ON DOMINATING SETS AND THE DOMINATION POLYNOMIAL

by

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Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy

at

Dalhousie University
Halifax, Nova Scotia
August 2021

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Abstract

A dominating set S of a graph G of order n is a subset of the vertices of G such that every vertex is either in S or adjacent to a vertex of S, and the domination number G, denoted $\gamma(G)$, is the cardinality of the smallest dominating set of G. The domination polynomial is defined by $D(G,x) = \sum_{\gamma(G)}^{n} d_i(G)x^i$ where $d_i(G)$ is the number of dominating sets in G with cardinality i. In this thesis we will consider four problems related to the domination polynomial. We begin by studying the optimality of domination polynomials. We will investigate the average order of dominating sets of graphs. We will explore the unimodality of the domination polynomials. Finally we will analyse the roots of domination polynomials.

List of Abbreviations and Symbols Used

$E(G)$ .... Edge set of a graph G (p. 4)

$V(G)$ .... Vertex set of a graph G (p. 4)

$N_G[v]$ .... Closed neighbourhood of vertex v on a graph G (p. 4)

$N_G(v)$ .... Open neighbourhood of vertex v on a graph G (see p. 4)

$\deg_G(v)$ .... The degree of a vertex v in a graph G (p. 4)

$\delta(G)$ .... The minimum degree of a graph G (p. 4)

$\Delta(G)$ .... The Maximum degree of a graph G (p. 4)

$\overline{G}$ .... Complement of a graph G (p. 4)

P_n .... Path graph on n vertices (p. 5)

K_n .... Complete graph on n vertices (p. 4)

C_n .... Cycle graph on n vertices (p. 5)

$K_{n_1,n_2,\ldots,n_k}$ .... Complete multipartite graph (p. 5)

$G \cup H$ .... Disjoint union of graphs G and H (p. 5)

$G \vee H$ .... Join of graphs G and H (p. 6)

$G \circ H$ .... Corona of graphs G and H (p. 6)

$G \diamond H$ .... Edge corona of graphs G and H (p. 6)

$G[H]$ .... The lexicographic product of graphs G and H (p. 6)

$\gamma(G)$ .... Domination number of a graph G (p. 6)

$D(G,x)$ .... Domination polynomial of a graph G (p. 8)

$\mathcal{D}(G)$ .... The set of all dominating sets of a graph G (p. 29)

$\mathcal{D}_k(G)$ .... The set of all dominating k-sets in a graph G (p. 38)

$\mathcal{D}_{+v}(G)$ .... All dominating sets containing v in a graph G (p. 36)

$\mathcal{D}_{-v}(G)$ .... All dominating sets not containing v in a graph G (p. 36)

$\mathrm{av}(\mathcal{A})$ .... The average order of a collection of sets $\mathcal{A}$ (p. 33)

$\mathrm{avd}(G)$ .... The average order of dominating sets in G (p. 29)

$\widehat{\mathrm{avd}}(G)$ .... The normalized average order of dominating sets in G (p. 52)

$p_v(G)$ ... The dominating sets of $G-N[v]$ which also dominate $G-v$ (p. 38)

$p_v(G,k)$ .... All k-subsets of $p_v(G)$ (p. 38)

$\mathrm{Priv}_S(v)$ .... The private neighbours of v with respect to S (p. 37)

$a(S)$ .... All $v \in S$ such that $S-v$ is not dominating (p. 36)

$a_1(S)$ ..... The subset of $a(S)$ which have private neighbours not in S (p. 37)

$a_2(S)$ .. The subset of $a(S)$ which have no private neighbours not in S (p. 37)

$N_1(S)$ .... The subset of $V-S$ with exactly one neighbour in S (p. 37)

$N_2(S)$ .... The subset of $V-S$ with two or more neighbours in S (p. 37)

$r_k(G)$ ... The proportion of k-subsets of vertices which are dominating (p. 65)

Acknowledgements

I would first like to thank my supervisor, Dr. Jason Brown, for your tremendous support and guidance during the past few years. Your expertise in combinatorics and many other fields was invaluable during my time at Dalhousie. I would like to thank you not only introducing me to the beauty of graph polynomials, but also the many other researchers you have influenced during your tenure. Because of you there are many other active researchers of graph polynomials who I have been able to collaborate with such as Danielle, Ben, and Lucas.

Thank you to Dr. Jeanette Janssen and Dr. Dorette Pronk for taking the time to read this thesis and providing me with helpful feedback.

Thank you as well to Dr. Bruce Sagan for being my external examiner. I appreciate the time you took to read the thesis and your helpful suggestions to improve it.

Thanks to everyone else at Dalhousie that I met along the way. Special thanks to Ben for our research collaboration and to be there to stop me before using 64 cases in a proof. Others not yet named who have enhanced my time at Dal include Abdullah, Ethan, Jonathan, Giuseppe, and Marie.

Thank you to Dalhousie University for financial support.

Chapter 1

Introduction

1.1 Overview

A subset of the vertices S of a graph G is a dominating set if every vertex in G is either in S or adjacent to at least one vertex in S. Dominating sets is a well-studied topic in graph theory. A 1991 bibliography on domination in graphs [53] by Hedetniemi and Laskar traced domination back to the graph theory texts of König (1950), Berge (1958) and Ore (1962). Dominating sets can be applied to the problem of preserving energy in wireless sensor network [74]. A wireless sensor network is a network of spatially dispersed sensors that monitor and record the physical conditions of a geographical location. At all times the active sensors must cover the entire geographical location. However some sensors can be left inactive for a period of time so long as a dominating set of sensors is left active. Dominating sets can also be used to summarize text documents [79]. One can consider a text document as a graph where the sentences of the document are vertices and two vertices are joined by an edge if the corresponding sentences are related. A dominating set in this graph would then be a collection of sentences which collectively relate to all other sentences in the document. One could also reduce the redundancy of the text summary by imposing an additional restriction to ensure no two sentences in the dominating set relate to each other. This would form what is called an independent dominating set in the graph.

Early problems in the research on dominating sets were related to determining the domination number; the cardinality of the smallest dominating set. For a graph G, the domination number of G is denoted $\gamma(G)$. In 1968, Vizing [87] posed one of the longest standing conjectures regarding the domination number of the Cartesian product of graphs. Vizing's conjecture posits that for two graphs G and H that

$$\gamma(G \square H) \geq \gamma(G)\gamma(H),$$

where $G\Box H$ denotes the Cartesian product of G and H. Vizing's conjecture has been shown to hold if G and H have special properties. Some of these properties include: one of G or H is a has domination number 1 or 2, one of G or H is a path or cycle, both of G and H are chordal. In 2000 Clark and Suen [39] showed for any two graphs G and H that $\gamma(G\Box H) \geq \frac{\gamma(G)\gamma(H)}{2}$. To date this is the best known bound for graphs without any special properties. See [83] for a survey of results regarding Vizing's conjecture.

Another salient open problem regards the domination number of maximal planar graphs. A graph is considered *planar* if it can be drawn in two dimensions without two edges crossing. Furthermore a graph is *maximally* planar if the addition of any edge makes the resultant graph no longer planar. In 1996, Matheson and Tarjan [71] proved any maximal planar graph of order n has a dominating number at most $\frac{n}{3}$. In the same paper, Matheson and Tarjan conjectured that every sufficiently large maximal planar graph of order n has a dominating number at most $\frac{n}{4}$. In 2010, King and Pelsmajer [57] proved this conjecture for graphs of maximum degree at most 6. More recently in 2020, Špacapan [82] improved the upper bound to $\frac{17n}{53}$ for all graphs of order $n > 6$.

Rather than studying the cardinality of the smallest dominating set, one can consider counting the number of dominating sets of each cardinality. One generating polynomial which encodes the number of dominating sets of each cardinality is the domination polynomial. The domination polynomial was introduced independently by Arocha and Llano in 2000 [21] and in 2008 by Alikhani and Peng [13]. In the past decade the domination polynomial has been well-studied. A natural area of interest is computing the domination polynomial [8, 9, 13, 14, 17, 21, 67]. Another area of interest is identifying which non-isomorphic graphs have the same domination polynomial [1,3,4,7,11,16,20,62]. Analytical properties of the domination polynomial such as the location of the roots of domination polynomials have also been researched [2, 5, 37, 73].

This thesis discusses four problems related to the domination polynomial. In Chapter 2, we discuss optimizing the domination polynomial. We consider a graph G optimal if the domination polynomial of G evaluated at x is greater than or equal to the domination polynomial of H evaluated at x for all $x \geq 0$ and all graphs H in a particular class of graphs. We investigate optimal graphs in all of the classes of graphs which have a fixed number of edges and vertices. We consider each class of graphs over the domain $[0, \infty)$ and completely classify when an optimal graph exists. In Chapter 3 we discuss the average cardinality of the dominating sets in a graph. Most graphs have many different dominating sets of varying cardinalities. The average cardinality of the dominating sets in a graph is simply the sum of all the cardinalities of all dominating set divided by the total number of dominating sets. For a graph G, the average cardinality of the dominating sets in G can be determined by the logarithmic derivative of the domination polynomial of G evaluated at 1. For a graph G with n vertices, we will show that the average cardinality of a dominating set in G is at least $\frac{n}{2}$. If G has no isolated vertices then we show that the average cardinality of a dominating set is at most $\frac{3n}{4}$ but conjecture a tighter upper bound of $\frac{2n}{3}$. If the minimum degree of G is at least $2\ln_2(n)$ we show that the average cardinality of a dominating set is at most $\frac{n+1}{2}$. In Chapter 4 we present certain families for which the domination polynomial is unimodal. A polynomial $f(x) = a_0 + a_1x + \cdots + a_nx^n$ is considered unimodal if its sequence of coefficients is non-decreasing and then non-increasing. That is, $f(x)$ is unimodal if there exists a k such that

$$a_0 \leq \cdots \leq a_{k-1} \leq a_k \geq a_{k-1} \geq \cdots \geq a_n.$$

In this case we would say k is a mode of $f(x)$. Note by this definition, $f(x)$ may have multiple modes and still be unimodal. This definition is also similar to the notion of unimodality in statistics for discrete distributions. Alikani and Peng [17] conjectured that all domination polynomials are unimodal. We provide significant evidence by showing that the domination polynomials of almost all graphs are unimodal. In Chapter 5, we investigate the real roots of domination polynomials. Brown and Tufts [37] showed that the collection of all roots of all domination polynomials are dense in the complex plane. Despite this, one can observe that no domination polynomial has a real root in the interval $(0, \infty)$. We will show that there are no other zero-free intervals on the real line by showing the real roots of the domination polynomial are dense on the interval $(-\infty, 0]$. Finally in Chapter 6 we conclude with some discussion and open problems.

1.2 Graph Theory Definitions

The reader is directed to West's textbook [89] for standard graph theory definitions. In this thesis we will be considering only simple and undirected graphs (although multiple edges do not affect domination). We remark that in the context of dominating sets the assumption for the graph to be simple is not needed. However, only considering simple graphs will streamline our discussions. A graph $G = (V, E)$ is a set of vertices $V(G)$ together with an edge set $E(G)$ of unordered pairs of vertices. The cardinality of the vertex set $V(G)$ and edge set $E(G)$ is referred to as the *order* and *size* of G. Two vertices $u, v \in V(G)$ are said to be *adjacent* if there exists an edge $e \in E(G)$ with $e = \{u, v\}$. In such a case u and v are *incident* with e (e is incident with u and v). It is common for edge $\{u, v\}$ to be denoted uv. The *degree* of vertex $v \in V(G)$ is the number of edges incident with v, which is the same as the number of vertices adjacent to v. We denote the degree of v as $\deg(v)$. The maximum and minimum degree of any vertex in G are denoted $\Delta(G)$ and $\delta(G)$, respectively. If $\Delta(G) = \delta(G) = k$ we say the graph is *$k-$regular*. A graph is *connected* if there is a path between every pair of vertices in its vertex set and *disconnected* otherwise. Two graphs G and H are isomorphic if there is a bijection $f : V(G) \to V(H)$ such that u and v are adjacent if and only if $f(u)$ and $f(v)$ are adjacent. In this thesis we do not distinguish between two isomorphic graphs.

The set of vertices $N_G(v) = \{u : uv \in E(G)\}$ is called the *open neighbourhood* of v. Similarly $N_G[v] = N(v) \bigcup \{v\}$ is called the *closed neighbourhood* of v. It is common for the subscript G to be omitted from the notation when only referring to one graph. For $S \subseteq V(G)$, the closed neighbourhood $N[S]$ of S is simply the union of the closed neighbourhoods for each vertex in S. For vertices $u, v \in V(G)$, if v has degree 1 and $N(v) = \{u\}$ then we refer to v as a *leaf* vertex and u as a *stem* vertex. If $\deg(v) = 0$ then v is called *isolated*. If $\deg(v) = n - 1$ then v is called *universal*.

The *complement* of a graph G, denoted $\bar{G}$, has the same vertex set as G but $E(\bar{G}) = \{uv : u \neq v \text{ and } uv \notin E(G)\}$. There are many common families of graphs, here we define the families used in this thesis.

- The *complete* graph of order n, denoted K_n, is the graph on n vertices where every pair of vertices is adjacent.

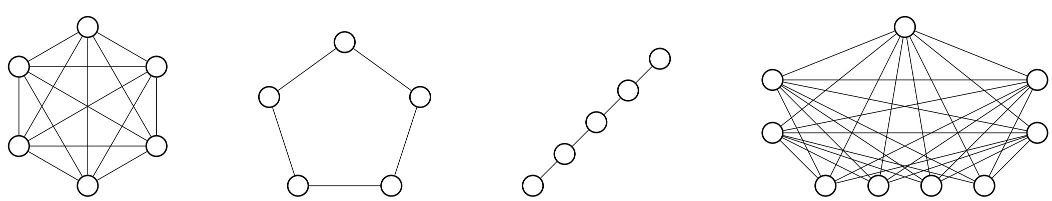
- The *empty* graph of order n, denoted $\overline{K_n}$, is the complement of K_n. That is, no two vertices of the empty graph are adjacent.

- The *cycle* graph of order n, denoted C_n, has the vertex set $V(C_n) = \{v_1, \ldots, v_n\}$ and edge set $E(C_n) = \{v_i v_{i+1} : 1 \leq i \leq n-1\} \cup \{v_1 v_n\}$.

- The *path* graph of order n, denoted P_n, has the vertex set $V(P_n) = \{v_1, \ldots, v_n\}$ and edge set $E(P_n) = \{v_i v_{i+1} : 1 \leq i \leq n-1\}$. Equivalently, a P_n can be obtained by removing any edge from C_n.

- A *complete multipartite* graph, denoted $K_{n_1,n_2,\ldots,n_k}$, has the vertex set $\{v_{i,j} : 1 \leq i \leq k, 1 \leq j \leq n_k\}$ where $v_{i,j}$ and $v_{k,\ell}$ are adjacent if and only if $i \neq k$. Equivalently the vertices of the k-partite graph $K_{n_1,n_2,\ldots,n_k}$ are partitioned into to k sets of size $n_1, n_2, ..., n_k$ respectively and edges are added between each pair of vertices except pairs of vertices in the same set. A complete multipartite graph with two sets is called *complete bipartite*. A *star* graph, denoted $K_{1,n}$, is a special case of a complete bipartite graph where one of the subsets of the partition has exactly one vertex.

Examples of some of the graphs listed above are shown in Figure 1.2.



(a) K_6 (b) C_5 (c) P_5 (d) $K_{1,2,2,4}$

Figure 1.1: Examples of common families of graphs

It is common to form a new graph from two (or more) other graphs. This process is typically referred to as a graph product. We will now define several graph products which will be used in this thesis. In each case we consider two disjoint graphs G and H.

- The *disjoint union* of G and H, denoted $G \cup H$, has vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. The disjoint union of k copies of the graph G is denoted kG. If G is the disjoint union of connected graphs $G_1 \cup G_2 \cdots \cup G_k$ we call each G_i subgraph a *component* of G. Note that a connected graph only has one component.

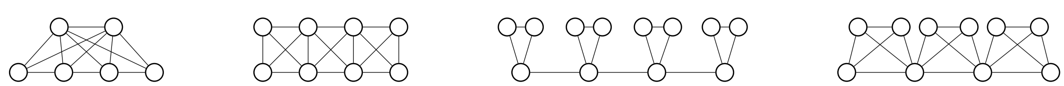
- The *join* of G and H is denoted $G \vee H$, with vertex set $V(G) \cup V(H)$, and edge set $E(G \vee H) = E(G) \bigcup E(H) \cup \{uv : u \in V(G), v \in V(H)\}$.

- The *lexicographic* product (or graph substitution) is defined as follows. Let G and H be graphs. The graph $G[H]$, formed by substituting a copy of H for every vertex of G, is constructed by taking a disjoint copy H_v of H, for each vertex v of G, and joining every vertex in H_u to every vertex in H_v if and only if u is adjacent to v in G. For example, the complete bipartite graph $K_{n,n}$ is the same as $K_2[\overline{K}_n]$.

- The *corona* of two disjoint graphs G and H, as defined by Frucht and Harary in [47] and denoted $G \circ H$, is one copy of G and $|V(G)|$ copies of H where each vertex v of G is joined to every vertex in a unique copy H_v of H.

- The *edge corona* of two disjoint graphs G and H is denoted $G \diamond H$. Hou and Shiu [59] defined $G \diamond H$ as the graph obtained by taking G and $|E(G)|$ copies of H and joining the two end vertices of the i^{th} edge of G to every vertex in the i^{th} copy of H. Note in the case where G has no edges, $G \diamond H \cong G$.

Examples of some of the operations listed above are shown in Figure 1.2.



(a) $P_4 \vee K_2$ (b) $P_4[K_2]$ (c) $P_4 \circ K_2$ (d) $P_4 \diamond K_2$

Figure 1.2: Examples of graph products

For a graph G, $S \subseteq V(G)$ is a *dominating set* of G if the closed neighbourhood of S, $N[S]$, is the entire vertex set, $V(G)$. That is to say, if S is a dominating set, then for each $v \in V(G)$, either $v \in S$ or there exists $u \in S$ which is adjacent to v. The *domination number* of G, denoted $\gamma(G)$, is the cardinality of the smallest dominating set of G. A dominating set with cardinality $\gamma(G)$ is called a *minimum dominating set*.

For example, consider the graph G in Figure 1.3, and a subset of its vertices, $S = \{v_1, v_2, v_5, v_7\}$. As $v_1, v_2, v_5, v_7 \in S$ and $v_3, v_4, v_6 \in N[v_7]$, S is a dominating set. Alternatively, $N[v_1] = \{v_1, v_2, v_3\}$, $N[v_2] = \{v_1, v_2, v_4, v_7\}$, $N[v_5] = \{v_4, v_5, v_6\}$, $N[v_7] = \{v_2, v_3, v_4, v_6\}$. So $N[S] = N[v_1] \cup N[v_2] \cup N[v_5] \cup N[v_7] = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\} = V(G)$. S is not a minimum dominating set as $\{v_2, v_6\}$ is also a dominating set. The domination number of G is 2 as we have a dominating set of cardinality 2 and there is no vertex in G which is adjacent to all other vertices, and hence G has no dominating set of cardinality 1.

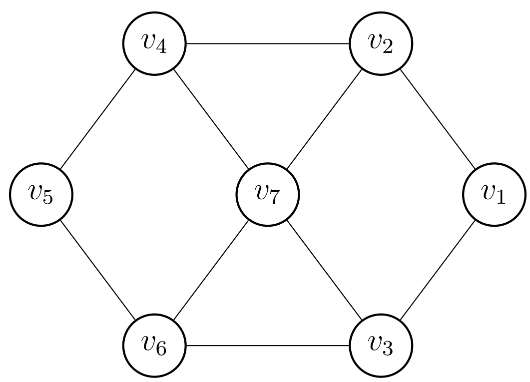


Figure 1.3: A graph on seven vertices

1.3 The Domination Polynomial

In general, graph polynomials have been of interest since 1912 when Birkhoff first defined the chromatic polynomial [25]. The chromatic polynomial, $P(G, \lambda)$ is a function which counts, for each positive integer λ, the number of ways to assign λ colours to each vertex such that adjacent vertices receive different colours. Birkhoff defined the chromatic polynomial in an attempt to prove the *Four Colour Conjecture*, which claimed that any planar graph could be coloured with four colours. Using Birkhoff's definition, proving the Four Colour Conjecture was equivalent to proving that no planar graph has a chromatic polynomial with a root at $\lambda = 4$. Although this approach was unsuccessful, study of the chromatic polynomial became interesting in its own right. Areas of interest for the chromatic polynomial include computing the chromatic polynomial for graphs, locating the roots of chromatic polynomial, finding non-isomorphic graphs with the same chromatic polynomial, and optimizing the chromatic polynomial. See [43] for a text on the chromatic polynomial.

Another graph theory problem, *all-terminal reliability*, also involves graph polynomials. All-terminal reliability was introduced to model robustness of a network. The model has vertices which are always operational but has edges which are operational independently with probability $p \in [0, 1]$. The all-terminal reliability model asks for the probability the operational edges form a spanning connected subgraph. The function which gives this probability, $Rel(G, p)$, is in fact a single variable polynomial. See [40] for an early book on all-terminal reliability.

Though the previous two polynomials are defined by their output, many graph polynomials have been introduced as generating functions. One such polynomial is the *independence polynomial*, $I(G, x)$. For a graph G, an *independent set* is a subset of vertices $S \subseteq V(G)$ such that no two vertices in V are adjacent. The coefficients of the independence polynomial enumerate the number of independent sets of each cardinality. That is, for a graph G, the coefficient of x^k in $I(G, x)$ is the number of independent sets of cardinality k. Gutman and Harary [49] were the first to investigate the independence polynomial in 1983 and it has been well studied ever since. See [70] for a survey on the results regarding the independence polynomial.

Although independent sets and dominating sets are both well studied areas of graph theory, an analogous polynomial for dominating sets was only introduced 17 years after the independence polynomial. The domination polynomial was introduced independently by Arocha and Llano in 2000 [21] and in 2008 by Alikhani and Peng [13]. We will now define the domination polynomial, which algebraically encodes the number of dominating sets of each cardinality.

Definition 1.3.1 *The domination polynomial $D(G, x)$ of G is defined as*

$$D(G, x) = \sum_{i=\gamma(G)}^{|V(G)|} d_i(G) x^i$$

where $\gamma(G)$ is the domination number of G and $d_i(G)$ is the number of dominating sets of G with cardinality i.

Consider every subset of vertices for the path of length three shown in Figure 1.4. The empty set is not dominating so $d_0(P_3) = 0$. For subsets of size one: $\{v_2\}$ is dominating but $\{v_1\}$ and $\{v_3\}$ are not, so $d_1(P_3) = 1$. For subsets of size two: $\{v_1, v_2\}$, $\{v_2, v_3\}$ and $\{v_1, v_3\}$ are all dominating hence $d_2(P_3) = 3$. The only subset of size three is the set of all vertices and hence dominating thus $d_3(P_3) = 1$. We conclude that $D(P_3, x) = x^3 + 3x^2 + x$.

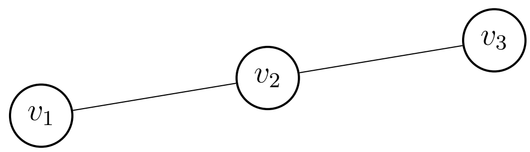


Figure 1.4: A path on three vertices

The exhaustive approach of checking if each subset of vertices is dominating is clearly not efficient. Unfortunately, in general, there seems to be no alternative that is significantly better. However, the domination polynomial is known explicitly for some families of graphs. Furthermore, we can deduce some coefficients based on particular properties of the graphs. For example see Lemma 2.2.6 and Lemma 2.2.7 which together show that the minimum degree of the graph is encoded by the domination polynomial.

Consider once more the graph G in Figure 1.3. The order of G is 7, so manually checking each of its $2^7 = 128$ subsets of vertices would be rather time consuming. However $\delta(G) = 2$, so for each vertex in G the size of its closed neighbourhood is at least three. If a subset omits fewer than three vertices of $V(G)$, it must intersect the closed neighbourhood of each vertex in $V(G)$ and hence dominate G. Thus $d_7(G) = \binom{7}{0} = 1$, $d_6(G) = \binom{7}{1} = 7$, and $d_5(G) = \binom{7}{2} = 21$. For a subset of size four there are only two vertices v_1 and v_5 with closed neighbourhoods of size three. As those two neighbourhoods do not contain the same vertices, the only subsets of cardinality four which do not dominate G are missing exactly the closed neighbourhoods of those two vertices. Thus $d_4(G) = \binom{7}{3} - 2 = 33$. For a subset of size three, we will again count the number of subsets which are not dominating sets. As we are omitting four vertices then any vertex which is not dominated must have degree two or three. For the vertices of degree two; v_5 and v_6, there are four subsets of cardinality three which omit the closed neighbours of v_5 and v_6 respectively (for a total of eight). For each of the vertices of degree three; v_2, v_3, v_4 and v_6, there is exactly one subset of cardinality three which omits their closed neighbours respectively (for a total of four). Hence $d_3(G) = \binom{7}{4} - 4 - 2 \cdot 4 = 23$. As stated earlier $\gamma(G) = 2$, so $d_0(G) = d_1(G) = 0$. It is easy enough to see that the only dominating sets of size 2 are $\{v_2, v_6\}$ and $\{v_3, v_4\}$ so $d_2(G) = 2$ and $D(G, x) = x^7 + 7x^6 + 21x^5 + 33x^4 + 23x^3 + 2x^2$.

