers, but all the numbers are at most $n-1$). Since $a_n = 1$, by the inequality given in (3.1) we obtain

$$\rho(g) \leq 2 \max \left\{ a_{n-r}(G)^{1/r} \right\}_{2 \leq r \leq n-k}.$$

Also, by Lemma 3.1.6, we get

$$a_{n-r}(G)^{1/r} \leq \left(\frac{\left(\binom{n}{2} - m\right)^r}{r!} \right)^{1/r} = \frac{\binom{n}{2} - m}{(r!)^{1/r}}.$$

Now, $(r!)^{1/r}$ increases as r increases. Therefore, $a_{n-r}(G)^{1/r} \leq \frac{1}{\sqrt{2}}\left(\binom{n}{2} - m\right)$ for $2 \leq r \leq n-k$. Thus, $\rho(g) \leq \sqrt{2}\left(\binom{n}{2} - m\right)$ and the results follow. $\square$

Graph G	Brown $\lvert z\rvert \leq m-n+2$	Sokal $\lvert z\rvert \leq 7.9\Delta(G)$	Fernandez-Procacci $\lvert z\rvert \leq 6.9\Delta(G)$	New bound $\lvert z\rvert \leq n-1+\sqrt{2}\left(\binom{n}{2}-m\right)$
$\overline{G}$ is a tree	$\binom{n}{2}-2n+3$	$7.964(n-2)$	$6.908(n-2)$	$2.414(n-1)$
$\overline{G}$ is a cycle	$\binom{n}{2}-2n+2$	$7.964(n-3)$	$6.908(n-3)$	$2.414n-1$
$\overline{G}$ is a theta graph	$\binom{n}{2}-2n+1$	$7.964(n-3)$	$6.908(n-3)$	$2.414n+0.414$
$\overline{G}$ is 3-regular	$\binom{n}{2}-\frac{5}{2}n+2$	$7.964(n-4)$	$6.908(n-4)$	$3.121n-1$
$\overline{G}$ is 4-regular	$\binom{n}{2}-3n+2$	$7.964(n-5)$	$6.908(n-5)$	$3.828n-1$

Table 3.1: Comparison of bounds for the chromatic roots of a graph G of order n and size m whose complement $\overline{G}$ is a cycle, tree, 3-regular graph or theta graph.

The proof of Theorem 3.2.2 shows the following.

Corollary 3.2.3. *Let G be a graph of order n and size m. If z is a root of $\pi(G,z)$ then*

$$|\Im(z)| \leq \sqrt{2}\left(\binom{n}{2}-m\right),$$

$$\Re(z) \leq n-1+\sqrt{2}\left(\binom{n}{2}-m\right).$$

□

Table 3.1 compares our new bound on the moduli to previously known bounds, for a variety of dense of graphs. Note the significant improvement in the constant in linear upper bounds. In particular, for any family of r-regular graphs with $r \geq n-8$, our bounds are asymptotically much better than the others.

3.2.2 Real chromatic roots and the real parts of complex chromatic roots

While the real chromatic roots have been extensively studied and well understood, little is known about the *real parts* of chromatic roots. It is not difficult to see that the largest real chromatic root of a graph with n vertices is $n-1$. The *tree-width* of a graph G is the minimum integer k such that G is a subgraph of a k-tree (given $q \in \mathbb{N}$, the class of *q-trees* is defined recursively as follows: any complete graph K_q is a q-tree, and any q-tree of order $n+1$ is a graph obtained from a q-tree G of order n, where $n \geq q$, by adding a new vertex and joining it to each vertex of a K_q in G). Indeed, it is known that the largest real chromatic root of a graph is at most the tree-width of the graph. Analogous to these facts, it was conjectured in [24] that the real parts of chromatic roots are also bounded above by both $n-1$ and the tree-width of the graph.

In this section we show that for all $k \geq 2$ there exist infinitely many graphs G with tree-width k such that G has non-real chromatic roots z with $\Re(z) > k$. We also discuss the weaker conjecture and prove it for graphs G with $\chi(G) \geq n-3$.

Another approach has been to study the *real* chromatic roots of graphs. It is not difficult to see that if r is a real chromatic root of G then $r \leq n-1$ with equality if and only if G is a complete graph, since $\pi(G,x) = \sum a_i(G)\ (x)_{\downarrow i}$. In [21] it was proven that among all real chromatic roots of graphs with order $n \geq 9$, the largest non-integer real chromatic root is $\dfrac{n-1-\sqrt{(n-3)(n-7)}}{2}$, and extremal graphs were determined. Moreover, Dong et al. [22,23] showed that real chromatic roots are bounded above by $5.664\Delta(G)$ and $\max\{\Delta(G), \lfloor n/3 \rfloor - 1\}$.

The problem of finding the largest *real part* of complex chromatic roots seems more difficult. In [24] the following conjectures on the real part of complex chromatic roots were proposed.

Conjecture 3.2.4. [24, pg. 299] Let G be a graph with tree-width k. If z is a root of $\pi(G, x)$ then $\Re(z) \leq k$.

Conjecture 3.2.5. [24, pg. 299] Let G be a graph of order n. If z is a root of $\pi(G, x)$ then $\Re(z) \leq n - 1$.

Conjecture 3.2.4 is reasonable given that Thomassen [52] proved that the real chromatic roots are bounded above by the tree-width of the graph. It is clear that the Conjecture 3.2.5 is weaker than Conjecture 3.2.4. In this work, first we present infinitely many counterexamples to Conjecture 3.2.4 for every $k \geq 2$ (Theorem 3.2.9). Then, we consider Conjecture 3.2.5 and prove it for all graphs G with $\chi(G) \geq n - 3$ (Theorem 3.2.15). (Our numerical computations suggest that graphs which have large chromatic number are more likely to have chromatic roots whose real parts are close to n.)

A polynomial $f(x)$ in $\mathbb{C}[x]$ is called *(Hurwitz) quasi-stable* (resp. *(Hurwitz) stable*) if every $z \in \mathbb{C}$ such that $f(z) = 0$ satisfies $\Re(z) \leq 0$ (resp. $\Re(z) < 0$), that is, the roots of f lie in the left half (resp. open left half) plane. Observe that z is a root of $f(x)$ if and only if $z - c$ is a root of $f(x + c)$, so that every root z of a polynomial $f(x)$ satisfies $\Re(z) \leq c$ (resp. $\Re(z) < c$) if and only if the polynomial $f(x + c)$ is quasi-stable (resp. stable). Thus, bounding the real parts of roots of polynomials is closely related to the Hurwitz stability of polynomials. In the sequel, we will make use of this observation to prove both of our main results.

Tree-width and the real part of complex chromatic roots

It is straightforward to check that the tree-width of the complete bipartite graph $K_{p,q}$ is equal to $\min(p, q)$, and our counterexamples to Conjecture 3.2.4 will be these graphs. Note that this conjecture clearly holds for $k = 1$ since the tree-width of a graph is equal to 1 if and only if the graph is a tree (which only has 0 and 1 as chromatic roots). Hence, our counterexamples are for $p \geq 2$.

We shall make use of a particular expansion of the chromatic polynomial. Let G be a graph of order n and size m. Suppose that $\beta : E(G) \to \{1, 2, \ldots, m\}$ is a bijection and C a cycle in G. Let e be the edge of C such that $\beta(e) > \beta(e')$ for any e' in $E(C) - \{e\}$. Then the path $C - e$ is called a *broken cycle* in G with respect to β. Whitney's Broken-Cycle Theorem (see, for example, [24]) states that

$$\pi(G, x) = \sum_{i=1}^{n} (-1)^{n-i} h_i(G) x^i,$$

where $h_i(G)$ is the number of spanning subgraphs of G that have exactly $n - i$ edges and that contain no broken cycles with respect to β.

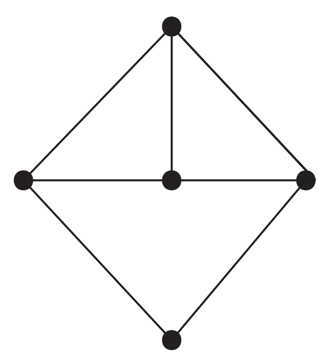

Figure 3.4: The graph H

Recall that for two graphs H and G, we denote by $\eta_G(H)$ (resp. $i_G(H)$) the number of subgraphs (respectively induced subgraphs) of G which are isomorphic to

H. The following result gives formulas for the first few coefficients of the chromatic polynomial by counting certain (induced) subgraphs of the graph.

Theorem 3.2.6. *[24, pg. 31-32] Let G be a graph of order n and size m, and let g be the girth of the graph. Then*

$$\pi(G,x) = \sum_{i=1}^{n} (-1)^{n-i} h_i(G) x^i$$

is a polynomial in x such that

$$\begin{aligned}
h_{n-i} &= \binom{m}{i} \text{ for } 0 \le i \le g-2, \\
h_{n-g+1} &= \binom{m}{g-1} - \eta_G(C_g), \quad (\text{in particular,} \quad h_{n-2} = \binom{m}{2} - \eta_G(C_3)) \\
h_{n-3} &= \binom{m}{3} - (m-2)\eta_G(K_3) - i_G(C_4) + 2\eta_G(K_4), \text{ and} \\
h_{n-4} &= \binom{m}{4} - \binom{m-2}{2}\eta_G(K_3) + \binom{\eta_G(K_3)}{2} - (m-3)i_G(C_4) \\
& \quad -(2m-9)\eta_G(K_4) - i_G(C_5) + i_G(K_{2,3}) + 2i_G(H) + 3i_G(W_5) - 6\eta_G(K_5),
\end{aligned}$$

where H is the graph shown in Figure 3.4 and W_5 is the wheel graph of order 5.

The first two items of Theorem 3.2.6 follow immediately from Whitney's Broken-Cycle Theorem and the expressions for h_{n-3} and h_{n-4} were obtained by Farrell in [28]. A direct application of the previous result yields explicit formulas for the first few coefficients of the chromatic polynomials of complete bipartite graphs.

Lemma 3.2.7. *Let $p, q \geq 2$, $n = p + q$ and $\pi(K_{p,q}, x) = \sum_{i=1}^{n}(-1)^{n-i}h_i(G)x^i$, then*

$$\begin{aligned}
h_n &= 1, \\
h_{n-1} &= pq, \\
h_{n-2} &= \binom{pq}{2}, \\
h_{n-3} &= \binom{pq}{3} - \binom{q}{2}\binom{p}{2}, \ \textit{and} \\
h_{n-4} &= \binom{pq}{4} - (pq-3)\binom{q}{2}\binom{p}{2} + \binom{q}{2}\binom{p}{3} + \binom{p}{2}\binom{q}{3}.
\end{aligned}$$

Proof. We apply Theorem 3.2.6 to find each coefficient. The girth of $K_{p,q}$ is 4 , so we get $h_{n-i} = \binom{pq}{i}$ for $0 \leq i \leq 2$. Also, we get the formula for h_{n-3} by noting that the number of C_4's in $K_{p,q}$ is equal to $\binom{q}{2}\binom{p}{2}$. Since bipartite graphs are odd cycle free, $K_{p,q}$ does not contain any K_3, K_4, C_5 H, W_5 or K_5. Moreover, the number of $K_{2,3}$'s in $K_{p,q}$ is equal to $\binom{q}{2}\binom{p}{3} + \binom{p}{2}\binom{q}{3}$. Thus, we obtain the formula for h_{n-4} and this completes the proof. □

A polynomial is called *standard* if it is either identically zero or has positive leading coefficient, and is said to have *only non-positive roots* if it is either identically zero or has all of its roots real and non-positive. Suppose that $f, g \in \mathbb{R}[x]$ both have only real roots, that those of f are $\zeta_1 \leq \cdots \leq \zeta_a$ and that those of g are $\theta_1 \leq \cdots \leq \theta_b$. We say that f *interlaces* g if deg $g = 1 +$ deg f and the roots of f and g satisfy

$$\theta_1 \leq \zeta_1 \leq \theta_2 \leq \cdots \leq \zeta_a \leq \theta_{a+1}.$$

We also say that f *alternates left of* g if deg $f =$ deg g and the roots of f and g satisfy

$$\zeta_1 \leq \theta_1 \leq \zeta_2 \leq \cdots \leq \zeta_a \leq \theta_a.$$

The notation $f \prec g$ stands for either f interlaces g or f alternates left of g. The following result which is known as Hermite-Biehler Theorem (see [63]) characterizes Hurwitz quasi-stable polynomials via the interlacing property.

Theorem 3.2.8 (Hermite-Biehler Theorem)**.** *Let $f(x) \in \mathbb{R}[x]$ be standard, and write $f(x) = f^e(x^2) + xf^o(x^2)$. Set $t = x^2$. Then $f(x)$ is Hurwitz quasi-stable if and only if both $f^e(t)$ and $f^o(t)$ are standard, have only non-positive roots, and $f^o(t) \prec f^e(t)$.*

We are now ready to show that many complete bipartite graphs have non-real chromatic roots with real parts greater than their tree-widths.

Theorem 3.2.9. *Suppose that $p \geq 2$ is fixed. Then, $\pi(K_{p,q})$ has a non-real root z with $\Re(z) > p$ for all sufficiently large q.*

Proof. Set $n = p + q$ and $\pi(K_{p,q}, x) = \sum_{i=1}^{n}(-1)^{n-i}h_i x^i$. We will show that

$$\pi(K_{p,q}, x+p) = \sum_{i=1}^{n}(-1)^{n-i}h_i(x+p)^i$$

is not Hurwitz quasi-stable when q is sufficiently large. Rewriting $\pi(K_{p,q}, x+p) = \sum_{i=1}^{n} a_i x^i$, we have

- $a_n = 1$;
- $a_{n-2} = \binom{n}{2}p^2 - (n-1)ph_{n-1} + h_{n-2}$;
- $a_{n-4} = \binom{n}{4}p^4 - \binom{n-1}{3}p^3 h_{n-1} + \binom{n-2}{2}p^2 h_{n-2} - (n-3)ph_{n-3} + h_{n-4}$.

Now we write $\pi(K_{p,q}, x+p) = f^e(x^2) + xf^o(x^2)$. First, we suppose that n is even and we look at the first three polynomials in the Sturm sequence $(f_0, f_1, f_2, \ldots)$ of $f^e(t)$:

$$\begin{aligned}
f_0 &= t^{n/2} + a_{n-2}t^{(n-2)/2} + a_{n-4}t^{(n-4)/2} + \ldots \\
f_1 &= \frac{n}{2}t^{(n-2)/2} + a_{n-2}\frac{n-2}{2}t^{(n-4)/2} + a_{n-4}\frac{n-4}{2}t^{(n-6)/2} + \ldots \\
f_2 &= -\frac{2}{n^2}\left(2na_{n-4} - (n-2)a_{n-2}^2\right)t^{(n-4)/2} + \ldots
\end{aligned}$$

We can write a_{n-4} and a_{n-2} in terms of p and q by using Lemma 3.2.7, and then we can write $2na_{n-4}-(n-2)a_{n-2}^2$ as a quartic polynomial in q where the coefficients are polynomial functions of p. More precisely, calculations show that $2na_{n-4}-(n-2)a_{n-2}^2$ is equal to

$$\begin{aligned}
&\left(\frac{1}{6}p^2-\frac{1}{6}p\right)q^4+\left(\frac{1}{2}p^4-\frac{5}{3}p^3+\frac{11}{6}p^2-\frac{2}{3}p\right)q^3\\
&+\left(-\frac{5}{6}p^5+\frac{5}{3}p^4-\frac{5}{6}p^3-\frac{1}{3}p^2+\frac{1}{3}p\right)q^2\\
&+\left(-\frac{1}{6}p^8+\frac{1}{3}p^6+\frac{1}{2}p^5-\frac{5}{6}p^4-\frac{1}{6}p^3+\frac{1}{3}p^2\right)q+\left(-\frac{1}{6}p^9+\frac{1}{2}p^8-\frac{1}{3}p^7\right).
\end{aligned}$$

Because $\frac{1}{6}p(p-1)>0$ for fixed $p\geq 2$, it follows that the leading coefficient of f_2 is negative for all sufficiently large q. Therefore, by Theorem 2.3.2, we find that f^e does not have all real roots and hence $\pi(K_{p,q},x+p)$ is not Hurwitz quasi-stable by Theorem 3.2.8. Thus, we obtain that $\pi(K_{p,q},x)$ has a root z with $\Re(z)>p$ for all sufficiently large q (that root cannot be a real number as we already noted that real chromatic roots are bounded by the tree-width of the graph). A similar argument works for n odd but in this case one would work with the Sturm sequence of f^o instead of f^e (we leave the details to the reader). $\square$

Since the tree-width of $K_{p,q}$ is equal to $\min(p,q)$, the following corollary follows immediately.

Corollary 3.2.10. *For any integer $k\geq 2$, there exist infinitely many graphs which have tree-width k and chromatic roots z with $\Re(z)>k$.*

Bounding the real part of complex chromatic roots by $n-1$

We now turn to proving that $n-1$ is an upper bound for the real part of chromatic roots of graphs with large chromatic number. We will need the following two elementary but useful results.

Let $\mathcal{G}(H)$ be the set of all subgraphs of G which are isomorphic to H.

Lemma 3.2.11. *Let H and K be two subgraphs of G, then*

$$\eta_G(H)\eta_G(K) \geq \eta_G(H \cup K). \qquad \square$$

Proof. The map $\psi : \mathcal{G}(H)\times\mathcal{G}(K) \to \mathcal{G}(H\cup K)$, which sends (H, K) to $H\cup K$ is an onto map, and therefore, $\eta_G(H)\eta_G(K) = |\mathcal{G}(H) \times \mathcal{G}(K)| \geq |\mathcal{G}(H \cup K)| = \eta_G(H \cup K)$. $\square$

Lemma 3.2.12. *Let $H_1, H_2, \ldots, H_k$ be disjoint subgraphs of G and $r = \sum_{i=1}^{k} |V(H_i)|$. Then,*

$$\eta_G(\cup_{i=1}^{k} H_i) \geq \eta_G(K_r). \qquad \square$$

Proof. Let $H = \cup_{i=1}^{k} H_i$. Let $\mathcal{G}(H)'$ be the set of all subgraphs of G which are isomorphic to H and which induce a complete graph. Let $\psi : \mathcal{G}(H)' \to \mathcal{G}(K_r)$ be the map which sends a subgraph H' in $\mathcal{G}(H)'$ to the complete graph induced by the vertex set of H'. Now ψ is an onto map and $\mathcal{G}(H)' \subseteq \mathcal{G}(H)$. Hence, the result follows. $\square$

(We remark that a natural question arising from Lemma 3.2.12 is whether the stronger statement that if H is a subgraph of K then $\eta_G(H) \geq \eta_G(K)$ is true. Unfortunately, the answer is negative. For example, let $G = K_4$, $H = 2K_2$ and K be the graph obtained from a triangle by adding a leaf. Clearly H is a subgraph of K but $\eta_G(H) = 3$ which is strictly less than $\eta_G(K) = 12$.)

As a consequence of the previous two lemmas, we obtain the following result which will be needed in the proofs of the next two theorems.

Lemma 3.2.13. *Let G be a graph of order n and $\sigma(G,x)=\sum a_i x^i$. Then*

$$a_{n-1}a_{n-2}+a_{n-1}^2 \geq a_{n-3}.$$

Proof. By Observation 2.1.13, we have

$$a_{n-1}a_{n-2}+a_{n-1}^2 = (\eta_{\overline{G}}(K_2))^2+\eta_{\overline{G}}(K_2)\eta_{\overline{G}}(K_3)+\eta_{\overline{G}}(K_2)\eta_{\overline{G}}(2K_2)$$

and

$$a_{n-3}=\eta_{\overline{G}}(K_4)+\eta_{\overline{G}}(K_3\mathbin{\dot\cup} K_2)+\eta_{\overline{G}}(3K_2).$$

Now by Lemma 3.2.11, it follows that

$$\eta_{\overline{G}}(K_2)\eta_{\overline{G}}(K_3)\geq \eta_{\overline{G}}(K_3\mathbin{\dot\cup} K_2)$$

and

$$\eta_{\overline{G}}(K_2)\eta_{\overline{G}}(2K_2)\geq \eta_{\overline{G}}(3K_2).$$

Also, by combining Lemma 3.2.11 and Lemma 3.2.12 we get

$$(\eta_{\overline{G}}(K_2))^2\geq \eta_{\overline{G}}(2K_2)\geq \eta_{\overline{G}}(K_4).$$

Therefore, the desired inequality is obtained.

□

For our next results, we shall also need specific conditions for a low degree polynomial to be stable (see, for example, [2, pg.181]).

Theorem 3.2.14 (Stability tests for polynomials of degree at most 4)**.** *The following conditions are necessary and sufficient for stability of polynomials of degree at most 4:*

- *A linear or quadratic polynomial is stable if and only if all the coefficients are of the same sign.*
- *A cubic monic polynomial $f(x) = x^3 + bx^2 + cx + d$ is stable if and only if all its coefficients are positive and $bc > d$.*
- *A quartic monic polynomial $f(x) = x^4 + ax^3 + bx^2 + cx + d$ is stable if and only if all its coefficients are positive and $abc > c^2 + a^2 d$.*

□

We are now ready to show that Conjecture 3.2.5 holds for graphs with chromatic number at least $n - 3$:

Theorem 3.2.15. *Let G be a graph with $\chi(G) \geq n-3$. If z is a root of $\pi(G, x)$ then $\Re(z) \leq n - 1$ with equality if and only if $\chi(G) = n$.*

Proof. If $\chi(G) = n$ then $G = K_n$, and if $\chi(G) = n - 1$ then $G - u \cong K_{n-1}$ for some vertex u of G since otherwise $\overline{G}$ contains an induced $2K_2$ and $\chi(G) \leq n - 2$. In both cases G is chordal and hence it has all integer chromatic roots. Therefore, the result follows as the largest integer chromatic root is always equal to $\chi(G) - 1$. So we assume that $\chi(G) \leq n - 2$. We show that $\pi(G, x + n - 1)$ is stable. First, we write

$$\pi(G, x + n - 1) = f(G, x) \prod_{i=1}^{\chi(G)} (x + n - i).$$

It suffices to show that $f(G, x)$ is Hurwitz stable. We set $\pi(G, x) = \sum a_i (x)_{\downarrow i}$.

If $\chi(G) = n - 2$, then

$$\begin{aligned} f(G,x) &= a_{n-2} + a_{n-1}(x+1) + (x+1)x \\ &= x^2 + (1 + a_{n-1})x + a_{n-1} + a_{n-2} \end{aligned}$$

Since all the coefficients are positive, the result is clear by Theorem 3.2.14. Now, if $\chi(G) = n - 3$, then

$$\begin{aligned} f(G,x) &= a_{n-3} + a_{n-2}(x+2) + a_{n-1}(x+2)(x+1) + (x+2)(x+1)x \\ &= x^3 + (3 + a_{n-1})x^2 + (2 + 3a_{n-1} + a_{n-2})x + 2a_{n-1} + 2a_{n-2} + a_{n-3} \end{aligned}$$

Because $f(G,x)$ is a cubic polynomial with all coefficients positive, by Theorem 3.2.14, $f(G,x)$ is Hurwitz stable if and only if

$$(3 + a_{n-1})(2 + 3a_{n-1} + a_{n-2}) > 2a_{n-1} + 2a_{n-2} + a_{n-3}$$

which is equivalent to

$$6 + 9a_{n-1} + a_{n-2} + 3a_{n-1}^2 + a_{n-1}a_{n-2} > a_{n-3}.$$

Now the latter inequality follows from Lemma 3.2.13. □

We now partially extend our results to graphs of chromatic number $n - 4$; such graphs' characterization were given in Theorem 2.4.1. We concentrate on two subfamilies of such graphs.