Simple combinatorial arguments can be used to calculate the domination polynomial for some families of graphs. For example, any non-empty subset of vertices of the complete graph K_n is a dominating set. Therefore, $d_0 = 0$ and $d_k(K_n) = \binom{n}{k}$ for $1 \leq k \leq n$. Using the binomial theorem we can easily obtain that $D(K_n, x) = (x + 1)^n - 1$. For another example consider the star graph $K_{1,n}$. Any subset of vertices which contains the only universal vertex of $K_{1,n}$ is dominating. Such dominating subsets are enumerated by the generating polynomial $x(x + 1)^n$. Alternatively, if a subset of vertices does not contain the universal vertex, then every other vertex must be in the subset in order to dominate $K_{1,n}$. Therefore $D(K_{1,n}, x) = x(x + 1)^n + x^n$.

Naturally when computing graph polynomials of product graphs we seek relationships with the graph polynomials of the smaller factor graphs. The domination polynomial is no different. Relationships for the disjoint union, join, lexicographic product, and corona of graphs are detailed in the next theorem.

Theorem 1.3.2 ([17, 37, 67]) *Let G and H be disjoint graphs on n_G and n_H vertices respectively.*

(i) $D(G \cup H, x) = D(G, x) \cdot D(H, x)$.

(ii) $D(G \vee H, x) = [(x + 1)^{n_G} - 1][(x + 1)^{n_H} - 1] + D(G, x) + D(H, x)$.

(iii) $D(G \circ H, x) = [D(K_1 \vee H, x)]^{n_G} = [x(x + 1)^{n_H} + D(H, x)]^{n_G}$.

(iv) $D(G[K_n], x) = D(G, (x + 1)^n - 1)$.

Interest in the domination polynomial since its introduction has focused on problems related to

- computing the domination polynomial [8, 9, 13, 14, 17, 21, 67]

- properties of the coefficient sequence [10, 15]
- properties of the roots of domination polynomial [2, 5, 37, 73]
- determining non-isomorphic graphs with equivalent domination polynomials [1, 3, 4, 7, 11, 16, 20, 62]

In this thesis we will discuss problems which are new in the context of the domination polynomial. However, each has been investigated for various other graph polynomials and graph parameters.

One problem we will discuss is the optimality of domination polynomials. For two graph G and H, G is said to (weakly) *improve* H if $D(G,x) \geq D(H,x)$ for all $x \geq 0$. Optimality has been studied for other graph polynomials such as independence polynomials [36] on the domain $[0,\infty)$, network reliability [22, 27, 28, 35, 48, 72] over the domain $[0,1]$, and chromatic polynomials over the natural numbers [77, 80].

Another problem we will discuss is the average order of dominating sets in a graph G, denoted $\text{avd}(G)$. For a graph G, $\text{avd}(G)$ can be determined by $\frac{D'(G,1)}{D(G,1)}$. Many other average graph parameters have been considered such as mean distance [44], mean subtree order [63], the average size of an independent set [78], the average size of a matching [19].

We will also consider the unimodality of domination polynomials. The domination polynomial of a graph G of order n is considered unimodal if for some $0 \leq k \leq n$ we have

$$d_0(G) \leq \cdots \leq d_{k-1}(G) \leq d_k(G) \geq d_{k-1}(G) \geq \cdots \geq d_n(G).$$

The unimodality of domination polynomials has been discussed in previous work (see [10, 17]). However that body of work pales in comparison to the work done on other graph polynomials. Typically other graph polynomials have been shown to be unimodal by showing a stronger condition. A graph polynomial $f(G,x) = \sum_{i=1}^{n} a_i x^i$ of a graph G of order n is *log-concave* if for every $1 \leq i \leq n-1$, $a_i(G)^2 \geq a_{i-1}(G)a_{i+1}(G)$. If a polynomial with all positive coefficients is log-concave then it is unimodal. All matching polynomials have been shown to be log-concave [54, 68]. The chromatic polynomial has also been shown to be log-concave [60]. In general, independence polynomials are not log-concave or even unimodal. However, the independence polynomials of claw-free graphs have been shown to be log-concave [38, 50].

This thesis is structured as follows. In Chapter 2 we will study the optimality of domination polynomials. In Chapter 3 we determine the extremal graphs for the average order of dominating sets of graphs of order n. We develop bounds for the average order of domination sets for connected graphs, as well as for trees. We also introduce a normalized version of the parameter, describe the distribution of these parameters, and consider the values for Erdös-Renyi random graphs. In Chapter 4 we extend the families for which unimodality of the domination polynomial is known to paths, cycles and complete multipartite graphs. More significantly, we will also show that almost all domination polynomials are unimodal with mode $\lceil \frac{n}{2} \rceil$. In Chapter 5 we prove that the closure of the real domination roots is the entire nonpositive real axis. Finally in Chapter 6 we conclude with some discussion and open problems.

Chapter 2

Optimal Domination Polynomials

2.1 Background

Consider a graph G with vertex set $V(G)$ and edge set $E(G)$ (we assume throughout that all graphs are *simple*, that is, without loops and multiple edges, as neither of these affect domination). Let S be a subset of vertices or edges such that S has a particular graph property, P. Perhaps P is that S is independent, complete, a dominating set or a matching. The sequences of the number of sets of varying cardinality that have property P have been studied, particularly through the associated generating polynomials (which are *graph polynomials*). Independence, clique, domination and matching polynomials have all arisen and been studied in this setting.

If the number of vertices n and edges m are fixed, one can ask whether there exist *optimal* graphs with respect to a property. In this chapter we will discuss optimal graphs with respect to domination. Let $\mathcal{S}_{n,m}$ denote the set of (simple) graphs of order n and size m (that is, with n vertices and m edges). Before we determine if an optimal graph exists we must define what it means for a graph to be optimal. We say $G \in \mathcal{S}_{n,m}$ is (n,m)*-optimal* (with respect to domination) if $D(G,x) \geq D(H,x)$ for all graphs $H \in \mathcal{S}_{n,m}$ and *all* $x \geq 0$ (for any particular value of $x \geq 0$, of course, there is such a graph G, as the number of graphs of order n and size m is finite, but we are interested in *uniformly* optimal graphs). For two graphs G and H, we define the reflexive and transitive relation $H \preceq G$ if $D(H,x) \leq D(G,x)$ for all $x \geq 0$. Additionally we say G (weakly) *improves* H if $H \preceq G$. If G *improves* H but for some x we have $D(H,x) < D(G,x)$ then we say G *strongly* improves H.

Now that we have defined a (n,m)-optimal graph, you may be wondering why use this definition? In the case of domination polynomials, $D(G,1)$ yields the total number of dominating sets in G. A natural notion of optimality may be to determine a graph $G \in \mathcal{S}_{n,m}$ which maximizes $D(G,1)$. However, our definition is a stronger notion of optimality. The evaluation $D(G,x)$ at various values of x does not always yield meaningful results. However, for two graphs G and H, if $D(G,x) \geq D(H,x)$ for values of x which approach infinity then G has more *large* dominating sets than H. Conversely, if $D(G,x) \geq D(H,x)$ for positive values of x which approach 0 then G has more *small* dominating sets than H. Of course, if there is a graph G such that the counts for dominating sets are each greater than or equal to that for any other graph of the same order n and size m, that graph will be (n,m)-optimal. However, our definition of an (n,m)-optimal graph is slightly more general than simply maximizing the coefficients of the domination polynomial.

Optimality, in this sense, has been studied for independence polynomials. Brown and Cox [36] showed that an (n,m)-optimal graph always exists. A (n,m)-optimal graph is formed by fixing a linear order $\preceq$ of the vertices, $v_1 \preceq v_2 \preceq \cdots \preceq v_n$ and select the m largest edges in lexicographic order.

Optimality of network reliability (over the domain $[0,1]$) has also be well-studied [22,27,28,35,48,66,72]. Network reliability distinguishes between the family of simple graphs with n vertices and m edges, $\mathcal{S}_{n,m}$, and the family of all graphs with n vertices and m edges $\mathcal{G}_{n,m}$. In the context of dominating sets, we only consider all graphs as simple because additional edges between a pair of adjacent vertices does change how a graph is dominated. However, in the context of network reliability multiple edges between a pair of vertices can dramatically increase the reliability of the network. For example, let G be a simple graph where the probability of each edge being operational is independent and identically $p \in [0,1]$. Let G_k be the graph G where each of its edges replaced with k identical edges. In this case, the reliability of G_k is similar to the reliability of G. In fact, $Rel(G_k,p) = Rel(G, 1-(1-p)^k)$ as the probability that at least one of k edges in a bundle is operational is $1-(1-p)^k$. In network reliability, a graph $H \in \mathcal{G}_{n,m}$ ($H \in \mathcal{S}_{n,m}$) is $\mathcal{G}_{n,m}$-optimal ($\mathcal{S}_{n,m}$-optimal) if $Rel(H,p) \geq Rel(G,p)$ for all graphs $G \in \mathcal{G}_{n,m}$ ($G \in \mathcal{S}_{n,m}$) and all $p \in [0,1]$. It was once conjectured that given m and n, there always exists a $\mathcal{G}_{n,m}$-optimal graph and an $\mathcal{S}_{n,m}$-optimal graph. For simple graphs it was shown that the conjecture held for $m \leq n+3$ [27] and $m \geq \binom{n}{2} - \lfloor \frac{n}{2} \rfloor$ [66]. Despite this, the conjecture for simple graphs was shown to be false [66, 72] for $m = \binom{n}{2} - \frac{n+2}{2}$ for even $n \geq 6$ and $m = \binom{n}{2} - \frac{n+5}{2}$ for odd $n > 7$. Brown and Cox [35] gave several more values of m where an $\mathcal{S}_{n,m}$-optimal graph does not exists. Brown and Cox also gave values of n and m where $\mathcal{G}_{n,m}$-optimal graphs do not exist. It remains an open question to characterize the values of n and m where $\mathcal{G}_{n,m}$-optimal graphs (or $\mathcal{S}_{n,m}$-optimal graphs) exist.

Optimality of chromatic polynomials has also been discussed [69, 77, 80] but with a modified notion of optimality. Simonelli [80] defined a graph $G \in \mathcal{S}_{n,m}$ as optimal if there does not exist another graph $H \in \mathcal{S}_{n,m}$ with $P(G,\lambda) \leq P(H,\lambda)$ for all natural numbers λ and $P(G,\lambda) < P(H,\lambda)$ for at least one λ. For this definition of optimality, a necessary condition for a graph $G \in \mathcal{S}_{n,m}$ to be optimal is that there exists a λ such that $P(G,\lambda) > P(H,\lambda)$ for all $H \in \mathcal{S}_{n,m}$. Lazebnik [69] determined the graphs which maximize $P(G,2)$ for each $\mathcal{S}_{n,m}$. Additionally Simonelli [80] determined necessary conditions for bipartite graphs to be optimal.

In this chapter we will study the optimality of domination polynomials. We will completely characterize the values of n and m for which (n,m)-optimal graphs exist.

2.2 Optimality for Domination Polynomials

We begin our study by observing (n,m)-optimal graphs of small order. Table 2.1 gives all (n,m)-optimal graphs up to order 3.

Order n	Size m	(n,m)-optimal graph
1	0	K_1
2	0	$\overline{K_2}$
2	1	K_2
3	0	$\overline{K_3}$
3	1	$K_1 \cup K_2$
3	2	$K_{1,2}$
3	3	K_3

Table 2.1: The (n,m)-optimal graphs up to order 3

Upon first inspection it may appear that an (n,m)-optimal graph always exists. However, there is only one simple graph in $\mathcal{S}_{n,m}$ for $n \leq 3$ and is hence (n,m)-optimal. Table 2.2 gives all (n,m)-optimal graphs of order 4 were we can see no $(4,3)$-optimal graph exists. A dash $-$ represents when an (n,m)-optimal graph does not exist for a given order and size.

Order n	Size m	(n, m)-optimal graph
4	0	$\overline{K_4}$
4	1	$\overline{K_2} \cup K_2$
4	2	$K_2 \cup K_2$
4	3	$-$
4	4	$-$
4	5	$K_4 - e$
4	6	K_4

Table 2.2: The (n, m)-optimal graphs of order 4

For $n = 4$ consider the cases when $m = 2$ and $m = 3$. For $m = 2$, note that $K_2 \cup K_2$ and $K_{1,2} \cup K_1$ are the only simple graphs in $G_{4,3}$. Furthermore, we have

$$D(K_2 \cup K_2, x) = x^4 + 4x^3 + 4x^2$$
$$D(K_{1,2} \cup K_1, x) = x^4 + 3x^3 + x^2$$

Each coefficient of $D(K_2 \cup K_2, x)$ is greater than or equal to each corresponding coefficient of $D(K_{1,2} \cup K_1, x)$. Therefore we can conclude that $D(K_2 \cup K_2, x) \geq D(K_{1,2} \cup K_1, x)$ for all $x \geq 0$ and hence $K_2 \cup K_2$ is $(4, 2)$-optimal.

For $n = 4$ and $m = 3$, note that P_4, $K_{1,3}$, and $K_3 \cup K_1$ are the only simple graphs in $G_{4,3}$. Furthermore, we have

$$D(P_4, x) = x^4 + 4x^3 + 4x^2$$
$$D(K_{1,3}, x) = x^4 + 4x^3 + 3x^2 + x$$
$$D(K_3 \cup K_1, x) = x^4 + 3x^3 + 3x^2$$

Each coefficient of $D(K_3 \cup K_1, x)$ is less than or equal to each corresponding coefficient of both $D(P_4, x)$ and $D(K_{1,3}, x)$. Therefore we can conclude that $D(K_3 \cup K_1, x) \leq D(P_4, x)$ and $D(K_3 \cup K_1, x) \leq D(K_{1,3}, x)$ for all $x \geq 0$. Now let $f(x) = D(P_4, x) - D(K_{1,3}, x) = x^2 - x$. Note that $f(x) > 0$ for $x > 1$ and $f(x) < 0$ for $0 < x < 1$. Therefore $D(P_4, x) > D(K_{1,3}, x) \geq D(K_3 \cup K_1, x)$ for $x > 1$ and $D(K_{1,3}, x) > D(P_4, x) \geq D(K_3 \cup K_1, x)$ for $0 < x < 1$ and hence no $(4, 3)$-optimal graphs exist.

The following useful observation compares the coefficients of the domination polynomials of two graphs to determine which domination polynomial is larger when evaluated at sufficiently large and small values of x.

Observation 2.2.1 *Suppose that G and H are graphs with*

$$D(G,x) = \sum_{j=1}^{|V(G)|} d_j(G)x^j,$$

and

$$D(H,x) = \sum_{j=1}^{|V(H)|} d_j(H)x^j.$$

Then

- *if $d_j(G) = d_j(H)$ for $j < \ell$ but $d_\ell(G) > d_\ell(H)$, then $D(G,x) > D(H,x)$ for x sufficiently small positive values of x and*
- *if $d_j(G) = d_j(H)$ for $j > t$ but $d_t(G) > d_t(H)$, then $D(G,x) > D(H,x)$ for x sufficiently large.*

The reason why this observation holds is the following. If $p(x) = a_l x^l + a_{l+1}x^{l+1} + \cdots + a_{l+k}x^{l+k}$ is a real polynomial with a_l and a_{l+k} nonzero, then by writing

$$\begin{aligned} p(x) &= x^l\left(a_l + a_{l+1}x + \cdots + a_{l+k-1}x^{k-1} + a_{l+k}x^k\right) \\ &= x^{l+k}\left(a_{l+k} + \frac{a_{l+k-1}}{x} + \cdots + \frac{a_l}{x^k}\right) \end{aligned}$$

we see that for small positive values of x, the sign of $p(x)$ is the same as the sign of a_l, and for large positive values of x, the sign of $p(x)$ is the same as the sign of a_{l+k} (we then apply this to the polynomial $D(G,x) - D(H,x)$ with $t = l + k$).

It follows from Observation 2.2.1 that if for two graphs G and H we have $d_j(G) \geq d_j(H)$ for all j then G improves H. In this case we call G *coefficient-wise greater* than H. This leads us to a sufficient condition to determine if an (n,m)-optimal graph exists. If for some graph $G \in \mathcal{S}_{n,m}$ we have that G is coefficient-wise greater than all $H \in \mathcal{S}_{n,m}$ then G is (n,m)-optimal. This was the case observed previously when $n = 4$ and $m = 2$.

For general polynomials, $f(x)$ and $g(x)$, we can have $f(x) \geq g(x)$ for all $x \geq 0$ without having $f(x)$ being coefficient-wise greater than g. For example, $5x^2+x+5 \geq x^2+4x+1$ for all $x \geq 0$. Despite this there are no known examples of two graphs G and H where G improves H without also being coefficient-wise greater than H.

Our first result will be regarding the existence of optimal sparse graphs. The following lemma describes an operation that always increases the domination polynomial on $[0, \infty)$.

Lemma 2.2.2 *Let G be a graph on $n \geq 3$ vertices with at least one isolated vertex x and at least one edge $e = uv$. Let H be the graph $(G - e) \cup ux$. Then*

$$D(H, x) \geq D(G, x) \text{ for } x \geq 0.$$

Moreover, if v has degree at least 2, then

$$D(H, x) > D(G, x) \text{ for } x > 0.$$

Proof. We begin by showing that there is an injection from the set of dominating sets of size i in G into the set of dominating sets of size i in H.

Let S_i be a dominating set of size i of G. Note that since x is an isolated vertex, it appears in every dominating set of G.

- Case 1: If both u and v are in S_i then S_i dominates in H.
- Case 2: If $u \in S_i$, $v \notin S_i$ then $(S_i - x) \cup \{v\}$ is a dominating set of size i in H which does not dominate in G.
- Case 3: If $u \notin S_i$, $v \in S_i$ then S_i dominates in H as $x \in S_i$ and $u \in N[x]$.
- Case 4: If neither u nor v are an element of S_i both u and v must be dominated in $G - e$, and therefore S_i a dominating set of H as well.

Thus, every dominating set of size i of G corresponds to a dominating set of H of size i. Moreover, it is not hard to verify that the dominating sets of H produced are different. Hence $d_i(H) \geq d_i(G)$ for $i \geq 1$ and so $D(H, x) \geq D(G, x)$ for $x \geq 0$ as was to be shown.

Moreover, if v has degree at least 2, it has another vertex $w \neq u$ adjacent to it. Consider the set $S = V(G) - \{v, x\}$. Then S is not a dominating set of G (as it does not contain x) but it is a dominating set in H. Moreover, S is not a result of any of the cases above, and hence the mapping above is not onto. It follows that $d_{n-2}(H) > d_{n-2}(G)$, and so $D(H, x) > D(G, x)$ for $x > 0$. □

We will now apply this lemma to show the following.

Corollary 2.2.3 *Let G be a graph on $n \geq 3$ vertices and $m \geq \lceil \frac{n}{2} \rceil$ edges. If G has an isolated vertex, then there exists a graph H of the same order and size with no isolated vertices such that $D(H, x) > D(G, x)$ for $x > 0$.*

Proof. Let G' be the graph with no isolated vertices such that $G = G' \cup rK_1$ where $r \geq 1$ is the number of isolated vertices in G. Then G' has $n - r$ vertices and $m \geq \lceil \frac{n}{2} \rceil$ edges. We will now show $\Delta(G') \geq 2$. Suppose not – that is, suppose $\Delta(G') < 2$. Then $\Delta(G') = \delta(G') = 1$ and G' must be the graph mK_2. However, then G' has $2m \geq n > n - r$ edges which is a contradiction as $r \geq 1$. Thus there indeed exists a vertex $v \in G'$ with degree two or more.

Let $u \in N(v)$ and H be the graph constructed in Lemma 2.2.2 by removing the edge uv from G and adding an edge from u to an isolated vertex. By Lemma 2.2.2, $D(H, x) > D(G, x)$ for $x > 0$ and H has one less isolated vertex. Hence by iterating this process we will find a graph with no isolated vertices which improves G. □

Using the previous result, we can now prove that optimal sparse graphs exist. Two non-isomorphic graphs can have the same domination polynomial, thus it is possible for two graphs from $\mathcal{S}_{n,m}$ to both be (n, m)-optimal. If $G \in \mathcal{S}_{n,m}$ is the only (n, m)-optimal graph in $\mathcal{S}_{n,m}$ we call it the *unique (n, m)-optimal* graph.

Corollary 2.2.4 *For a given $n \geq 2$ and $m = \lceil \frac{n}{2} \rceil$, the unique (n, m)-optimal graph is mK_2 if n is even and $(m - 2)K_2 \cup K_{1,2}$ if n is odd.*

Proof. Let G be a graph on n vertices and $m = \lceil \frac{n}{2} \rceil$ edges. By Corollary 2.2.3, if G has an isolated vertex, there exists a graph H with n vertices, m edges, and no isolated vertices which improves G. Depending on parity of n, as $m = \lceil \frac{n}{2} \rceil$ there is only one graph with no isolated vertices: mK_2 if n is even and $(m-2)K_2 \cup K_{1,2}$ if n is odd. Hence these graphs must be the unique (n,m)-optimal graphs in their class $\mathcal{S}_{n,m}$. $\square$

Theorem 2.2.5 *Let $n \geq 2$ and $m < \lceil \frac{n}{2} \rceil$. Then the unique (n,m)-optimal graph is $mK_2 \cup rK_1$ where $r = n - 2m$.*

Proof. Any such graph G with n vertices and $m < \lceil \frac{n}{2} \rceil$ must have at least one isolated vertex. Moreover, by Lemma 2.2.2, if G has a vertex of degree at least 2 then G can be strongly improved by a graph with one less isolated vertex. It follows that there is a unique (n,m)-optimal graph which is the one with no vertices of degree at least 2, namely $mK_2 \cup rK_1$ where $r = n - 2m$. $\square$

The previous results show that if $m \leq \lceil \frac{n}{2} \rceil$, a unique (n,m)-optimal graph exists. To contrast, we will now show that in general optimal graphs need not exist. To do so, we will need the following lemmas regarding the minimum degree of G.

Lemma 2.2.6 ([3]) *Let G be a graph of order n then*

$$d_{n-j}(G) = \binom{n}{j} \text{ for all } j \leq \delta(G)$$

Lemma 2.2.7 *Let G be a graph with n vertices. Then*

$$d_{n-\delta(G)-1}(G) = \binom{n}{\delta(G)+1} - |\{N[v] : \deg(v) = \delta(G)\}|.$$

Proof. For any k it is clear that $\binom{n}{k} - d_k(G)$ counts the number of subsets of V which do not dominate G. Therefore by Lemma 2.2.6 we have that $\binom{n}{\delta(G)+1} - d_{n-\delta(G)-1}(G)$ counts the largest subsets of V which do not dominate G. A subset $S \subseteq V$ is a dominating set if and only if for every vertex $v \in V$, $N[v] \cap S \neq \emptyset$. Therefore the maximum non-dominating subsets of V are of the form $\{V - N[v] : \deg(v) = \delta(G)\}$. As $|\{V - N[v] : \deg(v) = \delta(G)\}| = |\{N[v] : \deg(v) = \delta(G)\}|$ we get our result. $\square$

For a graph G let M_G be the collection of all minimum closed neighbours in G. That is,

$$M_G = \{N_G[v] : \deg_G(v) = \delta(G)\}.$$

Note that if two minimum degree vertices u and v in G have the same closed neighbourhood in G then their closed neighbours $N[u]$ and $N[v]$ would be the same element in M_G.

Lemma 2.2.8 *Let G and H be two graphs on n vertices.*
Then

(*i*) *If $\delta(G) > \delta(H)$ then $D(G, x) > D(H, x)$ for sufficiently large values of x.*

(*ii*) *If $\delta(G) = \delta(H)$ and $|M_G| < |M_H|$ then $D(G, x) > D(H, x)$ for sufficiently large values of x.*

Proof. To show (i), suppose $\delta(G) > \delta(H)$. Then by Lemma 2.2.6 and Lemma 2.2.7 we have that $d_{n-j}(G) = d_{n-j}(H)$ for $j \leq \delta(G)$ but $d_{n-\delta(G)-1}(G) = \binom{n}{\delta(G)+1} > d_{n-\delta(G)-1}(H)$. Therefore by Observation 2.2.1 $D(G', x) > D(G, x)$ for sufficiently large values of x.

To show (ii), suppose $\delta(G) = \delta(H)$ and $|M_G| < |M_H|$. It again follows from Lemma 2.2.6, Lemma 2.2.7 and Observation 2.2.1 that $D(G', x) > D(G, x)$ for sufficiently large values of x. $\square$

Theorem 2.2.9 *Let $\lceil \frac{n}{2} \rceil < m \leq n - 1$. Then for $n \geq 4$ an (n, m)-optimal graph does not exist.*

Proof. To reach a contradiction suppose there exists an (n, m)-optimal graph G with n vertices with $n - r$ edges where $1 \leq r < \lfloor \frac{n}{2} \rfloor$. Consider the domination number of G. By Observation 2.2.1, there is no graph with the same order and size of G but of smaller domination number. This holds because if H had a smaller domination number than G then $d_i(G) = 0$ for $i < \gamma(H)$, $d_{\gamma(H)}(G) = 0$ while $d_{\gamma(H)}(H) > 0$, which by Observation 2.2.1 implies that G is not (n, m)-optimal for small positive values of x, a contradiction.

Let $H = (r - 1)K_2 \cup K_{1,n-2r+1}$. As H has n vertices, $n - r$ edges and $\gamma(H) = r$, it follows that $\gamma(G) \leq r$. Furthermore $\gamma(G)$ is bounded below by the number of components in G. As G has n vertices and $n-r$ edges, G has at least r components. Therefore $\gamma(G) \geq r$, and so $\gamma(G) = r$. It follows that G must be a disjoint union of r graphs, each with a universal vertex. As G has $n-r$ edges, G must be a forest consisting of r star graphs.

As $\gamma(G) = r$ then $d_i(G) = 0$ for $i < r$. Therefore it follows from Observation 2.2.1 that $d_r(G) \geq d_r(F)$ for every graph F with the same order and size as G. Recall $H = (r-1)K_2 \cup K_{1,n-2r+1}$ and note that $d_r(H) = 2^{r-1}$. Thus $d_r(G) \geq 2^{r-1}$. Now $d_r(G)$ is the number of minimum dominating sets in G, and thus is equal to the product of the number of minimum dominating sets for each of its r components. However the only star graph with more than one minimum dominating set is K_2, which has two. Now $m > \lceil \frac{n}{2} \rceil$ implies $G \ncong rK_2$, so G has at most $(r-1)$ K_2 components. It follows that $d_r(G) \leq 2^{r-1}$. So $d_r(G) = 2^{r-1}$ and $G \cong H = (r-1)K_2 \cup K_{1,n-2r+1}$ as the last component must also be a star. Furthermore as $m = n - r$ and $m > \lceil \frac{n}{2} \rceil$ then $n - r \geq \frac{n}{2} + 1$ which implies $n - 2r + 1 \geq 3$.

We will now show that a star graph $K_{1,k}$ is not $(k+1,k)$-optimal for $k \geq 3$. This will imply that any G which has a star component $K_{1,n-2r+1}$ with $n-2r+1 \geq 3$, cannot be (n,m)-optimal. Consider P_{k+1}. By Lemma 2.2.7, $d_{k-1}(P_{k+1}) = \binom{k+1}{2} - 2$, while $d_{k-1}(K_{1,k}) = \binom{k+1}{2} - k$, and hence $d_{k-1}(P_k) > d_{k-1}(K_{1,k-1})$ for $k \geq 3$. Thus by Observation 2.2.1, a star graph $K_{1,k}$ is not $(k+1,k)$-optimal for $k \geq 3$. Thus there cannot exist an (n,m)-optimal graph for $\lceil \frac{n}{2} \rceil < m \leq n-1$. □

Now, we will show that (n,m)-optimal graphs do not exist for most values of $m \geq n-1$. We require the following lemma

Lemma 2.2.10 ([17]) *Let G be a graph of order n. Then*

$$d_1(G) = |\{v \in V(G) : deg(v) = n-1\}|.$$

Before we begin our next lemma, recall from Theorem 1.3.2 (*ii*) that for a graph G on n vertices

$$D(K_r \vee G, x) = ((x+1)^r - 1)(x+1)^n + D(G,x).$$

Lemma 2.2.11 *If a graph G of order n and size $m \geq n-1$ is (n,m)-optimal, then G is of the form $K_r \vee H$, the join of K_r and H, where $1 \leq r \leq n$ and H is optimal on $n-r$ vertices and at most $m_H = n-r-2$ edges.*

Proof. Suppose G is (n,m)-optimal. By Observation 2.2.1, G must both minimize $\gamma(G)$ and maximize $d_{\gamma(G)}(G)$. As $m \geq n-1$ then there exists a graph in $\mathcal{S}_{n,m}$ with domination number 1 and hence $\gamma(G)=1$. By Lemma 2.2.10 to maximize $d_1(G)$ we need to maximize the number of degree $n-1$ vertices. Let r be the maximum number of degree $n-1$ vertices G could have with m edges and n vertices. That is,

$$r = \max\left(k : m \geq \binom{k}{2} + k(n-k)\right).$$

As $m \geq n-1$ it follows that $1 \leq r$. Moreover we have $r \leq n$ and $G = K_r \vee H$ where H has $n-r$ vertices. Furthermore, H does not have enough edges to form a degree $n-r-1$ vertex, otherwise such a vertex would have degree $n-1$ in G contradicting that r is the maximum number of degree $n-1$ vertices G could have with m edges and n vertices. Thus, H has at most $n-r-2$ edges.

Finally we show H is $(n-r, m_H)$-optimal where $m_H \leq n-r-2$ edges. Let H' be any another graph of equal order and size to H. As G is (n,m)-optimal, $D(G,x) = D(K_r \vee H, x) \geq D(K_r \vee H', x)$ for all $x \geq 0$. By Theorem 1.3.2 (ii),

$$\begin{aligned} D(K_r \vee H, x) &= ((x+1)^r - 1)(x+1)^{n-r} + D(H,x) \\ D(K_r \vee H', x) &= ((x+1)^r - 1)(x+1)^{n-r} + D(H',x) \end{aligned}$$

Thus $D(H,x) \geq D(H',x)$ for all $x \geq 0$ and H is optimal. □

Theorem 2.2.12 *For $n \geq 6$ vertices and $n-1 \leq m < \binom{n}{2} - 6$ there does not exist an (n,m)-optimal graph for the domination polynomial.*

Proof. To show a contradiction suppose a graph G is (n,m)-optimal. By Lemma 2.2.11, G is the join of K_r and H for some $r \geq 0$ and optimal graph H with $n-r$ vertices and at most $n-r-2$ edges. Let m_H be the number of edges in H; then $m = m_H + \binom{r}{2} + r(n-r) \geq \binom{r}{2} + r(n-r)$. It follows from the bounds $n-1 \leq m < \binom{n}{2} - 6$ and $m \geq \binom{r}{2} + r(n-r)$ that $1 \leq r < n-4$ and hence $|H| = n-r > 4$. We will show G is not (n,m)-optimal by using Lemma 2.2.8 to eliminate the following three cases: $m_H < \lceil \frac{n-r}{2} \rceil$, $m_H = \lceil \frac{n-r}{2} \rceil$, and $m_H > \lceil \frac{n-r}{2} \rceil$.

Case 1: $m_H < \lceil \frac{n-r}{2} \rceil$.

In this case, H is an $(n-r, m_H)$-optimal graph on $n-r$ vertices and less than $\lceil \frac{n-r}{2} \rceil$ edges. Using Theorem 2.2.5, H must be the following $(n-r, m_H)$-optimal graph

$$H = m_H K_2 \cup (n - r - 2m_H)K_1.$$

Note that $n - r - 2m_H > 0$, so $\delta(G) = r$. Furthermore no two vertices of degree r are adjacent. Therefore

$$|M_G| = |\{v \in V(G) : \deg_G(v) = r\}| = n - r - 2m_H.$$

Recall that $1 \leq r < n-4$ and $|H| = n-r > 4$. Let u be a vertex of minimum degree in G, v be any other vertex in H, and x be a universal vertex in G. Further, let G' be the graph formed by replacing the edge vx in G with the edge uv. The graphs G and G' have the same size, order and $\delta(G') \geq \delta(G)$. As G is (n, m)-optimal then it follows from Lemma 2.2.8 (i) that $\delta(G') = \delta(G)$, otherwise $D(G', x) > D(G, x)$ for sufficiently large x. Note that every vertex in G', other than x and u, has the same degree as they did in G. Furthermore $\deg_{G'}(x) = n-2 > r$ and $\deg_{G'}(u) = \deg_G(u)+1 = r+1$. Therefore

$$|M_{G'}| = |\{v \in V(G') : \deg_{G'}(v) = r\}| = n - r - 2m_H - 1,$$

and hence $|M_G| > |M_{G'}|$. It follows from Lemma 2.2.8 (ii) that $D(G', x) > D(G, x)$ for sufficiently large x which contradicts G being an (n, m)-optimal graph.

Case 2: $m_H = \lceil \frac{n-r}{2} \rceil$.

In this case H has $n-r$ vertices and is $(n-r, m_H)$-optimal. By Corollary 2.2.4, $H = m_H K_2$ is uniquely $(n-r, m_H)$-optimal if $n-r$ is even and $H = (m_H-2)K_2 \cup K_{1,2}$ is uniquely $(n-r, m_H)$-optimal if $n-r$ is odd. Also $\delta(G) = r+1$, regardless of parity.

Case 2a: $n-r$ is even.

Recall $n-r > 4$ so $n-r \geq 6$. Without loss of generality let $G = K_r \vee H$ where $H = m_H K_2$ with $m_H \geq 3$. Note that the vertices of degree $r+1$ are exactly the vertices of H and each degree $r+1$ vertex in H shares its closed neighbourhood with its only neighbour in H. Therefore $|M_G| = m_H$.

Let u_1, u_2, v_1, v_2 and x be vertices in G such that x is a universal vertex in G and u_1, u_2 and v_1, v_2 each induce K_2 components in H. Note $N_G[u_1] = N_G[u_2] \in M_G$ and $N_G[v_1] = N_G[v_2] \in M_G$. Let G' be the graph formed by replacing the edges xu_1, xu_2, xv_1 and xv_2 with v_1u_1, v_1u_2, v_2u_1 and v_2u_2. Note the degree of u_1, u_2, v_1 and v_2 have all increased from G to G', whereas $\deg_{G'}(x) = \deg_G(x) - 4 = n - 5 \geq r + 1$. Furthermore the closed neighbourhood of every other vertex is unchanged and thus $\delta(G') = \delta(G) = r + 1$. Moreover, the closed neighbourhoods $N_G[u_1] = N_G[u_2]$ and $N_G[u_1] = N_G[u_2]$ are in $M_G - M_{G'}$ whereas the only closed neighbourhood possibly in $M_{G'} - M_G$ is $N_{G'}[x]$. Therefore $|M_G| > |M_{G'}|$. It follows from Lemma 2.2.8 (*ii*) that $D(G', x) > D(G, x)$ for sufficiently large x which contradicts G being an (n, m)-optimal graph.

Case 2b: $n - r$ is odd.

Then $n - r \geq 5$ and without loss of generality let $G = K_r \vee H$ where $H = (m_H - 2)K_2 \cup K_{1,2}$ with $m_H - 2 \geq 1$. Let u_1, u_2, v and x be vertices in G such that x is a universal vertex in G, $\{u_1, u_2\}$ induces a K_2 component in H and v is a leaf in the $K_{1,2}$ component of H. Note $N_G[u_1] = N_G[u_2] \in M_G$ and $N_G[v] \in M_G$. Let G' be the graph formed by replacing the edges xu_1 and xu_2 with vu_1, vu_2. The degrees of u_1 and u_2 remain $r+1$ while $\deg_{G'}(x) = \deg_G(x) - 2 = n - 3 > r + 1$ and $\deg_{G'}(v) = \deg_G(v) + 2 = r + 3$. The closed neighbourhood of every other vertex is unchanged and therefore $\delta(G') = \delta(G) = r + 1$. Furthermore $N_{G'}[u_1] = N_{G'}[u_2] \in M_{G'}$ and $N_{G'}[v] \notin M_{G'}$. As the closed neighbourhood of every other vertex is unchanged, $|M_G| > |M_{G'}|$. It follows from Lemma 2.2.8 (*ii*) that $D(G', x) > D(G, x)$ for sufficiently large x which contradicts G being an (n, m)-optimal graph.

Case 3: $m_H > \lceil \frac{n-r}{2} \rceil$.

By Lemma 2.2.11, H is an $(n - r, m_H)$-optimal graph on $n - r$ vertices and $m_H > \lceil \frac{n-r}{2} \rceil$ edges, where $m_H \leq n - r - 2 < n - r - 1$. As in case 1, $n - r \geq 5$. By Theorem 2.2.9, there is no $(n - r, m_H)$-optimal graph on $n - r$ vertices and $n - r - 1 > m_H > \lceil \frac{n-r}{2} \rceil$ edges. Thus this case is a contradiction. □

Clearly for $m = \binom{n}{2}$ and $m = \binom{n}{2} - 1$, unique (n, m)-optimal graphs exist, since there is only one graph in each case, but we now show that (n, m)-optimal graphs do not exist for the remaining values for m.

Theorem 2.2.13 *Let $n \geq 6$ and $m = \binom{n}{2} - k$ for $2 \leq k \leq 6$. Then an (n, m)-optimal graph does not exist.*

Proof. By Observation 2.2.1 and Lemma 2.2.10 we know that an (n, m)-optimal graph must have the highest number of universal vertices. Additionally, by Observation 2.2.1, Lemma 2.2.6, and Lemma 2.2.7 we know that an (n, m)-optimal graph must have the maximum minimum degree amongst all graphs in $\mathcal{S}_{n,m}$. For each $k = 2, 3, 4, 5, 6$ we will show any graph $G \in \mathcal{S}_{n,m}$ which maximizes the number of universal vertices will not maximize the minimum degree.

- For $k = 2$ there are two graphs with two edges removed. Let G and H be the graph K_n with the edges of a P_3 and $2K_2$ removed respectively. G has $n - 3$ universal vertices and minimum degree $n - 3$ whereas H has $n - 4$ universal vertices and minimum degree $n - 2$. Thus no (n, m)-optimal graph exists when $k = 2$.

- For $k = 3$ any graph in $\mathcal{S}_{n,m}$ has at most $n - 3$ universal vertices and this is uniquely achieved by the graph K_n with the edges of a K_3 removed. This graph has $n - 3$ universal vertices and minimum degree $n - 3$. However, the graph K_n with the edges of a $3K_2$ removed has minimum degree $n - 2$. Thus no (n, m)-optimal graph exists when $k = 3$.

- For $k = 4$ any graph in $\mathcal{S}_{n,m}$ has at most $n - 4$ universal vertices which is achieved by two graphs in $\mathcal{S}_{n,m}$. These two graph are K_n with the edges of a C_4 and $K_1 \vee (K_2 \cup K_1)$, removed respectively. Of those two graphs the graph K_n with the edges of a C_4 removed has the larger minimum degree of $n - 3$. Hence the graph K_n with the edges of a C_4, which we will call G, must be (n, m)-optimal should one exists. However, for $n \geq 8$, the graph K_n with the edges of a $4K_2$ removed has minimum degree $n - 2$ and thus no (n, m)-optimal graph exists. For $n = 6, 7$ and $k = 4$ we were able to verify via Maple that the graph K_n with the edges of a $2P_3$ removed is not improved by G and thus no (n, m)-optimal graph exists.

- For $k = 5$ any graph in $\mathcal{S}_{n,m}$ has at most $n-4$ universal vertices which is uniquely achieved by the graph K_n with the edges of a $K_2 \vee 2K_1$ removed. This graph has $n-4$ universal vertices and minimum degree $n-4$. However, the graph K_n with the edges of a $P_3 \cup K_3$ removed has minimum degree $n-3$. Thus no (n,m)-optimal graph exists when $k = 5$.

- Lastly, for $k = 6$ any graph in $\mathcal{S}_{n,m}$ has at most $n-4$ universal vertices, and this is uniquely achieved by the graph K_n with the edges of a K_4 removed. This graph has $n-4$ universal vertices and minimum degree $n-4$. However, the graph K_n with the edges of a $2K_3$ removed has minimum degree $n-3$. Thus no (n,m)-optimal graph exists when $k = 6$.

Therefore by the above arguments our assertion is true for each $2 \leq k \leq 6$. □

Corollary 2.2.14 *For graphs of order $n \geq 6$,*

- *$mK_2 \cup rK_1$ (where $r = n - 2m$) is (n,m)-uniquely optimal when $m < \lceil \frac{n}{2} \rceil$.*
- *mK_2 is uniquely (n,m)-optimal when n is even and $m = \lceil \frac{n}{2} \rceil$.*
- *$(m-2)K_2 \cup K_{1,2}$ is uniquely (n,m)-optimal when n is odd and $m = \lceil \frac{n}{2} \rceil$.*
- *No (n,m)-optimal graph exists for $\lceil \frac{n}{2} \rceil < m < \binom{n}{2} - 1$.*
- *$K_n - e$ is uniquely (n,m)-optimal for $m = \binom{n}{2} - 1$, for $e \in E(G)$.*
- *K_n is uniquely (n,m)-optimal for $m = \binom{n}{2}$.* □

In fact, via some calculations in Maple, Corollary 2.2.14 can been seen to hold for $n < 6$ as well, with the exception of $K_1 \vee 2K_2$ which is the unique (n,m)-optimal graph on five vertices and six edges. Appendix A gives all (n,m)-optimal graphs up to order 7.

In [42] the domination reliability polynomial was defined as follows. For a given graph G we assume that vertices are independently operational with probability $p \in [0,1]$; the *domination reliability* $Drel(G,p)$ of G is the probability that the operational vertices form a dominating set of the graph. Note that for a graph G of order n we have

$$Drel(G,p) = \sum_{i=\gamma(G)}^{n} d_i(G)p^i(1-p)^{n-i} = (1-p)^n \sum_{i=\gamma(G)}^{n} d_i(G)\left(\frac{p}{1-p}\right)^i.$$

As for all-terminal reliability, the existence of optimal reliability polynomials is an open area of study. Given that $Drel(G,p) = (1-p)^n \cdot D(G, \frac{p}{1-p})$ then from Corollary 2.2.14 we obtain a complete characterization of values of n and m for which optimal graphs exist for domination reliability.

Corollary 2.2.15 *For $n \in \mathbb{N}$ and $m \leq \lceil \frac{n}{2} \rceil$ uniquely (n,m)-optimal graphs exist for domination reliability. For $\lceil \frac{n}{2} \rceil < m < \binom{n}{2} - 1$ there are no (n,m)-optimal graphs for domination reliability with the exception of when $n = 5$ and $m = 6$ where a uniquely (n,m)-optimal graph exists. For $m = \binom{n}{2} - 1$ and $m = \binom{n}{2}$ uniquely optimal graphs exist for domination reliability.*

We have now completely determined all (n,m)-optimal graphs for both the domination polynomial and domination reliability. Although many (n,m)-optimal graph exists, most values of n and m yield no (n,m)-optimal graph. This greatly contrasts the results found for the independence polynomial where (n,m)-optimal graphs exist for every n and m. The network reliability and chromatic polynomial each have (n,m)-optimal graphs; however, it remains an open question for most values of n and m whether an (n,m)-optimal graph exists. In Chapter 6 we discuss future directions for this problem. In the next chapter we will pivot our focus from the optimality of the domination polynomial to a new parameter which can be determined via the domination polynomial.

Chapter 3

The Average Order of Dominating Sets of a Graph

3.1 Background

In the previous chapter we determined which graphs optimize the domination polynomial. Part of optimizing the domination polynomial was maximizing the domination number $\gamma(G)$. In this chapter we turn our focus to an alternative parameter, *average order of a dominating set*, which can be calculated via the domination polynomial.

Recall that $\mathcal{D}(G)$ denotes the collection of dominating sets of G. Then the average order of dominating sets in G, denoted $\text{avd}(G)$, is

$$\text{avd}(G) = \frac{1}{|\mathcal{D}(G)|} \sum_{S \in \mathcal{D}(G)} |S|,$$

that is, the average cardinality of a dominating set of G.

For graphs with few dominating sets $\text{avd}(G)$ is relatively easy to compute using the above formula. For example, the empty graph $\overline{K_n}$ has exactly one dominating set of order n, hence $\text{avd}(\overline{K_n}) = n$. However, if G has many dominating sets, then other techniques may be more appropriate to compute $\text{avd}(G)$. The average order of dominating sets in G can be computed as the logarithmic derivative of $D(G, x)$ evaluated at 1, that is,

$$\text{avd}(G) = \frac{d}{dx} \ln(D(G, x))\bigg|_{x=1} = \frac{D'(G, 1)}{D(G, 1)}. \tag{1}$$

This allows us to compute $\text{avd}(G)$ quickly when $D(G, x)$ is readily available. For example, recall the following graph from Chapter 1.

The graph in Figure 3.1 has domination polynomial $x^7 + 7x^6 + 21x^5 + 33x^4 + 23x^3 + 2x^2$. Using that domination polynomial, one can easily compute the average order of dominating sets in the graph in Figure 1.3 to be $\frac{359}{87} \approx 4.126$. Moreover as,

$$D(K_n, x) = (x + 1)^n - 1 \quad \text{and} \quad D(K_{1,n-1}, x) = x(x + 1)^{n-1} + x^{n-1},$$

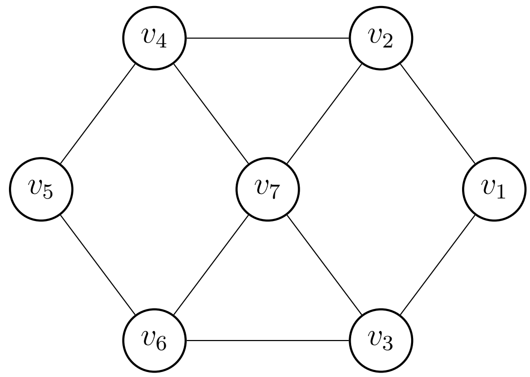


Figure 3.1: A graph on seven vertices

we have that

$$\operatorname{avd}(K_n) = \frac{n2^{n-1}}{2^n - 1} \quad \text{and} \quad \operatorname{avd}(K_{1,n-1}) = \frac{(n+1)2^{n-2} + n - 1}{2^{n-1} + 1}.$$

It follows from Theorem 1.3.2 (*i*) that $D(G \cup H, x) = D(G, x)D(H, x)$. From this we can obtain a fundamental result which states that the average order of dominating sets is additive over components.

Lemma 3.1.1 *Let G and H be graphs. Then* $\operatorname{avd}(G \cup H) = \operatorname{avd}(G) + \operatorname{avd}(H)$*.*

Proof. As $D(G \cup H, x) = D(G, x)D(H, x)$, it follows that $D'(G \cup H, x) = D'(G, x)D(H, x) + D(G, x)D'(H, x)$. Therefore,

$$\begin{aligned}
\operatorname{avd}(G \cup H) &= \frac{D'(G,1)D(H,1) + D(G,1)D'(H,1)}{D(G,1)D(H,1)} \\
&= \frac{D'(G,1)}{D(G,1)} + \frac{D'(H,1)}{D(H,1)} \\
&= \operatorname{avd}(G) + \operatorname{avd}(H),
\end{aligned}$$

which is what we wished to show. □

Although the average order of dominating sets is a novel area of research, there has been work done on several other graph invariants that are calculated as averages:

- The *mean distance* (between vertices) in a graph was introduced in 1977 by Doyle and Graver [44]. Doyle and Graver showed that among all connected graphs of order n (that is, with n vertices), the mean distance is maximized by a path, with mean distance $(n+1)/3$, and minimized by the complete graph, with mean distance 1.

- The *mean subtree order* of a graph was introduced in 1983 by Jamison [63]. Jamison showed for any tree T on n vertices, the average number of vertices in a subtree of T is at least $(n+2)/3$, with that minimum achieved if and only if T is a path. As the mean subtree order of T is at most n, Jamison naturally defined the mean subtree order of T divided by n to be the *density* of T, and showed that there are trees whose density approaches 1 as $n \to \infty$. Jamison conjectured that the tree with maximum density is some caterpillar graph. Additionally, the mean subtree order has been subject to a fair amount of recent work [52, 64, 86, 88]. The average order of a subtree of a tree was recently extended to more general graphs by considering induced connected subgraphs [85].

- The *average size of an independent set* in a graph was introduced in 1985 by Linial and Saks [78]. Linial and Saks proved a lower bound on the average size of an independent set in any bipartite graph. The average size of an independent set also arises in statistical physics, as the occupancy fraction of the hard-core model at fugacity 1. Recently, Andriantiana, Misanantenaina, and Wagner [18] showed that the average number of vertices of an independent set in a graph of order n is maximized by the empty graph and minimized by the complete graph. They also showed that the average number of vertices of an independent set in a tree of order n is maximized by P_n and minimized by $K_{1,n-1}$.

- In 2020, Andriantiana et al. [19] introduced the *average size of a matching* in a graph. Andriantiana et al. showed that the average number of edges in a matching of a graph of order n is minimized by the empty graph and maximized by the complete graph. They also showed that the average number of edges in a matching in a tree of order n is maximized by P_n and minimized by $K_{1,n-1}$.

- In 2004, Henning [55] introduced the *average domination number* of a graph to be the average size, over all vertices, of the smallest dominating set containing each vertex. For a graph G, despite the similar name, the average domination number of G is only tangentially related to the average order of dominating sets of G.