Theorem 3.2.16. *Let G be a graph of order n and chromatic number $n - 4$ whose complement belongs to M_1 or M_2 families depicted in Figure 2.11 and Figure 2.12 respectively. If z is a root of $\pi(G,x)$ then $\Re(z) < n - 1$.*

Proof. We will show that $\pi(G, x+n-1)$ is Hurwitz-stable. Let

$$\pi(G, x+n-1) = f(G, x)\prod_{i=1}^{n-4}(x+n-i).$$

Then,

$$f(G,x) = x^4 + (a_{n-1}+6)x^3 + (a_{n-2}+6a_{n-1}+11)x^2 + (a_{n-3}+5a_{n-2}+11a_{n-1}+6)x \\ + a_{n-4}+3a_{n-3}+6a_{n-2}+6a_{n-1}.$$

is a monic quartic polynomial with positive coefficients. Hence, by Theorem 3.2.14, the stability condition is that

$$(a_{n-1}+6)(a_{n-2}+6a_{n-1}+11)(a_{n-3}+5a_{n-2}+11a_{n-1}+6)$$

is strictly larger than

$$(a_{n-3}+5a_{n-2}+11a_{n-1}+6)^2 + (a_{n-1}+6)^2(a_{n-4}+3a_{n-3}+6a_{n-2}+6a_{n-1}).$$

Expanding the terms, we find that this condition is equivalent to

$$a_{n-1}a_{n-2}a_{n-3} + 3a_{n-1}^2a_{n-3} + 5a_{n-1}a_{n-2}^2 + 35a_{n-1}^2a_{n-2} + 5a_{n-2}^2 + 125a_{n-1}a_{n-2} \\ +60a_{n-1}^3 + 360a_{n-1}^2 + 660a_{n-1} + 90a_{n-2} + 360$$

being strictly larger than

$$a_{n-1}^2a_{n-4} + 12a_{n-1}a_{n-4} + 11a_{n-1}a_{n-3} + 36a_{n-4} + 54a_{n-3} + 4a_{n-2}a_{n-3} + a_{n-3}^2.$$

By Theorems 2.4.4 and 2.4.7, the sequence $\langle 1, a_{n-1}, a_{n-2}, a_{n-3}, a_{n-4}\rangle$ is logconcave and hence unimodal. Furthermore, again by Theorems 2.4.4 and 2.4.7 we know that $a_{n-3} > a_{n-4}$. So, there are three cases we need to consider.

Case 1: $1 = a_n \leq a_{n-1} \geq a_{n-2} \geq a_{n-3} > a_{n-4}$.

In this case we have the following three inequalities

$$\begin{aligned} a_{n-1}a_{n-2}a_{n-3} &\geq a_{n-3}^2, \\ 125a_{n-1}a_{n-2} &\geq 12a_{n-1}a_{n-4} + 11a_{n-1}a_{n-3} + 36a_{n-4} + 54a_{n-3} + 4a_{n-2}a_{n-3}, \\ 3a_{n-1}^2a_{n-3} &\geq a_{n-3}^2 \end{aligned}$$

where all the inequalities follow from the assumption. Now, clearly the stability condition is satisfied.

Case 2: $1 = a_n \leq a_{n-1} \leq a_{n-2} \geq a_{n-3} > a_{n-4}$.

In this case we have the following three inequalities

$$\begin{aligned} 3a_{n-1}^2a_{n-3} &\geq a_{n-1}^2a_{n-4}, \\ 125a_{n-1}a_{n-2} &\geq 12a_{n-1}a_{n-4} + 11a_{n-1}a_{n-3} + 36a_{n-4} + 54a_{n-3}, \\ 5a_{n-2}^2 &\geq a_{n-3}^2 \end{aligned}$$

Now it follows that the stability condition is satisfied.

Case 3: $1 = a_n \leq a_{n-1} \leq a_{n-2} \leq a_{n-3} > a_{n-4}$.

First note that $a_{n-1} \geq 6$ since G is in M_1 or M_2 family. Now, by multiplying both sides of the inequality given in Lemma 3.2.13 by a_{n-3}, we obtain $a_{n-1}a_{n-2}a_{n-3}+a_{n-1}^2a_{n-3} \geq a_{n-3}^2$. Moreover, $2a_{n-1}^2a_{n-3} \geq 12a_{n-1}a_{n-4}$ as $a_{n-1} \geq 6$. Hence, we obtain

$$a_{n-1}a_{n-2}a_{n-3} + 3a_{n-1}^2a_{n-3} \geq 12a_{n-1}a_{n-4} + a_{n-3}^2. \tag{3.3}$$

Also, by the log-concavity of $\sigma(G,x)$, we obtain that $a_{n-1}^2 \geq a_{n-2}a_n = a_{n-2}$ and $a_{n-2}^2 \geq a_{n-1}a_{n-3}$. Therefore,

$$\begin{aligned} 5a_{n-1}a_{n-2}^2 &\geq 5a_{n-1}^2 a_{n-3} \\ &= a_{n-1}^2 a_{n-3} + 4a_{n-1}^2 a_{n-3} \\ &\geq a_{n-1}^2 a_{n-4} + 4a_{n-2}a_{n-3} \end{aligned}$$

and we get

$$5a_{n-1}a_{n-2}^2 \geq a_{n-1}^2 a_{n-4} + 4a_{n-2}a_{n-3}. \tag{3.4}$$

Lastly, again by the log-concavity of $\sigma(G,x)$, we have $a_{n-1}^2 \geq a_{n-2}a_n = a_{n-2}$. Therefore,

$$\begin{aligned} 35a_{n-1}^2 a_{n-2} &\geq 35a_{n-2}^2 \\ &\geq 35a_{n-1}a_{n-3} \\ &= 11a_{n-1}a_{n-3} + 24a_{n-1}a_{n-3} \\ &\geq 11a_{n-1}a_{n-3} + 144a_{n-3} \\ &\geq 11a_{n-1}a_{n-3} + 36a_{n-4} + 54a_{n-3} \end{aligned}$$

and we get

$$35a_{n-1}^2 a_{n-2} \geq 11a_{n-1}a_{n-3} + 36a_{n-4} + 54a_{n-3}. \tag{3.5}$$

Now, combining the inequalities (3.3), (3.4) and (3.5) we obtain again that the stability condition is satisfied. $\square$

As we already mentioned, among all real chromatic roots of graphs with order $n \geq 9$, the largest non-integer real chromatic root is $\dfrac{n-1-\sqrt{(n-3)(n-7)}}{2}$ [21]. It seems that the largest real part of a chromatic root is much larger than this value. In fact, we can show that there exist chromatic roots whose real parts are in $(n-3, n-2)$.

On the other hand, we do not know of any chromatic root whose real part is in the interval $(n-2, n-1)$

Proposition 3.2.17. *Let $2 \leq q \leq 4$. Then, $\pi(K_n - qK_2)$ has a non-real root z such that $n-2 > \Re(z) > n-3$.*

Proof. The complement of the graph $K_n - qK_2$ is qK_2. So, it is easy to see that $a_{n-i}(K_n - qK_2) = \binom{q}{i}$. Now,

$$\pi(K_n - qK_2, x) = \sum_{i=0}^{q} a_{n-i}(K_n - qK_2)(x)_{\downarrow n-i} = \sum_{i=0}^{q} \binom{q}{i} (x)_{\downarrow n-i}.$$

The polynomial $\pi(K_n - qK_2, x)$ has trivial factor of $(x)_{\downarrow n-q}$. So, $\pi(K_n - qK_2, x)/(x)_{\downarrow n-q}$ is a quadratic, cubic and quartic polynomial for $q = 2, 3, 4$ respectively. Now shifting the polynomial by an appropriate amount, we can eliminate n and apply the Hurwitz-stability criterion to obtain the result. $\square$

We pose the following question:

Question 3.2.18. Among all non-real chromatic roots of graphs with order n, what is the largest real part of a chromatic root of a graph of order n?

This problem seems more difficult and the answer must be at least $n - 5/2$ (which is much bigger than the largest non-integer real root) as we have seen that the graph $K_n - 2K_2$ has non-real chromatic roots with real part equal to $n - 5/2$. Indeed, we believe that this should be the true value.

Obviously, the bound $\Re(z) \leq n-1$ in Conjecture 3.2.5 is sharp with complete graph being an extremal graph. We believe that the equality holds if and only if G is a complete graph. Also, we note that there is a stronger conjecture than Conjecture 3.2.5 posed by Sokal which states that if z is a root of $\pi(G, x)$ then $\Re(z) \leq \Delta(G)$. Equality $\Re(z) = \Delta(G)$ holds if the graph is either a complete graph or an odd cycle.

Another trivial related question is the following:

Question 3.2.19. Let G be a graph of order n. Is it true that if z is a chromatic root of G then $|z| \leq n-1$?

Chapter 4

Restrained Chromatic Polynomials

4.1 Introduction and Preliminaries

There are variants of vertex colourings that have been of interest. In a *list colouring*, for each vertex v there is a finite set $L(v)$ of colours available for use, and then one wishes to properly colour the vertices such that the colour of v is from $L(v)$. If $|L(v)| = k$ for every vertex v, then a list colouring is called a *k-list colouring*. There is a vast literature on list colourings (see, for example, [1], [15], Section 9.2 and [61]). We are going to consider a complementary problem, namely colouring the vertices of a graph G where each vertex v has a *forbidden* finite set of colours, $r(v) \subset \mathbb{N}$ (we allow $r(v)$ to be equal to the empty set); we call the function r a *restraint* on the graph G.

For a positive integer n, let $[n]$ stand for $\{1, \ldots, n\}$. Also, for $k \geq 1$ let us define $\binom{[n]}{k} := \{\, A \mid A \subseteq [n] \text{ and } |A| = k \,\}$. For example, $\binom{[n]}{1} = \{\{1\}, \ldots, \{n\}\}$ and $\binom{[3]}{2} = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$. Let G be a graph with n vertices. We say that r is a *k-restraint* on G if $|r(u)| = k$ and $r(u) \in \binom{[kn]}{k}$ for every $u \in V(G)$. If $k = 1$ (that is, we forbid exactly one colour at each vertex) we omit k from the notation and use the word *simple* when discussing such restraints. If the vertices of G are ordered as $v_1, v_2 \ldots v_n$, then we usually write r in the form $[r(v_1), r(v_2) \ldots r(v_n)]$.

A k-colouring c of G is *permitted* by restraint r (or c is a colouring *with respect to* r) if for all vertices of v of G, $c(v) \notin r(v)$. Restrained colourings arise in a natural way as a graph is sequentially coloured, since the colours already assigned to vertices induce a set of forbidden colours on their uncoloured neighbours. Restrained colourings can also arise in scheduling problems where certain time slots are unavailable for certain nodes (c.f. [38]). Moreover, restraints are of use in the construction of critical graphs (with respect to colourings) [53]; a k-chromatic graph $G = (V, E)$ is said to be *k-amenable* if every non-constant simple restraint $r : V \to [k]^1$ permits a k-colouring [14, 44]. Finally, observe that if each vertex v of a graph G has a list of available colours $L(v)$, and, without loss,

$$L = \bigcup_{v \in V(G)} L(v) \subseteq [N]$$

then setting $r(v) = [N] - L(v)$ we see that G is list colourable with respect to the lists $L(v)$ if and only if G has an N-colouring permitted by r.

Given a restraint r on graph G, we define the *restrained chromatic polynomial* of G with respect to r, denoted by $\pi_r(G, x)$, to be the number of x-colourings permitted by restraint r [11]. Note that this function extends the definition of chromatic polynomial, as if $r(v) = \emptyset$ for every vertex v then $\pi_r(G, x) = \pi(G, x)$. Now the use of the terminology begs the question as to whether the function is actually a polynomial in x, and the answer is 'yes', *provided x is sufficiently large*. In order to prove that this function is a polynomial function of x for large enough x, we need to prove some preliminary results.

Note that, unlike the chromatic polynomial, this function is not always a polynomial function of x. For instance, consider the path P_4 with $V(P_4) = \{v_1, v_2, v_3, v_4\}$ and $E(P_4) = \{v_i v_{i+1} \,|\, 1 \leq i \leq 3\}$. Let $r = [\{1\}, \{2\}, \{3\}, \{4\}]$ be a simple restraint on P_4. Then,

$$\pi_r(P_4,x) = \begin{cases} 0 & \text{if } x = 1 \\ 1 & \text{if } x = 2 \\ 8 & \text{if } x = 3 \\ x^4 - 7\,x^3 + 21\,x^2 - 32\,x + 21 & \text{if } x \geq 4 \end{cases}$$

and so $\pi_r(P_4,x)$ is a polynomial function of x when $x \geq 4$.

Restrained chromatic polynomials satisfy an edge addition-contraction formula like chromatic polynomials which is as follows:

Lemma 4.1.1. *Let r be any restraint on G, and $u,v \in V(G)$ be such that $uv \notin E(G)$. Suppose that u and v are replaced by w in the contraction $G \cdot uv$. Then*

$$\pi_r(G,x) = \pi_r(G+uv,x) + \pi_{r_{uv}}(G \cdot uv, x)$$

where

$$r_{uv}(a) = \begin{cases} r(a) & \textit{if } a \neq w \\ r(u) \cup r(v) & \textit{if } a = w \end{cases}$$

for each $a \in V(G \cdot uv)$.

Proof. The x-colourings of G that are permitted by r can be partitioned into two sets – those that assign the same colour to u and v and those that assign different colours to u and v. The former are the x-colourings of $G \cdot uv$ permitted by r_{uv}, and latter are the x-colourings of $G+uv$ that are permitted by r. □

Let $A = [x_1, \ldots, x_n]$ be a sequence of variables. Then recall that the i^{th} elementary symmetric function on A is equal to

$$S_i(A) = \sum_{1 \leq k_1 < \cdots < k_i \leq n} x_{k_1} \ldots x_{k_i}.$$

Also, given a restraint function r on a graph G, let $M_{G,r}$ be the maximum value in $\bigcup\limits_{v \in V(G)} r(v)$ if the set is nonempty and 0 otherwise.

Example 4.1.1. Let r be a restraint function on the empty graph $G = \overline{K_n}$. Then for all $x \geq M_{G,r}$,

$$\pi_r(G, x) = \prod_{v \in V(G)} (x - |r(v)|) = \sum_{i=0}^{n} (-1)^{n-i} S_i(A) x^{n-i}$$

where $A = [\ |r(v)|\ :\ v \in V(G)\ ]$.

Using the edge deletion-contraction formula, we can now show that the restrained chromatic polynomial $\pi_r(G, x)$ is a polynomial function of x for x sufficiently large, and like chromatic polynomials, the restrained chromatic polynomial of a graph G of order n is monic of degree n with integer coefficients that alternate in sign.

Theorem 4.1.2. *Let G be a graph of order n and r be a restraint on G. Then for all $x \geq M_{G,r}$, the function $\pi_r(G, x)$ is a monic polynomial of degree n with integer coefficients that alternate in sign.*

Proof. We proceed by induction on the number of edges. If G has no edges then the result is clear by Example 4.1.1. Suppose that G has at least one edge, say e, then note that $M_{G,r} = M_{G-e,r} = M_{G \cdot e, r_e}$. Now, it follows that the result holds for both $\pi_r(G - e, x)$ and $\pi_{r_e}(G \cdot e, x)$ by induction hypothesis. Thus, the result is established as $\pi_r(G, x) = \pi_r(G - e, x) - \pi_{r_e}(G \cdot e, x)$ by Lemma 4.1.1. $\square$

Observe that, unlike chromatic polynomials, the constant term of this polynomial need not be 0. For example, the constant term for any restraint r on $\overline{K_n}$ is $(-1)^n \prod_{v \in V(G)} |r(v)|$.

Let G be a graph of order n. If r_1 and r_2 are two restraints on G such that $r_1(v) \subseteq r_2(v)$ for each $v \in V(G)$ then it is clear that $\pi_{r_2}(G, x) \leq \pi_{r_1}(G, x)$ for every nonnegative integer x. Also, $\pi_r(G,x) \le (x-k)^n$ for any k-restraint r on G when x is sufficiently large.

If r is a restraint on G and H is a subgraph of G then $r|_H$, *the restriction of* r *to* H, denotes the restraint function induced by r on the vertex set of H. Observe that if H is a subgraph of G such that $V(H) = V(G)$ then $\pi_{r|_H}(H,x) \ge \pi_{r|_G}(G,x)$ since every x-colouring of G permitted by the restraint $r|_G$ is also an x-colouring of H permitted by the restraint $r|_H$. Also, if G is a graph with $V_1 \uplus \cdots \uplus V_t$ being a partition of the vertex set $V(G)$, then $G' = G_{V_1} \uplus \cdots \uplus G_{V_t}$ is a subgraph of G such that $V(G) = V(G')$. Therefore, $\pi_{r|_{G'}}(G',x) \ge \pi_{r|_G}(G,x)$. Since $G_{V_1}, \cdots, G_{V_t}$ are connected components of G', we have $\pi_{r|_{G'}}(G',x) = \prod_{i=1}^{t} \pi_{r|_{G_{V_i}}}(G_{V_i},x)$. Hence, it follows that for any restraint r on G we have $\prod_{i=1}^{t} \pi_{r|_{G_{V_i}}}(G_{V_i},x) \ge \pi_r(G,x)$ for all x.

Definition 4.1.1. Let r and r' be two restraints on G. We say that r and r' are *equivalent* restraints, denoted by $r \simeq r'$, if there exists a graph automorphism ϕ of G and a bijective function $f : \bigcup_{u \in V(G)} r(u) \mapsto \bigcup_{u \in V(G)} r'(u)$ such that

$$f(r(u)) = r'(\phi(u))$$

for every vertex u of G. If r and r' are not equivalent then we call them nonequivalent restraints and write $r \not\simeq r'$.

Example 4.1.2. Let $G = P_3$ and $v_1, v_2, v_3 \in V(G)$ such that $v_i v_{i+1} \in E(G)$. Consider the restraints $r_1 = [\{1\},\{2\},\{3\}]$, $r_2 = [\{2\},\{1\},\{4\}]$, $r_3 = [\{1\},\{1\},\{2\}]$ and $r_4 = [\{3\},\{2\},\{2\}]$ (see Figure 4.1). Then $r_1 \simeq r_2$, $r_3 \simeq r_4$ and $r_1 \not\simeq r_3$.

If r and r' are two equivalent restraints, then $\pi_r(G,x) = \pi_{r'}(G,x)$ for all x sufficiently large. Thus if $N = \sum_{v \in V(G)} |r(v)|$ then we can assume (as we shall do for the rest of this thesis) that each $r(v) \subseteq [N]$, and so there are only finitely many restrained

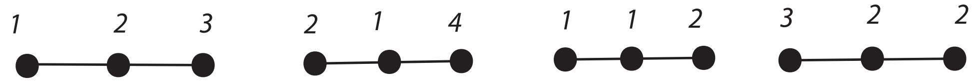

Figure 4.1: Some restraints on P_3.

chromatic polynomials on a given graph G. Hence past some point (past the roots of all of the differences of such polynomials), one polynomial exceeds (or is less) than all of the rest, no matter what x is.

Remark 4.1.1. There exist graphs for which two nonequivalent restraints permit the same number of colourings. For example, consider the graph P_4 with $V(P_4) = \{v_1, v_2, v_3, v_4\}$ and $E(P_4) = \{v_i v_{i+1} \,|\, 1 \leq i \leq 3\}$. It is trivial that $r = [\{1\}, \{2\}, \{2\}, \{1\}]$ and $r' = [\{1\}, \{2\}, \{3\}, \{3\}]$ are two nonequivalent restraints on P_4. However,

$$\pi_r(P_4, x) = \pi_{r'}(P_4, x) = x^4 - 7\,x^3 + 20\,x^2 - 28\,x + 16$$

for all large enough x.

4.2 Extremal Restraints

Our focus in this section will be on the following interesting question:

Question 4.2.1. Given a graph G and x large enough, among all k-restraints on G what restraint permits the largest/smallest number of x-colourings?

In this section, we first give a complete answer to the minimization part of this question, by describing such restraints for all graphs. We then turn our attention to the more difficult maximization problem in the case of some important graph families such as complete graphs and bipartite graphs, and describe the k-restraints which permit the largest number of colourings. Moreover, we prove that extremal restraints are unique; in other words, the number of colourings permitted by an extremal restraint is strictly larger (or smaller) than the number of colourings permitted by any other restraint which is not equivalent to that extremal restraint.

Example 4.2.1. Consider the cycle C_3. There are essentially three nonequivalent simple restraints on C_3, namely $r_1 = [\{1\}, \{1\}, \{1\}]$, $r_2 = [\{1\}, \{2\}, \{1\}]$ and $r_3 = [\{1\}, \{2\}, \{3\}]$. For $x \geq 3$, the restrained chromatic polynomials with respect to these restraints can be calculated as

$$\begin{aligned} \pi_{r_1}(C_3, x) &= (x-1)(x-2)(x-3), \\ \pi_{r_2}(C_3, x) &= (x-2)(x^2-4x+5), \text{ and} \\ \pi_{r_3}(C_3, x) &= 2(x-2)^2 + (x-2)(x-3) + (x-3)^3. \end{aligned}$$

where $\pi_{r_1}(C_3, x) < \pi_{r_2}(C_3, x) < \pi_{r_3}(C_3, x)$ holds for $x > 3$. Hence, r_3 permits the largest number of x-colourings whereas r_1 permits the smallest number of x-colourings for large enough x.

4.2.1 Restraints permitting the smallest number of colourings

A restraint function on a graph G is called *constant* k-restraint, denoted by r_c^k, if $r_c^k(u) = \{1, 2, \ldots, k\}$ for every vertex u of G. We will show that r_c^k permits the smallest number of colourings for every graph G. Observe that

$$\pi_{r_c^k}(G, x) = \pi(G, x-k)$$

for all $x \geq k$.

To prove the main results of this section, we will make use of the information about the second and third coefficients of the restrained chromatic polynomial. Hence, first we give interpretations for these coefficients.

Theorem 4.2.2. *Let $x \geq M_{G,r}$ and $\pi_r(G,x) = \sum_{i=0}^{n}(-1)^{n-i}a_i(G,r)x^i$. Then,*

$$a_{n-1}(G,r) = m_G + \sum_{u \in V(G)} |r(u)|.$$

In particular, if r is a k-restraint then $a_{n-1}(G,r) = m_G + nk$.