We remark that if the domination polynomial has all real roots, the average order of dominating sets of a graph G can also determine the largest coefficient (i.e. the mode of the coefficients) of $D(G,x)$. The mode of the coefficients will be discussed in more detail in Chapter 4. In general a positive sequence $(a_0, a_1, \cdots, a_n)$ can be expressed as a generating polynomial $f(x) = a_0 + a_1x + \cdots + a_nx^n$. Darroch [41] showed that if $f(x)$ has all real roots, then its mode is at either $\left\lfloor \frac{f'(1)}{f(1)} \right\rfloor$ or $\left\lceil \frac{f'(1)}{f(1)} \right\rceil$. Therefore by (1), if $D(G,x)$ has all real roots then it mode is at $\lfloor \mathrm{avd}(G) \rfloor$ or $\lceil \mathrm{avd}(G) \rceil$. Oboudi [73] showed that there is an infinite family of graphs G such that $D(G,x)$ has all real roots. This family includes, for example, K_2, P_3, $G \circ K_1$ for any graph G, and $G \circ \overline{K_2}$ for any graph G.

This chapter is structured as follows. In Section 3.2, we determine the extremal graphs for the average order of dominating sets of graphs of order n. That is, those that have the largest and smallest average order of a dominating set. In Section 3.3 and Section 3.4, we develop bounds for the average order of dominating sets for connected graphs, as well as for trees. Section 3.5, introduces a normalized version of the parameter $\widehat{\mathrm{avd}}(G)$ by dividing $\mathrm{avd}(G)$ by the order of the graph G. We proceed to describe the distribution of $\widehat{\mathrm{avd}}(G)$ over all graph G of order n, and consider $\widehat{\mathrm{avd}}(G)$ for Erdös-Renyi random graphs.

3.2 Extremal Graphs

For a graph G on n vertices, it is clear that $\mathrm{avd}(G) \leq n$ as every dominating set has cardinality at most n. This bound is achieved by $\overline{K_n}$, and this graph is the unique extremal graph, as every other graph of order n has a dominating set of cardinality smaller than n. On the other hand, what about the *minimum* value of $\mathrm{avd}(G)$ over all graphs G of order n? As one might expect, the complete graph K_n is the unique extremal graph in this case, but the argument will be more involved, and that is what we shall pursue now.

We shall first need some technical results about the average cardinality of sets in collections of sets. Let X be a nonempty finite set and $\mathcal{P}(X)$ its power set. For any nonempty subset $\mathcal{A} \subseteq \mathcal{P}(X)$ we define the average order of $\mathcal{A}$, denoted $\mathrm{av}(\mathcal{A})$ to be

$$\mathrm{av}(\mathcal{A}) = \frac{1}{|\mathcal{A}|} \sum_{A \in \mathcal{A}} |A|.$$

For simplicity, we denote $\sum_{A \in \mathcal{A}} |A|$ by $S(\mathcal{A})$. Therefore $\mathrm{av}(\mathcal{A}) = \frac{S(\mathcal{A})}{|\mathcal{A}|}$.

Lemma 3.2.1 *For a nonempty finite set X, let $\mathcal{A} \subseteq \mathcal{P}(X)$. If there exists $r_1, r_2 \in \mathbb{R}$ and a partition $\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_k$ of $\mathcal{A}$ such that $r_1 \leq \mathrm{av}(\mathcal{A}_i) \leq r_2$ for all $1 \leq i \leq k$, then $r_1 \leq \mathrm{av}(\mathcal{A}) \leq r_2$.*

Proof. Now

$$\mathrm{av}(\mathcal{A}) = \frac{S(\mathcal{A})}{|\mathcal{A}|} = \frac{\sum_{i=1}^{k} S(\mathcal{A}_i)}{|\mathcal{A}|} = \frac{\sum_{i=1}^{k} |\mathcal{A}_i| \mathrm{av}(\mathcal{A}_i)}{|\mathcal{A}|} \geq \frac{\sum_{i=1}^{k} |\mathcal{A}_i| r_1}{|\mathcal{A}|} = \frac{r_1 \sum_{i=1}^{k} |\mathcal{A}_i|}{|\mathcal{A}|} = r_1$$

and

$$\mathrm{av}(\mathcal{A}) = \frac{S(\mathcal{A})}{|\mathcal{A}|} = \frac{\sum_{i=1}^{k} S(\mathcal{A}_i)}{|\mathcal{A}|} = \frac{\sum_{i=1}^{k} |\mathcal{A}_i| \mathrm{av}(\mathcal{A}_i)}{|\mathcal{A}|} \leq \frac{\sum_{i=1}^{k} |\mathcal{A}_i| r_2}{|\mathcal{A}|} = \frac{r_2 \sum_{i=1}^{k} |\mathcal{A}_i|}{|\mathcal{A}|} = r_2,$$

which is what we wished to show. □

Lemma 3.2.2 *For a nonempty finite set X, let $\mathcal{A} \subset \mathcal{B} \subseteq \mathcal{P}(X)$. Then*

$$\mathrm{av}(\mathcal{B}) \leq \mathrm{av}(\mathcal{A}) \quad \textit{if and only if} \quad \mathrm{av}(\mathcal{B} - \mathcal{A}) \leq \mathrm{av}(\mathcal{A}).$$

Proof. Now

$$\begin{aligned}
& \mathrm{av}(\mathcal{B}) \leq \mathrm{av}(\mathcal{A}) \\
\Leftrightarrow \quad & \frac{S(\mathcal{B})}{|\mathcal{B}|} \leq \frac{S(\mathcal{A})}{|\mathcal{A}|} \\
\Leftrightarrow \quad & \frac{S(\mathcal{A}) + S(\mathcal{B} - \mathcal{A})}{|\mathcal{A}| + |\mathcal{B} - \mathcal{A}|} \leq \frac{S(\mathcal{A})}{|\mathcal{A}|} \\
\Leftrightarrow \quad & S(\mathcal{A})|\mathcal{A}| + S(\mathcal{B} - \mathcal{A})|\mathcal{A}| \leq S(\mathcal{A})|\mathcal{A}| + S(\mathcal{A})|\mathcal{B} - \mathcal{A}| \\
\Leftrightarrow \quad & S(\mathcal{B} - \mathcal{A})|\mathcal{A}| \leq S(\mathcal{A})|\mathcal{B} - \mathcal{A}| \\
\Leftrightarrow \quad & \frac{S(\mathcal{B} - \mathcal{A})}{|\mathcal{B} - \mathcal{A}|} \leq \frac{S(\mathcal{A})}{|\mathcal{A}|}
\end{aligned}$$

$$\Leftrightarrow \qquad \mathrm{av}(\mathcal{B}-\mathcal{A}) \leq \mathrm{av}(\mathcal{A}),$$

which is what we wished to show. □

A *simplicial complex* $\mathcal{A}$ is a subset of $\mathcal{P}(X)$ such that $\emptyset \in \mathcal{A}$ and $A \in \mathcal{A}$ implies $\mathcal{P}(A) \subseteq \mathcal{A}$. Simplicial complexes have numerous applications in combinatorics and algebraic topology (See [33] for various applications). Here we will need a result on the average size of a set in a simplicial complex.

Proposition 3.2.3 *Let $\mathcal{A}$ be a simplicial complex on a nonempty finite set X with n elements. Then for all $k \leq \frac{n}{2}$, we have*

$$|\mathcal{A}_k| \geq |\mathcal{A}_{n-k}|,$$

where $\mathcal{A}_k = \{A \in \mathcal{A} : |A| = k\}$. Hence $\mathrm{av}(\mathcal{A}) \leq \frac{n}{2}$.

Proof. Consider the bipartite graph with bipartition $(\mathcal{A}_{n-k}, \mathcal{A}_k)$ where $A \in \mathcal{A}_{n-k}$ and $B \in \mathcal{A}_k$ are adjacent if and only if $B \subseteq A$. As $\mathcal{A}$ is a simplicial complex, the degree of each $A \in \mathcal{A}_{n-k}$ is $\binom{n-k}{k}$ and the degree of each vertex $B \in \mathcal{A}_k$ is at most $\binom{n-k}{n-2k} = \binom{n-k}{k}$. Therefore there are exactly $|\mathcal{A}_{n-k}|\binom{n-k}{k}$ edges incident with the vertices of $\mathcal{A}_{n-k}$ and at most $|N(\mathcal{A}_{n-k})|\binom{n-k}{k}$ edges incident to the vertices of $N(\mathcal{A}_{n-k})$. As the number of edges incident to the vertices of $\mathcal{A}_{n-k}$ must equal the number of edges incident to the vertices of $N(\mathcal{A}_{n-k})$, $|\mathcal{A}_{n-k}|\binom{n-k}{k} \leq |N(\mathcal{A}_{n-k})|\binom{n-k}{k}$. Therefore $|\mathcal{A}_{n-k}| \leq |N(\mathcal{A}_{n-k})| \leq |\mathcal{A}_k|$.

Now let $\mathcal{B}_k = \mathcal{A}_{n-k} \cup \mathcal{A}_k$. Note that $\mathrm{av}(\mathcal{B}_k) \leq \frac{n}{2}$ and $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_{\lfloor \frac{n}{2} \rfloor}$ is a partition of $\mathcal{A}$. It follows from Lemma 3.2.1 that $\mathrm{av}(\mathcal{A}) \leq \frac{n}{2}$. □

Finally, recall Lemma 2.2.6 which states for a graph G of order n,

$$d_{n-k}(G) = \binom{n}{k}$$

for all $k \leq \delta(G)$, where $\delta(G)$ is the minimum degree of G.

Theorem 3.2.4 *Let G be a graph of order n. Then* $\mathrm{avd}(G) \geq \frac{n2^{n-1}}{2^n-1}$ *with equality if and only if $G \cong K_n$.*

Proof. Let $\overline{\mathcal{D}(G)}$ be the collection of subsets $S \subseteq V(G)$ such that $V(G) - S$ is a dominating set of G. Note $\overline{\mathcal{D}(G)}$ is a simplicial complex. Therefore by Proposition 3.2.3 for all $k \leq \frac{n}{2}$,

$$d_{n-k} = |\{S \in \overline{\mathcal{D}(G)} : |S| = k\}| \geq |\{S \in \overline{\mathcal{D}(G)} : |S| = n-k\}| = d_k.$$

Now consider the mean order of all dominating sets except for the dominating set $V(G)$. Let $\mathcal{D}^*(G) = \mathcal{D}(G) - \{V(G)\}$. Note that

$$\operatorname{av}(\mathcal{D}^*(G)) = \frac{D'(G,1) - n}{D(G,1) - 1}.$$

As $d_{n-k} \geq d_k$ for all $k \leq \frac{n}{2}$ it follows that

$$\frac{D'(G,1) - n}{D(G,1) - 1} = \operatorname{av}(\mathcal{D}^*(G)) \geq \frac{n}{2}.$$

Now suppose $G \ncong K_n$. Note that $D(G,1) < 2^n - 1$ as G must have at least one non-universal vertex, and hence at least two subsets which are not dominating. Then

$$\begin{aligned}
\operatorname{avd}(G) &= \frac{n + D'(G,1) - n}{D(G,1)} \\
&= \frac{n}{D(G,1)} + \left(\frac{D(G,1) - 1}{D(G,1) - 1}\right)\frac{D'(G,1) - n}{D(G,1)} \\
&= \frac{n}{D(G,1)} + \left(\frac{D(G,1) - 1}{D(G,1)}\right)\frac{D'(G,1) - n}{D(G,1) - 1} \\
&\geq \left(\frac{1}{D(G,1)}\right)n + \left(\frac{D(G,1) - 1}{D(G,1)}\right)\frac{n}{2}.
\end{aligned}$$

Now we have a convex combination of n and $\frac{n}{2}$. As $D(G,1) < 2^n - 1$ we can shift the weight in the convex combination closer to the smaller quantity $\frac{n}{2}$.

$$\begin{aligned}
\operatorname{avd}(G) &> \left(\frac{1}{2^n - 1}\right)n + \left(\frac{2^n - 2}{2^n - 1}\right)\frac{n}{2} \\
&= \frac{n}{2^n - 1} + \frac{n(2^{n-1} - 1)}{2^n - 1} \\
&= \frac{n2^{n-1}}{2^n - 1} = \operatorname{avd}(K_n).
\end{aligned}$$

Therefore if $G \ncong K_n$ then $\operatorname{avd}(G) > \operatorname{avd}(K_n)$. Clearly if $G \cong K_n$ then $\operatorname{avd}(G) = \operatorname{avd}(K_n)$. Therefore $\operatorname{avd}(G) = \operatorname{avd}(K_n)$ if and only if $G \cong K_n$. $\square$

3.3 Upper bounds based on minimum degree

For a graph G on n vertices, we have seen that $\operatorname{avd}(G) \leq n$, with the bound achieved uniquely by $\overline{K_n}$. However, can we say more if we insist on the graph being connected? Or even just having no isolated vertices? We shall do so first in terms of δ, the minimum degree.

For a dominating set S of a graph G, let

$$a(S) = \{v \in S : S - v \notin \mathcal{D}(G)\},$$

the set of *critical* vertices of S with respect to domination (in that their removal makes the set no longer dominating). This parameter is key to improving the upper bound. We will first need an expression for the sum of $|a(S)|$ over all dominating sets. Before we begin we will partition $\mathcal{D}(G)$. Let $\mathcal{D}_{+v}(G)$ denote the collection of dominating sets which contain v. Moreover $\mathcal{D}_{-v}(G)$ denote the collection of dominating sets which do not contain v. That is:

$$\mathcal{D}_{+v}(G) = \{S \in \mathcal{D}(G) : v \in S\}$$
$$\mathcal{D}_{-v}(G) = \{S \in \mathcal{D}(G) : v \notin S\}.$$

Lemma 3.3.1 *Let G be a graph of order n. Then*

$$\sum_{S \in \mathcal{D}(G)} |a(S)| = 2D'(G,1) - nD(G,1).$$

Proof. For a vertex $v \in V(G)$ let $a_v(G) = \{S \in \mathcal{D}(G) : S - v \notin \mathcal{D}(G)\}$. We will now show that there is a one-to-one correspondence between $\mathcal{D}_{+v}(G) - a_v(G)$ and $\mathcal{D}_{-v}(G)$. For any $S \in \mathcal{D}_{+v}(G) - a_v(G)$, we have $S - v \in \mathcal{D}(G)$ so clearly $S - v \in \mathcal{D}_{-v}(G)$. Furthermore, if $S \in \mathcal{D}_{-v}(G)$, then $S \cup \{v\} \in \mathcal{D}_{+v}(G)$ and $S \cup \{v\} \notin a_v(G)$. As the maps are injective, it follows that $|\mathcal{D}_{+v}(G) - a_v(G)| = |\mathcal{D}_{-v}(G)|$ and as $a_v(G) \subseteq \mathcal{D}_{+v}(G)$, we have $|a_v(G)| = |\mathcal{D}_{+v}(G)| - |\mathcal{D}_{-v}(G)|$.

Now consider $\sum_{v \in V(G)} |\mathcal{D}_{+v}(G)|$. Every dominating set of cardinality i is counted once for every vertex it contains (i.e. i times). Therefore

$$\sum_{v \in V(G)} |\mathcal{D}_{+v}(G)| = \sum_{i=1}^{n} i \cdot d_i(G) = D'(G,1) \tag{2}$$

Now consider $\sum_{v \in V(G)} |\mathcal{D}_{-v}(G)|$. Every dominating set of cardinality i is counted once for every vertex it does not contains (i.e. $n-i$ times). Therefore

$$\sum_{v \in V(G)} |\mathcal{D}_{-v}(G)| = \sum_{i=1}^{n} (n-i) \cdot d_i(G) = nD(G,1) - D'(G,1). \tag{3}$$

Therefore

$$\sum_{S \in \mathcal{D}(G)} |a(S)| = \sum_{v \in V(G)} |a_v(G)| = \sum_{v \in V(G)} (|\mathcal{D}_{+v}(G)| - |\mathcal{D}_{-v}(G)|) = 2D'(G,1) - nD(G,1),$$

which is what we wished to show. □

In order to get to our upper bound, we need to partition $a(S)$. Let S be a dominating set of G containing the vertex v. By definition $v \in a(S)$ if and only if $S - v$ is not a dominating set in G. Therefore $v \in a(S)$ if and only if there exists $u \in N[v]$ such that among the vertices of S, u is only dominated by v (u could very well be v). We will call such a vertex u a *private neighbour* of v with respect to S. Let $\mathrm{Priv}_S(v)$ denote the collection of all private neighbours of v with respect to S, that is,

$$\mathrm{Priv}_S(v) = \{u \in N[v] : N[u] \cap S = \{v\}\}.$$

Note that $v \in a(S)$ if and only if $\mathrm{Priv}_S(v) \neq \emptyset$. Moreover, for $v \in a(S)$, note that $\mathrm{Priv}_S(v) \cap S \subseteq \{v\}$. We now partition $a(S) = a_1(S) \cup a_2(S)$, where

$$a_1(S) = \{v \in a(S) : \mathrm{Priv}_S(v) \cap (V - S) \neq \emptyset\}$$
$$a_2(S) = \{v \in a(S) : \mathrm{Priv}_S(v) = \{v\}\}.$$

(We allow either to be empty.) Note that if $v \in a_2(S)$ then $N(v) \subseteq V - S$. We can partition $V - S = N_1(S) \cup N_2(S)$, where

$$N_1(S) = \{v \in V - S : |N[v] \cap S| = 1\}$$
$$N_2(S) = \{v \in V - S : |N[v] \cap S| \geq 2\}.$$

That is, $N_1(S)$ is the set of those vertices outside of S that have a single neighbour in S, and $N_2(S)$ are those that have more than one neighbour in S. (Again, we allow either to be empty.)

As an example consider the labelled P_5 in Figure 3.2. Let S be the dominating set $S = \{v_2, v_3, v_5\}$. Now $a(S) = \{v_2, v_5\}$ with $a_1(S) = \{v_2\}$ and $a_2(S) = \{v_5\}$. Furthermore $N_1(S) = \{v_1\}$ and $N_2(S) = \{v_4\}$. Alternatively, let $S' = \{v_1, v_3, v_5\}$. Now $a(S') = \{v_1, v_3, v_5\}$ with $a_1(S') = \emptyset$ and $a_2(S') = \{v_1, v_3, v_5\}$. Additionally $N_1(S') = \emptyset$ and $N_2(S') = \{v_2, v_4\}$.

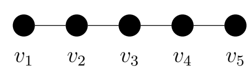


Figure 3.2: A vertex labelled P_5

Lemma 3.3.2 *Let G be a graph. For any $S \in \mathcal{D}(G)$, $|a_1(S)| \leq |N_1(S)|$.*

Proof. For any $v \in N_1(S)$, $N[v] \cap S \in a_1(S)$. By definition, for every $u \in a_1(S)$ we have $\mathrm{Priv}_S(u) \cap (V - S) \neq \emptyset$. Fix any $v \in \mathrm{Priv}_S(u) \cap (V - S)$. Note $v \in N_1(S)$ such that $N[v] \cap S = \{u\}$. Therefore the map $f : N_1(S) \to a_1(S)$ where $f(v) = N[v] \cap S$ is surjective, so $|N_1(S)| \geq |a_1(S)|$. $\square$

For a graph G containing a vertex v, let $p_v(G)$ denote the collection of subsets of $V - N[v]$ which dominate $G - v$ (and hence they dominate $G - N[v]$ as well). Now let $p_v(G, i)$ be the collection all i-subsets of $p_v(G)$. Moreover let $\mathcal{D}_i(G)$ denotes the collection of dominating sets of order i. In the next Lemma we will show there is a bijection from $\sum_{S \in \mathcal{D}_i(G)} |a_2(S)|$ to $\sum_{v \in V(G)} |p_v(G, i-1)|$. This together with the inequality $|a_1(S)| \leq |N_1(S)|$ will allow us to bound $\sum_{S \in \mathcal{D}(G)} |a(S)|$. This will then allow us to use inequality (7) to determine a segment of non-increasing coefficients.

Lemma 3.3.3 *Let G be a graph. Then*

$$\sum_{S \in \mathcal{D}_i(G)} |a_2(S)| = \sum_{v \in V(G)} |p_v(G, i-1)|.$$

Proof. To begin let

$$A_{i,2} = \bigcup_{S \in \mathcal{D}_i(G)} \{(v, S) : v \in a_2(S)\} \quad \text{and} \quad P_{i-1} = \bigcup_{v \in V(G)} \{(v, S) : S \in p_v(G, i-1)\}.$$

Note that $|A_{i,2}| = \sum_{S \in \mathcal{D}_i(G)} |a_2(S)|$ and $|P_{i-1}| = \sum_{v \in V(G)} |p_v(G, i-1)|$. Therefore it suffices to show there is a bijection from $A_{i,2}$ to P_{i-1}. Consider the mapping $f(v, S) = (v, S - v)$. We will first show $f : A_{i,2} \to P_{i-1}$. For any $(v, S) \in A_{i,2}$ as $v \in a_2(S)$ then by definition $S - v \notin \mathcal{D}_{i-1}(G)$ and some vertex in G is not dominated by $S - v$. In order to show $(v, S - v) \in P_{i-1}$ it suffices to show that v is the only vertex not dominated by $S - v$ (and hence $S - v \in p_v(G, i-1)$). As S is a dominating set, then any vertex not dominated by $S - v$ must have been dominated by v and hence is in $N[v]$. As $v \in a_2(S)$ then by definition $N[v] \cap N_1(S) = \emptyset$ and hence every vertex in $V - S$ which was dominated by v is also dominated by some other vertex in S. Therefore the only vertex which could possibly not be dominated by $S - v$ is v itself. Therefore v must be the only vertex not dominated by $S - v$ and $(v, S - v) \in P_{i-1}$.

We now begin showing f is bijective by first showing it is injective. Suppose that there exists $(v, S), (v', S') \in A_{i,2}$ such that $f(v, S) = f(v', S')$. Then $(v, S - v) = (v', S' - v')$ and hence $v = v'$. Furthermore $(S - v) \cup \{v\} = (S' - v') \cup \{v'\}$ and thus $S = S'$. Therefore $(v, S) = (v', S')$ and hence f is injective. It remains to show f is surjective. For any $(v, S') \in P_{i-1}$ we have $S' \in p_v(G, i-1)$. By definition of $p_v(G, i-1)$, $S' \notin \mathcal{D}(G)$ but the only vertex not dominated by S' is v. Therefore $S = S' \cup \{v\}$ is a dominating set of cardinality i with $v \in a(S)$. However every neighbour of v is already dominated by $S - v$; therefore, $N(v) \cap N_1(S) = \emptyset$ and $v \in a_2(S)$. Thus $f(v, S) = (v, S')$ so f is surjective and hence bijective. $\square$

We are now ready to improve our upper bound on the average order of dominating sets for a graph with no isolated vertices.

Theorem 3.3.4 *Let G be a graph of order $n \geq 2$ and minimum degree $\delta \geq 1$. Then*

$$\operatorname{avd}(G) \leq \frac{2n(2^\delta - 1) + n}{3(2^\delta - 1) + 1},$$

and so $\operatorname{avd}(G) \leq \frac{3n}{4}$.

Proof. By summing the equality in Lemma 3.3.3 over all i we can obtain

$$\sum_{S\in\mathcal{D}(G)} |a_2(S)| = \sum_{v\in V(G)} |p_v(G)|. \tag{4}$$

We will now show $(2^{\deg(v)}-1)|p_v(G)| \leq |\mathcal{D}_{-v}(G)|$. For now fix $v \in V(G)$. By definition every $S \in p_v(G)$ dominates $G-v$ but does not contain any vertices of $N[v]$. Therefore for any non-empty $T \subseteq N(v)$, we have $S \cup T \in \mathcal{D}_{-v}(G)$. Let $A_v = \{(S,T) : S \in p_v(G), T \subseteq N(v), \text{ and } T \neq \emptyset\}$ and note that $|A_v| = (2^{\deg(v)}-1)|p_v(G)|$. We will now show the mapping $f : A_v \to \mathcal{D}_{-v}(G)$ defined by $f((S,T)) = S \cup T$ is injective and hence $|A_v| \leq |\mathcal{D}_{-v}(G)|$. Suppose $(S_1,T_1),(S_2,T_2) \in A_v$. Then if $f(S_1,T_1) = f(S_2,T_2)$ then $S_1 \cup T_1 = S_2 \cup T_2$. However by the definition of the sets in $p_v(G)$, $S_1, S_2 \subseteq V - N[v]$ and hence $S_1 \cap T_1 = \emptyset$ and $S_2 \cap T_2 = \emptyset$. As $S_1 \cup T_1 = S_2 \cup T_2$ then $S_1 = S_2$, $T_1 = T_2$ and $(S_1,T_1) = (S_2,T_2)$. Therefore f is injective and $|A_v| \leq |\mathcal{D}_{-v}(G)|$. As $|A_v| = (2^{\deg(v)}-1)|p_v(G)|$ then together with (3) and (4) we obtain

$$\begin{aligned}
\sum_{S\in\mathcal{D}(G)} |a_2(S)| &= \sum_{v\in V(G)} |p_v(G)| \\
&\leq \sum_{v\in V(G)} \frac{|\mathcal{D}_{-v}(G)|}{2^{\deg(v)}-1} \\
&\leq \sum_{v\in V(G)} \frac{|\mathcal{D}_{-v}(G)|}{2^{\delta}-1} \\
&= \frac{nD(G,1) - D'(G,1)}{2^{\delta}-1}.
\end{aligned}$$

By Lemma 3.3.2, $|a_1(S)| \leq |N_1(S)|$. So together with (3) we obtain

$$\begin{aligned}
\sum_{S\in\mathcal{D}(G)} |a_1(S)| &\leq \sum_{S\in\mathcal{D}(G)} |N_1(S)| \\
&\leq \sum_{S\in\mathcal{D}(G)} |V - S| \\
&= \sum_{v\in V(G)} |\mathcal{D}_{-v}(G)| \\
&= nD(G,1) - D'(G,1).
\end{aligned}$$

By Lemma 3.3.1, $\sum_{S\in\mathcal{D}(G)} |a(S)| = 2D'(G,1) - nD(G,1)$, and hence from

$$\sum_{S\in\mathcal{D}(G)} |a(S)| = \sum_{S\in\mathcal{D}(G)} |a_1(S)| + \sum_{S\in\mathcal{D}(G)} |a_2(S)|$$

we have that

$$2D'(G,1) - nD(G,1) \leq nD(G,1) - D'(G,1) + \frac{nD(G,1) - D'(G,1)}{2^\delta - 1}.$$

From this it follows that

$$\frac{D'(G,1)}{D(G,1)} \leq \frac{2n(2^\delta - 1) + n}{3(2^\delta - 1) + 1}.$$

Finally, one can verify that as $\delta \geq 1$,

$$\frac{2n(2^\delta - 1) + n}{3(2^\delta - 1) + 1} \leq \frac{3n}{4},$$

and we are done. □

Theorem 3.3.4 shows that all graphs G with no isolated vertices have $\mathrm{avd}(G) \leq \frac{3n}{4}$. However, for $\delta \geq 4$ the bound can be improved again, if we are even more careful with our counting. Again, we shall need a couple of technical lemmas first.