Proof. We proceed by induction on the number of edges. If G has no edges then $a_{n-1}(G,r) = \sum_{u \in V(G)} |r(u)|$ and the result clearly holds. Suppose that G has at least one edge, say e. Then by the induction hypothesis on $G - e$,

$$\pi_r(G-e,x) = x^n - \left(m_G - 1 + \sum_{u \in V(G)} |r(u)| \right) x^{n-1} + \ldots$$

holds. Now since $\pi_{r_e}(G \cdot e, x)$ is a monic polynomial of degree $n-1$, the result follows from Lemma 4.1.1. □

Theorem 4.2.3. *Let $x \geq M_{G,r}$ and $\pi_r(G,x) = \sum_{i=0}^{n}(-1)^{n-i}a_i(G,r)x^i$. Also, let $V(G) = \{u_1, \ldots u_n\}$. Then, $a_{n-2}(G,r)$ is equal to*

$$\binom{m_G}{2} - \eta_G(C_3) + \sum_{i<j} |r(u_i)|\ |r(u_j)|\ + m_G \sum_{u_i \in V(G)} |r(u_i)|\ - \sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)|.$$

In particular, if r is a k-restraint then

$$a_{n-2}(G,r) = \binom{m_G}{2} - \eta_G(C_3) + k^2\binom{n}{2} + nkm_G - \sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)|.$$

Proof. We proceed by induction on the number of edges. If G has no edges then $a_{n-2}(G,r) = \sum_{i<j} |r(u_i)|\ |r(u_j)|$ and the result is clear. Suppose that G has at least one edge, say $e = uv$. By the induction hypothesis on $G - e$, the coefficient of x^{n-2}

in $\pi_r(G-e,x)$ is equal to

$$\binom{m_G-1}{2} \;-\; \eta_{G-e}(C_3) \;+\; \sum_{i<j} |r(u_i)|\;|r(u_j)| \;+\; (m_G-1)\sum_{u_i\in V(G)} |r(u_i)|$$
$$-\sum_{u_iu_j\in E(G)\setminus\{e\}} |r(u_i)\cap r(u_j)|.$$

Also, by Theorem 4.2.2, the coefficient of x^{n-2} in $\pi_r(G\cdot e,x)$ is equal to

$$-m_{G\cdot e}-\sum_{w\in V(G\cdot e)} |r_e(w)|.$$

Observe that $m_{G\cdot e}=m_G-1-|N_G(u)\cap N_G(v)|$ and $|N_G(u)\cap N_G(v)|$ is equal to the number of triangles which contain the edge uv. Also, $\eta_{G-e}(C_3)$ is the number of triangles of G which do not contain the edge uv. Therefore,

$$\binom{m_G-1}{2}-\eta_{G-e}(C_3)+m_{G\cdot e}=\binom{m_G}{2}-\eta_G(C_3).$$

Now,

$$\begin{aligned}\sum_{w\in V(G\cdot e)} |r_e(w)| &= \sum_{u_i\in V(G)\setminus\{u,v\}} |r(u_i)| \;+\; |r(u)\cup r(v)|\\ &= \sum_{u_i\in V(G)\setminus\{u,v\}} |r(u_i)| \;+\; |r(u)|+|r(v)|-|r(u)\cap r(v)|\\ &= \sum_{u_i\in V(G)} |r(u_i)|-|r(u)\cap r(v)|\end{aligned}$$

Thus,

$$(m_G-1)\sum_{u_i\in V(G)} |r(u_i)| \;-\; \sum_{u_iu_j\in E(G)\setminus\{e\}} |r(u_i)\cap r(u_j)| \;+\; \sum_{w\in V(G\cdot e)} |r_e(w)|$$

is equal to

$$m_G \sum_{u_i \in V(G)} |r(u_i)| - \sum_{u_i u_j \in E(G)} |r(u_i) \cap r(u_j)|.$$

Hence, the result follows from Lemma 4.1.1. $\square$

Now we are ready to answer the question of which k-restraint permits the smallest number of colourings, for a large enough number of colours.

Theorem 4.2.4. *Let G be a connected graph of order n. Let also r be a k-restraint on G such that $r \not\cong r_c^k$. Then,*

$$\pi_{r_c^k}(G, x) < \pi_r(G, x)$$

provided x is sufficiently large.

Proof. Both $\pi_{r_c^k}(G, x)$ and $\pi_r(G, x)$ are monic polynomials. Also, the coefficient of the term x^{n-1} is the same for these polynomials by Theorem 4.2.2. Therefore, $\pi_r(G, x) - \pi_{r_c^k}(G, x)$ is a polynomial of degree $n - 2$. Now, by Theorem 4.2.3, the leading coefficient of $\pi_r(G, x) - \pi_{r_c^k}(G, x)$ is equal to

$$k\, m_G - \sum_{uv \in E(G)} |r(u) \cap r(v)|$$

which is clearly strictly positive. Thus, the desired inequality is obtained. $\square$

Remark 4.2.1. One can give an alternative proof for the fact that $\pi_r(G, x) \geq \pi_{r_c^k}(G, x)$ for large enough x by using some earlier results regarding list colourings. But first let us summarize some related work. Kostochka and Sidorenko [37] showed that if a chordal graph G has a list of l available colours at each vertex, then the number of list colourings is at least $\pi(G, l)$ for every natural number l. It is known that there exist graphs G (see, for example, Example 1 in [25]) for which the number of list colourings is strictly less than $\pi(G,l)$ for some natural number l. On the other hand, Thomassen [51] and Donner [25] independently proved that for any graph G, the number of list colourings is at least $\pi(G,l)$ when l is sufficiently large compared to the number of vertices of the graph. In particular, Thomassen [51] proved the result for $l \geq n^{10}$ where n is the order of the graph.

As we already pointed out, given a k-restraint r on a graph G and a natural number $x \geq kn$, we can consider an x-colouring permitted by r as a list colouring L where each vertex v has a list $L(v) = [x] - r(v)$ of $x-k$ available colours. Therefore, we derive that for a k-restraint r on graph G, $\pi_r(G,x) \geq \pi(G,x-k)$ for any natural number $x \geq n^{10} + kn$. But since $\pi_{r_c^k}(G,x)$ is equal to $\pi(G,x-k)$, it follows that $\pi_r(G,x) \geq \pi_{r_c^k}(G,x)$ for $x \geq n^{10} + kn$.

4.2.2 Restraints permitting the largest number of colourings

The k-restraints that permit the smallest number of colourings are easy to describe, and are, in fact, the same for all graphs. The more difficult question is which k-restraints permit the largest number of colourings; even for special families of graphs, it appears difficult, so we will focus on this question. As we shall see, the extremal k-restraints differ from graph to graph.

Let $R_{\max}(G,k)$ be the set of extremal k-restraints on G permitting the largest number of colourings for sufficiently large number of colours. More precisely, $R_{\max}(G,k)$ is the set of k-restraints r on G such that for every k-restraint r' on G, $\pi_{r'}(G,x) \geq \pi_r(G,x)$ for all large enough x.

In this section, we are going to present three results (Theorems 4.2.5, 4.2.8 and 4.2.12) which give necessary conditions for a restraint to be in $R_{\max}(G,k)$. Theorem 4.2.5 and Theorem 4.2.8 apply to all graphs and Theorem 4.2.12 applies to all (C_3,C_4)-free graphs. The necessary conditions given in Theorem 4.2.5 and Theorem 4.2.8 become sufficient to determine $R_{\max}(G,k)$ when G is a complete graph and bipartite graph respectively. In order to obtain these results, we will give combinatorial interpretations to the coefficients of x^{n-3} and x^{n-4} of the restrained chromatic polynomial (Theorem 4.2.7 and Theorem 4.2.11).

The first necessary condition for a restraint to be in $R_{\max}(G, k)$

A restraint r on graph a G is called a *proper restraint* if $r(u) \cap r(v) = \emptyset$ for every $uv \in E(G)$. We begin with showing that restraints in $R_{\max}(G, k)$ must be proper restraints.

Theorem 4.2.5. *If $r \in R_{\max}(G, k)$ then r is a proper restraint.*

Proof. For k-restraints, the coefficients of x^n and x^{n-1} of the restrained chromatic polynomial do not depend on the restraint function. So, in order to maximize the restrained chromatic polynomial, one needs to maximize the coefficient of x^{n-2}. By Theorem 4.2.3, it is clear that this coefficient is maximized when $|r(u) \cap r(v)| = 0$ for every edge uv of the graph. $\square$

Theorem 4.2.5 allows us to determine the extremal restaint for complete graphs. We deduce that for complete graphs the extremal restraint is unique and such restraint is the one where no two vertices have a common restrained colour.

Theorem 4.2.6. *Let r^* be the k-restraint on K_n such that $r^*(u) \cap r^*(v) = \emptyset$ for every $u, v \in V(K_n)$. Then, for any k-restraint r on G such that $r \not\simeq r^*$, we have $\pi_r(G, x) < \pi_{r^*}(G, x)$ for all large enough x.*

Proof. If r^* is a proper k restraint on K_n then $r^*(u) \cap r^*(v) = \emptyset$ for every $u, v \in V(K_n)$. Thus, the result follows by Theorem 4.2.5. $\square$

In general Theorem 4.2.5 is not sufficient to determine the extremal restraint. However it is very useful to narrow the possibilities for extremal restraints down to a smaller number of restraints. In the next example, we illustrate this on a cycle of length 4.

Example 4.2.2. Let $G = C_4$. Then there are exactly seven nonequivalent simple restraints on G and these restraints are namely

$$\begin{aligned}
r_1 &= [\{1\}, \{1\}, \{1\}, \{1\}],\\
r_2 &= [\{1\}, \{1\}, \{1\}, \{2\}],\\
r_3 &= [\{1\}, \{1\}, \{2\}, \{2\}],\\
r_4 &= [\{1\}, \{2\}, \{1\}, \{2\}],\\
r_5 &= [\{1\}, \{1\}, \{2\}, \{3\}],\\
r_6 &= [\{1\}, \{2\}, \{1\}, \{3\}],\\
r_7 &= [\{1\}, \{2\}, \{3\}, \{4\}].
\end{aligned}$$

Now, among these seven restraints, there are only three proper restraints and these are namely r_4, r_6 and r_7. Therefore, by Theorem 4.2.5, the possibilities for nonequivalent restraints in $R_{\max}(G, k)$ reduce to r_4, r_6 and r_7.

The second necessary condition for a restraint to be in $R_{\max}(G, k)$

Theorem 4.2.7. *Let $x \geq M_{G,r}$ and $\pi_r(G, x) = \sum_{i=0}^{n}(-1)^{n-i}a_i(G, r)x^i$. Also, let $V(G) = \{u_1, \ldots u_n\}$. Then,*

$$a_{n-3}(G, r) = A_0(G) \;+\; \sum_{i=1}^{8} A_i(G, r)$$

where

$$A_0(G) = \binom{m_G}{3} - (m_G - 2)\eta_G(C_3) - i_G(C_4) + 2\eta_G(K_4);$$

$$A_1(G, r) = \sum_{i<j<k} |r(u_i)|\ |r(u_j)|\ |r(u_k)|;$$

$$A_2(G,r) = (m_G - 1)\sum_{i<j} |r(u_i)|\ |r(u_j)|;$$

$$A_3(G,r) = \sum_{u_iu_j \notin E(G)} |r(u_i)|\ |r(u_j)|;$$

$$A_4(G,r) = -\sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)| \sum_{k \notin \{i,j\}} |r(u_k)|;$$

$$A_5(G,r) = \left(\binom{m_G}{2} \ - \ \eta_G(C_3)\right) \sum_{1 \le i \le n} |r(u_i)|;$$

$$A_6(G,r) = -(m_G - 1) \sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)|;$$

$$A_7(G,r) = A_7'(G,r) + A_7''(G,r) \quad \textit{where}$$

$$A_7'(G,r) = \sum_{u_iu_j \in E(G)} |N_G(u_i) \cap N_G(u_j)|\ |r(u_i) \cap r(u_j)|,$$

$$A_7''(G,r) = -\sum_{u_i \in V(G)} \sum_{\substack{u_j, u_k \in N_G(u_i) \\ j<k}} |r(u_j) \cap r(u_k)|;$$

$$A_8(G,r) = A_8'(G,r) + A_8''(G,r) \quad \textit{where}$$

$$A_8'(G,r) = \frac{1}{2} \sum_{u_iu_j \in E(G)} \sum_{\substack{k \notin \{i,j\} \\ u_k \in N_G(u_i) \cup N_G(u_j)}} |r(u_i) \cap r(u_j) \cap r(u_k)|$$

$$A_8''(G,r) = \frac{1}{6} \sum_{u_iu_j \in E(G)} \sum_{u_k \in N_G(u_i) \cap N_G(u_j)} |r(u_i) \cap r(u_j) \cap r(u_k)|.$$

Proof. We proceed by induction on the number of edges. First suppose that G is an empty graph. We know that $a_{n-3}(G,r) = A_1(G,r)$ by the formula given in Example 4.1.1. Also, it is easy to see that $A_i(G,r) = 0$ for $i \notin \{1,2,3\}$, $A_2(G,r) = -\sum_{i<j} |r(u_i)|\ |r(u_j)|$ and $A_3(G,r) = \sum_{i<j} |r(u_i)|\ |r(u_j)|$. So the result holds for empty graphs. Suppose now that G has at least one edge, say $e = u_1u_2$. First, let us define

$$B_0(G,e) = \binom{m_{G\cdot e}}{2} - \eta_{G\cdot e}(C_3);$$

$$B_1(G,r,e) = 0;$$

$$B_2(G,r,e) = \sum_{i<j} |r(u_i)||r(u_j)|;$$

$$B_3(G,r,e) = -|r(u_1)||r(u_2)|;$$

$$B_4(G,r,e) = -|r(u_1)\cap r(u_2)| \sum_{i\notin\{1,2\}} |r(u_i)|;$$

$$B_5(G,r,e) = (m_G - 1 - |N_G(u_1)\cap N_G(u_2)|) \sum_{1\le i\le n} |r(u_i)|;$$

$$B_6(G,r,e) = -(m_G-1)|r(u_1)\cap r(u_2)| - \sum_{u_iu_j\in E(G-e)} |r(u_i)\cap r(u_j)|;$$

$$B_7(G,r,e) = |N_G(u_1)\cap N_G(u_2)||r(u_1)\cap r(u_2)| - \sum_{\substack{i,j\in\{1,2\}\\ i\neq j}} \sum_{u\in N_G(u_i)\setminus N_G[u_j]} |r(u_j)\cap r(u)|;$$

$$B_8(G,r,e) = \sum_{\substack{u_i\in N_G(u_1)\cup N_G(u_2)\\ i\notin\{1,2\}}} |r(u_1)\cap r(u_2)\cap r(u_i)|.$$

First, we shall prove that

$$a_{n-3}(G\cdot e, r_e) = B_0(G,e) + \sum_{i=1}^{8} B_i(G,r,e).$$

Since $G\cdot e$ has $n-1$ vertices, by Theorem 4.2.3, the coefficient of x^{n-3} in $\pi_{r_e}(G\cdot e, x)$ is equal to

$$\binom{m_{G\cdot e}}{2} - \eta_{G\cdot e}(C_3) \;+ \sum_{\substack{u\neq v\\ u,v\in V(G\cdot e)}} |r_e(u)||r_e(v)| \;+\; m_{G\cdot e} \sum_{u\in V(G\cdot e)} |r_e(u)|$$
$$- \sum_{uv\in E(G\cdot e)} |r_e(u)\cap r_e(v)|.$$

Now,

$$\begin{aligned}
\sum_{\substack{u\neq v\\ u,v\in V(G\cdot e)}} |r_e(u)||r_e(v)| &= \sum_{3\leq i<j\leq n} |r(u_i)||r(u_j)| + \sum_{i\notin\{1,2\}} |r(u_1)\cup r(u_2)||r(u_i)| \\
&= \sum_{3\leq i<j\leq n} |r(u_i)||r(u_j)| + \sum_{k\in\{1,2\}} \sum_{i\notin\{1,2\}} |r(u_k)||r(u_i)| \\
&\quad -|r(u_1)\cap r(u_2)| \sum_{i\notin\{1,2\}} |r(u_i)| \\
&= B_2(G,r,e) + B_3(G,r,e) + B_4(G,r,e).
\end{aligned}$$

Also, $m_{G\cdot e} \sum_{u\in V(G\cdot e)} |r_e(u)|$ is equal to

$$(m_G - 1 - |N_G(u_1)\cap N_G(u_2)|)\left(\left(\sum_{1\leq i\leq n} |r(u_i)|\right) - |r(u_1)\cap r(u_2)|\right)$$

since $m_{G\cdot e} = m_G - 1 - |N_G(u_1)\cap N_G(u_2)|$.

Lastly, $-\sum_{uv\in E(G\cdot e)} |r_e(u)\cap r_e(v)|$ is equal to

$$-\sum_{\substack{u_iu_j\in E(G)\\ i,j\notin\{1,2\}}} |r(u_i)\cap r(u_j)| - \sum_{\substack{u_i\in N_G(u_1)\cup N_G(u_2)\\ i\notin\{1,2\}}} |(r(u_1)\cup r(u_2))\cap r(u_i)|$$

which can be rearranged as

$$\begin{aligned}
&-\sum_{\substack{u_iu_j\in E(G)\\ i,j\notin\{1,2\}}} |r(u_i)\cap r(u_j)| \\
&-\sum_{\substack{u_i\in N_G(u_1)\cup N_G(u_2)\\ i\notin\{1,2\}}} \sum_{k\in\{1,2\}} |r(u_k)\cap r(u_i)| \\
&+\sum_{\substack{u_i\in N_G(u_1)\cup N_G(u_2)\\ i\notin\{1,2\}}} |r(u_1)\cap r(u_2)\cap r(u_i)|
\end{aligned}$$

or equivalently

$$
\begin{aligned}
&- \sum_{u_i u_j \in E(G-e)} |r(u_i) \cap r(u_j)| \\
&- \sum_{\substack{k,l \in \{1,2\} \\ k \neq l}} \sum_{u_i \in N_G(u_k) \setminus N_G[u_l]} |r(u_i) \cap r(u_l)| \\
&+ \sum_{\substack{u_i \in N_G(u_1) \cup N_G(u_2) \\ i \notin \{1,2\}}} |r(u_1) \cap r(u_2) \cap r(u_i)|.
\end{aligned}
$$

Thus, by combining all these together we obtain that $a_{n-3}(G \cdot e, r_e)$ is equal to $B_0(G,e) + \sum_{i=1}^{8} B_i(G,r,e)$.

Finally, by the edge deletion-contraction formula, it suffices to show that

$$
\begin{aligned}
A_0(G) &= A_0(G-e) + B_0(G,e) \quad \text{and} \\
A_i(G,r) &= A_i(G-e,r) + B_i(G,r,e) \quad \text{for} \quad 1 \leq i \leq 8.
\end{aligned}
$$

Claim 1: $A_0(G) = A_0(G-e) + B_0(G,e)$.

Proof of Claim 1. Recall that $A_0(G) = \binom{m_G}{3} - (m_G - 2)\eta_G(C_3) - i_G(C_4) + 2\eta_G(K_4)$,

$A_0(G-e) = \binom{m_{G-e}}{3} - (m_{G-e} - 2)\eta_{G-e}(C_3) - i_{G-e}(C_4) + 2\eta_{G-e}(K_4)$ and

$B_0(G,e) = \binom{m_{G \cdot e}}{2} - \eta_{G \cdot e}(C_3)$.

By Theorem 3.2.6, the coefficient of x^{n-3} in the chromatic polynomial $\pi(G,x)$ of G is equal to $-A_0(G)$. Since $G \cdot e$ has $n-1$ vertices, by Theorem 3.2.6, the coefficient of x^{n-3} in the chromatic polynomial $\pi(G \cdot e, x)$ of $G \cdot e$ is equal to $B_0(G,e)$. The chromatic polynomial satisfies the edge deletion-contraction formula, $\pi(G,x) = \pi(G-e,x) - \pi(G \cdot e, x)$. Therefore $-A_0(G) = -A_0(G-e) - B_0(G,e)$ and the result follows.

Claim 2: $A_1(G,r) = A_1(G-e,r) + B_1(G,r,e)$.

Proof of Claim 2. Recall that $A_1(G,r) = A_1(G-e,r) = \sum_{i<j<k} |r(u_i)|\,|r(u_j)|\,|r(u_k)|$ and $B_1(G,r,e) = 0$. Since G and $G-e$ have the same vertices, $A_1(G,r)$ is equal to $A_1(G-e,r)$. Now the result follows since $B_1(G,r,e) = 0$.

Claim 3: $A_2(G,r) = A_2(G-e,r) + B_2(G,r,e)$.

Proof of Claim 3. Recall that $A_2(G,r) = (m_G - 1)\sum_{i<j} |r(u_i)|\,|r(u_j)|$,

$$A_2(G-e,r) = (m_{G-e} - 1)\sum_{i<j} |r(u_i)|\,|r(u_j)| \text{ and } B_2(G,r,e) = \sum_{i<j} |r(u_i)||r(u_j)|.$$

Now, $A_2(G-e,r)$ is equal to $(m_G - 2)\sum_{i<j} |r(u_i)|\,|r(u_j)|$ since $G-e$ has $m_G - 1$ edges.

Claim 4: $A_3(G,r) = A_3(G-e,r) + B_3(G,r,e)$.

Proof of Claim 4. Recall that $A_3(G,r) = \sum_{u_iu_j \notin E(G)} |r(u_i)|\,|r(u_j)|$,

$$A_3(G-e,r) = \sum_{u_iu_j \notin E(G-e)} |r(u_i)|\,|r(u_j)| \text{ and } B_3(G,r,e) = -|r(u_1)||r(u_2)|.$$

The result holds because $E(G) = E(G-e) \cup \{e\}$ and the vertices of e are u_1 and u_2.

Claim 5: $A_4(G,r) = A_4(G-e,r) + B_4(G,r,e)$.

Proof of Claim 5. Recall that $A_4(G,r) = -\sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)| \sum_{k \notin \{i,j\}} |r(u_k)|$,

$$A_4(G-e,r) = -\sum_{u_iu_j \in E(G-e)} |r(u_i) \cap r(u_j)| \sum_{k \notin \{i,j\}} |r(u_k)| \text{ and}$$

$$B_4(G,r,e) = -|r(u_1) \cap r(u_2)| \sum_{i \notin \{1,2\}} |r(u_i)|.$$

Again, as in the previous case, the result holds because $E(G) = E(G-e) \cup \{e\}$ and the vertices of e are u_1 and u_2.

Claim 6: $A_5(G,r) = A_5(G-e,r) + B_5(G,r,e)$:

Proof of Claim 6. Recall that $A_5(G,r) = \left(\binom{m_G}{2} - \eta_G(C_3) \right) \sum_{1 \le i \le n} |r(u_i)|$,

$$A_5(G-e,r) = \left(\binom{m_{G-e}}{2} - \eta_{G-e}(C_3) \right) \sum_{1 \le i \le n} |r(u_i)| \text{ and}$$

$$B_5(G,r,e) = (m_G - 1 - |N_G(u_1) \cap N_G(u_2)|) \sum_{1 \le i \le n} |r(u_i)|.$$

The number of triangles in G is equal to $\eta_G(C_3)$. Observe that $\eta_{G-e}(C_3)$ is the number of triangles in G which does not contain the edge e and $|N_G(u_1) \cap N_G(u_2)|$ is the number of triangles in G which contains the edge e. Therefore, $\eta_G(C_3)$ is equal to $\eta_{G-e}(C_3) + |N_G(u_1) \cap N_G(u_2)|$. Also, it is easy to check that $\binom{m_G}{2}$ is equal to $\binom{m_{G-e}}{2} + m_G - 1$ as m_{G-e} is equal to $m_G - 1$. Hence, the equality is obtained.