Lemma 3.3.5 *For any graph G,*

$$\sum_{S\in\mathcal{D}(G)} |N_1(S)| = \sum_{e\in E(G)} |\mathcal{D}(G) - \mathcal{D}(G-e)|.$$

Proof. It suffices to show that for every dominating set $S \in \mathcal{D}(G)$, there are exactly $|N_1(S)|$ edges $e = \{u, v\}$ in G such that $S \notin \mathcal{D}(G-e)$. For every $S \in \mathcal{D}(G)$ consider the edge e in G. If e goes from a vertex $v \in N_1(S)$ to some vertex in S then v is not dominated by S in $G-e$, so $S \in \mathcal{D}(G) - \mathcal{D}(G-e)$.

Conversely suppose e does not go from a vertex in $N_1(S)$ to some vertex in S; we need to show that $S \notin \mathcal{D}(G) - \mathcal{D}(G-e)$. Note that in $G-e$, the set S necessarily dominates every vertex other than possibly u and v. Therefore $S \in \mathcal{D}(G-e)$ if and only if S dominates both u and v in $G-e$. Consider the following 3 cases:

Case 1: $u, v \in S$. Then both u and v dominate themselves in S, so S is a dominating set in $G-e$. Therefore $S \notin \mathcal{D}(G) - \mathcal{D}(G-e)$.

Case 2: $u, v \notin S$. As S is a dominating set of G, there exist vertices $x, y \in S$ (possibly $x = y$) such that x and y are adjacent to u and v respectively in G. Note that x and y are still adjacent to u and v respectively in $G - e$. Therefore S is a dominating set in $G - e$ and $S \notin \mathcal{D}(G) - \mathcal{D}(G - e)$.

Case 3: Either $u \in S$ and $v \notin S$, or $u \notin S$ and $v \in S$. Without loss of generality suppose $u \in S$ and $v \notin S$. As e does not go from a vertex in $N_1(S)$ to some vertex in S then $v \notin N_1(S)$ and therefore $v \in N_2(S)$. By definition of $N_2(S)$, there exists at least one other vertex $x \in S$ adjacent to v. Therefore x is still adjacent to v in $G - e$ and S is a dominating set in $G - e$. Therefore $S \notin \mathcal{D}(G) - \mathcal{D}(G - e)$.

Therefore for every dominating set $S \in \mathcal{D}(G)$, the number of edges e in G which have $S \in \mathcal{D}(G) - \mathcal{D}(G - e)$ is exactly the number of edges from $N_1(S)$ to S. By definition of $N_1(S)$, each vertex in $N_1(S)$ is adjacent to exactly one vertex in S. Therefore, the number of edges e in G which have $S \in \mathcal{D}(G) - \mathcal{D}(G - e)$ is exactly $|N_1(S)|$. □

Lemma 3.3.6 ([67]) *Let G be a graph. For every edge $e = \{u, v\}$ of G,*

$$|\mathcal{D}(G) - \mathcal{D}(G - e)| = |p_u(G - e)| + |p_v(G - e)| - |p_u(G)| - |p_v(G)|.$$

□

We are now ready to prove another upper bound for $\mathrm{avd}(G)$.

Theorem 3.3.7 *For any graph G with no isolated vertices,*

$$\mathrm{avd}(G) \leq \frac{n}{2} + \sum_{v \in V(G)} \frac{\deg(v)}{2^{\deg(v)+1} - 2}.$$

Proof. By Lemma 3.3.2, Lemma 3.3.5, and Lemma 3.3.6, we obtain

$$\begin{aligned} \sum_{S \in \mathcal{D}(G)} |a_1(S)| &\leq \sum_{e \in E(G)} (|p_u(G - e)| + |p_v(G - e)| - |p_u(G)| - |p_v(G)|) \\ &= \sum_{v \in V(G)} \sum_{u \in N(v)} (|p_v(G - uv)| - |p_v(G)|). \end{aligned}$$

Together with (4) we obtain

$$\begin{aligned}\sum_{S\in\mathcal{D}(G)}|a(S)| &= \sum_{S\in\mathcal{D}(G)}(|a_1(S)|+|a_2(S)|)\\ &\le \sum_{v\in V(G)}\sum_{u\in N(v)}|p_v(G-uv)| - \sum_{v\in V(G)}(\deg(v)-1)|p_v(G)|.\end{aligned}$$

Furthermore as G has no isolated vertices we obtain

$$\sum_{S\in\mathcal{D}(G)}|a(S)| \le \sum_{v\in V(G)}\sum_{u\in N(v)}|p_v(G-uv)|. \tag{5}$$

For each $v\in V(G)$ and $e=\{u,v\}\in E(G)$ consider $S\in p_v(G-e)$. For any nonempty $T\subseteq N[v]-\{u\}$, we have $S\cup T\in\mathcal{D}(G-e)\subseteq\mathcal{D}(G)$ and all such sets are distinct. Therefore $(2^{\deg(v)}-1)|p_v(G-e)|\le|\mathcal{D}(G)|$ (where the degree is in the graph G) and together with Lemma 3.3.1 and (5) we obtain

$$2D'(G,1)-nD(G,1)=\sum_{S\in\mathcal{D}(G)}|a(S)|\le\sum_{v\in V(G)}\frac{\deg(v)\cdot D(G,1)}{2^{\deg(v)}-1},$$

from which it follows that

$$\frac{D'(G,1)}{D(G,1)}\le\frac{n}{2}+\sum_{v\in V(G)}\frac{\deg(v)}{2^{\deg(v)+1}-2},$$

which is what we wished to show. □

Corollary 3.3.8 *For a graph G with minimum degree $\delta\ge 1$, we have*

$$\operatorname{avd}(G)\le\frac{n}{2}\left(1+\frac{\delta}{2^{\delta}-1}\right).$$

In particular, if $\delta\ge 2\log_2(n)$, then $\operatorname{avd}(G)<\frac{n+1}{2}$.

Proof. Let $f(x)=\frac{x}{2^{x+1}-2}$. It is not hard to verify that for $x\ge 1$, $f(x)$ is a decreasing function. Therefore for all $v\in V(G)$, $f(\deg(v))\le f(\delta)$, and by Theorem 3.3.7

$$\operatorname{avd}(G)\le\frac{n}{2}+\sum_{v\in V(G)}\frac{\deg(v)}{2^{\deg(v)+1}-2}\le\frac{n}{2}+\frac{n\cdot\delta}{2^{\delta+1}-2}=\frac{n}{2}\left(1+\frac{\delta}{2^{\delta}-1}\right).$$

Now suppose $\delta \geq 2\log_2(n)$. As $\delta \leq n-1$, we know that $2\log_2(n) \leq n-1$. Again, one can verify that $2f(\delta) = \delta/(2^\delta - 1)$ is decreasing for $\delta \geq 1$, so

$$\begin{aligned}
\operatorname{avd}(G) &\leq \frac{n}{2}\left(1 + \frac{\delta}{2^\delta - 1}\right) \\
&\leq \frac{n}{2}\left(1 + \frac{2\log_2(n)}{2^{2\log_2(n)} - 1}\right) \\
&\leq \frac{n}{2}\left(1 + \frac{n-1}{n^2 - 1}\right) \\
&= \frac{n}{2}\left(1 + \frac{1}{n+1}\right) \\
&< \frac{n}{2}\left(1 + \frac{1}{n}\right) \\
&= \frac{n+1}{2},
\end{aligned}$$

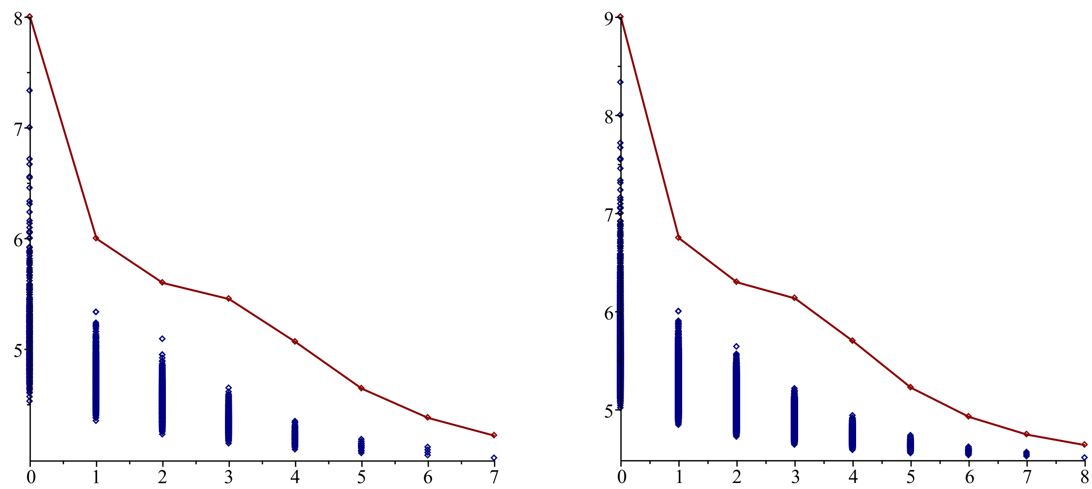
which is what we wished to show. □

Theorem 3.3.4 and Corollary 3.3.8 give two different upper bounds for $\operatorname{avd}(G)$ based on $\delta(G)$. Figure 3.3 plots $\operatorname{avd}(G)$ sorted by minimum degree for all graphs of order $n = 8$ and $n = 9$, respectively. The curve in Figure 3.3 is the minimum of the two bounds of Theorem 3.3.4 and Corollary 3.3.8 evaluated for each integer $0 \leq \delta \leq n$ and linearly interpolated between each point.

Our best upper bound for all isolate-free graphs remains $\operatorname{avd}(G) \leq \frac{3n}{4}$. However by Corollary 3.3.8 if $\delta(G) \geq 4$ then $\operatorname{avd}(G) \leq \frac{19n}{30} < \frac{2n}{3}$. In fact, all graphs up to order 9 with no isolated vertices have $\operatorname{avd}(G) \leq \frac{2n}{3}$. This leads us to the following conjecture.

Conjecture 3.3.9 *Let G be a graph with $n \geq 2$ vertices. If G has no isolated vertices (so, in particular, if G is connected) then* $\operatorname{avd}(G) \leq \frac{2n}{3}$.

We can show that the upper bound in Conjecture 3.3.9 is achieved for all $n \geq 2$: For $n = 2$ and $n = 3$, $\operatorname{avd}(K_2) = \frac{4}{3}$ and $\operatorname{avd}(K_{1,2}) = 2$. For any $n \geq 4$, there exist non-negative integers k and ℓ such that $n = 2k + 3\ell$. Then by Lemma 3.1.1 any graph of the form $H = kK_2 \cup \ell K_{1,2}$ will have $\operatorname{avd}(H) = \frac{2n}{3}$. These graphs are not connected, but one can insist on connectivity as follows. Let G be any connected graph on $k + \ell$



(a) Graphs of order 8 (b) Graphs of order 9

Figure 3.3: The bounds from Theorem 3.3.4 and Corollary 3.3.8 compared to $\text{avd}(G)$ for $n = 8$ and $n = 9$.

vertices, and let G' be the graph obtained by adding one leaf to k vertices of G and two leaves to the other ℓ vertices of G. Note that G' is connected. Oboudi [73] showed that $D(G', x) = D(H, x)$ and therefore $\text{avd}(G') = \text{avd}(H) = \frac{2n}{3}$.

While we are unable to prove Conjecture 3.3.9, we can provide some evidence for it. A graph G is called *quasi-regularizable* if one can replace each edge of G with a nonnegative number of parallel copies, so as to obtain a nonempty graph where every vertex has the same degree with possibly multiple edges between pairs of vertices (i.e. a nonempty regular multigraph). In particular, any graph which contains a spanning subgraph which is both regular and nonempty is quasi-regularizable. More specifically, any graph which has a perfect matching or is Hamiltonian (i.e. contains a spanning cycle) will also be quasi-regularizable. Berge [24] characterized quasi-regularizable graphs as those for which $|S| \leq |N(S)|$ holds for every independent set S of G. We will now show that for quasi-regularizable graphs, Conjecture 3.3.9 holds.

Theorem 3.3.10 *If G is a quasi-regularizable graph, then* $\text{avd}(G) \leq \frac{2n}{3}$.

Proof. We begin by showing that $|a(S)| \leq n - |S|$ for every $S \in \mathcal{D}(G)$. By Lemma 3.3.2, $|a_1(S)| \leq |N_1(S)|$. Therefore it suffices to show that $|a_2(S)| \leq |N_2(S)|$. For every $v \in a_2(S)$, we have $N(v) \subseteq V - S$, as otherwise $\text{Priv}_S(v) \neq \{v\}$. Furthermore,

$N(v) \subseteq N_2(S)$ as otherwise $v \in a_1(S)$. Therefore $a_2(S)$ is an independent set with $N(a_2(S)) \subseteq N_2(S)$. As G is a quasi-regularizable graph then $|a_2(S)| \leq |N(a_2(S))| \leq |N_2(S)|$, so

$$|a(S)| = |a_1(S)| + |a_2(S)| \leq |N_1(S)| + |N_2(S)| = n - |S|.$$

Finally, as $|a(S)| \leq n - |S|$ then $\sum_{S \in \mathcal{D}(G)} |a(S)| \leq nD(G,1) - D'(G,1)$. Thus together with Lemma 3.3.1 we obtain

$$2D'(G,1) - nD(G,1) \leq nD(G,1) - D'(G,1) \Rightarrow \operatorname{avd}(G) = \frac{D'(G,1)}{D(G,1)} \leq \frac{2n}{3},$$

which is what we wished to show. □

We will now extend a weaker version of the previous result. A matching in a graph is subset of edges such that no two edges are incident to the same vertex. Let $\nu(G)$ denote the matching number of G, that is, the largest cardinality of a matching. We alter the proof of the previous theorem to put $\operatorname{avd}(G)$ in terms of $\nu(G)$. This will not improve the bound from Theorem 3.3.10 for graphs with perfect matchings. However there are graphs which contain near perfect matchings which are not quasi-regularizable and therefore not subject to the bound in Theorem 3.3.10, for example paths of odd order. However, we can get an upper bound via the matching number.

Theorem 3.3.11 *Let G be a graph of order n. Then* $\operatorname{avd}(G) \leq n - \frac{2\nu(G)}{3}$.

Proof. We begin by showing that $|a(S)| \leq 2(n - \nu(G)) - |S|$ for every $S \in \mathcal{D}(G)$. By Lemma 3.3.2, $|a_1(S)| \leq |N_1(S)|$. Therefore, it suffices to show that $|a_2(S)| \leq |N_2(S)| + n - 2\nu(G)$. For every $v \in a_2(S)$, we have $N(v) \subseteq V - S$ otherwise $\operatorname{Priv}_S(v) \neq \{v\}$. Furthermore, $N(v) \subseteq N_2(S)$ otherwise $v \in a_1(S)$. Fix a maximum matching in G. Each vertex in $a_2(S)$ is either unmatched or matched with a vertex in $N_2(S)$. Note that there are exactly $n - 2\nu(G)$ unmatched vertices in G. Therefore $|a_2(S)| \leq |N_2(S)| + n - 2\nu(G)$.

Finally, as $|a(S)| \leq 2(n - \nu(G)) - |S|$ we have

$$\sum_{S \in \mathcal{D}(G)} |a(S)| \leq 2(n - \nu(G))D(G,1) - D'(G,1).$$

Thus together with Lemma 3.3.1 we obtain

$$2D'(G,1) - nD(G,1) \leq 2(n - \nu(G))D(G,1) - D'(G,1),$$

which implies

$$\operatorname{avd}(G) = \frac{D'(G,1)}{D(G,1)} \leq n - \frac{2\nu(G)}{3}.$$

This completes the proof. □

3.4 Lower bounds for trees

In this section we turn to trees (which are connected and, if they are nontrivial, have $\delta \geq 1$). For every $n \geq 2$ there is a tree T of order n with $\operatorname{avd}(T) = \frac{2n}{3}$, satisfying the upper bound from Conjecture 3.3.9 for isolate-free graphs. Such trees are constructed as follows. Let $n = 2k + 3\ell$ for $k, \ell \geq 0$ and T be a tree on $k + \ell$ vertices. Now let T' be the tree obtained by adding one leaf to k vertices of T and two leaves to the other ℓ vertices of T. Now we have that $\operatorname{avd}(T') = \frac{2n}{3}$ as T' is in the family of graphs described following Conjecture 3.3.9. We can classify trees T' as being a tree such that every non-leaf vertex has exactly one or two leaf neighbours. Recently, Erey [46] proved that the upper bound from Conjecture 3.3.9 was in fact the upper bound for trees (and forests). That is if T is a tree of order n then $\operatorname{avd}(T) \leq \frac{2n}{3}$. Furthermore Erey showed that $\operatorname{avd}(T) = \frac{2n}{3}$ if and only if every non-leaf vertex in T has exactly one or two leaf neighbours.

However, what about the lower bound? In Theorem 3.2.4, we showed that the lower bound for a graph G of order n is $\frac{n2^{n-1}}{2^n-1}$, which is achieved only by K_n, but these graphs are far from being trees. We show now that $\operatorname{avd}(T) \geq \operatorname{avd}(K_{1,n-1})$, and the argument is even more involved than for the lower bound for general graphs. For this we require a result similar to that of Proposition 3.2.3. However the proof of this is considerably more involved. For a tree T of order n, recall that $\mathcal{D}(T)$ denotes the collection of all dominating sets in T. For now fix $S \in \mathcal{D}(T)$. Recall that in the proof of Proposition 3.2.3, it was important to bound the number of subsets $S' \subseteq S$ where S' is also a dominating set and $|S'| = k$. Let

$$\mathrm{dom}_k(S) = |\{S' \subseteq S : S' \in \mathcal{D}(T) \text{ and } |S'| = k\}|.$$

The trivial upper bound, which was used in the proof of Proposition 3.2.3, is simply $\mathrm{dom}_k(S) \leq \binom{|S|}{k}$, but we need something stronger for trees. Recall that $a(S) = \{v \in S : S - v \notin \mathcal{D}(T)\}$. Therefore for any $S' \subseteq S$, if $S' \in \mathcal{D}(T)$ then $a(S) \subseteq S'$. Therefore $\mathrm{dom}_k(S) \leq \binom{|S|-|a(S)|}{k-|a(S)|}$. However this is only useful if $a(S) \neq \emptyset$. On the other hand, when $a(S) = \emptyset$, S is a *double dominating set* [51], that is, a subset $S \subseteq V(G)$ such that for every vertex $v \in V(G)$, $|N[v] \cap S| \geq 2$. The order of the smallest double dominating set is denoted $\gamma_{\times 2}(G)$. Note that for a dominating set S of a tree T, if $|S| < \gamma_{\times 2}(T)$ then $a(S) \neq \emptyset$ and so $|a(S)| \geq 1$. In the next lemma we will show $\gamma(T) + \gamma_{\times 2}(T) \geq n + 1$. Then $|S| > \gamma_{\times 2}(T)$ will imply that $n + 1 - |S| < \gamma(T)$ and hence $\mathrm{dom}_k(S) = 0$ for $k \leq n + 1 - |S|$. This will be crucial in proving Lemma 3.4.3 which implies $\mathrm{avd}(T) \geq \frac{n+1}{2}$.

Theorem 3.4.1 *If T is a nontrivial tree then $\gamma_{\times 2}(T) + \gamma(T) \geq n + 1$.*

Proof. We can assume that $n \geq 3$, as if $n = 2$, then $T = K_2$ and so $\gamma_{\times 2}(T) = 2$, $\gamma(T) = 1$ and the result holds. Set $V(T) = V$. It is sufficient to show that for any double dominating set S, we have $\gamma(T) \geq n - |S| + 1$. Note any dominating set must contain at least one vertex from each closed neighbourhood in G. If m vertices $v_1, \ldots, v_m$ have pairwise disjoint closed neighbourhoods, then $\gamma(T) \geq m$. Therefore it is sufficient to show that for any double dominating set S, there exists a collection of $|V - S| + 1$ vertices with pairwise disjoint closed neighbourhoods. We will induct on the number of vertices in $V - S$. For $v \in V$ and $u \in N(v)$ let $B(T, v, u)$ denote the set of vertices in the same component as u in $T - v$ (See Figure 3.4).

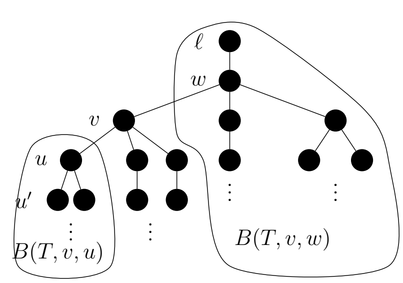


Figure 3.4: An example of $B(T, v, u)$ and $B(T, v, w)$.

Let S be a double dominating set. This implies that S contains every leaf and stem of T (as a *stem* in a tree is a vertex adjacent to a leaf). Our inductive hypothesis is as follows: there exists a collection of $|V - S| + 1$ vertices with pairwise disjoint closed neighbourhoods. The case where $|V - S| = 0$ is clearly true for any nontrivial tree. Assume for any nontrivial tree and some $k \geq 0$ that if $|V - S| \leq k$, then our inductive hypothesis holds. Now let S be a double dominating set so that $|V - S| = k + 1$. Note that for any leaf in T, both it and its *stem* (i.e., the leaf's only neighbour) must both be in S, otherwise S is not a double dominating set. Fix a leaf $\ell \in V$. Now choose a vertex $v \notin S$ which is at maximum distance from ℓ. Note that v is not a leaf nor a stem, as otherwise $v \in S$ which contradicts $v \notin S$. Therefore $\deg(v) \geq 2$ and $v \neq \ell$.

Let $w \in N(v)$ be the only neighbour of v which is closer to ℓ than v (See Figure 3.4). Note that $w \neq \ell$, as otherwise v would be a stem and hence belongs to S. As $\deg(v) \geq 2$, we can choose $u \in N(v) - \{w\}$. Note that every vertex in $B(T, v, u)$ is further from ℓ than v and therefore $B(T, v, u) \subseteq S$. Moreover, as v is not a stem, $\deg(u) \geq 2$. Therefore, we can choose $u' \in N(u) - \{v\}$. Note that $N[u'] \subseteq B(T, v, u)$ (as in Figure 3.4). Now set $T' = B(T, v, w)$ and $S' = S \cap B(T, v, w)$. Clearly T' is a nontrivial tree as $w, \ell \in T'$. Note that $N_T[w] = N_{T'}[w] \cup \{v\}$, and that for every other vertex $x \in V(T')$, we have $N_T[x] = N_{T'}[x]$. As $v \notin S$, $|N_{T'}[x] \cap S'| = |N_T[x] \cap S| \geq 2$ for all $x \in V(T')$. Therefore S' is a double dominating set of T'. Finally, the only vertex in $V(T) - V(T')$ which was not in S was v, as v was the furthest vertex from ℓ which was not in S. Therefore $|V(T') - S'| = |V(T) - S| - 1 = k$ and by our induction hypothesis there exists a collection of $k + 1$ vertices with disjoint closed neighbourhoods in T'. Let P denote this collection. As $v \notin N_T[u']$, we have $N_T[x] \cap N_T[u'] = \emptyset$ for all $x \in V(T')$. Therefore $P \cup \{u'\}$ is a collection of $k + 2 = |V - S| + 1$ vertices with pairwise disjoint closed neighbourhoods in T. □

We need three additional lemmas on the way to finding the tree of order n with the least average order of dominating sets. The first is due to Blidia et al.