Claim 7: $A_6(G,r) = A_6(G-e,r) + B_6(G,r,e)$:

Proof of Claim 7. Recall that $A_6(G,r) = -(m_G - 1) \sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)|$,

$$A_6(G-e,r) = -(m_{G-e} - 1) \sum_{u_iu_j \in E(G-e)} |r(u_i) \cap r(u_j)| \text{ and}$$

$$B_6(G,r,e) = -(m_G - 1)|r(u_1) \cap r(u_2)| - \sum_{u_iu_j \in E(G-e)} |r(u_i) \cap r(u_j)|$$

The reason why the equality holds is the same as in the proofs of Claims 4 and 5.

Claim 8: $A_7(G,r) = A_7(G-e,r) + B_7(G,r,e)$:

Proof of Claim 8. Recall that $A_7(G,r)$ is equal to

$$\sum_{u_iu_j \in E(G)} |N_G(u_i) \cap N_G(u_j)|\ |r(u_i) \cap r(u_j)| - \sum_{u_i \in V(G)} \sum_{\substack{u_j,u_k \in N_G(u_i) \\ j<k}} |r(u_j) \cap r(u_k)|,$$

$A_7(G-e,r)$ is equal to

$$\sum_{u_iu_j \in E(G-e)} |N_{G-e}(u_i) \cap N_{G-e}(u_j)|\ |r(u_i) \cap r(u_j)| - \sum_{u_i \in V(G-e)} \sum_{\substack{u_j,u_k \in N_{G-e}(u_i) \\ j<k}} |r(u_j) \cap r(u_k)|$$ and

$B_7(G,r,e)$ is equal to

$$|N_G(u_1) \cap N_G(u_2)||r(u_1) \cap r(u_2)| - \sum_{\substack{i,j \in \{1,2\} \\ i \ne j}} \sum_{u \in N_G(u_i) \setminus N_G[u_j]} |r(u_j) \cap r(u)|.$$

Observe that $N_G(u_i) = N_{G-e}(u_i)$ for $i \notin \{1,2\}$. Also, $N_G(u_1) \setminus N_{G-e}(u_1) = \{u_2\}$ and $N_G(u_2) \setminus N_{G-e}(u_2) = \{u_1\}$.

Therefore, $\sum_{u_iu_j \in E(G)} |N_G(u_i) \cap N_G(u_j)||r(u_i) \cap r(u_j)|$ is equal to

$$\begin{aligned}
&\sum_{u_iu_j \in E(G-e)} |N_{G-e}(u_i) \cap N_{G-e}(u_j)||r(u_i) \cap r(u_j)| \\
&+ \sum_{u \in N_G(u_1) \cap N_G(u_2)} (|r(u) \cap r(u_1)| + |r(u) \cap r(u_2)|) \\
&+ |N_G(u_1) \cap N_G(u_2)| \; |r(u_1) \cap r(u_2)|.
\end{aligned}$$

Moreover, $\sum_{u_i \in V(G)} \sum_{\substack{u_j, u_k \in N_G(u_i) \\ j<k}} |r(u_j) \cap r(u_k)|$ is equal to

$$\sum_{u_i \in V(G-e)} \sum_{\substack{u_k, u_j \in N_{G-e}(u_i) \\ j<k}} |r(u_k) \cap r(u_j)| + \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u \in N_G(u_s) \setminus \{u_t\}} |r(u) \cap r(u_t)|.$$

Hence, the result follows since

$$\sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u \in N_G(u_s) \setminus \{u_t\}} |r(u) \cap r(u_t)| - \sum_{u \in N_G(u_1) \cap N_G(u_2)} (|r(u) \cap r(u_1)| + |r(u) \cap r(u_2)|)$$

is equal to $\sum_{\substack{i,j \in \{1,2\} \\ i \neq j}} \sum_{u \in N_G(u_i) \setminus N_G[u_j]} |r(u_j) \cap r(u)|$.

Claim 9: $A_8(G, r) = A_8(G - e, r) + B_8(G, r, e)$:

Proof of Claim 9. Recall that $A_8(G, r)$ is equal to

$$\begin{aligned}
&\frac{1}{2} \sum_{u_iu_j \in E(G)} \sum_{\substack{k \notin \{i,j\} \\ u_k \in N_G(u_i) \cup N_G(u_j)}} |r(u_i) \cap r(u_j) \cap r(u_k)| \\
&+ \frac{1}{6} \sum_{u_iu_j \in E(G)} \sum_{u_k \in N_G(u_i) \cap N_G(u_j)} |r(u_i) \cap r(u_j) \cap r(u_k)|,
\end{aligned}$$

$A_8(G - e, r)$ is equal to

$$\begin{aligned}
&\frac{1}{2} \sum_{u_iu_j \in E(G-e)} \sum_{\substack{k \notin \{i,j\} \\ u_k \in N_{G-e}(u_i) \cup N_{G-e}(u_j)}} |r(u_i) \cap r(u_j) \cap r(u_k)| \\
&+ \frac{1}{6} \sum_{u_iu_j \in E(G-e)} \sum_{u_k \in N_{G-e}(u_i) \cap N_{G-e}(u_j)} |r(u_i) \cap r(u_j) \cap r(u_k)|
\end{aligned}$$

and $B_8(G,r,e)$ is equal to $\displaystyle\sum_{\substack{u_i \in N_G(u_1)\cup N_G(u_2)\\ i\notin\{1,2\}}} |r(u_1)\cap r(u_2)\cap r(u_i)|$.

We need to observe two equalities. First,

$$\frac{1}{2}\sum_{u_iu_j\in E(G)}\ \sum_{\substack{k\notin\{i,j\}\\ u_k\in N_G(u_i)\cup N_G(u_j)}} |r(u_i)\cap r(u_j)\cap r(u_k)|$$

is equal to

$$\begin{aligned}
&\frac{1}{2}\sum_{u_iu_j\in E(G-e)}\ \sum_{\substack{k\notin\{i,j\}\\ u_k\in N_{G-e}(u_i)\cup N_{G-e}(u_j)}} |r(u_i)\cap r(u_j)\cap r(u_k)|\\
&+\sum_{\substack{k\notin\{1,2\}\\ u_k\in(N_G(u_1)\cup N_G(u_2))\setminus(N_G(u_1)\cap N_G(u_2))}} |r(u_1)\cap r(u_2)\cap r(u_k)|\\
&+\frac{1}{2}\sum_{u\in N_G(u_1)\cap N_G(u_2)} |r(u_1)\cap r(u_2)\cap r(u)|.
\end{aligned}$$

Secondly,

$$\frac{1}{6}\sum_{u_iu_j\in E(G)}\ \sum_{u_k\in N_G(u_i)\cap N_G(u_j)} |r(u_i)\cap r(u_j)\cap r(u_k)|$$

is equal to

$$\begin{aligned}
&\frac{1}{6}\sum_{u_iu_j\in E(G-e)}\ \sum_{u_k\in N_{G-e}(u_i)\cap N_{G-e}(u_j)} |r(u_i)\cap r(u_j)\cap r(u_k)|\\
&+\frac{1}{2}\sum_{u\in N_G(u_1)\cap N_G(u_2)} |r(u_1)\cap r(u_2)\cap r(u)|.
\end{aligned}$$

Therefore, the result is established. □

Theorem 4.2.8. *Let G be any graph. If $r^*\in R_{\max}(G,k)$ then r^* satisfies both of the following.*

(i) r^* is a proper restraint,

(ii) $A''_7(G,r^*) = \min\{A''_7(G,r) : $ *r is a proper k-restraint on G*$\}$. *In other words,*

$$\sum_{u\in V(G)} \sum_{\substack{v,w\in N_G(u)\\ v\neq w}} |r^*(v)\cap r^*(w)| \geq \sum_{u\in V(G)} \sum_{\substack{v,w\in N_G(u)\\ v\neq w}} |r(v)\cap r(w)|$$

for every proper k-restraint r on G.

Proof. By Theorem 4.2.5, we know that r^* is a proper restraint. So we shall prove the statement in (ii). Let r be a proper k-restraint on G. Note that $a_n(G,r) = a_n(G,r^*) = 1$ as the restrained chromatic polynomial is a monic polynomial. By Theorem 4.2.2, we have $a_{n-1}(G,r) = a_{n-1}(G,r^*) = m_G + nk$. Also, since r and r^* are proper restraints we have $\sum_{uv\in E(G)} |r(u)\cap r(v)| = 0$. So, $a_{n-2}(G,r) = a_{n-2}(G,r^*) = \binom{m_G}{2} - \eta_G(C_3) + k^2\binom{n}{2} + nkm_G$ by Theorem 4.2.3. Since the coefficient of x^{n-3} of the restrained chromatic polynomial is negative, we must have $a_{n-3}(G,r) \geq a_{n-3}(G,r^*)$. Recall that $a_{n-3}(G,r) = A_0(G) + \sum A_i(G,r)$ where $A_i(G,r)$'s are as in the statement of Theorem 4.2.7. First note that $A_0(G)$ does not depend on the restraint function. Furthermore, since r and r^* are k-restraints, $A_i(G,r) = A_i(G,r^*)$ for $i = 1,2,3,5$. Also, since r and r^* are proper restraints, we have $A_i(G,r) = A_i(G,r^*) = 0$ for $i = 4,6,8$ and $A'_7(G,r) = A'_7(G,r^*) = 0$. Thus, $0 \leq a_{n-3}(G,r) - a_{n-3}(G,r^*) = A''_7(G,r) - A''_7(G,r^*)$ and the result follows. $\square$

In the next theorem, we will show that in the case of bipartite graphs, the necessary conditions in Theorem 4.2.8 become sufficient to determine the extremal restraints.

Suppose G is a connected bipartite graph with bipartition (A_1, A_2). Then a k-restraint is called an *alternating restraint*, denoted r_{alt}, if r_{alt} is constant on both A_1 and A_2 individually (that is, $r_{alt}(a) = r_{alt}(a')$ for every $a, a' \in A_i$ for $i = 1,2$), and $r_{alt}(u)\cap r_{alt}(v) = \emptyset$ for every $u \in A_1$ and $v \in A_2$.

Theorem 4.2.9. *Let G be a connected bipartite graph. Then, $r \in R_{\max}(G,k)$ if and only if $r \simeq r_{alt}$.*

Proof. By Theorem 4.2.8, it suffices to show that for any proper k-restraint r such that $r \not\simeq r_{alt}$,

$$\sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r_{alt}(v) \cap r_{alt}(w)| > \sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(v) \cap r(w)|.$$

Let r be a proper k-restraint such that $r \not\simeq r_{alt}$. Then there exist vertices u, v, w such that $v, w \in N_G(u)$, $v \neq w$ and $|r(v) \cap r(w)| < k$, as G is a connected graph. Thus, the result follows since $|r(v) \cap r(w)| = k$ for every u, v, w such that $v, w \in N_G(u)$, $v \neq w$. □

(C_3, C_4)-free graphs

We have seen that the conditions given in Theorem 4.2.8 are sufficient to determine $R_{\max}(G,k)$ when G is a bipartite graph. However these conditions are not sufficient in general to determine the extremal restraints. For example, let G be equal to C_7. It is easy to check that if r is a proper simple restraint on G then $|A_7''(G,r)| \leq 4$. Furthermore, for a simple proper restraint r on G, $|A_7''(G,r)| = 4$ if and only if r is equivalent to either $r_1 = [\{1\},\{2\},\{1\},\{2\},\{1\},\{2\},\{3\}]$ or $r_2 = [\{1\},\{2\},\{1\},\{2\},\{3\},\{1\},\{3\}]$ (see Figure 4.2). Computations show that

$$\pi_{r_1}(G,x) = x^7 - 14\,x^6 + 91\,x^5 - 353\,x^4 + 879\,x^3 - 1404\,x^2 + 1333\,x - 581$$

and

$$\pi_{r_2}(G,x) = x^7 - 14\,x^6 + 91\,x^5 - 353\,x^4 + 880\,x^3 - 1411\,x^2 + 1352\,x - 600.$$

Therefore, $\pi_{r_2}(G,x) > \pi_{r_1}(G,x)$ for all large enough x and $R_{\max}(G,1)$ consists of restraints which are equivalent to r_2. Thus, Theorem 4.2.8 cannot determine $R_{\max}(G,1)$ when G is equal to C_7.

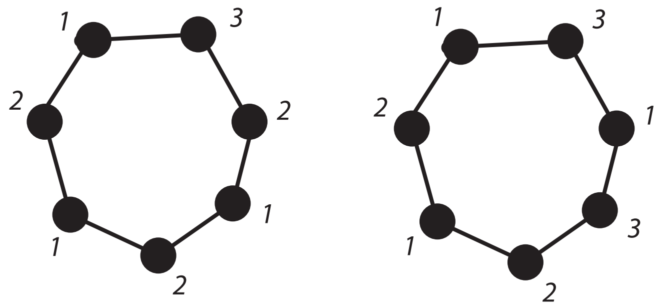

Figure 4.2: Two nonequivalent restraints $r_1 = [\{1\}, \{2\}, \{1\}, \{2\}, \{1\}, \{2\}, \{3\}]$ (left) and $r_2 = [\{1\}, \{2\}, \{1\}, \{2\}, \{3\}, \{1\}, \{3\}]$ (right) on C_7.

In the next theorem, we will make use of the following remark.

Remark 4.2.2. Let G be a $(C_3, C_4)-$free graph and e be an edge of G. Then, $G - e$ is also $(C_3, C_4)-$free and $G \cdot e$ is C_3-free.

Given two graphs G and H, recall that $\mathcal{G}(H)$ denotes the set of all subgraphs of G which are isomorphic to H.

Lemma 4.2.10. *Let G be a $(C_3, C_4)-$free graph and $x \geq M_{G,r}$. Also, let $\pi_r(G, x) = \sum_{i=0}^{n}(-1)^{n-i}a_i(G, r)x^i$ and $V(G) = \{u_1, \ldots u_n\}$. Suppose that $e = u_1u_2 \in E(G)$. Then*

$$a_{n-4}(G \cdot e, r_e) = D_0(G, e) + \sum_{i=1}^{19} D_i(G, r, e)$$

where $D_0(G, e) = A_0(G \cdot e)$ and $D_i(G, r, e)$ are defined for $i = 1, \ldots, 19$ as follows:

$$D_1(G, r, e) = 0;$$

$$D_2(G, r, e) = \frac{1}{m_G}C_2(G, r);$$

$$D_3(G, r, e) = -|r(u_1)||r(u_2)| \sum_{3 \leq i \leq n} |r(u_i)|;$$

$$D_4(G, r, e) = -|r(u_1) \cap r(u_2)| \sum_{3 \leq i < j \leq n} |r(u_i)||r(u_j)|;$$

$$D_5(G,r,e) = D_5'(G,r,e) + D_5''(G,r,e) \quad \textit{where}$$

$$D_5'(G,r,e) = (m_G - 2)\left(\left(\sum_{1\le i<j\le n} |r(u_i)|\,|r(u_j)|\right) - |r(u_1)||r(u_2)|\right);$$

$$D_5''(G,r,e) = \sum_{uv\notin E(G)} |r(u)||r(v)|$$

$$D_6(G,r,e) = -\sum_{\substack{s,t\in\{1,2\}\\ s\neq t}} |r(u_s)| \sum_{u_i\in N_G(u_t)\setminus\{u_s\}} |r(u_i)|;$$

$$D_7(G,r,e) = D_7'(G,r,e) + D_7''(G,r,e) \;\textit{with}$$

$$D_7'(G,r,e) = -(m_G - 2)|r(u_1)\cap r(u_2)| \sum_{3\le i\le n} |r(u_i)|$$

$$D_7''(G,r,e) = -\sum_{u_iu_j\in E(G-e)} |r(u_i)\cap r(u_j)| \sum_{k\notin\{i,j\}} |r(u_k)|;$$

$$D_8(G,r,e) = D_{10}'(G,r,e) + D_{10}'(G,r,e) \;\textit{with}$$

$$D_8'(G,r,e) = -|r(u_1)\cap r(u_2)| \sum_{v\notin N_G(u_1)\cup N_G(u_2)} |r(v)|$$

$$D_8''(G,r,e) = \sum_{\substack{s,t\in\{1,2\}\\ s\neq t}} |r(u_s)| \sum_{u_i\in N_G(u_t)\setminus\{u_s\}} |r(u_i)\cap r(u_t)|;$$

$$D_9(G,r,e) = -\sum_{\substack{s,t\in\{1,2\}\\ s\neq t}} \sum_{u_i\in N_G(u_t)\setminus\{u_s\}} |r(u_s)\cap r(u_i)| \sum_{j\notin\{1,2,i\}} |r(u_j)|;$$

$$D_{10}(G,r,e) = |r(u_1)\cap r(u_2)| \sum_{\substack{u_iu_j\in E(G)\\ i,j\notin\{1,2\}}} |r(u_i)\cap r(u_j)|;$$

$$D_{11}(G,r,e) = \sum_{\substack{u_i\in N_G(u_1)\cup N_G(u_2)\\ i\notin\{1,2\}}} |r(u_1)\cap r(u_2)\cap r(u_i)| \sum_{j\notin\{1,2,i\}} |r(u_j)|;$$

$$D_{12}(G,r,e) = \binom{m_G - 1}{2} \sum_{1\le i\le n} |r(u_i)|;$$

$$D_{13}(G,r,e) = D_{13}'(G,r,e) + D_{13}''(G,r,e) \;\textit{with}$$

$$D_{13}'(G,r,e) = -\binom{m_G - 1}{2} |r(u_1)\cap r(u_2)| \;\textit{and}$$

$$D''_{13}(G,r,e) = -(m_G - 2) \sum_{u_i u_j \in E(G-e)} |r(u_i) \cap r(u_j)|;$$

$$D_{14}(G,r,e) = D'_{14}(G,r,e) + D''_{14}(G,r,e) \text{ with}$$

$$D'_{14}(G,r,e) = -(m_G - 2) \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u_i \in N_G(u_s) \setminus \{u_t\}} |r(u_t) \cap r(u_i)| \text{ and}$$

$$D''_{14}(G,r,e) = -\sum_{u_i \in V(G)} \sum_{\substack{u_j, u_k \in N_{G-e}(u_i) \\ j<k}} |r(u_j) \cap r(u_k)|;$$

$$D_{15}(G,r,e) = -\sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u \in N_G(u_s) \setminus \{u_t\}} \sum_{v \in N_G(u) \setminus \{u_s\}} |r(u_t) \cap r(v)|$$

$$- \sum_{\substack{u_i \in N_G(u_1) \setminus \{u_2\} \\ u_j \in N_G(u_2) \setminus \{u_1\}}} |r(u_i) \cap r(u_j)|;$$

$$D_{16}(G,r,e) = D'_{16}(G,r,e) + D''_{16}(G,r,e) \text{ with}$$

$$D'_{16}(G,r,e) = (m_G - 2) \sum_{\substack{u_i \in N_G(u_1) \cup N_G(u_2) \\ i \notin \{1,2\}}} |r(u_1) \cap r(u_2) \cap r(u_i)|,$$

$$D''_{16}(G,r,e) = \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{v,w \in N_G(u_s) \setminus \{u_t\}} |r(u_s) \cap r(v) \cap r(w)|$$

$$+ \sum_{\substack{u \in V(G) \\ u \notin \{u_1,u_2\}}} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(u) \cap r(v) \cap r(w)|$$

$$D_{17}(G,r,e) = \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u_i,u_j \in N_G(u_s) \setminus \{u_t\}} |r(u_t) \cap r(u_i) \cap r(u_j)|;$$

$$D_{18}(G,r,e) = D'_{18}(G,r,e) + D''_{18}(G,r,e) \text{ with}$$

$$D'_{18}(G,r,e) = \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u \in N_G(u_s) \setminus \{u_t\}} \sum_{v \in N_G(u) \setminus \{u_s\}} |r(u_1) \cap r(u_2) \cap r(v)|,$$

$$D''_{18}(G,r,e) = \sum_{\substack{u_i \in N_G(u_1) \setminus \{u_2\} \\ u_j \in N_G(u_2) \setminus \{u_1\}}} \sum_{k \in \{1,2\}} |r(u_k) \cap r(u_i) \cap r(u_j)|$$

$$+ \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{u \in N_G(u_s) \setminus \{u_t\}} \sum_{v \in N_G(u) \setminus \{u_1,u_2\}} |r(u) \cap r(v) \cap r(u_t)|;$$

$$D_{19}(G,r,e) = -\sum_{\substack{u_i,u_j\in N_G(u_1)\cup N_G(u_2)\\ i,j\notin\{1,2\}}} |r(u_1)\cap r(u_2)\cap r(u_i)\cap r(u_j)|$$

$$-\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}} \sum_{v\in N_G(u)\setminus\{u_1,u_2\}} |r(u_1)\cap r(u_2)\cap r(u)\cap r(v)|$$

Proof. Recall that $a_{n-4}(G\cdot e, r_e) = A_0(G)+\sum_{i=1}^{8} A_i(G\cdot e, r_e)$ by Theorem 4.2.7. So, it suffices to verify the following eight claims.

Claim 1: $A_1(G\cdot e, r_e) = D_2(G,r,e) + D_3(G,r,e) + D_4(G,r,e)$.

Proof of Claim 1:

$$\begin{aligned}
A_1(G\cdot e, r_e) &= \sum_{3\le i<j\le n} |r(u_1)\cup r(u_2)|\,|r(u_i)|\,|r(u_j)| \\
&= \sum_{3\le i<j\le n} \left(|r(u_1)|+|r(u_2)|-|r(u_1)\cap r(u_2)|\right)\,|r(u_i)|\,|r(u_j)| \\
&= \sum_{3\le i<j\le n} |r(u_1)||r(u_i)|\,|r(u_j)| + \sum_{3\le i<j\le n} |r(u_2)|\,|r(u_i)|\,|r(u_j)| \\
&\quad - \sum_{3\le i<j\le n} |r(u_1)\cap r(u_2)|\,|r(u_i)|\,|r(u_j)| \\
&= \sum_{1\le i<j<k\le n} |r(u_i)|\,|r(u_j)|\,|r(u_k)| - |r(u_1)|\,|r(u_2)| \sum_{3\le i\le n} |r(u_i)| \\
&\quad -|r(u_1)\cap r(u_2)| \sum_{3\le i<j\le n} |r(u_i)|\,|r(u_j)| \\
&= D_2(G,r,e)+D_3(G,r,e)+D_4(G,r,e).
\end{aligned}$$

Claim 2: $A_2(G\cdot e, r_e) = D_5'(G,r,e) + D_7'(G,r,e)$

Proof of Claim 2: Since G is a triangle-free graph, we have $m_{G\cdot e} = m_G - 1$. So,

$$\begin{aligned}
A_2(G\cdot e, r_e) &= (m_G-2)\sum_{i\geq 3}|r(u_1)\cup r(u_2)|\,|r(u_i)| \\
&= (m_G-2)\sum_{i\geq 3}(|r(u_1)|+|r(u_2)|-|r(u_1)\cap r(u_2)|)\,|r(u_i)| \\
&= (m_G-2)\left(\sum_{i\geq 3}(|r(u_1)||r(u_i)| + \sum_{3\leq i\leq n}|r(u_2)||r(u_i)|\right) \\
&\quad -(m_G-2)|r(u_1)\cap r(u_2)|\sum_{3\leq i\leq n}|r(u_i)| \\
&= (m_G-2)\sum_{1\leq i<j\leq n}|r(u_i)||r(u_j)| - (m_G-2)|r(u_1)||r(u_2)| \\
&\quad -(m_G-2)|r(u_1)\cap r(u_2)|\sum_{3\leq i\leq n}|r(u_i)| \\
&= D_5'(G,r,e)+D_7'(G,r,e).
\end{aligned}$$

Claim 3: $A_3(G\cdot e, r_e) = D_5''(G,r,e) + D_6(G,r,e) + D_8'(G,r,e)$

Proof of Claim 3:

$$\begin{aligned}
A_3(G\cdot e, r_e) &= \sum_{\substack{u_iu_j\notin E(G)\\ 3\leq i<j\leq n}}|r(u_i)||r(u_j)| + \sum_{u\notin N_G(u_1)\cup N_G(u_2)}|r(u_1)\cup r(u_2)||r(u)| \\
&= \sum_{\substack{u_iu_j\notin E(G)\\ 3\leq i<j\leq n}}|r(u_i)||r(u_j)| + \sum_{u\notin N_G(u_1)\cup N_G(u_2)}(|r(u_1)|+|r(u_2)|)|r(u)| \\
&\quad -|r(u_1)\cap r(u_2)|\sum_{u\notin N_G(u_1)\cup N_G(u_2)}|r(u)| \\
&= \sum_{\substack{u_iu_j\notin E(G)\\ 1\leq i<j\leq n}}|r(u_i)||r(u_j)| - \sum_{u\in N_G(u_2)\setminus\{u_1\}}|r(u_1)||r(u)| \\
&\quad -\sum_{u\in N_G(u_1)\setminus\{u_2\}}|r(u_2)||r(u)| - |r(u_1)\cap r(u_2)|\sum_{u\notin N_G(u_1)\cup N_G(u_2)}|r(u)| \\
&= D_5''(G,r,e)+D_6(G,r,e)+D_8'(G,r,e).
\end{aligned}$$

Claim 4: $A_4(G\cdot e, r_e) = D_7''(G,r,e) + D_8''(G,r,e) + \sum_{i\in\{9,10,11\}} D_i(G,r,e)$

Proof of Claim 4: By the definition, $A_4(G \cdot e, r_e)$ is equal to

$$-\sum_{\substack{u_i \in N_G(u_1) \cup N_G(u_2) \\ i \notin \{1,2\}}} |(r(u_1) \cup r(u_2)) \cap r(u_i)| \sum_{j \notin \{1,2,i\}} |r(u_j)| \tag{4.1}$$

$$-\sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)| \, |r(u_1) \cup r(u_2)| \tag{4.2}$$

$$-\sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)| \sum_{k \notin \{1,2,i,j\}} |r(u_k)| \tag{4.3}$$

Since $|(r(u_1) \cup r(u_2)) \cap r(u_i)| = |r(u_1) \cap r(u_i)| + |r(u_2) \cap r(u_i)| - |r(u_1) \cap r(u_2) \cap r(u_i)|$, the expression in (4.1) is equal to

$$-\sum_{\substack{u_i \in N_G(u_1) \cup N_G(u_2) \\ i \notin \{1,2\}}} |r(u_1) \cap r(u_i)| \sum_{j \notin \{1,2,i\}} |r(u_j)| \tag{4.4}$$

$$-\sum_{\substack{u_i \in N_G(u_1) \cup N_G(u_2) \\ i \notin \{1,2\}}} |r(u_2) \cap r(u_i)| \sum_{j \notin \{1,2,i\}} |r(u_j)| \tag{4.5}$$

$$-\sum_{\substack{u_i \in N_G(u_1) \cup N_G(u_2) \\ i \notin \{1,2\}}} |r(u_1) \cap r(u_2) \cap r(u_i)| \sum_{j \notin \{1,2,i\}} |r(u_j)| \tag{4.6}$$

Note that the expression in (4.6) is equal to $D_{11}(G, r, e)$. Also, since $|r(u_1) \cup r(u_2)| = |r(u_1)| + |r(u_2)| - |r(u_1) \cap r(u_2)|$, the expression in (4.2) is equal to

$$\begin{aligned} &-|r(u_1)| \sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)| - |r(u_2)| \sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)| \\ &+|r(u_1) \cap r(u_2)| \sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)|. \end{aligned}$$

Note that $|r(u_1) \cap r(u_2)| \sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)|$ is equal to $D_{10}(G, r, e)$. Furthermore, the expression in (4.3) and $-|r(u_1)| \sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)| - |r(u_2)| \sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap$

$r(u_j)|$ add up to $-\sum_{\substack{u_iu_j\in E(G)\\ ij,\notin\{1,2\}}} |r(u_i)\cap r(u_j)| \sum_{k\notin\{i,j\}} |r(u_k)|$. Now, the expression in (4.4) is equal to

$$\begin{aligned}
&-\sum_{u_i\in N_G(u_1)\setminus\{u_2\}} |r(u_1)\cap r(u_i)| \sum_{j\notin\{1,i\}} |r(u_j)| \\
&+|r(u_2)| \sum_{u_i\in N_G(u_1)\setminus\{u_2\}} |r(u_1)\cap r(u_i)| \\
&-\sum_{u_i\in N_G(u_2)\setminus\{u_1\}} |r(u_1)\cap r(u_i)| \sum_{j\notin\{1,2,i\}} |r(u_j)|.
\end{aligned}$$

Similarly, the expression in (4.5) is equal to

$$\begin{aligned}
&-\sum_{u_i\in N_G(u_2)\setminus\{u_1\}} |r(u_2)\cap r(u_i)| \sum_{j\notin\{2,i\}} |r(u_j)| \\
&+|r(u_1)| \sum_{u_i\in N_G(u_2)\setminus\{u_1\}} |r(u_2)\cap r(u_i)| \\
&-\sum_{u_i\in N_G(u_1)\setminus\{u_2\}} |r(u_2)\cap r(u_i)| \sum_{j\notin\{1,2,i\}} |r(u_j)|.
\end{aligned}$$

Now,

$$\begin{aligned}
&-\sum_{\substack{u_iu_j\in E(G)\\ ij,\notin\{1,2\}}} |r(u_i)\cap r(u_j)| \sum_{k\notin\{i,j\}} |r(u_k)| \\
&-\sum_{u_i\in N_G(u_1)\setminus\{u_2\}} |r(u_1)\cap r(u_i)| \sum_{j\notin\{1,i\}} |r(u_j)| \\
&-\sum_{u_i\in N_G(u_2)\setminus\{u_1\}} |r(u_2)\cap r(u_i)| \sum_{j\notin\{2,i\}} |r(u_j)|
\end{aligned}$$

is equal to $D_7''(G,r,e)$. Also,

$$\left(|r(u_2)| \sum_{u_i\in N_G(u_1)\setminus\{u_2\}} |r(u_1)\cap r(u_i)|\right) + \left(|r(u_1)| \sum_{u_i\in N_G(u_2)\setminus\{u_1\}} |r(u_2)\cap r(u_i)|\right)$$

is equal to $D''_8(G,r,e)$. Lastly,

$$-\sum_{u_i\in N_G(u_2)\setminus\{u_1\}}|r(u_1)\cap r(u_i)|\sum_{j\notin\{1,2,i\}}|r(u_j)|$$
$$-\sum_{u_i\in N_G(u_1)\setminus\{u_2\}}|r(u_2)\cap r(u_i)|\sum_{j\notin\{1,2,i\}}|r(u_j)|$$

is equal to $D_9(G,r,e)$. Thus, the proof of Claim 4 is complete.

Claim 5: $A_5(G\cdot e,r_e)=D_{12}(G,r,e)+D'_{13}(G,r,e)$

Proof of Claim 5: By the definition, $A_5(G\cdot e,r_e)$ is equal to

$$\left(\binom{m_{G\cdot e}}{2}-\eta_{G\cdot e}(C_3))\right)\sum_{u\in V(G\cdot e)}|r_e(u)|.$$

Since the graphs G and $G\cdot e$ are triangle-free, $m_{G\cdot e}=m_G-1$ and $\eta_{G\cdot e}(C_3))=0$. Also, $\sum_{u\in V(G\cdot e)}|r_e(u)|=\sum_{1\le i\le n}|r(u_i)|\,-\,|r(u_1)\cap r(u_2)|$. Therefore,

$$\begin{aligned}
A_5(G\cdot e,r_e) &= \binom{m_G-1}{2}\left(\sum_{1\le i\le n}|r(u_i)|\,-\,|r(u_1)\cap r(u_2)|\right)\\
&= \binom{m_G-1}{2}\sum_{1\le i\le n}|r(u_i)|\,-\,\binom{m_G-1}{2}|r(u_1)\cap r(u_2)|\\
&= D_{12}(G,r,e)+D'_{13}(G,r,e).
\end{aligned}$$

Claim 6: $A_6(G\cdot e,r_e)=D''_{13}(G,r,e)+D'_{14}(G,r,e)+D'_{16}(G,r,e)$

Proof of Claim 6: By the definition, $A_6(G\cdot e,r_e)$ is equal to

$$-(m_G-2)\sum_{uv\in E(G\cdot e)}|r_e(u)\cap r_e(v)|.$$

Note that $\sum_{uv\in E(G\cdot e)}|r_e(u)\cap r_e(v)|$ is equal to

$$\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}}|(r(u_1)\cup r(u_2))\cap r(u)|+\sum_{\substack{u_iu_j\in E(G)\\ i,j\notin\{1,2\}}}|r(u_i)\cap r(u_j)|.$$

Now, we rewrite $\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}}|(r(u_1)\cup r(u_2))\cap r(u)|$ as

$$\sum_{\substack{u \in N_G(u_1) \cup N_G(u_2) \\ u \notin \{u_1,u_2\}}} (|r(u_1) \cap r(u)| + |r(u_2) \cap r(u)| - |r(u_1) \cap r(u_2) \cap r(u)|)$$

which is equal to

$$\begin{aligned} & \sum_{u \in N_G(u_1) \setminus \{u_2\}} |r(u_1) \cap r(u)| + \sum_{u \in N_G(u_2) \setminus \{u_1\}} |r(u_1) \cap r(u)| \\ & + \sum_{u \in N_G(u_1) \setminus \{u_2\}} |r(u_2) \cap r(u)| + \sum_{u \in N_G(u_2) \setminus \{u_1\}} |r(u_2) \cap r(u)| \\ & - \sum_{\substack{u \in N_G(u_1) \cup N_G(u_2) \\ u \notin \{u_1,u_2\}}} |r(u_1) \cap r(u_2) \cap r(u)|. \end{aligned}$$

Observe that $\sum_{\substack{u_i u_j \in E(G) \\ i,j \notin \{1,2\}}} |r(u_i) \cap r(u_j)|$ and

$$\sum_{u \in N_G(u_1) \setminus \{u_2\}} |r(u_1) \cap r(u)| + \sum_{u \in N_G(u_2) \setminus \{u_1\}} |r(u_2) \cap r(u)|$$

add up to $\sum_{u_i u_j \in E(G-e)} |r(u_i) \cap r(u_j)|$. Therefore, we obtain that

$$\begin{aligned} A_6(G \cdot e, r_e) &= -(m_G - 2) \sum_{u_i u_j \in E(G-e)} |r(u_i) \cap r(u_j)| \\ &\quad +(m_G - 2) \sum_{\substack{u \in N_G(u_1) \cup N_G(u_2) \\ u \notin \{u_1,u_2\}}} |r(u_1) \cap r(u_2) \cap r(u)| \\ &\quad -(m_G - 2) \left(\sum_{u \in N_G(u_2) \setminus \{u_1\}} |r(u_1) \cap r(u)| \right) \\ &\quad -(m_G - 2) \left(\sum_{u \in N_G(u_1) \setminus \{u_2\}} |r(u_2) \cap r(u)| \right) \\ &= D''_{13}(G,r,e) + D'_{16}(G,r,e) + D'_{14}(G,r,e). \end{aligned}$$

Claim 7: $A_7(G \cdot e, r_e) = D''_{14}(G,r,e) + D_{15}(G,r,e) + D'_{18}(G,r,e)$

Proof of Claim 7: Recall that $A_7(G \cdot e, r_e) = A'_7(G \cdot e, r_e) + A''_7(G \cdot e, r_e)$. By the definition, $A'_7(G \cdot e, r_e)$ is equal to

$$\sum_{uv\in E(G\cdot e)} |N_{G\cdot e}(u)\cap N_{G\cdot e}(v)|\,|r_e(u)\cap r_e(v)|.$$

But since $G\cdot e$ is a triangle-free graph, $N_{G\cdot e}(u)\cap N_{G\cdot e}(v)=\emptyset$ for every $uv\in E(G\cdot e)$. Therefore, it follows that $A_7'(G\cdot e, r_e)=0$. So, it suffices to show that $A_7''(G,r,e) = D_{14}''(G,r,e)+D_{15}(G,r,e)+D_{18}'(G,r,e)$. By the definition, $A_7''(G,r,e)$ is equal to

$$-\sum_{u\in V(G\cdot e)}\ \sum_{\substack{v,w\in N_{G\cdot e}(u)\\ v\neq w}} |r_e(v)\cap r_e(w)|$$

which is equal to

$$-\sum_{\substack{u,v\in N_G(u_1)\cup N_G(u_2)\\ u,v\notin\{u_1,u_2\}}} |r(u)\cap r(v)| \tag{4.7}$$

$$-\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}}\ \sum_{\substack{v\in N_G(u)\\ v\notin\{u_1,u_2\}}} |(r(u_1)\cup r(u_2))\cap r(v)| \tag{4.8}$$

$$-\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}}\ \sum_{\substack{v,w\in N_G(u)\\ v,w\notin\{u_1,u_2\}}} |r(v)\cap r(w)| \tag{4.9}$$

$$-\sum_{u\notin N_G(u_1)\cup N_G(u_2)}\ \sum_{v,w\in N_G(u)} |r(v)\cap r(w)|. \tag{4.10}$$

The expression in (4.7) can be rewritten as

$$-\sum_{u,v\in N_G(u_1)\setminus\{u_2\}} |r(u)\cap r(v)| - \sum_{u,v\in N_G(u_2)\setminus\{u_1\}} |r(u)\cap r(v)| \tag{4.11}$$

$$-\sum_{\substack{u\in N_G(u_1)\setminus\{u_2\}\\ v\in N_G(u_2)\setminus\{u_1\}}} |r(u)\cap r(v)| \tag{4.12}$$

Also, the expression in (4.8) can be rewritten as

$$
\begin{aligned}
&- \sum_{\substack{s,t\in\{1,2\}\\ s\neq t}} \sum_{u\in N_G(u_s)\setminus\{u_t\}} \sum_{v\in N_G(u)\setminus\{1,2\}} |r(u_s)\cap r(v)| && (4.13)\\
&- \sum_{\substack{s,t\in\{1,2\}\\ s\neq t}} \sum_{u\in N_G(u_s)\setminus\{u_t\}} \sum_{v\in N_G(u)\setminus\{1,2\}} |r(u_t)\cap r(v)| && (4.14)\\
&+ \sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}} \sum_{\substack{v\in N_G(u)\\ v\notin\{u_1,u_2\}}} |r(u_1)\cap r(u_2)\cap r(v)|. && (4.15)
\end{aligned}
$$

Now, the expressions in (4.11), (4.13), (4.9) and (4.10) add up to $D''_{14}(G,r,e)$. Furthermore, the expressions in (4.12) and (4.14) add up to $D_{15}(G,r,e)$. Lastly, the expression in (4.15) is equal to $D'_{18}(G,r,e)$. Thus, the proof of Claim 7 is complete.

Claim 8: $A_8(G\cdot e, r_e) = D''_{16}(G,r,e) + D_{17}(G,r,e) + D''_{18}(G,r,e) + D_{19}(G,r,e)$

Proof of Claim 8: Recall that $A_8(G\cdot e, r_e) = A'_8(G\cdot e, r_e) + A''_8(G\cdot e, r_e)$. Since $G\cdot e$ is a triangle free graph, $N_{G\cdot e}(u)\cap N_{G\cdot e}(v) = \emptyset$ for every $uv\in E(G\cdot e)$. Therefore,

$$A''_8(G\cdot e, r_e) = \frac{1}{6}\sum_{uv\in E(G\cdot e)} \sum_{w\in N_{G\cdot e}(u)\cap N_{G\cdot e}(v)} |r(u)\cap r(v)\cap r(w)| = 0.$$

So, it suffices to show that $A'_8(G\cdot e, r_e) = D''_{16}(G,r,e) + D_{17}(G,r,e) + D''_{18}(G,r,e) + D_{19}(G,r,e)$. First, note that for every triangle free graph G we have

$$
\begin{aligned}
A'_8(G,r) &= \frac{1}{2}\sum_{uv\in E(G)} \sum_{\substack{w\in N_G(u)\cup N_G(v)\\ w\notin\{u,v\}}} |r(u)\cap r(v)\cap r(w)|\\
&= \sum_{u\in V(G)} \sum_{v,w\in N_G(u)} |r(u)\cap r(v)\cap r(w)|.
\end{aligned}
$$

Thus, $A'_8(G\cdot e, r_e)$ is

$$\sum_{u\in V(G\cdot e)} \sum_{v,w\in N_{G\cdot e}(u)} |r_e(u)\cap r_e(v)\cap r_e(w)|$$

which is equal to

$$\sum_{\substack{u,v\in N_G(u_1)\cup N_G(u_2)\\ u,v\notin\{u_1,u_2\}}} |(r(u_1)\cup r(u_2))\cap r(u)\cap r(v)| \tag{4.16}$$

$$+\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}}\ \sum_{\substack{v\in N_G(u)\\ v\notin\{u_1,u_2\}}} |(r(u_1)\cup r(u_2))\cap r(u)\cap r(v)| \tag{4.17}$$

$$+\sum_{\substack{u\in N_G(u_1)\cup N_G(u_2)\\ u\notin\{u_1,u_2\}}}\ \sum_{\substack{v,w\in N_G(u)\\ v,w\notin\{u_1,u_2\}}} |r(u)\cap r(v)\cap r(w)| \tag{4.18}$$

$$+\sum_{u\notin N_G(u_1)\cup N_G(u_2)}\ \sum_{v,w\in N_G(u)} |r(u)\cap r(v)\cap r(w)|. \tag{4.19}$$

Now since $|(r(u_1)\cup r(u_2))\cap r(u)\cap r(v)|$ is equal to

$$|r(u_1)\cap r(u)\cap r(v)|+|r(u_2)\cap r(u)\cap r(v)|-|r(u_1)\cap r(u_2)\cap r(u)\cap r(v)|$$

it is easy to check that the result holds. Thus, the proof of Claim 8 is complete.

□

Theorem 4.2.11. *Let G be a $(C_3, C_4)-$free graph and $x \geq M_{G,r}$. Also, let $\pi_r(G,x) = \sum_{i=0}^{n}(-1)^{n-i}a_i(G,r)x^i$ and $V(G)=\{u_1,\dots u_n\}$. Then,*

$$a_{n-4}(G,r) = C_0(G)+\sum_{i=1}^{19} C_i(G,r)$$

where

$$C_0(G)=\binom{m_G}{4}-i_G(C_5);$$

$$C_1(G,r)=\sum_{1\leq i<j<k<l\leq n}|r(u_i)||r(u_j)||r(u_k)||r(u_l)|;$$

$$C_2(G,r)=m_G\sum_{1\leq i<j<k\leq n}|r(u_i)||r(u_j)||r(u_k)|;$$

$$C_3(G,r)=-\sum_{uv\in E(G)}|r(u)||r(v)|\sum_{w\notin\{u,v\}}|r(w)|;$$

$$C_4(G,r) = -\sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)| \sum_{\substack{k,l \notin \{i,j\} \\ k \neq l}} |r(u_k)||r(u_l)|;$$

$$C_5(G,r) = \left(\binom{m_G}{2} \sum_{uv \notin E(G)} |r(u)||r(v)|\right) + \left(\binom{m_G - 1}{2} \sum_{uv \in E(G)} |r(u)||r(v)|\right);$$

$$C_6(G,r) = -\sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(v)||r(w)|;$$

$$C_7(G,r) = -(m_G - 2) \sum_{uv \in E(G)} |r(u) \cap r(v)| \sum_{w \notin \{u,v\}} |r(w)|;$$

$$C_8(G,r) = -\sum_{uv \in E(G)} |r(u) \cap r(v)| \sum_{w \notin N_G(u) \cup N_G(v)} |r(w)|;$$

$$C_9(G,r) = -\sum_{u_i \in V(G)} \sum_{\substack{u_j,u_k \in N_G(u_i) \\ j \neq k}} |r(u_j) \cap r(u_k)| \sum_{l \notin \{i,j,k\}} |r(u_l)|;$$

$$C_{10}(G,r) = \frac{1}{2} \sum_{u_iu_j \in E(G)} |r(u_i) \cap r(u_j)| \sum_{\substack{u_ku_l \in E(G) \\ k,l \notin \{i,j\}}} |r(u_k) \cap r(u_l)|;$$

$$C_{11}(G,r) = \sum_{u_i \in V(G)} \sum_{\substack{u_j,u_k \in N_G(u_i) \\ j \neq k}} |r(u_i) \cap r(u_j) \cap r(u_k)| \sum_{l \notin \{i,j,k\}} |r(u_l)|;$$

$$C_{12}(G,r) = \binom{m_G}{3} \sum_{1 \leq i \leq n} |r(u_i)|;$$

$$C_{13}(G,r) = -\binom{m_G - 1}{2} \sum_{uv \in E(G)} |r(u) \cap r(v)|;$$

$$C_{14}(G,r) = -(m_G - 2) \sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(v) \cap r(w)|;$$

$$C_{15}(G,r) = -\sum_{uv \in E(G)} \sum_{\substack{u' \in N_G(u) \setminus \{v\} \\ v' \in N_G(v) \setminus \{u\}}} |r(u') \cap r(v')|$$

$$C_{16}(G,r) = +(m_G - 2) \sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(u) \cap r(v) \cap r(w)|;$$

$$C_{17}(G,r) = \sum_{u_i \in V(G)} \sum_{\substack{u_j,u_k,u_l \in N_G(u_i) \\ j,k,l \text{ distinct}}} |r(u_j) \cap r(u_k) \cap r(u_l)|;$$

$$C_{18}(G,r) = \sum_{uv \in E(G)} \sum_{\substack{u' \in N_G(u)\setminus\{v\} \\ v' \in N_G(v)\setminus\{u\}}} |r(u) \cap r(u') \cap r(v')| + |r(v) \cap r(u') \cap r(v')|;$$

$$C_{19}(G,r) = -\sum_{H \in \mathcal{G}(P_4) \cup \mathcal{G}(K_{1,3})} |\bigcap_{u \in V(H)} r(u)|.$$

Proof. We proceed by induction on the number of edges. For the basis step, suppose that G is an empty graph. It is easy to check that $C_0(G) = C_i(G,r) = 0$ for $i \neq 1$. So, it follows that $a_{n-4}(G,r)$ is equal to $C_1(G,r)$. Hence, the result is clear by the formula given in Example 4.1.1 for the restrained chromatic polynomials of empty graphs.