Lemma 3.4.2 ([26]) *For every nontrivial tree T, we have $2\gamma(T) \leq \gamma_{\times 2}(T)$.* □

Lemma 3.4.3 *If T is a tree of order n, then $d_{n-k} \geq d_{k+1}$ for all k such that $k + 1 \leq \frac{n+1}{2}$.*

Proof. Fix k such that $k+1 \leq \frac{n+1}{2}$. If $k+1 < \gamma(T)$ then clearly $d_{n-k} \geq d_{k+1}$ holds as $d_{k+1} = 0$. So suppose for the remainder of this proof that $k+1 \geq \gamma(T)$. We will now use Hall's Theorem again. As before, let $\mathcal{D}_k$ denote the collection of all dominating sets of order k. We now construct a bipartite graph with bipartition $(\mathcal{D}_{k+1}, \mathcal{D}_{n-k})$; two vertices $A \in \mathcal{D}_{k+1}$ and $B \in \mathcal{D}_{n-k}$ are adjacent if $A \subseteq B$. As every superset of a dominating set remains dominating, the degree of each $A \in \mathcal{D}_{k+1}$ is $\binom{n-k-1}{n-2k-1} = \binom{n-k-1}{k}$. By the same argument used in the proof of Proposition 3.2.3, it suffices to show that for every $B \in \mathcal{D}_{n-k}$, there are at most $\binom{n-k-1}{k}$ subsets of B which are in $\mathcal{D}_{k+1}$.

By Theorem 3.4.1, we have $\gamma_{\times 2}(T)+\gamma(T) \geq n+1$ and hence $k+1 \geq n+1-\gamma_{\times 2}(T)$. We now consider two cases:

Case 1: Suppose that $k+1 > n+1-\gamma_{\times 2}(T)$, i.e., that $\gamma_{\times 2}(T) > n-k$. For any dominating set $B \in \mathcal{D}_{n-k}$ there exists a vertex $v \in T$ such that $N[v] \cap B$ contains exactly one vertex. Let $\{u\} = N[v] \cap B$. Then u is in every dominating set contained in B. Thus we must choose k other element from $B - u$ to get a dominating set in $\mathcal{D}_{k+1}$. Hence there are at most $\binom{n-k-1}{k}$ subsets of B which are also in $\mathcal{D}_{k+1}$.

Case 2: Suppose that $k+1 = n+1-\gamma_{\times 2}(T)$, i.e., that $\gamma_{\times 2}(T) = n-k$. As $\gamma_{\times 2}(T) + \gamma(T) \geq n+1$, we have $\gamma(T) \geq k+1$. Furthermore, as $\gamma(T) \leq k+1$, it follows that $k+1 = \gamma(T)$. For any dominating set $B \in \mathcal{D}_{n-k}$, if B is not a double dominating set, then by the argument of Case 1, there are at most $\binom{n-k-1}{k}$ subsets of B which are also in $\mathcal{D}_{k+1}$. So suppose B is a double dominating set. Let m be the number of stems in T. If $m = 1$ then $T = K_{1,n-1}$. It is easy to see that $k+1 = \gamma(K_{1,n-1}) = 1$, so $n-k = n$. Furthermore, $d_n(K_{1,n-1}) = d_1(K_{1,n-1}) = 1$, and therefore $d_n(K_{1,n-1}) \geq d_1(K_{1,n-1})$. Now suppose $m \geq 2$. Choose two stems s_1 and s_2 along with leaves ℓ_1 and ℓ_2 which are adjacent to s_1 and s_2 respectively. As B is a double dominating set we have $s_1, s_2, \ell_1, \ell_2 \in B$, otherwise ℓ_1 or ℓ_2 will not be double dominated. Furthermore if $A \subseteq B$ such that $A \in \mathcal{D}_{k+1}$, then A is a minimum dominating set. Therefore A contains exactly one of s_i or ℓ_i for each $i = 1, 2$ and the remaining $k-1$ vertices of A are chosen from the remaining $n-k-4$ vertices in B. Therefore there are at most $4\binom{n-k-4}{k-1}$ subsets $A \subseteq B$ such that $A \in \mathcal{D}_{k+1}$. It suffices to show that $4\binom{n-k-4}{k-1} \leq \binom{n-k-1}{k}$. Using Vandermonde's Convolution we obtain

$$\binom{n-k-1}{k} = \binom{n-k-4}{k} + 3\binom{n-k-4}{k-1} + 3\binom{n-k-4}{k-2} + \binom{n-k-4}{k-3}.$$

Note that $\binom{n-k-4}{k} + \binom{n-k-4}{k-2} \geq \binom{n-k-4}{k-1}$ when $n-k-4 \neq 0$. Therefore $4\binom{n-k-4}{k-1} \leq \binom{n-k-1}{k}$ when $n-k-4 \neq 0$. So suppose $n-k-4 = 0$. As $\gamma_{\times 2}(T) = n-k$, we have $\gamma_{\times 2}(T) = 4$. By Lemma 3.4.2, $2\gamma(T) \leq \gamma_{\times 2}(T)$. Therefore $\gamma(T) \leq 2$. Furthermore as T has two stems, $\gamma(T) \geq 2$ and therefore $\gamma(T) = 2$. Now $\gamma_{\times 2}(T) + \gamma(T) = n-k+k+1 = n+1$, so $n = 5$. There is exactly one tree, P_5, with $\gamma(T) = 2, \gamma_{\times 2}(T) = 4$ and $n = 5$. However, $D(P_5, x) = x^5 + 5x^4 + 8x^3 + 3x^2$ which satisfies $d_{n-k} \geq d_{k+1}$ for $k+1 \leq \frac{n+1}{2}$.

We have now shown for all trees of order n that $d_{n-k} \geq d_{k+1}$ for all k such that $k+1 \leq \frac{n+1}{2}$. □

Bród et al. proved the following useful fact.

Lemma 3.4.4 ([31]) *The star $K_{1,n-1}$ has the most dominating sets amongst all trees of order n.* □

Theorem 3.4.5 *If T is a tree of order n, then $\operatorname{avd}(T) \geq \operatorname{avd}(K_{1,n-1})$, with equality if and only if $T \cong K_{1,n-1}$.*

Proof. By Lemma 3.4.3, $\operatorname{avd}(T) \geq \frac{n+1}{2}$ and $d_{n-k} \geq d_{k+1}$ for $k+1 \leq \frac{n+1}{2}$. Suppose $T \ncong K_{1,n-1}$, so $\gamma(T) \geq 2$ and $d_1(T) = 0$. Now consider the mean order of all dominating sets except for the dominating set $V(T)$. Let $\mathcal{D}^*(T) = \mathcal{D}(T) - \{V(T)\}$. Note that

$$\operatorname{av}(\mathcal{D}^*(T)) = \frac{D'(T,1) - n}{D(T,1) - 1}$$

For $k+1 \leq \frac{n+1}{2}$ let $\mathcal{B}_k = \mathcal{D}_{n-k}(T) \cup \mathcal{D}_{k+1}(T)$. Note that $\operatorname{av}(\mathcal{B}_k) \geq \frac{n+1}{2}$ as $d_{n-k} \geq d_{k+1}$. Furthermore $\mathcal{B}_1, \ldots, \mathcal{B}_{\lfloor \frac{n+1}{2} \rfloor}$ is a partition of $\mathcal{D}^*(T)$. It follows from Lemma 3.2.1 that we have

$$\frac{D'(T,1) - n}{D(T,1) - 1} = \operatorname{av}(\mathcal{D}^*(T)) \geq \frac{n+1}{2}.$$

Therefore

$$\begin{aligned}\operatorname{avd}(T) &= \frac{n + D'(T,1) - n}{D(T,1)} \\ &= \frac{n}{D(T,1)} + \left(\frac{D(T,1)-1}{D(T,1)}\right)\frac{D'(T,1)-n}{D(T,1)-1} \\ &\geq \left(\frac{1}{D(T,1)}\right)n + \left(\frac{D(T,1)-1}{D(T,1)}\right)\frac{n+1}{2}.\end{aligned}$$

By Lemma 3.4.4, we have $D(T,1) \leq D(K_{1,n-1},1)$. Therefore we can shift the weight in the convex combination closer to the smaller quantity $\frac{n+1}{2}$

$$\begin{aligned}\operatorname{avd}(T) &\geq \left(\frac{1}{D(K_{1,n-1},1)}\right)n + \left(\frac{D(K_{1,n-1},1)-1}{D(K_{1,n-1},1)}\right)\frac{n+1}{2} \\ &> \left(\frac{1}{D(K_{1,n-1},1)}\right)(n-1) + \left(\frac{D(K_{1,n-1},1)-1}{D(K_{1,n-1},1)}\right)\frac{n+1}{2} \\ &= \frac{n-1}{2^{n-1}+1} + \left(\frac{2^{n-1}}{2^{n-1}+1}\right)\frac{n+1}{2} \\ &= \frac{n-1+2^{n-2}(n+1)}{2^{n-1}+1} = \operatorname{avd}(K_{1,n-1}).\end{aligned}$$

(In order to prove the second inequality above, we use the fact that if $A \geq a > 0$ and $1 \geq x \geq y > 0$, then $xA + (1-x)a \geq yA + a(1-y)$ with $A = n$, $a = (n+1)/2$, $x = 1/D(T,1)$ and $y = 1/D(K_{1,n-1},1)$.) $\square$

3.5 Distribution of Average Order of Dominating Sets

We've considered upper and lower bounds for $\operatorname{avd}(G)$. However, more generally, what are the possible values for $\operatorname{avd}(G)$? If G is a graph of order n, we showed in the previous section that $\operatorname{avd}(G) \in (\frac{n}{2}, n]$, but it seems unlikely that one can say precisely what values in the interval are average orders of dominating sets. A natural variant of $\operatorname{avd}(G)$ is $\widehat{\operatorname{avd}}(G) = \frac{\operatorname{avd}(G)}{n}$ which we shall refer to as the *normalized average order of dominating sets in G*. (Similar kinds of normalized graph parameters have been investigated throughout the literature – see [52, 63, 86], for example.)

We start with some examples. We say that a graph contains a *simple k-path* if there exist k vertices of degree two which induce a path in G.

For example, the path P_n contains a simple k-path for every $k \leq n-2$ (but not for $k \geq n-1$), and the cycle C_n contains a simple k-path for every $k \leq n-1$ (but not for $k = n$). The following holds for graphs which contain simple 3-paths.

Theorem 3.5.1 ([67]) *Suppose G is a graph with vertices u, v, w which form a simple 3-path. Then*

$$D(G,x) = x(D(G/u,x) + D(G/u/v,x) + D(G/u/v/w,x))$$

where G/u is the graph formed by joining every pair of neighbours of u and then deleting u. □

There is no known "nice" closed formula for all coefficients of $D(P_k,x)$ and $D(C_k,x)$ respectively. This makes determining the average order of dominating sets in paths and cycles difficult. We will now show that for a family of graphs satisfying a recurrence relation similar to that in Theorem 3.5.1, we can calculate the limit of the normalized average order of dominating sets as $n \to \infty$. First we shall put forward a way to calculate the limits of average values of functions of a certain type (which include those that arise from solving linear polynomial recurrences).

Theorem 3.5.2 *Suppose functions $f_n(x)$ satisfy*

$$f_n(x) = \alpha_1(x)(\lambda_1(x))^n + \alpha_2(x)(\lambda_2(x))^n + \cdots + \alpha_k(x)(\lambda_k(x))^n$$

where $\alpha_i(x)$ and $\lambda_i(x)$ are fixed non-zero analytic functions, such that $|\lambda_1(1)| > |\lambda_i(1)|$ for all $i > 1$. Then

$$\lim_{n\to\infty} \frac{f_n'(1)}{nf_n(1)} = \frac{\lambda_1'(1)}{\lambda_1(1)}.$$

Proof. As $|\lambda_1(1)| > |\lambda_i(1)|$ for all $i > 1$ then $\lim_{n\to\infty} \frac{\lambda_i(1)^n}{\lambda_1(1)^n} = 0$ for all $i > 1$. Furthermore,

$$\lim_{n\to\infty} \frac{f_n'(1)}{nf_n(1)} = \lim_{n\to\infty} \frac{\sum_{i=1}^{k} (\alpha_i'(1)\lambda_i(1)^n + n\alpha_i(1)\lambda_i(1)^{n-1}\lambda_i'(1))}{n\sum_{i=1}^{k} \alpha_i(1)\lambda_i(1)^n}$$

$$= \lim_{n\to\infty} \frac{\sum_{i=1}^{k} \frac{\alpha_i'(1)\lambda_i(1)^n + n\alpha_i(1)\lambda_i(1)^{n-1}\lambda_i'(1)}{\lambda_1(1)^n}}{n\sum_{i=1}^{k}\frac{\alpha_i(1)\lambda_i(1)^n}{\lambda_1(1)^n}}$$

$$= \lim_{n\to\infty} \frac{\alpha_1'(1) + \frac{n\alpha_1(1)\lambda_1'(1)}{\lambda_1(1)}}{n\alpha_1(1)}$$

$$= \lim_{n\to\infty} \frac{\alpha_1'(1)}{n\alpha_1(1)} + \frac{\lambda_1'(1)}{\lambda_1(1)} = \frac{\lambda_1'(1)}{\lambda_1(1)},$$

which is what we wished to show. □

Theorem 3.5.3 $\lim_{n\to\infty} \widehat{\mathrm{avd}}(P_n) = \lim_{n\to\infty} \widehat{\mathrm{avd}}(C_n) \approx 0.618419922.$

Proof. For both paths and cycles, we have a sequence of graphs $(G_n)_{n\geq 1}$ which satisfy the recurrence in Theorem 3.5.1,

$$D(G_n, x) = x(D(G_{n-1}, x) + D(G_{n-2}, x) + D(G_{n-3}, x)),$$

for all $n \geq 5$. As G_n follows the homogeneous linear recurrence relation $D(G_n, x) = x(D(G_{n-1}, x)+D(G_{n-2}, x)+D(G_{n-3}, x))$, we have $D(G_n, x) = \alpha_1(x)\lambda_1(x)^n+\alpha_2(x)\lambda_2(x)^n+\alpha_3(x)\lambda_3(x)^n$ where each $\lambda_i(x)$ satisfies

$$\lambda_i(x)^3 - x\lambda_i(x)^2 - x\lambda_i(x) - x = 0.$$

We solve this cubic polynomial (see also [8]). The solutions are

$$\begin{aligned}
\lambda_1(x) =& \frac{x}{3} + p(x) + q(x),\\
\lambda_2(x) =& \frac{x}{3} - p(x) - q(x) + \frac{\sqrt{3}}{2}\left(p(x) - q(x)\right) i,\\
\lambda_3(x) =& \frac{x}{3} - p(x) - q(x) - \frac{\sqrt{3}}{2}\left(p(x) - q(x)\right) i,
\end{aligned}$$

where

$$\begin{aligned}
p(x) =& \sqrt[3]{\frac{x^3}{27} + \frac{x^2}{6} + \frac{x}{2} + \sqrt{\frac{x^4}{36} + \frac{7x^3}{54} + \frac{x^2}{4}}},\\
q(x) =& \sqrt[3]{\frac{x^3}{27} + \frac{x^2}{6} + \frac{x}{2} - \sqrt{\frac{x^4}{36} + \frac{7x^3}{54} + \frac{x^2}{4}}}.
\end{aligned}$$

Note that $|\lambda_1(1)| \approx 1.83929 > |\lambda_2(1)| = |\lambda_3(1)| \approx 0.73735$.

Therefore by Theorem 3.5.2, we have $\lim_{n\to\infty} \frac{\operatorname{avd}(G_n)}{n} = \frac{\lambda_1'(1)}{\lambda_1(1)}$. It follows that

$$\begin{aligned}
\lim_{n\to\infty} \frac{\operatorname{avd}(G_n)}{n} &= \frac{\lambda_1'(1)}{\lambda_1(1)} \\
&= \frac{\frac{1}{3} + p'(1) + q'(1)}{\frac{1}{3} + p(1) + q(1)} \\
&= \frac{\frac{1}{3} + \frac{27\sqrt{33}+187}{66(19+3\sqrt{33})^{\frac{2}{3}}} - \frac{27\sqrt{33}-187}{66(19-3\sqrt{33})^{\frac{2}{3}}}}{\frac{1}{3} + \frac{(19+3\sqrt{33})^{\frac{1}{3}}}{3} + \frac{(19-3\sqrt{33})^{\frac{1}{3}}}{3}} \\
&= \frac{1}{3} + \frac{(88-8\sqrt{33})(19+3\sqrt{33})^{\frac{1}{3}}}{1056} + \frac{(55-7\sqrt{33})(19+3\sqrt{33})^{\frac{2}{3}}}{1056},
\end{aligned}$$

which we will denote by r. By Theorem 3.5.1, both C_n and P_n satisfy the same recurrence as G_n and hence $\lim_{n\to\infty} \frac{\operatorname{avd}(P_n)}{n} = \lim_{n\to\infty} \frac{\operatorname{avd}(C_n)}{n} = r \approx 0.618419922$. $\square$

For all graphs of order 9 we counted the number of graphs with $\widehat{\operatorname{avd}}(G) \in [\frac{1}{2} + \frac{k}{20n}, \frac{1}{2} + \frac{k+1}{20n})$ for each integer $0 \le k \le 10n-1$. Figure 3.5 shows the linearly interpolated distribution of $\widehat{\operatorname{avd}}(G)$ for all graphs of order 9. The distribution appears to be skewed towards $\frac{1}{2}$. However, our next result shows that $\widehat{\operatorname{avd}}(G)$ can be arbitrarily close to any value in $\left[\frac{1}{2}, 1\right]$.

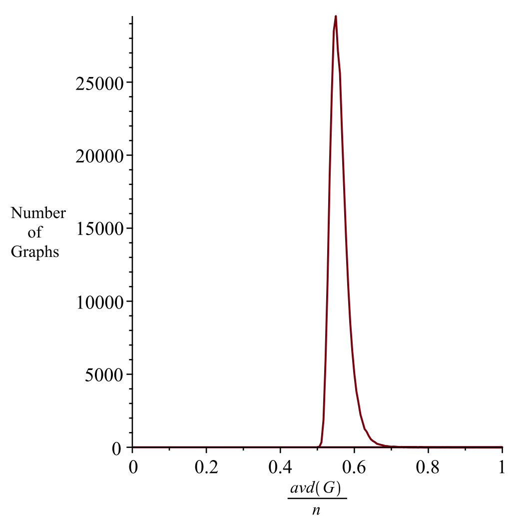


Figure 3.5: Distribution of $\widehat{\operatorname{avd}}(G)$ for all graphs of order 9

Proposition 3.5.4 *The set* $\left\{\widehat{\operatorname{avd}}(G) : G \textit{ is a graph}\right\}$ *is dense in* $[\frac{1}{2}, 1]$.

Proof. It suffices to show that for every rational number $\frac{a}{b} \in [\frac{1}{2}, 1]$ (a and b positive), there exists a sequence of graphs $(G_k)_{k\geq 1}$, where G_k has order n_k, such that $\lim_{k\to\infty} n_k = \infty$ and $\lim_{k\to\infty} \frac{\text{avd}(G_k)}{n_k} = \frac{a}{b}$. Let $G_k = (2b-2a)K_k \cup (2a-b)\overline{K_k}$. Note that such a graph exists as $\frac{a}{b} \in [\frac{1}{2}, 1]$ and hence $a \leq b \leq 2a$. Additionally, G_k has order $(2b-2a)k + (2a-b)k = bk$. Recall that $D(K_k, x) = (x+1)^k - 1$ and $D(\overline{K_k}, x) = x^k$. Therefore

$$\lim_{k\to\infty} \frac{\text{avd}(K_k)}{k} = \lim_{k\to\infty} \frac{k2^{k-1}}{k(2^k-1)} = 0.5 \quad \text{and} \quad \lim_{k\to\infty} \frac{\text{avd}(\overline{K_k})}{k} = 1.$$

Therefore by Lemma 3.1.1, we have

$$\begin{aligned}
\lim_{k\to\infty} \frac{\text{avd}(G_k)}{bk} &= \lim_{k\to\infty} \frac{(2b-2a)\text{avd}(K_k) + (2a-b)\text{avd}(\overline{K_k})}{bk} \\
&= \lim_{i\to\infty} \frac{(2b-2a)\text{avd}(K_k)}{bk} + \lim_{k\to\infty} \frac{(2a-b)\text{avd}(\overline{K_k})}{bk} \\
&= \frac{(2b-2a)\cdot 0.5}{b} + \frac{2a-b}{b} = \frac{a}{b},
\end{aligned}$$

which is what we wished to show. □

While we have shown that the closure of the normalized average order of dominating sets is the interval $[1/2, 1]$, where do most values lie? Let $\mathcal{G}(n, p)$ denote the sample space of random graphs on n vertices where each edge is independently present with probability p (any such graph is often called an Erdös-Renyi graph). We will now show that with probability tending to 1, the normalized average order of dominating sets of a random graph approaches $\frac{1}{2}$ (even if the graph is sparse with p close to 0); this explains the "bundling up" of values near $n/2$ in Figure 3.5. First we require Hoeffding's well known bound on the tail of a binomial distribution.

Theorem 3.5.5 ([56]) *Let $X = X_1 + \cdots + X_n$ where $X_1, \ldots, X_n$ are identical independent Bernoulli random variables each with probability of success p. Then we have*

$$\mathit{Prob}\,(X \leq (p-\varepsilon)n)) \leq e^{-2\varepsilon^2 n},$$

where $\varepsilon > 0$. □

Theorem 3.5.6 *Let $G_n \in \mathcal{G}(n,p)$ for $p \in (0,1)$. Then with probability tending to 1,*

$$\frac{1}{2} \leq \widehat{\mathrm{avd}}(G_n) \leq \frac{1}{2} + \frac{1}{2n}.$$

Proof. It follows from Theorem 3.2.4 that $\widehat{\mathrm{avd}}(G_n) \geq \frac{1}{2}$. Therefore it is sufficient to show that $\widehat{\mathrm{avd}}(G_n) \leq \frac{1}{2} + \frac{1}{2n}$.

The degree of any vertex v of G_n has a binomial distribution X_v with $N = n-1$, and hence has mean $p(n-1)$. From Theorem 3.5.5 it follows that for any fixed $\varepsilon > 0$,

$$\mathrm{Prob}\left(X_v \leq (p-\varepsilon)(n-1)\right) \leq e^{-2\varepsilon^2(n-1)}.$$

Thus

$$\mathrm{Prob}\left(\bigcup_v (X_v \leq (p-\varepsilon)(n-1))\right) \leq ne^{-2\varepsilon^2(n-1)} \to 0.$$

It follows that $\delta(G_n) > (p-\varepsilon)(n-1) > 2\log_2(n)$ with probability tending to 1. By Corollary 3.3.8, if $\delta(G_n) \geq 2\log_2(n)$ then $\mathrm{avd}(G_n) \leq \frac{n+1}{2}$. Therefore with probability tending to 1,

$$\widehat{\mathrm{avd}}(G_n) \leq \frac{n+1}{2n} = \frac{1}{2} + \frac{1}{2n},$$

and we are done. □

The result in Theorem 3.5.6 states that for $G_n \in \mathcal{G}(n,p)$ with constant $p \in (0,1)$ then almost surely $\widehat{\mathrm{avd}}(G_n) \to \frac{1}{2}$ as $n \to \infty$. We remark that it is unlikely, but not impossible that the randomly selected graph is $\overline{K_n}$ in which case $\widehat{\mathrm{avd}}(G_n) = 1$ and the theorem fails. Furthermore we remark that p need not be constant for the theorem to hold. In fact p only needs to satisfy $(p-\varepsilon)(n-1) > 2\log_2(n)$ for some $\epsilon > 0$ which satisfies $ne^{-2\varepsilon^2(n-1)} \to 0$ as $n \to \infty$. This can be achieved by choosing, for example, $p = 2\sqrt{\frac{\ln(n)}{n-1}}$ and $\epsilon = \sqrt{\frac{\ln(n)}{n-1}}$. In this case

$$ne^{-2\varepsilon^2(n-1)} = ne^{-2\ln(n)} = \frac{1}{n} \to 0.$$

and $(p-\varepsilon)(n-1) = \sqrt{(n-1)\ln(n)} > 2\log_2(n)$ for large enough n.

In this chapter we defined a new graph parameter, $\mathrm{avd}(G)$. For any graph G on n vertices we showed $\frac{n}{2} < \mathrm{avd}(G) \leq n$ while giving tighter bounds $\frac{n+1}{2} < \mathrm{avd}(G) \leq \frac{2n}{3}$ when G is a tree. Additionally we introduced $\widehat{\mathrm{avd}}(G)$ and showed that although the values of $\widehat{\mathrm{avd}}(G)$ were dense in $[\frac{1}{2}, 1]$, almost all graphs have $\widehat{\mathrm{avd}}(G) = \frac{1}{2}$. In Chapter

6 we will discuss future directions of research for this average parameter. In the next chapter we will investigate the unimodality of the domination polynomial. Many techniques from this chapter will be used in next chapter. This will be most evident in Section 4.4

Chapter 4

On the Unimodality of Domination Polynomials

4.1 Background

A question for any graph polynomial is: what is the shape of the coefficient sequence? Beyond increasing or decreasing it is next natural to inquire whether or not the sequence of coefficients is unimodal: a polynomial with real coefficients $a_0 + a_1x + \cdots + a_nx^n$ is said to be *unimodal* if there exists $0 \leq k \leq n$, such that

$$a_0 \leq \cdots \leq a_{k-1} \leq a_k \geq a_{k-1} \geq \cdots \geq a_n$$

(in such a case, we call the location(s) of the largest coefficient the *mode*). To show a polynomial is unimodal, it has often been helpful (and easier) to show a stronger condition, called log-concavity, holds, as the latter does not require knowing where the peak might be located. A polynomial is *log-concave* if for every $1 \leq i \leq n-1$, $a_i^2 \geq a_{i-1}a_{i+1}$. It is not hard to see that a polynomial with positive coefficients that is log-concave is also unimodal, and log-concavity has the advantage over unimodality that the peak need not be specified.