Now suppose that G has at least one edge, say $e = u_1u_2$. Let us define $D_0(G,e)$ and $D_i(G,r,e)$ for $i = 1,\ldots,19$ as in Lemma 4.2.10. By the edge deletion-contraction formula, $a_{n-4}(G,r)$ is equal to $a_{n-4}(G-e,r) + a_{n-4}(G \cdot e, r_e)$. Hence, it suffices to prove the following two claims:

Claim 1: $a_{n-4}(G \cdot e, r_e) = D_0(G,e) + \sum_{i=1}^{21} D_i(G,r,e)$.

Claim 2: $C_0(G) = C_0(G-e) + D_0(G)$ and $C_i(G,r) = C_i(G-e,r) + D_i(G,r,e)$ for $i = 1,\ldots,19$.

The proof of Claim 1 immediately follows from Lemma 4.2.10. So let us prove Claim 2.

Proof of Claim 2. Since G is a (C_3, C_4)-free graph, By Theorem 3.2.6, it is clear that $C_0(G) = C_0(G-e) + D_0(G)$. So, we shall show that $C_i(G,r) = C_i(G-e,r) + D_i(G,r,e)$ for $i = 1,\ldots,19$.

Subclaim 1: $C_1(G,r) = C_1(G-e,r) + D_1(G,r,e)$.

Proof of Subclaim 1. The result is trivial as $V(G) = V(G-e)$.

Subclaim 2: $C_2(G,r) = C_2(G-e,r) + D_2(G,r,e)$.

Proof of Subclaim 2. The result is trivial as $m_G = m_{G-e} + 1$.

Subclaim 3: $C_3(G,r) = C_3(G-e,r) + D_3(G,r,e)$.

Proof of Subclaim 3. The result is trivial as $E(G) = E(G-e) \cup \{u_1u_2\}$.

Subclaim 4: $C_4(G,r) = C_4(G-e,r) + D_4(G,r,e)$.

Proof of Subclaim 4. The result is trivial again as $E(G) = E(G-e) \cup \{u_1u_2\}$.

Subclaim 5: $C_5(G,r) = C_5(G-e,r) + D_5(G,r,e)$.

Proof of Subclaim 5. By the induction hypothesis, $C_5(G-e,r)$ is equal to

$$\left(\binom{m_G-1}{2}\sum_{uv\notin E(G-e)}|r(u)||r(v)|\right) + \left(\binom{m_G-2}{2}\sum_{uv\in E(G-e)}|r(u)||r(v)|\right).$$

If $m_G = 1$ then $C_5(G,r) = C_5(G-e,r) = 0$ and

$$D_5'(G,r,e) = -\left(\left(\sum_{1\le i<j\le n}|r(u_i)|\,|r(u_j)|\right) - |r(u_1)||r(u_2)|\right),$$

$$D_5''(G,r,e) = \sum_{uv\notin E(G)}|r(u)||r(v)| = -D_5'(G,r,e).$$

Hence, $D_5(G,r,e) = 0$ and the result is clear. So, we may assume that $m_G \ge 2$. We rewrite $C_5(G-e,r)$ as

$$\binom{m_G-1}{2}\left(\left(\sum_{uv\notin E(G)}|r(u)||r(v)|\right) + |r(u_1)||r(u_2)|\right)$$
$$+\binom{m_G-2}{2}\left(\left(\sum_{uv\in E(G)}|r(u)||r(v)|\right) - |r(u_1)||r(u_2)|\right).$$

Note that $D_5'(G,r,e)$ is equal to

$$(m_G-2)\left(\left(\sum_{uv\in E(G)}|r(u)||r(v)|\right)+\left(\sum_{uv\notin E(G)}|r(u)||r(v)|\right)-|r(u_1)||r(u_2)|\right).$$

Now the result follows since $\binom{m_G}{2}=\binom{m_G-1}{2}+m_G-1$ and $\binom{m_G-1}{2}=\binom{m_G-2}{2}+m_G-2$ for $m_G\geq 2$.

Subclaim 6: $C_6(G,r)=C_6(G-e,r)+D_6(G,r,e)$.

Proof of Subclaim 6: The result is trivial as $V(G)=V(G-e)$ and $E(G)=E(G-e)\cup\{u_1u_2\}$.

Subclaim 7: $C_7(G,r)=C_7(G-e,r)+D_7(G,r,e)$.

Proof of Subclaim 7: By the induction hypothesis, $C_7(G-e,r)$ is equal to

$$-(m_G-3)\sum_{uv\in E(G-e)}|r(u)\cap r(v)|\sum_{w\notin\{u,v\}}|r(w)|.$$

So, the sum of $C_7(G-e,r)$ and $D_7''(G,r,e)$ is equal to

$$-(m_G-2)\sum_{uv\in E(G-e)}|r(u)\cap r(v)|\sum_{w\notin\{u,v\}}|r(w)|.$$

Now, adding $D_7'(G,r,e)$ to the latter expression yields $C_7(G,r)$ and we are done.

Subclaim 8: $C_8(G,r)=C_8(G-e,r)+D_8(G,r,e)$.

Proof of Subclaim 8: We consider the terms which contribute to $C_8(G,r)$ but $C_8(G-e,r)$, and vice versa. So we need to consider the edges which are incident with u_1 or

u_2. Obviously, the edge u_1u_2 contributes nothing to $C_8(G-e,r)$ and it contributes

$$-|r(u_1)\cap r(u_2)| \sum_{w\notin N_G(u_1)\cup N_G(u_2)} |r(w)|$$

to $C_8(G,r)$. Now we consider the edges which are incident with exactly one of u_1 or u_2. From such edges, $C_8(G-e,r)$ gains the extra term

$$-\left(|r(u_2)| \sum_{u\in N_G(u_1)\setminus\{u_2\}} |r(u_1)\cap r(u)|\right) - \left(|r(u_1)| \sum_{u\in N_G(u_2)\setminus\{u_1\}} |r(u_2)\cap r(u)|\right)$$

which is not in $C_8(G,r)$. Thus the result follows.

Subclaim 9: $C_9(G,r) = C_9(G-e,r) + D_9(G,r,e)$.

Proof of Subclaim 9: By the induction hypothesis, $C_9(G-e,r)$ is equal to

$$-\sum_{u\in V(G)} \sum_{\substack{v,w\in N_{G-e}(u)\\ v\neq w}} |r(v)\cap r(w)| \sum_{z\notin\{u,v,w\}} |r(z)|.$$

Since $N_G(u) = N_{G-e}(u)$ for every vertex $u\notin\{u_1,u_2\}$, we rewrite $C_9(G-e,r)$ as

$$-\sum_{\substack{u\in V(G)\\ u\notin\{u_1,u_2\}}} \sum_{\substack{v,w\in N_G(u)\\ v\neq w}} |r(v)\cap r(w)| \sum_{z\notin\{u,v,w\}} |r(z)| \tag{4.20}$$

$$-\sum_{u\in\{u_1,u_2\}} \sum_{\substack{v,w\in N_{G-e}(u)\\ v\neq w}} |r(v)\cap r(w)| \sum_{z\notin\{u,v,w\}} |r(z)|. \tag{4.21}$$

Now it is easy to check that the expression in (4.21) and $D_9(G,r,e)$ add up to

$$-\sum_{u\in\{u_1,u_2\}} \sum_{\substack{v,w\in N_G(u)\\ v\neq w}} |r(v)\cap r(w)| \sum_{z\notin\{u,v,w\}} |r(z)|.$$

Thus the proof of Subclaim 9 is complete.

Subclaim 10: $C_{10}(G, r) = C_{10}(G - e, r) + D_{10}(G, r, e)$.

Proof of Subclaim 10: We rewrite $C_{10}(G, r)$ as

$$\frac{1}{2} \sum_{u_i u_j \in E(G-e)} |r(u_i) \cap r(u_j)| \sum_{\substack{u_k u_l \in E(G) \\ k,l \notin \{i,j\}}} |r(u_k) \cap r(u_l)|$$
$$+\frac{1}{2} |r(u_1) \cap r(u_2)| \sum_{\substack{u_k u_l \in E(G) \\ k,l \notin \{1,2\}}} |r(u_k) \cap r(u_l)|$$

Now it is clear that the difference between $C_{10}(G, r)$ and $C_{10}(G - e, r)$ is equal to $D_{10}(G, r, e)$.

Subclaim 11: $C_{11}(G, r) = C_{11}(G - e, r) + D_{11}(G, r, e)$.

Proof of Subclaim 11: By the induction hypothesis, $C_{11}(G - e, r)$ is equal to

$$\sum_{u \in V(G)} \sum_{\substack{v,w \in N_{G-e}(u) \\ v \neq w}} |r(u) \cap r(v) \cap r(w)| \sum_{z \notin \{u,v,w\}} |r(z)|.$$

Since $N_G(u) = N_{G-e}(u)$ for every $u \notin \{u_1, u_2\}$, $C_{11}(G - e, r)$ is equal to

$$\sum_{u \in V(G) \setminus \{u_1,u_2\}} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(u) \cap r(v) \cap r(w)| \sum_{z \notin \{u,v,w\}} |r(z)| \tag{4.22}$$
$$+ \sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{v,w \in N_G(u_s) \setminus \{u_t\}} |r(u_s) \cap r(v) \cap r(w)| \sum_{z \notin \{u_s,v,w\}} |r(z)|. \tag{4.23}$$

Now it is easy to check that the expression (4.23) in plus $D_{11}(G, r, e)$ is equal to

$$\sum_{u \in \{u_1,u_2\}} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(u) \cap r(v) \cap r(w)| \sum_{z \notin \{u,v,w\}} |r(z)|.$$

Thus the result follows.

Subclaim 12: $C_{12}(G,r) = C_{12}(G-e,r) + D_{12}(G,r,e)$.

Proof of Subclaim 12: The result holds since $m_{G-e} = m_G - 1$ and $\binom{m_G}{3} = \binom{m_G-1}{3} + \binom{m_G-1}{3}$ for $m_G \geq 1$.

Subclaim 13: $C_{13}(G,r) = C_{13}(G-e,r) + D_{13}(G,r,e)$.

Proof of Subclaim 13: If $m_G = 1$ then it is clear that $C_{13}(G,r) = C_{13}(G-e,r) = D'_{13}(G,r,e) = 0$ and $D''_{13}(G,r,e) = 0$ as $E(G-e) = \emptyset$. So we may assume that $m_G \geq 2$. By the induction hypothesis, $C_{13}(G-e,r)$ is equal to

$$-\binom{m_G-2}{2} \sum_{uv\in E(G-e)} |r(u)\cap r(v)|.$$

Since $\binom{m_G-2}{2} + (m_G-2) = \binom{m_G-1}{2}$ for $m_G \geq 2$, we obtain that the sum of $D''_{13}(G,r,e)$ and $C_{13}(G-e,r)$ is equal to

$$-\binom{m_G-1}{2} \sum_{uv\in E(G-e)} |r(u)\cap r(v)|.$$

Now adding $D'_{13}(G,r,e)$ to the latter expression we obtain $C_{13}(G,r)$.

Subclaim 14: $C_{14}(G,r) = C_{14}(G-e,r) + D_{14}(G,r,e)$.

Proof of Subclaim 14: By the induction hypothesis, $C_{14}(G-e,r)$ is equal to

$$-(m_G-3) \sum_{u\in V(G)} \sum_{\substack{v,w\in N_{G-e}(u)\\ v\neq w}} |r(v)\cap r(w)|.$$

Now, the sum of $C_{14}(G-e,r)$ and $D''_{14}(G,r,e)$ is equal to

$$-(m_G-2) \sum_{u\in V(G)} \sum_{\substack{v,w\in N_{G-e}(u)\\ v\neq w}} |r(v)\cap r(w)|. \tag{4.24}$$

Note that $N_G(u) = N_{G-e}(u)$ for every $u \neq u_1, u_2$. Also, the set of all pairs v, w such that $v, w \in N_{G-e}(u_1)$ is equal to the set of all pairs v, w having $v, w \in N_G(u_1) \setminus \{u_2\}$. Similarly, the same is true when u_1 and u_2 are switched. Therefore, the sum of the expression in (4.24) and $D'_{14}(G, r, e)$ is equal to $C_{14}(G, r)$ and the proof of Subclaim 14 is complete.

Subclaim 15: $C_{15}(G, r) = C_{15}(G - e, r) + D_{15}(G, r, e)$.

Proof of Subclaim 15: Note that in $C_{15}(G, r)$, we sum the size of the intersection of the restraints on the end-vertices of all paths of order four in the graph. Obviously, every path in $G - e$ is also in G. So we consider the extra terms which are in $C_{15}(G, r)$ but not in $C_{15}(G - e, r)$. By considering the paths of order four whose midedge is u_1u_2, we find the extra term

$$-\sum_{\substack{u \in N_G(u_1) \setminus \{u_2\} \\ v \in N_G(u_2) \setminus \{u_1\}}} |r(u) \cap r(v)|.$$

Also, by considering the paths of order four whose pendant edge is u_1u_2, we find the extra term

$$-\left(\sum_{u \in N_G(u_1) \setminus \{u_2\}} \sum_{v \in N_G(u) \setminus \{u_1\}} |r(u_2) \cap r(v)|\right) - \left(\sum_{u \in N_G(u_2) \setminus \{u_1\}} \sum_{v \in N_G(u) \setminus \{u_2\}} |r(u_1) \cap r(v)|\right).$$

Now it is clear that these extra terms add up to $D_{15}(G, r, e)$ and the result follows.

Subclaim 16: $C_{16}(G, r) = C_{16}(G - e, r) + D_{16}(G, r, e)$.

Proof of Subclaim 16: By the induction hypothesis, $C_{16}(G - e, r)$ is equal to

$$(m_G - 3) \sum_{u \in V(G)} \sum_{\substack{v, w \in N_{G-e}(u) \\ v \neq w}} |r(u) \cap r(v) \cap r(w)|.$$

Since $N_G(u) = N_{G-e}(u)$ for every vertex $u \notin \{u_1, u_2\}$, we can rewrite $C_{16}(G-e, r)$ as

$$\begin{aligned}&(m_G - 3) \sum_{\substack{u \in V(G)\\ u \notin \{u_1,u_2\}}} \sum_{\substack{v,w \in N_G(u)\\ v \neq w}} |r(u) \cap r(v) \cap r(w)|\\ &+(m_G - 3) \sum_{\substack{s,t \in \{1,2\}\\ s \neq t}} \sum_{\substack{v,w \in N_G(u_s)\setminus\{u_t\}\\ v \neq w}} |r(u_s) \cap r(v) \cap r(w)|.\end{aligned}$$

Now it is clear that the sum of $C_{16}(G-e, r)$ and $D_{16}(G, r, e)$ is equal to $C_{16}(G, r)$.

Subclaim 17: $C_{17}(G, r) = C_{17}(G-e, r) + D_{17}(G, r, e)$.

Proof of Subclaim 17: It is clear that $N_G(u) = N_{G-e}(u)$ for every vertex $u \notin \{u_1, u_2\}$. Also, $N_{G-e}(u_1) = N_G(u_1) \setminus \{u_2\}$ and $N_{G-e}(u_2) = N_G(u_2) \setminus \{u_1\}$. So, every term contributing to $C_{17}(G-e, r)$ also contributes to $C_{17}(G, r)$. Furthermore, the extra term which contributes to $C_{17}(G, r)$ but $C_{17}(G-e, r)$ is equal to

$$\left(\sum_{\substack{u,v \in N_G(u_1)\setminus\{u_2\}\\ u \neq v}} |r(u) \cap r(v) \cap r(u_2)| \right) + \left(\sum_{\substack{u,v \in N_G(u_2)\setminus\{u_1\}\\ u \neq v}} |r(u) \cap r(v) \cap r(u_1)| \right).$$

Thus the proof of Subclaim 17 is complete.

Subclaim 18: $C_{18}(G, r) = C_{18}(G-e, r) + D_{18}(G, r, e)$.

Proof of Subclaim 18: It is clear that every term which contributes to $C_{18}(G-e, r)$ also contributes to $C_{18}(G, r)$. So we need to find the terms which are in $C_{18}(G, r)$ but $C_{18}(G-e, r)$. Such terms can arise only when we sum over an edge which is incident with u_1 or u_2. By considering the edge u_1u_2, we find an extra term

$$\sum_{\substack{u' \in N_G(u_1)\setminus\{u_2\}\\ v' \in N_G(u_2)\setminus\{u_1\}}} |r(u_1) \cap r(u') \cap r(v')| + |r(u_2) \cap r(u') \cap r(v')|.$$

Also, by the considering the edges which are incident with exactly one of u_1 or u_2, we find two extra terms which are

$$\sum_{u \in N_G(u_1)\backslash\{u_2\}} \sum_{u' \in N_G(u)\backslash\{u_1\}} |r(u) \cap r(u') \cap r(u_2)| + |r(u_1) \cap r(u_2) \cap r(u')| \text{ and}$$

$$\sum_{u \in N_G(u_2)\backslash\{u_1\}} \sum_{u' \in N_G(u)\backslash\{u_2\}} |r(u) \cap r(u') \cap r(u_1)| + |r(u_1) \cap r(u_2) \cap r(u')|.$$

Now all these extra terms add up to $D_{18}(G, r, e)$ and the result follows.

Subclaim 19: $C_{19}(G, r) = C_{19}(G - e, r) + D_{19}(G, r, e)$.

Proof of Subclaim 19: As in the previous cases, every term which contributes to $C_{19}(G - e, r)$ also contributes to $C_{19}(G, r)$. So we need to find the terms which are in $C_{19}(G, r)$ but $C_{19}(G - e, r)$. First let us considers the terms which come from summing over the subgraphs that are isomorphic to P_4. By considering the P_4's whose mid-edge is equal to u_1u_2, we obtain the extra term

$$-\sum_{\substack{u \in N_G(u_1)\backslash\{u_2\} \\ v \in N_G(u_2)\backslash\{u_1\}}} |r(u_1) \cap r(u_2) \cap r(u) \cap r(v)|.$$

Furthermore, by considering the P_4's whose pendant edge is equal to u_1u_2, we obtain the extra term

$$-\sum_{\substack{u \in N_G(u_1) \cup N_G(u_2) \\ u \notin \{u_1, u_2\}}} \sum_{v \in N_G(u)\backslash\{u_1, u_2\}} |r(u_1) \cap r(u_2) \cap r(u) \cap r(v)|.$$

Finally, the extra terms which arises from summing over the subgraphs which are isomorphic to $K_{1,3}$ is equal to

$$-\sum_{\substack{s,t \in \{1,2\} \\ s \neq t}} \sum_{\substack{u,v \in N_G(u_s)\backslash\{u_t\} \\ u \neq v}} |r(u_1) \cap r(u_2) \cap r(u) \cap r(v)|.$$

Thus the sum of all these extra terms add up to $D_{19}(G, r, e)$ and the proof is complete.

$\square$

Now, by Theorem 4.2.11, we derive a necessary condition for a restraint r on a (C_3, C_4)-free graph to be in $R_{\max}(G, k)$.

Theorem 4.2.12. *Let G be a (C_3, C_4)-free graph and $G \not\cong K_2$. If $r^* \in R_{\max}(G, k)$ then r^* satisfies all of the following.*

(i) *r^* is a proper restraint,*

(ii) *$A''_7(G, r^*) = \min\{A''_7(G, r) : r$ is a proper k-restraint on $G\}$. In other words,*

$$\sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r^*(v) \cap r^*(w)| \geq \sum_{u \in V(G)} \sum_{\substack{v,w \in N_G(u) \\ v \neq w}} |r(v) \cap r(w)|$$

for every proper k-restraint on G.

(iii) *If there exists a proper k-restraint r' on G with $r' \not\cong r^*$ such that $A''_7(G, r^*) = A''_7(G, r')$ then for every proper k-restraint r on G such that $A''_7(G, r^*) = A''_7(G, r)$ we have*

$$C_{15}(G, r^*) + C_{17}(G, r^*) \geq C_{15}(G, r) + C_{17}(G, r),$$

that is,

$$\sum_{u \in V(G)} \sum_{\substack{v,w,t \in N_G(u) \\ v,w,t\, distinct}} |r^*(v) \cap r^*(w) \cap r^*(t)| - \sum_{uv \in E(G)} \sum_{\substack{u' \in N_G(u) \setminus \{v\} \\ v' \in N_G(v) \setminus \{u\}}} |r^*(u') \cap r^*(v')|$$

is larger than or equal to

$$\sum_{u \in V(G)} \sum_{\substack{v,w,t \in N_G(u) \\ v,w,t\, distinct}} |r(v) \cap r(w) \cap r(t)| - \sum_{uv \in E(G)} \sum_{\substack{u' \in N_G(u) \setminus \{v\} \\ v' \in N_G(v) \setminus \{u\}}} |r(u') \cap r(v')|.$$

Proof. We follow a similar argument as in the proofs of Theorems 4.2.5 and 4.2.8. It suffices to show that $a_{n-4}(G,r^*) \geq a_{n-4}(G,r)$ holds for every proper k-restraint r on G such that $A_7''(G,r^*) = A_7''(G,r)$. Let r be a such restraint. Recall that $a_{n-4}(G,r) = C_0(G)+\sum C_i(G,r)$. Note that $C_0(G)$ does not depend on the restraint function. Now, since r and r^* are k-restraints we find that $C_i(G,r) = C_i(G,r^*)$ for $i = 1,2,3,5,6,12$. Furthermore, $C_i(G,r) = C_i(G,r^*) = 0$ for $i = 4,7,8,10,11,13,16,18,19$ as r and r^* are proper restraints. Lastly, $C_i(G,r) = C_i(G,r^*)$ for $i = 9,14$ since $A_7''(G,r^*) = A_7''(G,r)$ by the assumption. $\square$

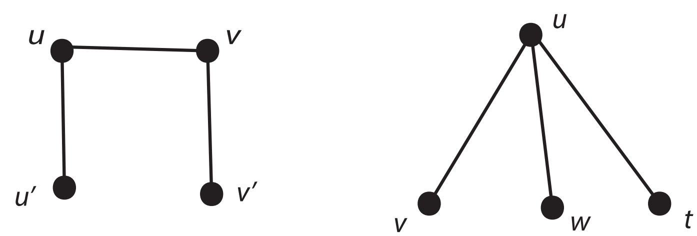

Figure 4.3: A P_4 (left) and a claw (right)

Example 4.2.3. Let $G = C_7$. We apply Theorem 4.2.12 to determine $R_{\max}(G,1)$. As we already mentioned, by Theorem 4.2.8, if $r \in R_{\max}(G,1)$ then r must be equivalent to $r_1 = [\{1\},\{2\},\{1\},\{2\},\{1\},\{2\},\{3\}]$ or $r_2 = [\{1\},\{2\},\{1\},\{2\},\{3\},\{1\},\{3\}]$. First note that $C_{17}(G,r) = 0$ for every restraint r on G because cycles are claw-free graphs. Now we find that $C_{15}(G,r_1) = 2$ and $C_{15}(G,r_2) = 1$. Therefore, by Theorem 4.2.12, $R_{\max}(G,1)$ consists of restraints which are equivalent to r_2.

Bounding the number of colours x

All of the previous results find the extremal restraints, but only for sufficiently large x. How large does x need to be? This is a seemingly difficult problem, but for complete graphs and trees we will show that the results hold for $x \geq nk$.

Given a restraint function r on G and a vertex v of G, we define $\pi_r(G, x, v \to j)$ as the number of x-colourings of G permitted by r such that the vertex v is assigned the colour j.

Theorem 4.2.13. *Let T be a tree on $n \geq 2$ vertices and r be a k-restraint on T. Then, for $x \geq nk$*

$$\pi_r(T, x) \leq \pi_{r_{alt}}(T, x).$$

Furthermore, the strict inequality holds if $r \not\simeq r_{alt}$.

Proof. We proceed by induction on n. Let u be a leaf of T and v be the neighbour of u. For the basis step $n = 2$, the only tree with two vertices is K_2. Let r be any k-restraint on T. If v gets a colour from $r(u) \setminus r(v)$ (respectively $[x] \setminus (r(u) \cup r(v))$) then u has $x - k$ (respectively $x - k - 1$) choices. Hence,

$$\begin{aligned}
\pi_r(K_2, x) &= (x-k)|r(u) \setminus r(v)| + (x-k-1)|[x] \setminus (r(u) \cup r(v))| \\
&= (x-k-1)(|r(u) \setminus r(v)| + |[x] \setminus (r(u) \cup r(v))|) + |r(u) \setminus r(v)| \\
&= (x-k-1)(x-k) + |r(u) \setminus r(v)|.
\end{aligned}$$

Now, $|r(u) \setminus r(v)| = k$ if and only if $r \simeq r_{alt}$. Therefore, $\pi_r(G, x)$ achieves its maximum value if and only if $r \simeq r_{alt}$.

Now suppose that $n \geq 3$ and let $v_1, \ldots, v_l$ be the vertices of the set $N(v) \setminus \{u\}$. Also, let $T' = T - u$, $T'' = T - \{u, v\}$ and T^i be the connected component of T'' which contains the vertex v_i. Given a k-restraint r on T, we consider again two cases: either v gets a colour from $r(u) \setminus r(v)$ or $[x] \setminus (r(u) \cup r(v))$. If v is assigned a colour from $r(u) \setminus r(v)$ (respectively $[x] \setminus (r(u) \cup r(v))$), once all the vertices of T' are coloured with respect to $r|_{T'}$ the vertex u has $x-k$ (respectively $x-k-1$) choices. Therefore,

$$\pi_r(T, x) = (x-k) \sum_{j \in r(u) \setminus r(v)} \pi_{r|_{T'}}(T', x, v \to j) + (x-k-1) \sum_{j \in r(u) \setminus r(v)} \pi_{r|_{T'}}(T', x, v \to j).$$

Rewriting the equation above, we have

$$\pi_r(T,x) = (x-k-1)\sum_{j\in[x]\setminus r(v)} \pi_{r|_{T'}}(T',x,v\to j) + \sum_{j\in r(u)\setminus r(v)} \pi_{r|_{T'}}(T',x,v\to j).$$

Thus,

$$\pi_r(T,x) = (x-k-1)\pi_{r|_{T'}}(T',x) + \sum_{j\in r(u)\setminus r(v)} \pi_{r|_{T'}}(T',x,v\to j). \tag{4.25}$$

Also, given $j\in r(u)\setminus r(v)$, let us define a restraint function $r_i^j : V(T^i) \to [n]^k \cup [n]^{k+1}$ on each component T^i for $i=1,\dots,l$ as follows:

$$r_i^j(w) := \begin{cases} r(v_i)\cup\{j\} & \text{if } w = v_i \\ r(w) & \text{if } w \in V(T^i)\setminus\{v_i\} \end{cases}$$

Now, it is not difficult to see that

$$\pi_{r|_{T'}}(T',x,v\to j) = \prod_{i=1}^{l} \pi_{r_i^j}(T^i,x).$$

Since $x \geq nk$, there exists a restraint function $r^* : V(T') \to [n-1]^k$ (which is obtained by permuting the colours of $r|_{T'}$) such that the number of x-colourings of T' with respect to $r|_{T'}$ is equal to the number of x-colourings of T' with respect to r^*. Therefore, by the induction hypothesis on T', $\pi_{r|_{T'}}(T',x)$ attains its maximum value if and only if r induces an alternating restraint on T'.

Moreover, since $r(V(T^i)) \subseteq r_i^j(V(T^i))$ and by the induction hypothesis on T^i, $\pi_{r_i^j}(T^i,x)$ is maximized when $j\in r(v_i)$ and r induces an alternating restraint on T^i for every $i=1,\dots,l$ and $j\in r(u)\setminus r(v)$. So, $\sum_{j\in r(u)\setminus r(v)} \pi_{r|_{T'}}(T',x,v\to j)$ attains its maximum value if and only if all of the following conditions are satisfied:

(i) $r(u)\cap r(v) = \emptyset$,

(ii) $j \in r(v_i)$ for each i and j, and

(iii) r induces an alternating restraint on T^i for each i.

Thus, Equation 4.25 and all these together imply that $\pi_r(T, x)$ is maximized if and only if r is an alternating restraint on T.

□

Note that in Theorem 4.2.13, the number of colours x must be at least nk and this bound is best possible. For example, let us consider the path graph P_3 whose vertices are v_1, v_2, v_3, and v_1 is the stem of the leaves v_2, v_3. Let $r = [\{1\}, \{2\}, \{3\}]$ and $r_{alt} = [\{1\}, \{2\}, \{2\}]$ be two simple restraints on P_3. Then,

$$\pi_r(P_3, 2) = \pi_{r_{alt}}(P_3, 2) = 1.$$

Moreover, one can find examples where $\pi_{r_{alt}}(T, x)$ is strictly less than $\pi_r(T, x)$ for some other restraint r when x is less than nk. For example, consider the star $K_{1,4}$ whose vertices are $v_1, \ldots, v_5$ and v_1 is its universal vertex. Let $r = [\{1\}, \{2\}, \{3\}, \{4\}, \{5\}]$ and $r_{alt} = [\{1\}, \{2\}, \{2\}, \{2\}, \{2\}]$, then

$$16 = \pi_r(K_{1,4}, 3) > \pi_{r_{alt}}(K_{1,4}, 3) = 9.$$

Observe that in the proof of Theorem 4.2.6, the extremal restraint on K_n does not determine how large x should be. In Theorem 4.2.14, we present another proof and determine that x should be at least nk. On the other hand, Theorem 4.2.6 has its own advantage that it proves the strict inequality in $\pi_r(G, x) < \pi_{r^*}(G, x)$ and this shows the uniqueness of the extremal restraint function.

Theorem 4.2.14. *Let $r : V(K_n) \to \binom{[kn]}{k}$ be a k-restraint on K_n. Also, let $r^* : V(K_n) \to \binom{[kn]}{k}$ be the k-restraint which satisfies $r^*(w) \cap r^*(w') = \emptyset$ for every w and*

w' in $V(K_n)$. Then, for all $x \geq nk$,

$$\pi_r(K_n, x) \leq \pi_{r^*}(K_n, x).$$

Proof. We show that if two vertices of a complete graph have a common forbidden colour, then one can modify the restraint function to get another restraint which permits greater or equal number of colourings, by replacing the common restraint at one of these vertices with a colour not forbidden elsewhere.

Let $r : V(K_n) \to [n]^k$ be a k-restraint such that there are two vertices u and v with $r(u) \cap r(v) \neq \emptyset$. Let i be a colour in $r(u) \cap r(v)$ and $x \geq nk$. So, there exist $j \in [nk]$ such that $j \notin r(w)$ for every vertex w of K_n. Let us define a restraint function r' on K_n as follows:

$$r'(w) := \begin{cases} \{j\} \cup (r(v) \setminus \{i\}) & \text{if } w = v \\ r(w) & \text{if } w \neq v \end{cases}$$

Let c be an x-colouring of K_n permitted by r. For each such c, we find another x-colouring c' of K_n permitted by r', in a 1-to-1 fashion. We consider three cases:

Case 1: $c(v) \neq j$.

The x-colouring c is also permitted by r', so we take $c' = c$.

Case 2: $c(v) = j$ and the colour i is not used by c.

We define c' as follows: $c'(v) = i$ and $c'(w) = c(w)$ for $w \neq v$. Since $i \notin r'(v)$ and $x \geq i$, it is clear that c' is an x-colouring of K_n permitted by r'.

Case 3: $c(v) = j$ and the colour i is used by c.

Let w be the vertex such that $c(w) = i$. Now we define c' as follows: $c'(v) = i$, $c'(w) = j$ and $c'(a) = c(a)$ for every vertex a not equal to v or w. Again this gives an x-colouring of K_n permitted by r'.

No colouring c' from one case is a colouring in another case and different colourings c give rise to different colourings c' within each case. Thus, $\pi_r(K_n, x) \leq \pi_{r'}(K_n, x)$ for all $x \geq nk$. Now, if $r'(w) \cap r'(w') = \emptyset$ for every $w \neq w'$ in $V(K_n)$, then $r^* = r'$. If not, then we repeat the same argument until we get such a restraint.

$\square$

Note that Theorem 4.2.14 was proven in [11] for the special case of simple restraints.

Chapter 5

Concluding Remarks

5.1 Some Concluding Results on σ-Polynomials

5.1.1 Nonreal roots of σ-polynomials

We have seen that many - almost all! - small graphs have all real σ-roots. The examples of graphs with nonreal σ-roots are few and far between. Of course, we can build larger graphs ones from smaller ones via joins, as σ-polynomials are multiplicative with respect to join but this will not give us new nonreal σ-roots. How to obtain infinitely many nonreal σ-roots? In this section, we study a family graphs which are good candidates to find infinitely many nonreal σ-roots and provide a recursive construction of this family.

Let $H^t_{n,k}$ be the graph K_n with a path of size t hanging off k vertices of the clique K_n. More precisely, $H^t_{n,k}$ is the graph on $n+kt$ vertices and $\binom{n}{2}+kt$ edges whose vertex set is equal to

$$\{u_i : 1 \le i \le n\} \cup \{v^j_i : 1 \le i \le t,\, 1 \le j \le k\}$$

and edge set is equal to

$$\{u_i u_j : 1 \le i < j \le n\} \cup \{u_i v^i_1 : 1 \le i \le k\} \cup \{v^j_i v^j_{i+1} : 1 \le i \le t-1,\, 1 \le j \le k\}.$$

For example, see Figure 5.1.

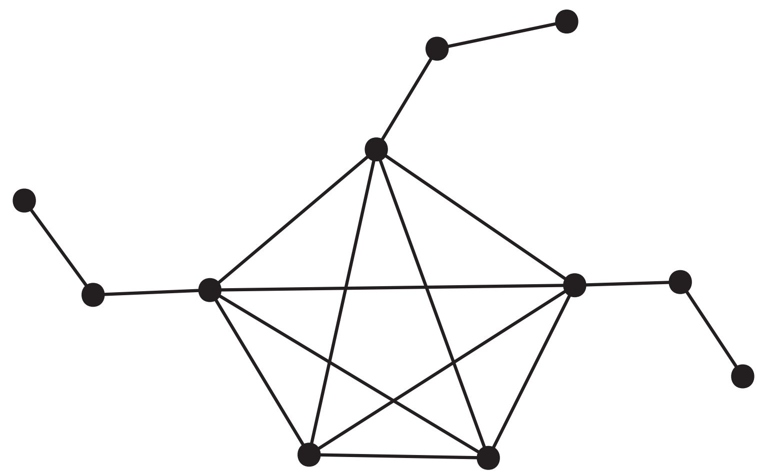

Figure 5.1: The graph $H^2_{5,3}$.

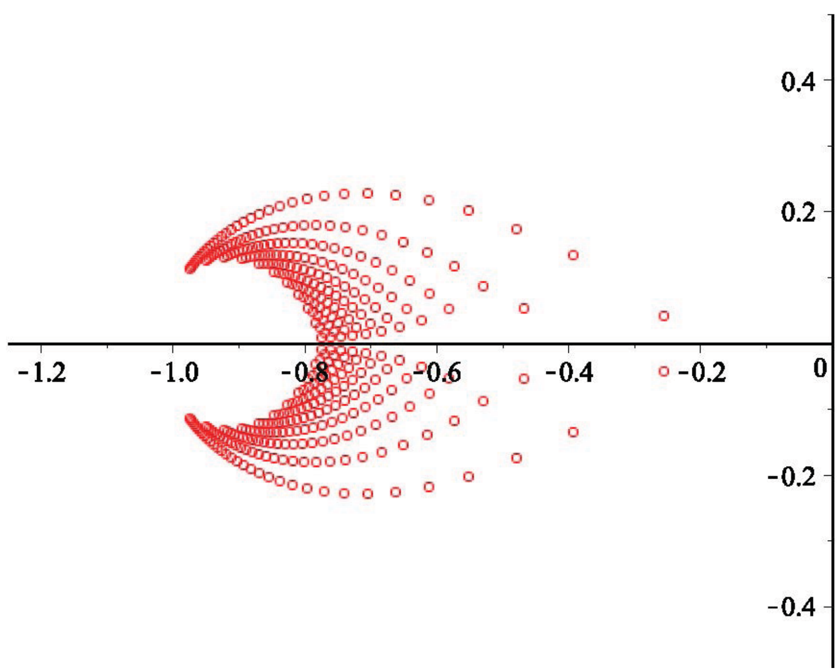

Figure 5.2: Nonreal roots of the adjoint polynomial of $H^2_{n,n}$ for $n = 1, \ldots, 35$.

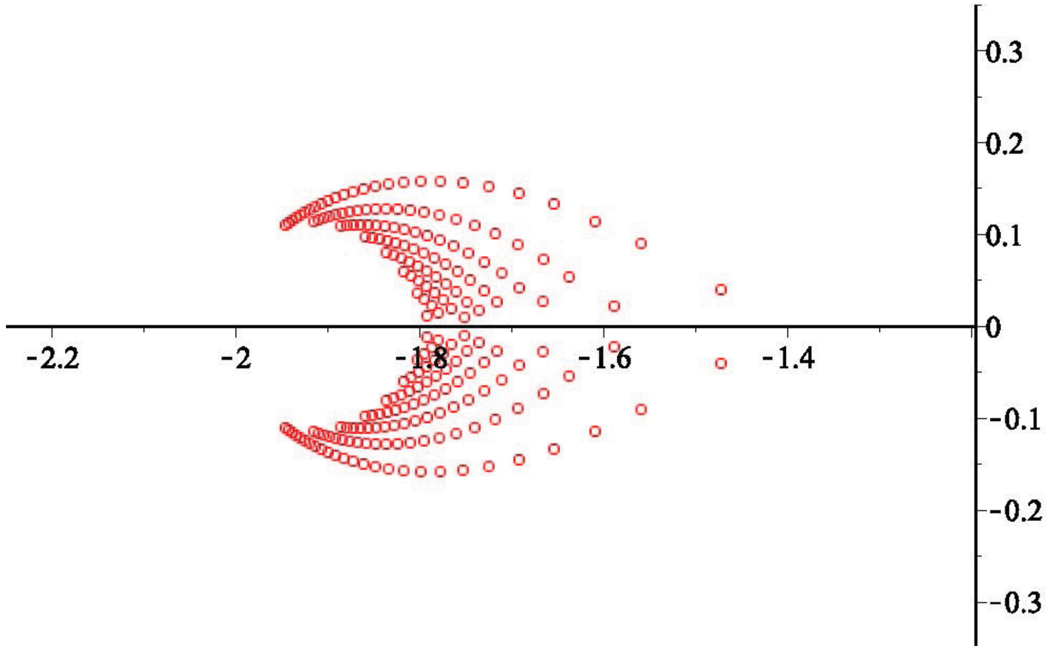

Figure 5.3: Nonreal roots of the adjoint polynomial of $H^3_{n,n}$ for $n = 1, \ldots, 30$.

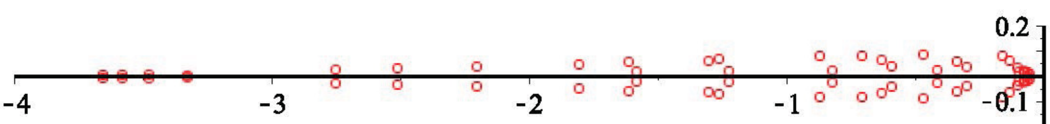

Figure 5.4: Nonreal roots of the adjoint polynomial of $H^n_{n,n}$ for $n = 1, \ldots, 10$.

Theorem 5.1.1. *The adjoint polynomial of $H^t_{n,k}$ satisfies the following recursion*

$$h(H^t_{n,k}, x) = h(P_t, x)\, h(H^t_{n,k-1}, x) + x\, h(P_{t-1}, x)\, h(H^t_{n-1,k-1}, x),$$

with initial conditions $h(H^t_{1,1}, x) = h(P_{t+1}, x)$ *and* $h(H^t_{n,0}, x) = h(H^0_{n,k}, x) = h(K_n, x)$.

Proof. First, note that $H^t_{1,1} \cong P_{t+1}$ and $H^t_{n,0} \cong H^0_{n,k} \cong K_n$, so the initial conditions are satisfied. By the recursive formula given in Equation (2.1), we get

$$h(H^t_{n,k}, x) = h(H^t_{n,k} - u_1v_1^1, x) + h(H^t_{n,k} \odot u_1v_1^1, x).$$

Since u_1 and v_1^1 have no common neighbors in $H^t_{n,k}$,

$$H^t_{n,k} - u_1v_1^1 \;\cong\; P_t \,\dot\cup\, H^t_{n,k-1}$$

and

$$H^t_{n,k} \odot u_1v_1^1 \;\cong\; K_1 \,\dot\cup\, P_{t-1} \,\dot\cup\, H^t_{n-1,k-1}.$$

Therefore,

$$h(H^t_{n,k} - u_1v_1^1, x) = h(P_t \,\dot\cup\, H^t_{n,k-1}, x) = h(P_t, x)\, h(H^t_{n,k-1}, x)$$

and

$$h(H^t_{n,k} \odot u_1v_1^1, x) = h(K_1 \,\dot\cup\, P_{t-1} \,\dot\cup\, H^t_{n-1,k-1}, x) = x\, h(P_{t-1}, x)\, h(H^t_{n-1,k-1}, x).$$

Thus, the proof is complete. $\square$

The complement of the graph $H_{n,k}^t$ appears to have nonreal σ-roots with large moduli (see Figures 5.2, 5.3 and 5.4) although we have not been able to prove it. Observe that these graphs are not the join of smaller graphs (as $H_{n,k}^t$ are all connected), and this points to why the nonreal roots are distinct.

5.1.2 Cycles and theta graphs

The *generalized theta graph*, denoted $\Theta_{s_1,\ldots,s_k}$, consists of a pair of endvertices joined by k internally disjoint paths of sizes $s_1, \ldots, s_k \geq 2$. Such graphs played an important role in the study of chromatic polynomials as Sokal used such graphs to show that chromatic roots are dense in the complex plane. In contrast to this fact, computations suggest that the σ-polynomials of these graphs have only real roots. In this section, we consider the σ-polynomial of the theta graph Θ_{s_1,s_2,s_3}.

Lemma 5.1.2. *The σ-polynomial of the theta graph Θ_{s_1,s_2,s_3} is given by the equality*

$$\sigma(\Theta_{s_1,s_2,s_3}, x) = \left(\frac{\sigma(C_{s_1+1}, x)}{x^2} * \frac{1}{x^2}\left(\frac{C_{s_2+1}}{x^2} * \frac{C_{s_3+1}}{x^2}\right)\right) + \left(\frac{\sigma(C_{s_1}, x)}{x} * \frac{1}{x}\left(\frac{C_{s_2}}{x} * \frac{C_{s_3}}{x}\right)\right)$$

Proof. Let u and v be the endvertices of the three disjoint paths. By applying the Cutset Theorem successively we obtain

$$\sigma(\Theta_{s_1,s_2,s_3} + uv, x) = \frac{\sigma(C_{s_1+1}, x)}{x^2} * \frac{1}{x^2}\left(\frac{C_{s_2+1}}{x^2} * \frac{C_{s_3+1}}{x^2}\right)$$

and

$$\sigma(\Theta_{s_1,s_2,s_3} \cdot uv, x) = \frac{\sigma(C_{s_1}, x)}{x} * \frac{1}{x}\left(\frac{C_{s_2}}{x} * \frac{C_{s_3}}{x}\right).$$

Thus, the desired equality follows from the edge addition-contraction formula. $\square$

Lemma 5.1.3. *The σ-polynomial of a cycle C_n satisfies the following*

$$\sigma(C_n, x) = \sum_{i=0}^{n-2} (-1)^i \sigma(P_{n-i}, x).$$

Proof. By applying the edge deletion-contraction formula repeatedly, we obtain

$$\begin{aligned}
\sigma(C_n, x) &= \sigma(P_n, x) - \sigma(C_{n-1}, x) \\
&= \sigma(P_n, x) - \sigma(P_{n-1}, x) + \sigma(C_{n-2}, x) \\
&= \sigma(P_n, x) - \sigma(P_{n-1}, x) + \sigma(P_{n-2}, x) - \sigma(C_{n-3}, x) \\
&\vdots \\
&= \sigma(P_n, x) - \sigma(P_{n-1}, x) + \cdots + (-1)^{n-3}\sigma(P_3, x) + (-1)^{n-2}\sigma(P_2, x).
\end{aligned}$$

□

Rolle's Theorem says that every polynomial f and its derivative f' interlace. Therefore, it is not difficult to see the following:

Lemma 5.1.4. *[17] If f and g are two compatible polynomials then their derivatives f' and g' are also compatible.*

Conjecture 5.1.5. For every $n \geq 3$, the polynomials $\sigma(C_n, x)$ and $\sigma(C_{n+1}, x)$ are compatible.

It is not possible to strengthen the conjecture above to interlacing property because $\sigma(C_n, x)$ and $\sigma(C_{n+1}, x)$ do not interlace when n is odd (see Table 5.2).