A variety of techniques have been used to show many graph polynomials are log-concave, and hence unimodal, including:

- real analysis (log-concavity of the matching polynomial [54] and the independence polynomial of claw-free graphs [38]),

- homological algebra (June Huh's proof of the log concavity of chromatic polynomials), and

- combinatorial arguments (the arguments of Krattenthaler [68] and Hamidoune [50] that reproved the log concavity of matching polynomials and independence polynomial of claw-free graphs, respectively, as well as Horrocks' [58] result that the dependent k-set polynomial is log-concave (a subset of vertices is *dependent* iff it contains an edge of the graph).

What can we say about the shape of the domination polynomial? For simplicity we say graph G is log-concave or unimodal if its domination polynomial is log-concave or unimodal respectively. Calculations show that every graph of order at most 8 is log-concave. However the domination polynomial of the graph on 9 vertices in Figure 4.1 is

$$D(G,x) = x^9 + 9x^8 + 35x^7 + 75x^6 + 89x^5 + 50x^4 + 7x^3 + x^2$$

which is not log-concave as $d_3(G)^2 = 49$ but $d_4(G)d_2(G) = 50$. Although not all domination polynomials are log-concave they are conjectured to be unimodal [17].

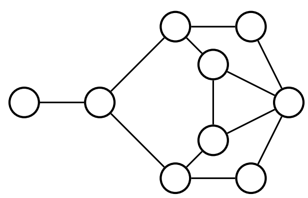


Figure 4.1: The only graph of order 9 which is not log-concave

Conjecture 4.1.1 ([17]) *The domination polynomial of any graph is unimodal.*

To date, only a little progress has been made on Conjecture 4.1.1. This progress is summarized in the following theorem

Theorem 4.1.2 ([10]) *For $n \geq 1$ and any graph G:*

(i) The friendship graph $F_n \cong K_1 \vee nK_2$ is unimodal.

(ii) The graph formed by adding a universal vertex to $nK_2 \cup K_1$ is unimodal.

(iii) $G \circ K_n$ is log-concave and hence unimodal.

(iv) $G \circ P_3$ is log-concave and hence unimodal.

n	$D(P_n, x)$	m_n
1	x	1
2	$x^2 + 2x$	1
3	$x^3 + 3x^2 + x$	2
4	$x^4 + 4x^3 + 4x^2$	3

n	$D(C_n, x)$	m_n
3	$x^3 + 3x^2 + 3x$	2
4	$x^4 + 4x^3 + 6x^2$	2
5	$x^5 + 5x^4 + 10x^3 + 5x^2$	3
6	$x^6 + 6x^5 + 15x^4 + 14x^3 + 3x^2$	4

Table 4.1: Domination polynomials for paths and cycles of small order together with the location of their mode m_n

In this chapter we extend the families for which unimodality of the domination polynomial is known to paths, cycles and complete multipartite graphs. We will also show almost all domination polynomials are unimodal with mode $\lceil \frac{n}{2} \rceil$. Finally we will discuss when the sequence of coefficients is non-increasing.

4.2 Paths, Cycles and Complete Multipartite Graphs

There is no useful closed formula for the coefficients of $D(P_n, x)$ and $D(C_n, x)$. However, recall the following recurrence relations from Theorem 3.5.1,

- $D(P_n, x) = x(D(P_{n-1}, x) + D(P_{n-2}, x) + D(P_{n-3}, x))$
- $D(C_n, x) = x(D(C_{n-1}, x) + D(C_{n-2}, x) + D(C_{n-3}, x))$

Now consider Table 4.1, which displays $D(P_n, x)$, $D(C_n, x)$, and their respective modes m_n.

Note that for both paths and cycles, consecutive modes differ by at most one in these small cases. We will now show that these observations for small n are sufficient to prove that the domination polynomials of all paths and cycles are unimodal.

Theorem 4.2.1 *Suppose we have a sequence of polynomials $(f_n)_{n\geq 1}$ with non-negative coefficients which satisfy*

$$f_n = x(f_{n-1} + f_{n-2} + f_{n-3}) \tag{6}$$

for $n \geq 4$. Let $\mathcal{P}_n$ denote the property that for all $i \in \{1, 2, \ldots, n\}$, f_i is unimodal and there exists a sequence of modes $m_1, \ldots, m_n$ of each f_i respectively such that $0 \leq m_i - m_{i-1} \leq 1$ for all $2 \leq i \leq n$. If $\mathcal{P}_4$ then $\mathcal{P}_n$ holds for all $n \geq 1$ (and so each f_n is unimodal).

Proof. We will prove our assertion via induction on $n \geq 4$. Our base case is satisfied by the assumption that $\mathcal{P}_4$ holds. For some $k \geq 4$, suppose $\mathcal{P}_k$ holds, and so $\mathcal{P}_j$ holds for all $1 \leq j \leq k$. To show $\mathcal{P}_{k+1}$ holds it suffices to show f_{k+1} is unimodal with a mode $m_{k+1} = m_k$ or $m_k + 1$. By our inductive hypothesis, f_k, f_{k-1}, and f_{k-2} are all unimodal with modes m_k, m_{k-1}, and m_{k-2} respectively. Additionally, $m_{k-1} \leq m_k \leq m_{k-1} + 1$ and $m_{k-2} \leq m_{k-1} \leq m_{k-2} + 1$. For simplicity let $m_k = m$. Note that $m - 2 \leq m_{k-2} \leq m_{k-1} \leq m_k = m$. Furthermore for each $n \geq 1$ let

$$f_n = \sum_{j=0}^{\infty} a_{n,j} x^j.$$

Therefore for $n = k, k-1, k-2$ we have

$$a_{n,0} \leq a_{n,1} \leq \cdots \leq a_{n,m-2} \text{ and } a_{n,m} \geq a_{n,m+1} \geq \cdots .$$

By the recursive relation (6) we see that $a_{k+1,0} = 0$ and for each $j \geq 1$

$$a_{k+1,j} = a_{k,j-1} + a_{k-1,j-1} + a_{k-2,j-1}.$$

Therefore

$$0 = a_{k+1,0} \leq a_{k+1,1} \leq \cdots \leq a_{k+1,m-1} \text{ and } a_{k+1,m+1} \geq a_{k+1,m+2} \geq \cdots .$$

We will now show $a_{k+1,m-1} \leq a_{k+1,m}$. Consider the following two cases:

Case 1: $m - 1 \leq m_{k-2} \leq m$

As $m - 1 \leq m_{k-2}$ then the modes of f_k, f_{k-1}, and f_{k-2} are each at least $m-1$. Thus $a_{k,m-2} \leq a_{k,m-1}$, $a_{k-1,m-2} \leq a_{k-1,m-1}$, and $a_{k-2,m-2} \leq a_{k-2,m-1}$. Therefore

$$\begin{aligned} a_{k+1,m-1} &= a_{k,m-2} + a_{k-1,m-2} + a_{k-2,m-2} \\ &\leq a_{k,m-1} + a_{k-1,m-1} + a_{k-2,m-1} \\ &= a_{k+1,m}. \end{aligned}$$

Case 2: $m_{k-2} = m - 2$

By the recursive relation the polynomials follow we obtain $a_{k,0} = 0$ and $a_{k,j} = a_{k-1,j-1} + a_{k-2,j-1} + a_{k-3,j-1}$ for each $j \geq 1$. Note $a_{k,m} \geq a_{k,m-1}$ because the mode of f_k is m. Therefore

$$a_{k-1,m-1} + a_{k-2,m-1} + a_{k-3,m-1} \geq a_{k-1,m-2} + a_{k-2,m-2} + a_{k-3,m-2}.$$

Let the mode of f_{k-3} be m_{k-3}. By our inductive hypothesis $m_{k-3} \leq m_{k-2} = m-2$, and therefore $a_{k-3,m-1} \leq a_{k-3,m-2}$. Furthermore

$$a_{k-1,m-1} + a_{k-2,m-1} \geq a_{k-1,m-2} + a_{k-2,m-2}.$$

Again the mode of f_k is m so $a_{k,m-1} \geq a_{k,m-2}$. Hence

$$\begin{aligned} a_{k+1,m-1} &= a_{k,m-2} + a_{k-1,m-2} + a_{k-2,m-2} \\ &\leq a_{k,m-1} + a_{k-1,m-1} + a_{k-2,m-1} \\ &= a_{k+1,m}. \end{aligned}$$

As $a_{k+1,m-1} \leq a_{k+1,m}$ then f_{k+1} is unimodal with mode at either m or $m+1$. Therefore $\mathcal{P}_{k+1}$ holds and by induction $\mathcal{P}_n$ holds for all $n \geq 1$. □

Note that for a vertex u in either P_n or C_n, $P_n/u \cong P_{n-1}$ and $C_n/u \cong C_{n-1}$. Thus by Theorem 3.5.1, the recursion for paths and cycles (which are stated at the beginning of Section 4.2) is equivalent to recursion relation (6). It follows from Theorem 4.2.1 and Table 4.1 that the following corollary holds.

Corollary 4.2.2 *For $n \in \mathbb{N}$ and $n \geq 3$, P_n and C_n are unimodal.* □

We remark that Theorem 4.2.1 can be leveraged to show many other families of graphs which contain simple k-paths are unimodal. For example, let L_n denote a path on $n-2$ vertices with a K_2 joined to one of the leaves (See Figure 4.2).

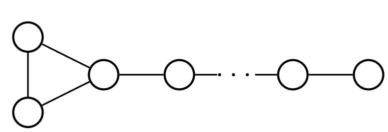


Figure 4.2: The graph L_n

n	$D(L_n, x)$	m_n
4	$x^4 + 4x^3 + 5x^2 + x$	2
5	$x^5 + 5x^4 + 9x^3 + 6x^2$	3
6	$x^6 + 6x^5 + 14x^4 + 14x^3 + 4x^2$	4
7	$x^7 + 7x^6 + 20x^5 + 27x^4 + 15x^3 + x^2$	4

Table 4.2: Domination polynomials for graphs L_n.

For $n \geq 5$, L_n contains a simple $n-4$-path and therefore by Theorem 3.5.1 follows the recurrence relation (6). Furthermore, Table 4.2 shows that the base condition in Theorem 4.2.1 holds for four consecutive values of n – 4,5,6 and 7. It follows that L_n is unimodal for $n \geq 4$.

We shall now show complete multipartite graphs are unimodal. We shall rely on an important result of Alikhani et al. that shows that the coefficients of the domination polynomial are non-decreasing up to $\frac{n}{2}$.

Proposition 4.2.3 ([17]) *Let G be a graph of order n. Then for every $0 \leq i < \frac{n}{2}$, we have $d_i(G) \leq d_{i+1}(G)$.*

We are now ready to proceed.

Theorem 4.2.4 *For $n_1, \ldots, n_k \in \mathbb{N}$, the complete multipartite graph $K_{n_1,\ldots,n_k}$ is unimodal.*

Proof. Set $G = K_{n_1,\ldots,n_k}$. Consider any subset of vertices $S \subseteq V(G)$ which is dependent. Therefore S contains two adjacent vertices u and v. Note that as G is complete multipartite, each of u and v are adjacent to every vertex in G except the other vertices in their respective parts. As u and v are adjacent, they are not in the same part of G and hence S dominates G. Let $f(x) = f_G(x)$ denote the dependent polynomial of G (the generating function of the number of dependent sets of cardinality k in G). As mentioned earlier, $f(x)$ is log-concave [58]. Furthermore

$$D(G, x) = f(x) + \sum_{i=1}^{k} x^{n_i},$$

as the only dominating sets which are not dependent sets consist of every vertex in one of the k parts of G. Let G have n vertices. By Proposition 4.2.3 $d_i(G) \leq d_{i+1}(G)$ for every $0 \leq i < \frac{n}{2}$. That is

$$d_1 \leq d_2(G) \leq \cdots \leq d_{\lceil \frac{n}{2} \rceil}$$

First suppose that every $n_j < \frac{n}{2}$. Then $d_i(G) = f_i$ for all $i \geq \frac{n}{2}$ where f_i is the coefficient of x^i in $f(x)$. Note that this means $d_{\lceil \frac{n}{2} \rceil} = f_{\lceil \frac{n}{2} \rceil}$. Furthermore as $f(x)$ is log-concave then $f(x)$ is unimodal and hence $D(G, x)$ is unimodal. So suppose there exists some $n_j \geq \frac{n}{2}$. Note that there is either exactly one $n_j \geq \frac{n}{2}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

First suppose there is exactly one $n_j \geq \frac{n}{2}$. Then $d_i(G) = f_i$ for all $i \geq \frac{n}{2}$ except for $d_j(G) = f_j + 1$. As the sequence $f(x)$ is log-concave and hence unimodal then the only way for the sequence to not be unimodal is for $f_j = f_{j+1} < f_{j+2}$ or $f_{j-2} > f_{j-1} = f_j$. However each case would contradict $f(x)$ being log-concave.

Now suppose $G \cong K_{\frac{n}{2},\frac{n}{2}}$. Note that every subset of vertices which contains at least $\frac{n}{2} + 1$ vertices is a dominating set as it necessarily contains vertices from both parts. Therefore $d_i(G) = \binom{n}{i}$ for all $i \geq \frac{n}{2} + 1$. Furthermore $d_i(G)$ is non-increasing for $i \geq \frac{n}{2} + 1$ and hence G is unimodal. $\square$

4.3 Almost all graphs are unimodal

In this section we will show that the domination polynomial of almost all graphs is unimodal with mode $\lceil \frac{n}{2} \rceil$, and hence that any counterexamples to unimodality are relatively rare.

We will now show graphs with minimum degree at least $2\log_2(n)$ are unimodal. We begin with a few preliminary definitions and observations. For a graph of order n, let $r_i(G)$ be the proportion of the subsets of vertices of G with cardinality i which are dominating. That is,

$$r_i(G) = \frac{d_i(G)}{\binom{n}{i}}.$$

Note that $0 \leq r_i(G) \leq 1$. For all $1 \leq i \leq n$, let $\mathcal{D}_i(G)$ denote the collection of dominating sets of cardinality exactly i. Note for any dominating set $S \in \mathcal{D}_i(G)$ and any vertex $v \in V - S$, $S \cup \{v\} \in \mathcal{D}_{i+1}(G)$. More specifically if we let $A_{i+1} = \{(v, S) :$

$S \in \mathcal{D}_{i+1}(G), v \in S\}$ and $B_i = \{(v, S) : S \in \mathcal{D}_i(G), v \notin S\}$ there is an injective mapping $f : B_i \to A_{i+1}$ defined as $f(v, S) = (v, S \cup \{v\})$. Therefore $|A_{i+1}| \geq |B_i|$ and equivalently $(i+1)d_{i+1}(G) \geq (n-i)d_i(G)$. Furthermore

$$r_{i+1}(G) = \frac{d_{i+1}(G)}{\binom{n}{i+1}} \geq \frac{(n-i)d_i(G)}{(i+1)\binom{n}{i+1}} = \frac{d_i(G)}{\binom{n}{i}} = r_i(G).$$

This allows us to obtain the following lemma.

Lemma 4.3.1 *Let G be a graph on n vertices, and $k \geq \frac{n}{2}$. If $r_k(G) \geq \frac{n-k}{k+1}$ then $d_{i+1}(G) \leq d_i(G)$ for all $i \geq k$. In particular, if $k = \lceil \frac{n}{2} \rceil$ then G is unimodal with mode $\lceil \frac{n}{2} \rceil$.*

Proof. Set $d_i = d_i(G)$ and $r_i = r_i(G)$ for all i. Note that

$$d_{i+1} \leq d_i \;\Leftrightarrow\; r_{i+1}\binom{n}{i+1} \leq r_i\binom{n}{i} \;\Leftrightarrow\; \frac{r_{i+1}}{r_i} \leq \frac{i+1}{n-i} \;\Leftrightarrow\; \frac{r_i}{r_{i+1}} \geq \frac{n-i}{i+1}.$$

Therefore for each i, if $r_i \geq \frac{n-i}{i+1}$ then $d_{i+1} \leq d_i$ as $r_{i+1} \leq 1$. So suppose for some $k \geq \frac{n}{2}$, $r_k(G) \geq \frac{n-k}{k+1}$. Then for any $i \geq k$ we have

$$r_i(G) \geq r_k(G) \geq \frac{n-k}{k+1} \geq \frac{n-i}{i+1}$$

and hence $d_{i+1} \leq d_i$. Finally, if $k = \lceil \frac{n}{2} \rceil$ then together with Proposition 4.2.3 we have

$$d_1 \leq d_2 \leq \cdots \leq d_{\lceil \frac{n}{2} \rceil} \geq \cdots \geq d_n,$$

which is what we wished to show. □

Theorem 4.3.2 *If G is a graph with n vertices with minimum degree $\delta(G) \geq 2\log_2(n)$ then $D(G, x)$ is unimodal with a mode at $\lceil \frac{n}{2} \rceil$.*

Proof. Set $\delta = \delta(G)$, $d_i = d_i(G)$ and $r_i = r_i(G)$ for all i. Let n_i denote the number of non-dominating subsets $S \subseteq V(G)$ of cardinality i. Note that $n_i = \binom{n}{i} - d_i$ and hence

$$r_i = 1 - \frac{n_i}{\binom{n}{i}}.$$

We will now show $n_i \leq n\binom{n-\delta-1}{i}$. For each vertex $v \in V$ let $n_i(v)$ denote the number of subsets which do not dominate v. A subset S does not dominate v if and only if it does not contain any vertices in $N[v]$. Therefore $n_i(v)$ simply counts every subset of $V(G)$ with i vertices which omits $N[v]$. Hence $n_i(v) = \binom{n-\deg(v)-1}{i}$. Furthermore any non-dominating set of order i must not dominate some vertex of G. Therefore

$$n_i \leq \sum_{v \in V} n_i(v) = \sum_{v \in V} \binom{n - \deg(v) - 1}{i} \leq \sum_{v \in V} \binom{n - \delta - 1}{i} = n\binom{n - \delta - 1}{i},$$

and

$$\begin{aligned} r_i =& 1 - \frac{n_i}{\binom{n}{i}} \\ \geq& 1 - \frac{n\binom{n-\delta-1}{i}}{\binom{n}{i}} \\ =& 1 - \frac{n(n-\delta-1)!}{i!(n-\delta-1-i)!} \cdot \frac{i!(n-i)!}{n!} \\ =& 1 - \frac{(n-1-\delta)!}{(n-1)!} \cdot \frac{(n-i)!}{(n-i-\delta-1)!} \\ \geq& 1 - \frac{(n-i)(n-i-1)(n-i-2)\cdots(n-i-\delta)}{(n-1)(n-2)\cdots(n-\delta)}. \end{aligned}$$

Note that for any $k \geq 0$, $\frac{n-i-k}{n-k} \geq \frac{n-i-k-1}{n-k-1}$ holds as $i \geq 0$. Therefore

$$\frac{n-i}{n} \geq \frac{n-i-1}{n-1} \geq \cdots \geq \frac{n-i-\delta}{n-\delta}.$$

and so

$$r_i \geq 1 - (n-i)\left(\frac{n-i}{n}\right)^{\delta}.$$

Now let $f(x,\delta) = 1-(n-x)\left(\frac{n-x}{n}\right)^{\delta}$ and $g(x) = \frac{n-x}{x+1}$ for $x, \delta \in [0,n]$. Note that $f(x,\delta)$ is an increasing function of both x and δ and $g(x)$ is also a decreasing function of x. By Lemma 4.3.1, it suffices to show $f(\frac{n}{2}, 2\log_2(n)) \geq g(\frac{n}{2})$. Note

$$f\left(\frac{n}{2}, 2\log_2(n)\right) = 1 - \frac{n}{2}\left(\frac{1}{2}\right)^{2\log_2(n)} = 1 - \frac{n}{2n^2} = 1 - \frac{1}{2n}$$

and

$$g\left(\frac{n}{2}\right) = \frac{\frac{n}{2}}{\frac{n}{2}+1} = \frac{n}{n+2} = 1 - \frac{2}{n+2}.$$

Therefore $f(\frac{n}{2}, 2\log_2(n)) \geq g(\frac{n}{2})$ if and only if $\frac{2}{n+2} \geq \frac{1}{2n}$ which holds for all $n \geq 1$. $\square$

Recall that $\mathcal{G}(n,p)$ denotes the Erdös-Rényi random graph model on n vertices (each edge is independently present with probability p).

Theorem 4.3.3 *Fix $p \in (0,1)$. Let $G_n \in \mathcal{G}(n,p)$. Then with probability tending to 1, $D(G_n, x)$ is unimodal with a mode at $\lceil \frac{n}{2} \rceil$.*

Proof. It follows from the proof of Theorem 3.5.6 that for sufficiently large n, $\delta(G_n) > 2\log_2(n)$ with probability tending to 1. By Theorem 4.3.2, it follows that, with probability tending to 1, $D(G_n, x)$ is unimodal with a mode at $\lceil \frac{n}{2} \rceil$. $\square$

4.4 A Non-increasing Segment of Coefficients

In light of not being able to prove domination polynomials are unimodal, we can focus on proving that various portions of the coefficient sequence are increasing or decreasing. For a graph G on n vertices, Proposition 4.2.3 states that

$$d_1(G) \leq d_2(G) \leq \cdots \leq d_{\lceil \frac{n}{2} \rceil - 1} \leq d_{\lceil \frac{n}{2} \rceil}.$$

Furthermore, Lemma 2.2.6 states that $d_{n-j}(G) = \binom{n}{j}$ for all $j \leq \delta(G)$. Therefore

$$d_{n-\delta(G)} \geq d_{n-\delta(G)+1} \geq \cdots \geq d_{n-1} \geq d_n.$$

In this section we will show if G has minimum degree $\delta(G) \geq 1$ then

$$d_{\lfloor \frac{3n}{4} \rfloor} \geq d_{\lfloor \frac{3n}{4} \rfloor + 1} \geq \cdots \geq d_{n-1} \geq d_n.$$

Note that this can fail when $\delta(G) = 0$ if G has sufficiently many isolated vertices. For example $D(K_{1,2} \cup 7K_1, x) = x^{10} + 3x^9 + x^8$.

Many of the techniques used in this section will mirror those used in Section 3.3. For a graph G, recall $\mathcal{D}(G)$ denotes the collection of dominating sets of G. Now let

$\mathcal{D}_i(G) = \{S \in \mathcal{D}(\mathcal{G}) : |S| = i\}$. For a dominating set S of G we have previously defined

$$a(S) = \{v \in S : S - v \notin \mathcal{D}(G)\},$$

the set of *critical* vertices of S with respect to domination (in that their removal makes the set no longer dominating). In Section 3.3 we showed $\mathrm{avd}(G)$ could be expressed in terms of the sum of $|a(S)|$ over all $S \in \mathcal{D}(G)$. For simplicity let $a(G,i)$ denote the sum of $|a(S)|$ over all $S \in \mathcal{D}_i(G)$. That is,

$$a(G,i) = \sum_{S \in \mathcal{D}_i(G)} |a(S)|.$$

In the next lemma we will now show the significance of $a(G,i)$.

Lemma 4.4.1 *For a graph G with n vertices.*

$$a(G,i) = \sum_{S \in \mathcal{D}_i(G)} |a(S)| = id_i(G) - (n-i+1)d_{i-1}(G).$$

Proof. Let

$$A_i = \bigcup_{S \in \mathcal{D}_i(G)} \{(v,S) : v \in a(S)\} \quad \text{and} \quad \overline{A}_i = \bigcup_{S \in \mathcal{D}_i(G)} \{(v,S) : v \in S - a(S)\}.$$

Note that $|A_i| = a(G,i)$. For every $S \in \mathcal{D}_i(G)$ and $v \in S$ either $(v,S) \in A_i$ or $(v,S) \in \overline{A}_i$. As $A_i \cap \overline{A}_i = \emptyset$ then $|A_i| + |\overline{A}_i| = id_i(G)$, that is, $a(G,i) = id_i(G) - |\overline{A}_i|$. Now let

$$\overline{D}_{i-1} = \bigcup_{S \in \mathcal{D}_{i-1}(G)} \{(v,S) : v \in V - S\}.$$

Note that $|\overline{D}_{i-1}| = (n-i+1)d_{i-1}(G)$ and hence it suffices to show $|\overline{D}_{i-1}| = |\overline{A}_i|$. For any $(v,S) \in \overline{A}_i$ as $v \in S - a(S)$ then by definition $S - v \in \mathcal{D}_{i-1}(G)$ and hence $(v, S-v) \in \overline{D}_{i-1}$. Now consider the map $f : \overline{A}_i \to \overline{D}_{i-1}$ where $f(v,S) = (v, S-v)$. It suffices to show f is bijective. For any two $(v,S),(u,T) \in \overline{A}_i$ suppose $f(v,S) = f(u,T)$. Then $u = v$, $S - u = T - v$ and hence $S = T$. Therefore f is injective.