Lemma 5.1.6. *The σ-polynomial of a cycle C_n satisfies the following recursion*

$$\sigma(C_n, x) = (x-2)\sigma(C_{n-1}, x) + x\frac{d}{dx}\sigma(C_{n-1}, x) + (x-1)\sigma(C_{n-2}, x) + x\frac{d}{dx}\sigma(C_{n-2}, x)$$

n	**Nonzero roots of** $\sigma(P_n, x)$
3	-1.0
4	$-2.618, -0.3820$
5	$-4.491, -1.343, -0.1658$
6	$-6.510, -2.652, -0.7622, -0.07600$
7	$-8.626, -4.181, -1.704, -0.4533, -0.03590$
8	$-10.81, -5.863, -2.890, -1.140, -0.2771, -0.01727$
9	$-13.05, -7.658, -4.257, -2.072, -0.7824, -0.1726, -0.008403$
10	$-15.33, -9.541, -5.760, -3.193, -1.519, -0.5458, -0.1089, -0.004121$
11	$-17.64, -11.49, -7.371, -4.463, -2.444, -1.130, -0.3854, -0.06933, -0.002032$
12	$-19.98, -13.50, -9.070, -5.854, -3.523, -1.897, -0.8503, -0.2746, -0.04449, -0.001006$
13	$-22.35, -15.56, -10.84, -7.344, -4.730, -2.818, -1.487, -0.6453, -0.1970, -0.02872, -0.0004990$
14	$-24.73, -17.66, -12.67, -8.918, -6.044, -3.869, -2.275, -1.176, -0.4930, -0.1422, -0.01862, -0.0002481$
15	$-27.14, -19.79, -14.56, -10.56, -7.449, -5.031, -3.193, -1.850, -0.9351, -0.3787, -0.1031, -0.01212, -0.0001236$

Table 5.1: Nonzero roots of the σ-polynomial of P_n for $n = 3, \ldots, 15$

n	**Nonzero roots of** $\sigma(C_n, x)$
4	$-1.0, -1.0$
5	$-3.618, -1.382$
6	$-5.886, -2.465, -0.5161, -0.1336$
7	$-8.135, -3.918, -1.511, -0.4360$
8	$-10.40, -5.594, -2.706, -1.053, -0.2156, -0.02796$
9	$-12.70, -7.402, -4.072, -1.954, -0.7128, -0.1594$
10	$-15.02, -9.302, -5.578, -3.063, -1.434, -0.5043, -0.09008, -0.006429$
11	$-17.37, -11.27, -7.195, -4.329, -2.348, -1.070, -0.3549, -0.06269$
12	$-19.74, -13.30, -8.901, -5.720, -3.421, -1.825, -0.8066, -0.2542, -0.03795, -0.001540$
13	$-22.12, -15.37, -10.68, -7.212, -4.625, -2.739, -1.433, -0.6130, -0.1824, -0.02569$
14	$-24.53, -17.48, -12.52, -8.789, -5.938, -3.785, -2.213, -1.134, -0.4688, -0.1320, -0.01614, -0.0003765$
15	$-26.94, -19.62, -14.41, -10.44, -7.343, -4.944, -3.125, -1.801, -0.9025, -0.3604, -0.09572, -0.01079$

Table 5.2: Nonzero roots of the σ-polynomial of C_n for $n = 4, \ldots, 15$

Proof. By applying Lemma 2.1.1 and Lemma 2.1.4, we obtain

$$
\begin{aligned}
\sigma(C_n,x) &= \sigma(P_n,x)-\sigma(C_{n-1},x)\\
&= \sigma(P_{n-1}\uplus K_1,x)-\sigma(P_{n-1},x)-\sigma(C_{n-1},x)\\
&= \sigma(C_{n-1}\uplus K_1,x)+\sigma(C_{n-2}\uplus K_1,x)\\
&\quad -(\sigma(C_{n-1},x)+\sigma(C_{n-2},x))-\sigma(C_{n-1},x)\\
&= \sigma(C_{n-1}\uplus K_1,x)+\sigma(C_{n-2}\uplus K_1,x)-2\sigma(C_{n-1},x)-\sigma(C_{n-2},x)\\
&= (x-2)\sigma(C_{n-1},x)+x\frac{d}{dx}\sigma(C_{n-1},x)+(x-1)\sigma(C_{n-2},x)\\
&\quad +x\frac{d}{dx}\sigma(C_{n-2},x).
\end{aligned}
$$

□

Lemma 5.1.7. *The σ-polynomial of a cycle C_n is given by the equality*

$$\sigma(C_n,x)=x^3\left(\frac{\sigma(C_{n-1},x)}{x^2}+\left(\frac{\sigma(C_{n-1},x)}{x^2}\right)'\right)+x^2\left(\frac{\sigma(C_{n-2},x)}{x}+\left(\frac{\sigma(C_{n-2},x)}{x}\right)'\right)$$

Proof. Let u and v be two nonadjacent vertices of C_n which have a common neighbor. By the edge addition-contraction formula, we have

$$\sigma(C_n,x)=\sigma(C_n+uv,x)+\sigma(C_n\cdot uv,x).$$

Now by applying the Complete Cutset Theorem we obtain

$$\frac{\sigma(C_n+uv,x)}{x^2}=\frac{\sigma(C_3,x)}{x^2}*\frac{\sigma(C_{n-1},x)}{x^2}=x*\frac{\sigma(C_{n-1},x)}{x^2}$$

and

$$\frac{\sigma(C_n\cdot uv,x)}{x}=\frac{\sigma(K_2,x)}{x}*\frac{\sigma(C_{n-2},x)}{x}=x*\frac{\sigma(C_{n-2},x)}{x}.$$

Since $x*f=x(f+f')$ for any polynomial f, the desired equality is obtained.

□

Having a better understanding of the roots of σ-polynomials of cycles might be useful to obtain results about the theta graphs. From some computations, we believe the following conjecture might hold.

Conjecture 5.1.8. The σ-polynomials of theta graphs have only real roots.

5.1.3 Average σ-polynomials

Let $\mathcal{G}_n$ be the set of all labeled graphs on $\{1, \ldots, n\}$. We define the *nth average σ-polynomial*, denoted by $\tilde{\sigma}_n(x)$, as the average of the σ-polynomials over all labeled graphs of order n. More precisely,

$$\tilde{\sigma}_n(x) = \frac{1}{2^{\binom{n}{2}}} \sum_{G \in \mathcal{G}_n} \sigma(G, x).$$

Let $\mathcal{P}(S)$ denote the power set of S. A *partition of S into k nonempty subsets* is a subset $\mathcal{A}$ of $\mathcal{P}(S) \setminus \{\emptyset\}$ such that $|\mathcal{A}| = k$, $S = \cup\mathcal{A}$ and $X \cap X' = \emptyset$ for every two distinct $X, X' \in \mathcal{A}$. Now, let *Part*(S,k) denote the set of all partitions of S into k nonempty subsets.

For example, Part$([4], 2)$ consists of

$$\{\{1,2\},\{3,4\}\},\ \{\{1,3\},\{2,4\}\},\ \{\{1,4\},\{2,3\}\},$$

$$\{\{1\},\{2,3,4\}\},\ \{\{2\},\{1,3,4\}\},\ \{\{3\},\{1,2,4\}\} \text{ and } \{\{4\},\{1,2,3\}\}.$$

Now we find that

$$\tilde{\sigma}_n(x) = \sum_{k=1}^{n} \sum_{\mathcal{A} \in \mathrm{Part}([n],k)} 2^{-\sum_{A \in \mathcal{A}} \binom{|A|}{2}} x^k$$

n	**Nonzero roots of** $\frac{d}{dx}\sigma(C_n, x)$
4	$-1.0, -0.5000$
5	$-3.0, -1.0$
6	$-5.056, -1.965, -0.3947, -0.08504$
7	$-7.181, -3.298, -1.206, -0.3152$
8	$-9.367, -4.867, -2.258, -0.8286, -0.1607, -0.01824$
9	$-11.60, -6.589, -3.512, -1.618, -0.5613, -0.1162$
10	$-13.88, -8.420, -4.927, -2.625, -1.183, -0.3955, -0.06674, -0.004240$
11	$-16.19, -10.33, -6.470, -3.802, -2.003, -0.8800, -0.2786, -0.04603$
12	$-18.53, -12.31, -8.113, -5.117, -2.992, -1.552, -0.6620, -0.1995, -0.02812, -0.001021$
13	$-20.89, -14.34, -9.839, -6.544, -4.121, -2.387, -1.215, -0.5026, -0.1433, -0.01896$
14	$-23.27, -16.42, -11.63, -8.065, -5.369, -3.362, -1.924, -0.9600, -0.3843, -0.1037, -0.01199, -0.0002502$
15	$-25.67, -18.53, -13.49, -9.665, -6.717, -4.458, -2.769, -1.563, -0.7634, -0.2955, -0.07535, -0.007998$

Table 5.3: Nonzero roots of the derivative of the σ-polynomial of C_n for $n = 4, \ldots, 15$.

n	$\tilde{\sigma}_n(x)$
1	x
2	$\frac{1}{2}\,x + x^2$
3	$\frac{1}{8}\,x + \frac{3}{2}\,x^2 + x^3$
4	$\frac{1}{64}\,x + \frac{5}{4}\,x^2 + 3\,x^3 + x^4$
5	$\frac{1}{1024}\,x + \frac{45}{64}\,x^2 + 5\,x^3 + 5\,x^4 + x^5$
6	$\frac{1}{32768}\,x + \frac{143}{512}\,x^2 + \frac{375}{64}\,x^3 + \frac{55}{4}\,x^4 + \frac{15}{2}\,x^5 + x^6$
7	$\frac{1}{2097152}\,x + \frac{2583}{32768}\,x^2 + \frac{5341}{1024}\,x^3 + \frac{1715}{64}\,x^4 + \frac{245}{8}\,x^5 + \frac{21}{2}\,x^6 + x^7$
8	$\frac{1}{268435456}\,x + \frac{4145}{262144}\,x^2 + \frac{29799}{8192}\,x^3 + \frac{5187}{128}\,x^4 + \frac{2835}{32}\,x^5 + \frac{119}{2}\,x^6 + 14\,x^7 + x^8$
9	$\frac{1}{68719476736}\,x + \frac{604425}{268435456}\,x^2 + \frac{1054825}{524288}\,x^3 + \frac{406245}{8192}\,x^4 + \frac{102543}{512}\,x^5 + \frac{7623}{32}\,x^6 + 105\,x^7$ $+18\,x^8 + x^9$
10	$\frac{1}{35184372088832}\,x + \frac{7818053}{34359738368}\,x^2 + \frac{237857325}{268435456}\,x^3 + \frac{13151615}{262144}\,x^4 + \frac{6081705}{16384}\,x^5 + \frac{191163}{256}\,x^6$ $+\frac{17745}{32}\,x^7 + \frac{345}{2}\,x^8 + \frac{45}{2}\,x^9 + x^{10}$
11	$\frac{1}{36028797018963968}\,x + \frac{573667083}{35184372088832}\,x^2 + \frac{21374449591}{68719476736}\,x^3 + \frac{11388932005}{268435456}\,x^4 + \frac{607302245}{1048576}\,x^5$ $+\frac{31619511}{16384}\,x^6 + \frac{1173711}{512}\,x^7 + \frac{37125}{32}\,x^8 + \frac{2145}{8}\,x^9 + \frac{55}{2}\,x^{10} + x^{11}$

Table 5.4: Average σ-polynomials for $n = 1, \ldots, 11$

A partition of an integer n into k integers is a nonincreasing sequence of k positive integers whose sum is equal to n. Let $\mathrm{InPart}(n, k)$ denote the set of all partitions of the integer n into k integers. For example,

$$\begin{aligned}
\mathrm{InPart}(5,1) &= \{(5)\} \\
\mathrm{InPart}(5,2) &= \{(4,1),(3,2)\} \\
\mathrm{InPart}(5,3) &= \{(3,1,1),(2,2,1)\} \\
\mathrm{InPart}(5,4) &= \{(2,1,1,1)\} \\
\mathrm{InPart}(5,5) &= \{(1,1,1,1,1)\}
\end{aligned}$$

Given a sequence τ of size k, we write $\tau = (\tau_1, \ldots, \tau_k)$. Let i be an integer then the number of repetitions of i in τ is denoted by $\mathrm{rep}(\tau, i)$. For example, if $\tau = (1,1,1,2,3,3)$ then $\mathrm{rep}(\tau,1) = 3$, $\mathrm{rep}(\tau,2) = 1$, $\mathrm{rep}(\tau,3) = 2$ and $\mathrm{rep}(\tau,4) = 0$. Also, let

$$\binom{n}{\tau_1, \ldots, \tau_k} = \binom{n}{\tau_1}\binom{n-\tau_1}{\tau_2}\cdots\binom{n-\tau_1-\cdots-\tau_{k-1}}{\tau_k} = \frac{n!}{\tau_1!\cdots\tau_k!}$$

be the multinomial coefficient. Now we find that

$$\tilde{\sigma}_n(x) = \sum_{k=1}^{n} \sum_{\tau \in \mathrm{InPart}(n,k)} \binom{n}{\tau_1, \ldots, \tau_k} \frac{1}{\prod_{i=1}^{n-k+1} \mathrm{rep}(\tau, i)!} \; \frac{1}{2^{\sum_{i=1}^{k} \binom{\tau_i}{2}}} \; x^k.$$

By computer aided computations we have verified that Conjecture 5.1.9 is true for every n at most 30.

Conjecture 5.1.9. The polynomial $\tilde{\sigma}_n(x)$ has only real roots for every n. Moreover, $\tilde{\sigma}_n(x)$ interlaces $\tilde{\sigma}_{n+1}(x)$. That is, if $r_1^n \leq r_2^n \leq \cdots \leq r_n^n$ are the roots of $\tilde{\sigma}_n(x)$ and $r_1^{n+1} \leq r_2^{n+1} \leq \cdots \leq r_{n+1}^{n+1}$ are the roots of $\tilde{\sigma}_{n+1}(x)$ then

$$r_1^{n+1} \leq r_1^n \leq r_2^{n+1} \leq r_2^n \leq \cdots \leq r_n^n \leq r_{n+1}^{n+1}.$$

n	Roots of $\tilde{\sigma}_n(x)$
1	0.0
2	$-0.5000, 0.0$
3	$-1.411, -0.08856, 0.0$
4	$-2.503, -0.4840, -0.01290, 0.0$
5	$-3.700, -1.132, -0.1661, -0.001403, 0.0$
6	$-4.967, -1.948, -0.5305, -0.05428, -0.0001095, 0.0$
7	$-6.284, -2.880, -1.073, -0.2463, -0.01648, -0.000006052, 0.0$
8	$-7.640, -3.898, -1.752, -0.5942, -0.1114, -0.004578, -0.0000002356, 0.0$
9	$-9.026, -4.982, -2.537, -1.079, -0.3265, -0.04866, -0.001152,$ $-0.000000006463, 0.0$
10	$-10.44, -6.118, -3.406, -1.677, -0.6645, -0.1766, -0.02039, -0.0002606,$ $-0.0000000001249, 0.0$
11	$-11.87, -7.298, -4.343, -2.369, -1.114, -0.4067, -0.09365, -0.008171,$ $-0.00005280, -1.702 \times 10^{-12}, 0.0$

Table 5.5: Roots of average σ-polynomials for $n = 1, \ldots, 11$

5.2 Concluding Remarks on Restrained Colourings

We determined the extremal restraints for bipartite graphs which includes all even cycles. A natural problem is to investigate the problem on odd cycles. Surprisingly, determining extremal restraints for odd cycles is more difficult than bipartite graphs. We believe that the necessary conditions for (C_3, C_4)–free graphs given in Theorem 4.2.12 are sufficient for odd cycles. Note that odd cycles are claw–free and therefore an immediate consequence of Theorem 4.2.12 for odd cycles is the following.

Corollary 5.2.1. *Let G be equal to an odd cycle. If $r^* \in R_{\max}(G,k)$ then r^* satisfies all of the following.*

(i) *r^* is a proper restraint,*

(ii) *$A_7''(G,r^*) = \min\{A_7''(G,r) :$ r is a proper k-restraint on $G\}$. In other words,*

$$\sum_{u\in V(G)} \sum_{\substack{v,w\in N_G(u)\\ v\neq w}} |r^*(v)\cap r^*(w)| \geq \sum_{u\in V(G)} \sum_{\substack{v,w\in N_G(u)\\ v\neq w}} |r(v)\cap r(w)|$$

for every proper k-restraint on G.

(iii) *If there exists a proper k-restraint r' on G with $r' \not\simeq r^*$ such that $A_7''(G,r^*) = A_7''(G,r')$ then for every proper k-restraint r on G such that $A_7''(G,r^*) = A_7''(G,r)$ we have*

$$C_{15}(G,r^*) \geq C_{15}(G,r),$$

that is,

$$\sum_{uv\in E(G)} \sum_{\substack{u'\in N_G(u)\setminus\{v\}\\ v'\in N_G(v)\setminus\{u\}}} |r^*(u')\cap r^*(v')| \leq \sum_{uv\in E(G)} \sum_{\substack{u'\in N_G(u)\setminus\{v\}\\ v'\in N_G(v)\setminus\{u\}}} |r(u')\cap r(v')|.$$

Conjecture 5.2.2. The conditions given in Corollary 5.2.1 are sufficient to determine $R_{\max}(G,k)$ when G is an odd cycle.

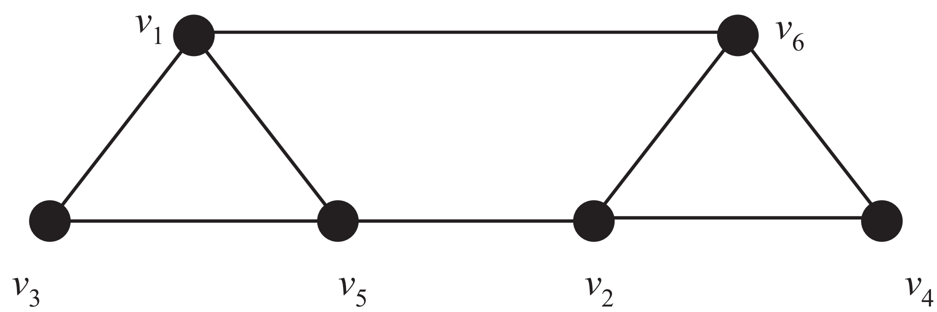

Figure 5.5: A nonchordal graph G whose simple restraint permitting the largest number of colourings is not a minimal colouring.

It is worth noting that for complete graphs and trees the simple restraints which maximize the restrained chromatic polynomials are all minimal colourings, that is, colourings with the smallest number of colours. One might wonder therefore whether this always holds, but unfortunately this is not always the case. For example, the graph G in Figure 5.5 has chromatic number 3, and there are exactly two different kinds of simple restraints which are minimal colourings of G, namely, $r_1 = [\{1\},\{1\},\{3\},\{3\},\{2\},\{2\}]$ and $r_2 = [\{1\},\{3\},\{3\},\{1\},\{2\},\{2\}]$. Now, for $r_3 = [\{1\},\{1\},\{3\},\{4\},\{2\},\{2\}]$ which is clearly not a minimal colouring of G, we have

$$\pi_{r_3}(G,x) - \pi_{r_1}(G,x) = 2\,x^2 - 14\,x + 26,$$

$$\pi_{r_3}(G,x) - \pi_{r_2}(G,x) = 3\,x^2 - 20\,x + 34$$

for all large enough x. It follows that the simple restraint which maximizes the restrained chromatic polynomial of G cannot be a minimal colouring of the graph.

So, one might hope for a generalization of the results for trees and complete graphs in a restricted family of graphs such as chordal graphs. But this is not possible either. For consider the chordal graph G in Figure 5.6 which has chromatic number 3. It is easy to see that there is essentially only one simple restraint ($r_2 = [\{1\},\{2\},\{3\},\{1\},\{2\},\{3\}]$) which is a proper colouring of the graph with three colours. If $r_1 = [\{1\}, \{2\}, \{3\}, \{1\}, \{2\}, \{4\}]$, then some direct computations show that

$$\pi_{r_1}(G, x) - \pi_{r_2}(G, x) = (x - 3)^2 > 0$$

for all x large enough.

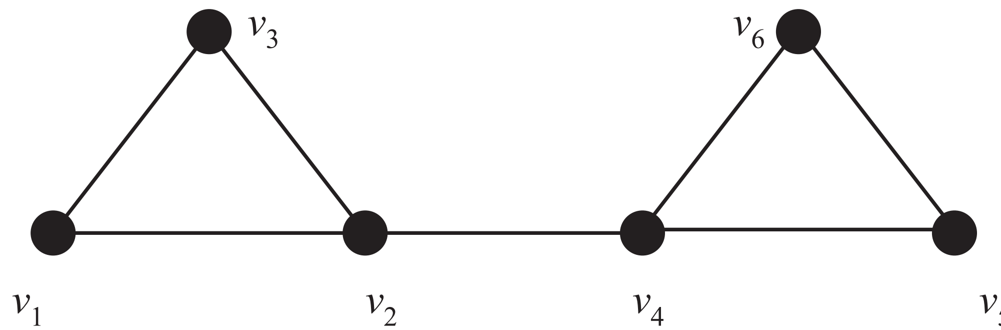

Figure 5.6: A chordal graph whose simple restraint permitting the largest number of colourings is not a minimal colouring.

Indeed, we know that among all graphs of order at most 6, there are only two graphs where the simple restraint which maximizes the restrained chromatic polynomial is not a minimal colouring of the graph. Therefore, we suggest the following interesting problem:

Problem 5.2.3. Is it true that for almost all graphs the simple restraint which maximizes the restrained chromatic polynomial is a minimal colouring of the graph?

Remark 5.2.1. As we already mentioned, the minimum number of l-list colourings on graph G is equal to $\pi(G, l)$ when l is large enough and this allows one to show that $r_c^k \in R_{\min}(G, k)$. Similarly one might wonder whether considering list colourings can be helpful to determine $R_{\max}(G, k)$. So a natural analogue of the extremal restraint problem is the following: what is the maximum number of l-list colourings on a graph G and which list colourings are extremal among all l-list colourings of G? This problem is trivial as the maximum number of l-list colourings is equal to l^n

and this value is achieved by an l-list colouring L if and only if $L(u) \cap L(v) = \emptyset$ for every $uv \in E(G)$. Obviously, knowing this does not help us to determine $R_{\max}(G, k)$ because when we consider the list colouring version of a restrained colouring, we are not able to produce all possible list colourings. For example, consider the graph $G = P_3$ with vertices v_1, v_2, v_3 such that v_1v_2, $v_2v_3 \in E(G)$. Let us consider a 3-colouring of G. Now there are four nonequivalent simple restraints on G. Such restraints and the corresponding list colourings are

$$\begin{array}{ll} r_1 = [\{1\}, \{2\}, \{3\}] & L_1 = [\{2,3\}, \{1,3\}, \{1,2\}] \\ r_2 = [\{1\}, \{2\}, \{1\}] & L_2 = [\{2,3\}, \{1,3\}, \{2,3\}] \\ r_3 = [\{1\}, \{1\}, \{2\}] & L_3 = [\{2,3\}, \{2,3\}, \{1,3\}] \\ r_4 = [\{1\}, \{1\}, \{1\}] & L_4 = [\{2,3\}, \{2,3\}, \{2,3\}] \end{array}$$

Obviously, 3-colourings permitted by the restraint r_i are the same as L_i-colourings. But the list colourings produced by the restraints do not include all possible list colourings. In particular when x is large enough, none of such list colourings will achieve the maximum value l^n.

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