For any $(v, S') \in \overline{D}_{i-1}$ note that $S' \cup \{v\} \in \mathcal{D}_i(G)$. Therefore $(v, S' \cup \{v\}) \in \overline{A}_i$ and $f(v, S' \cup \{v\}) = (v, S')$. Thus f is subjective and hence bijective. $\square$

It follows from Lemma 4.4.1 that if $d_i(G) \leq d_{i-1}(G)$ then

$$a(G, i) = id_i(G) - (n - i + 1)d_{i-1}(G) \leq (2i - n - 1)d_i(G).$$

Furthermore, if $d_i(G) > d_{i-1}(G)$ then

$$a(G, i) = id_i(G) - (n - i + 1)d_{i-1}(G) > (2i - n - 1)d_i(G).$$

Therefore we have that $d_i(G) \leq d_{i-1}(G)$ if and only if

$$a(G, i) \leq (2i - n - 1)d_i(G). \tag{7}$$

From Section 3.3, for a dominating set $S \in \mathcal{D}(\mathcal{G})$, we can partition $V - S$ as $N_1(S) \cup N_2(S)$, where

$$\begin{aligned} N_1(S) &= \{v \in V - S : |N[v] \cap S| = 1\} \\ N_2(S) &= \{v \in V - S : |N[v] \cap S| \geq 2\}. \end{aligned}$$

Furthermore, recall the partition $a(S) = a_1(S) \cup a_2(S)$, where

$$\begin{aligned} a_1(S) &= \{v \in a(S) : N[v] \cap N_1(S) \neq \emptyset\} \\ a_2(S) &= \{v \in a(S) : N[v] \cap N_1(S) = \emptyset\}; \end{aligned}$$

for any vertex $v \in a_2(S)$, it must be the case that $N(v) \subseteq N_2(S)$. Before we prove Theorem 4.4.2 we require the following inequality proven in Lemma 3.3.2. For a graph G and any $S \in \mathcal{D}(G)$,

$$|a_1(S)| \leq |N_1(S)|.$$

For graph G containing a vertex v recall that $p_v(G, k)$ denote the collection of k-subsets of $V - N[v]$ which dominate $G - v$ (and hence they dominate $G - N[v]$ as well). Equivalently $p_v(G, k)$ is the collection of k-subsets which dominate every vertex except v. We showed in Lemma 3.3.3 that

$$\sum_{S \in \mathcal{D}_i(G)} |a_2(S)| = \sum_{v \in V(G)} |p_v(G, i-1)|.$$

This together with the inequality $|a_1(S)| \leq |N_1(S)|$ will allow us to bound $a(G, i)$. This will then allow us to use inequality (7) to determine a segment of non-increasing coefficients.

Theorem 4.4.2 *Let G be a graph with $n \geq 2$ vertices and minimum degree $\delta \geq 1$. Then $d_i(G) \leq d_{i-1}(G)$ for all*

$$i \geq \frac{n(2\delta + 1) + \delta}{3\delta + 1}.$$

In particular $d_i(G) \leq d_{i-1}(G)$ for $i \geq \frac{3n+1}{4}$.

Proof. From Lemma 3.3.3 we have

$$\sum_{S \in \mathcal{D}_i(G)} |a_2(S)| = \sum_{v \in V(G)} |p_v(G, i-1)|. \tag{8}$$

We will now show the following inequality holds:

$$\sum_{v \in V(G)} \deg(v)|p_v(G, i-1)| \leq \sum_{S \in \mathcal{D}_i(G)} |a_1(S)|. \tag{8}$$

Let

$$A_{i,1} = \bigcup_{S \in \mathcal{D}_i(G)} \{(v, S) : v \in a_1(S)\},$$

and

$$P_{i-1,1} = \bigcup_{v \in V(G)} \{(u, S) : S \in p_v(G, i-1) \text{ and } u \in N(v)\}.$$

Note that $|A_{i,1}| = \sum_{S \in \mathcal{D}_i(G)} |a_1(S)|$ and $|P_{i-1,i}| = \sum_{v \in V(G)} \deg(v)|p_v(G, i-1)|$. Therefore it suffices to show there is a injection from $P_{i-1,1}$ to $A_{i,1}$. Consider the mapping $g(u, S) = (u, S \cup \{u\})$. We will first show $g : P_{i-1,1} \to A_{i,1}$. For any $(u, S) \in P_{i-1,1}$ there is exactly one $v \in V(G)$ such that $S \in p_v(G, i-1))$ and $u \in N(v)$. Note v is the only vertex not dominated by S. Furthermore $S \cup \{u\}$ is a dominating set of cardinality i where v is adjacent to exactly one neighbour, u, in S. Therefore $v \in N_1(S)$ and thus $u \in a_1(S)$. Therefore $g(u, S) = (u, S \cup \{u\}) \in A_{i,1}$.

We will now show that g is injective. Suppose that there exists $(u,S),(u',S') \in P_{i-1,1}$ such that $g(u,S) = g(u',S')$. Then $(u, S\cup\{u\}) = (u', S'\cup\{u'\})$ and hence $v = v'$. Furthermore $S\cup\{u\} = S'\cup\{u'\}$ and thus $S = S'$ as $u \notin S$ and $u' \notin S'$. Therefore $(u,S) = (u',S')$ and g is injective. Furthermore the inequality in (8) holds and together with (8) we obtain

$$\sum_{S\in\mathcal{D}_i(G)} \delta\cdot|a_2(S)| = \sum_{v\in V(G)} \delta\cdot|p_v(G,i-1)| \leq \sum_{v\in V(G)} \deg(v)|p_v(G,i-1))| \leq \sum_{S\in\mathcal{D}_i(G)} |a_1(S)|.$$

Furthermore

$$a(G,i) = \sum_{S\in\mathcal{D}_i(G)} |a(S)| = \sum_{S\in\mathcal{D}_i(G)} |a_1(S)| + \sum_{S\in\mathcal{D}_i(G)} |a_2(S)| \leq \sum_{S\in\mathcal{D}_i(G)} \left(1+\frac{1}{\delta}\right)|a_1(S)|.$$

By Lemma 3.3.2, $|a_1(S)| \leq |N_1(S)| \leq n-i$ for each $S \in \mathcal{D}_i(G)$ and hence

$$a(G,i) \leq \sum_{S\in\mathcal{D}_i(G)} \left(1+\frac{1}{\delta}\right)(n-i) = \left(1+\frac{1}{\delta}\right)(n-i)d_i(G).$$

From equation (7), $d_i(G) \leq d_{i-1}(G)$ if and only if $a(G,i) \leq (2i-n-1)d_i(G)$. One can see that provided $d_i(G) > 0$, then

$$\left(1+\frac{1}{\delta}\right)(n-i)d_i(G) \leq (2i-n-1)d_i(G)$$

is equivalent to

$$i \geq \frac{n(2\delta+1)+\delta}{3\delta+1}.$$

Note that when $\delta \geq 1$ and $n \geq 2$ then $\gamma(G) \leq \frac{n}{2}$ hence $d_i(G) > 0$ for $i \geq \frac{n}{2}$. As $\frac{n(2\delta+1)+\delta}{3\delta+1} \geq \frac{n}{2}$ then from equation (7) we have $d_i(G) \leq d_{i-1}(G)$ for $i \geq \frac{n(2\delta+1)+\delta}{3\delta+1}$.

Finally note that $\frac{a\delta+b}{c\delta+d}$ is a non-increasing function of δ if and only if $bc \geq ad$. Therefore $\frac{n(2\delta+1)+\delta}{3\delta+1} = \frac{(2n+1)\delta+n}{3\delta+1}$ is non-increasing if and only if $3n \geq 2n+1$, which is certainly true for $n \geq 2$. Therefore for all $\delta \geq 1$ we have $\frac{3n+1}{4} \geq \frac{n(2\delta+1)+\delta}{3\delta+1}$ and hence $d_i(G) \leq d_{i-1}(G)$ when $i \geq \frac{3n+1}{4}$. □

Theorem 4.4.2 and Theorem 4.2.3 imply that if a graph without isolated vertices is unimodal then its mode is between $\frac{n}{2}$ and $\frac{3n+1}{4}$. Using Maple we have verified that all graphs with up to 9 vertices are unimodal. Furthermore the modes of graphs with no isolated vertices were bounded above by $\frac{2n}{3}$. This leads to the following conjecture.

Conjecture 4.4.3 *Let G be a graph with $n \geq 2$ vertices. If G has no isolated vertices then $d_i(G) \leq d_{i-1}(G)$ for $i \geq \lceil \frac{2n}{3} \rceil$.*

If a graph G without isolated vertices is unimodal then Conjecture 4.4.3 puts an upper bound on the mode of $D(G, x)$. That is, Conjecture 4.4.3 posits that a unimodal domination polynomial $D(G, x)$ has mode at most $\lceil \frac{2n}{3} \rceil$. This parallels Conjecture 3.3.9 which puts forth that $\text{avd}(G) \leq \frac{2n}{3}$. Furthermore, the family of graphs with $\text{avd}(G) = \frac{2n}{3}$ given after Conjecture 3.3.9 are each unimodal with mode at either $\lceil \frac{2n}{3} \rceil$ or $\lfloor \frac{2n}{3} \rfloor$. Recall each graph G' in this family is obtained by taking any graph G on $k + \ell$ vertices and adding one leaf to k vertices of G and two leaves to the other ℓ vertices of G. The fact that each of these graphs are unimodal follows from the fact that they all have real roots [73]. Additionally, Darroch [41] showed that if $D(G, x)$ has all real roots then it has mode $\lfloor \text{avd}(G) \rfloor$ or $\lceil \text{avd}(G) \rceil$.

So far, most of this section has paralleled the results and techniques from Section 3.3. The remainder of this section will not be any different. We will show Conjecture 4.4.3 holds for quasi-regularizable graphs. Recall a quasi-regularizable graph can be characterized as a graph for which $|S| \leq |N(S)|$ holds for any independent set S of G. We will also show $d_i(G) \leq d_{i-1}(G)$ for $i \geq n - \frac{2\nu(G)+1}{3}$ where $\nu(G)$ denotes the matching number of G.

Theorem 4.4.4 *If G is a quasi-regularizable graph $d_i(G) \leq d_{i-1}(G)$ for $i \geq \frac{2n+1}{3}$.*

Proof. Let S be a dominating set of G. Recall from the proof of Theorem 3.3.10 that $|a(S)| \leq n - |S|$ because G is a quasi-regularizable graph. Therefore

$$a(G, i) = \sum_{S \in \mathcal{D}_i(G)} |a(S)| \leq \sum_{S \in \mathcal{D}_i(G)} (n - |S|) = (n - i)d_i(G).$$

From equation (7), we have $d_i(G) \leq d_{i-1}(G)$ if and only if $a(G, i) \leq (2i - n - 1)d_i(G)$. As the inequality $(n - i)d_i(G) \leq (2i - n - 1)d_i(G)$ is satisfied for $i \geq \frac{2n+1}{3}$, we are done. $\square$

As mentioned previously, any graph which contains a perfect matching is quasi-regularizable. Recall a matching in a graph is a subset of edges such that no two edges are incident to the same vertex. Let $\nu(G)$ denote the matching number of G, that is, the largest cardinality of a matching. We alter the proof of the previous theorem to bound the mode of $D(G,x)$ in terms of the matching number $\nu(G)$. This will not improve the bound from Theorem 4.4.4 for graphs with perfect matchings. However there are graphs which contain near perfect matchings, such as paths of odd order, which are not quasi-regularizable and therefore not subject to the bound in Theorem 4.4.4.

Theorem 4.4.5 *Let G be a graph with n vertices. Then $d_i(G) \leq d_{i-1}(G)$ for*

$$i \geq n - \frac{2\nu(G)-1}{3}.$$

Proof. Let S be a dominating set. We begin by showing that $|a(S)| \leq 2n - 2\nu(G) - |S|$ by showing $|a_1(S)| + |a_2(S)| \leq |N_1(S)| + |N_2(S)| + n - 2\nu(G)$. By Lemma 3.3.2, we have $|a_1(S)| \leq |N_1(S)|$. Therefore it suffices to show that $|a_2(S)| \leq |N_2(S)| + n - 2\nu(G)$.

From the proof of Theorem 4.4.4 we know that for every vertex $v \in a_2(S)$, it must be the case that $N(v) \subseteq N_2(S)$. Now, fix a maximum matching in G. Each vertex in $a_2(S)$ is either unmatched or matched with a vertex in $N_2(S)$. Note there are at most $n - 2\nu(G)$ unmatched vertices in G. Therefore $|a_2(S)| \leq |N_2(S)| + n - 2\nu(G)$. Furthermore

$$a(G,i) = \sum_{S \in \mathcal{D}_i(G)} |a(S)| \leq \sum_{S \in \mathcal{D}_i(G)} (2n - 2\nu(G) - |S|) = (2n - 2\nu(G) - i)d_i(G).$$

From equation (7), we have $d_i(G) \leq d_{i-1}(G)$ if and only if $a(G,i) \leq (2i-n-1)d_i(G)$. As $(2n - 2\nu(G) - i)d_i(G) \leq (2i - n - 1)d_i(G)$ is satisfied for $i \geq n - \frac{2\nu(G)-1}{3}$, we are done. $\square$

Although the unimodality conjecture remains open for domination polynomials, we have been able to show that almost all domination polynomials are unimodal. An old theorem from Newton (See [29]) states that a polynomial with positive coefficients is log-concave (and hence unimodal) if it is real-rooted, that is, it has all real roots. More generally, if the roots lie in the sector $\left\{z \in \mathbb{C} : \frac{2\pi}{3} < |\arg(z)| < \frac{4\pi}{3}\right\}$ the polynomial is also log-concave [30]. Thus the location of the roots of graph polynomials are of interest and this motivates our next chapter. In fact, in Section 5.2 we will show that for a particular family of graphs, the roots of their domination polynomials lie in $\left\{z \in \mathbb{C} : \frac{2\pi}{3} < |\arg(z)| < \frac{4\pi}{3}\right\}$ and are therefore log-concave.

Chapter 5

The Roots of Domination Polynomials

5.1 Background

For many graph polynomials, the location and nature of the roots have been (and continue to be) active areas of study. For example, the roots of chromatic polynomials (usually referred to as *chromatic roots*) have been of interest since the inception of chromatic polynomials, as the infamous Four Color Conjecture (now the Four Color Theorem) was equivalent to stating that 4 is never a chromatic root of a planar graph. While it is clear that the real chromatic roots are nonnegative (as the polynomial has coefficients that alternate in sign), it is not hard to show that $(0, 1)$ is always a root-free interval for chromatic roots. Are there others? In fact, a combination of results by Thomassen [84] and Jackson [61] proved that the closure of real chromatic roots is exactly the set $\{0, 1\} \cup [32/27, \infty)$ (and hence, surprisingly, $(1, 32/27)$ is chromatic root-free). For all-terminal reliability polynomials (the probability that a graph is connected, given that the edges are independently operational with probability p), the closure of their real roots [34] is precisely $\{0\} \cup [1, 2]$. We remark that, in contrast to the real case, the closure of the *complex* chromatic roots is the entire complex plane [81], while the closure of the complex all-terminal roots is not yet known (while it contains the unit disk centered at $z = 1$ [34], there are some roots just outside the disk [32, 75]).

In this chapter we investigate the roots of *domination polynomials*. The domination polynomials and their roots, *domination roots*) have been of significant interest over the last 10 years(c.f. [6]). Alikhani characterized graphs with two, three and four distinct domination roots [2,5]. In [73] Oboudi gave a degree dependent bound on the modulus of domination roots for a given graph. Brown and Tufts [37] showed that domination roots are dense in the complex plane. In this Chapter we will discuss two problems related to domination roots. In Section 5.2 we will provide a closed form of $D(C_n \diamond H, x)$ and then bound the roots of $D(C_n \diamond K_1, x)$. We will then use a classical result from Brenti [30] to show that the location of the roots of $D(C_n \diamond K_1, x)$ imply that $D(C_n \diamond K_1, x)$ is log-concave. In Section 5.3 we will show that the closure of the *real* domination roots is $(-\infty, 0]$.

5.2 Edges Coronas and Domination Polynomials

The edge corona is a graph product first introduced in 2010 by Hou and Shiu [59]. Hou and Shiu defined the edge corona as a variant to the corona of two graphs introduced by Frucht and Harary [47]. Hou and Shiu considered the edge corona in the context of the adjacency spectrum and Laplacian spectrum, while they also considered the number of spanning trees of edge coronas.

For two graphs G and H let m denote the number of edges in G. Recall the *edge corona* $G \diamond H$ of graphs G and H, $G \diamond H$, as the graph obtained by taking G and m copies of H and joining the two end vertices of the i^{th} edge of G to every vertex in the i^{th} copy of H. Note in the case where G has no edges $G \diamond H \cong G$. An example of $C_4 \diamond K_2$ is shown in Figure 5.1.

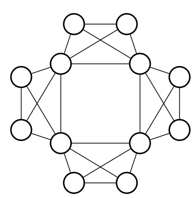


Figure 5.1: $C_4 \diamond K_2$

There is similar graph operation called the corona [47] $G \circ H$ which is defined by taking $|V(G)|$ copies of H and joining the i^th vertex in G to the i^th copy of H. The corona operation was shown to have nice properties with respect to domination. Particularly, for any pair of graphs G and H we have $\gamma(G \circ H) = |V(G)|$. The edge corona operation also behaves nicely with respect to domination. For any graph G and H we have $\gamma(G \diamond H) = |V(G)| - \alpha(G)$ were $\alpha(G)$ is the size of the largest independent set of G. Coronas of a graph have also been studied in the context of domination polynomials [67]. In particular, for any graph G the set of domination roots of $G \circ K_1$ is $\{0, 2\}$.

In this section we will study the domination polynomials of edge coronas. We will provide a closed form of $D(C_n \diamond H, x)$ in terms of $D(H, x)$. We will use the closed form of $D(C_n \diamond H, x)$ to show the log-concavity of $D(C_n \diamond K_1, x)$ via the location of their roots. Along the way we will also show $D(P_n \diamond H, x)$ satisfies a two term recurrence relation. We first require the following results.

For a graph G, a vertex $v \in V(G)$ is *domination-covered* if every dominating set of $G - v$ includes at least one vertex adjacent to v in G. Therefore if v is domination covered, the collection of dominating sets of G which do not contain v is exactly the collection of dominating sets of $G - v$. Kotek et al. classified all such vertices as follows.

Theorem 5.2.1 ([67]) *Let G be a graph. A vertex $v \in V(G)$ is domination-covered if and only if there is a vertex $u \in N(v)$ such that $N[u] \subseteq N[v]$.* □

For two graphs G and H, any non-isolated vertex v in G in the edge corona $G \diamond H$ contains the closed neighbourhood of every vertex in every copy of H for which v is joined. Therefore by Theorem 5.2.1, every vertex of G in $G \diamond H$ is domination-covered. This will be useful in the proofs of Theorem 5.2.2 and Theorem 5.2.6.

For graphs G and H on n_G and n_H vertices respectively, recall the following result from Theorem 1.3.2 (*ii*):

$$D(G \vee H, x) = ((1+x)^{n_G} - 1)((1+x)^{n_H} - 1) + D(G, x) + D(H, x).$$

We will require two special cases of Theorem 1.3.2 (*ii*):

- $D(G \vee K_1, x) = x(1+x)^{n_G} + D(G, x)$
- $D(G \vee K_2, x) = (x^2 + 2x)(1+x)^{n_G} + D(G, x)$.

We now provide a recursive formula for the corona of paths and any fixed graph G (we remark that in [12] Alikhani proved Theorem 5.2.2 for the restricted case of domination polynomials of cactus chains $P_n \diamond K_1$).

Theorem 5.2.2 *Let G be a graph with $r \geq 1$ vertices, and let $n \geq 4$. Then*

$$D(P_n \diamond G, x) = \beta_1 \cdot D(P_{n-1} \diamond G, x) + \beta_2 \cdot D(P_{n-2} \diamond G, x),$$

where

$$\beta_1 = x(1+x)^r + D(G, x)$$
$$\beta_2 = ((1+x)^r - D(G, x)) \cdot x(1+x)^r$$

Proof. Set $PG_n = P_n \diamond G$. Consider the labelling of PG_n in Figure 5.2 where $G_i \cong G$ for all $1 \leq i \leq n-1$.

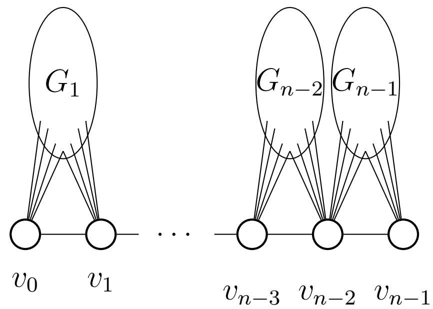


Figure 5.2: $P_n \diamond G$

For each $1 \leq i \leq n-1$ let H_i be the subgraph of PG_n induced by v_i and G_i. Note $H_i \cong G \vee K_1$ and $PG_n - H_{n-1}$ is isomorphic to PG_{n-1}. For a subset $S \subseteq V(PG_n)$ let $S[H_{n-1}]$ and $S[V - H_{n-1}]$ be the subset of S restricted to the vertices of H_{n-1} and $PG_n - H_{n-1}$, respectively.

We will now show $\beta_1 \cdot D(P_{n-1} \diamond G, x)$ and $\beta_2 \cdot D(P_{n-2} \diamond G, x)$ together are generating functions for all subsets S which are dominating. To do so we will consider whether or not $S[H_{n-1}]$ dominates H_{n-1}.

Case 1: $S[H_{n-1}]$ is a dominating set of H_{n-1}

As $S[H_{n-1}]$ is a dominating set of $H_{n-1} \cong G \vee K_1$, $S[H_{n-1}]$ is non-empty and v_{n-2} is also dominated by some vertex in $S[H_{n-1}]$. We will now show for this case that S dominates PG_n if and only if $S[V - H_{n-1}]$ dominates $V - H_{n-1}$. If $S[V - H_{n-1}]$ dominates $PG_n - H_{n-1}$ then clearly S is a dominating set of PG_n. So suppose $S[V - H_{n-1}]$ does not dominate $PG_n - H_{n-1}$. If S were to dominate PG_n, then $S[V - H_{n-1}]$ must be a dominating set of $PG_n - H_{n-1} - v_{n-2}$ which does not dominate v_{n-2}. However, because $r \geq 1$, we have that v_{n-2} is a domination-covered vertex of $PG_n - H_{n-1}$ and hence every dominating set of $PG_n - H_{n-1} - v_{n-2}$ must also dominate $PG_n - H_{n-1}$. Thus $S[V - H_{n-1}]$ dominates $PG_n - H_{n-1}$, which is a contradiction. Therefore S dominates PG_n if and only if $S[V - H_{n-1}]$ dominates $V - H_{n-1}$. Note the dominating sets of H_{n-1} are enumerated by $D(G \vee K_1, x)$ and the dominating sets of $PG_n - H_{n-1} \cong PG_{n-1}$ are enumerated by $D(P_{n-1} \diamond G, x)$. Therefore all dominating sets of PG_n for this case can be enumerated by

$$D(G \vee K_1, x)D(P_{n-1} \diamond G, x) = \beta_1 \cdot D(P_{n-1} \diamond G, x). \tag{5.1}$$

Case 2: $S[H_{n-1}]$ is not a dominating set of H_{n-1}

For this case it is easy to see that S dominates PG_n if and only if $S[V - H_{n-1}]$ dominates $V - H_{n-1}$ and $v_{n-2} \in S[V - H_{n-1}]$. To enumerate the dominating sets in PG_{n-1} that contain v_{n-2}, we notice that, for similar reasons, these are precisely the dominating sets in PG_{n-2} along with v_{n-2} and any subset of $V(G_{n-2})$. Note the non-dominating sets of H_{n-1} are enumerated by $(1+x)^{r+1} - D(G \vee K_1, x)$, the subsets of H_{n-2} containing v_{n-2} are enumerated by $x(1+x)^r$ and the dominating sets of PG_{n-2} are enumerated by $D(P_{n-2} \diamond G, x)$. Therefore all dominating sets of PG_n for this case can be enumerated by

$$((1+x)^{r+1} - D(G \vee K_1, x)) \cdot x(1+x)^r \cdot D(P_{n-2} \diamond G, x) = \beta_2 \cdot D(P_{n-2} \diamond G, x). \tag{5.2}$$

Which is what we wished to show. □

We will now prove that $C_n \diamond G$ also follows the same recursion as in Theorem 5.2.2. First we need a few minor results. For a graph G with vertex v let $D_{+v}(G, x)$ and $D_{-v}(G, x)$ denote the respective polynomials which enumerate the dominating sets which contain v and do not contain v, respectively. Note that $D(G, x) = D_{+v}(G, x) + D_{-v}(G, x)$. Now consider the dominating sets of $P_n \diamond G$ which do not contain v_0 (as labelled in Figure 5.2). For $n \geq 4$ the arguments in the proof of Theorem 5.2.2 are still satisfied for $D_{-v_0}(P_n \diamond G, x)$ and $D_{+v_0}(P_n \diamond G, x)$, yielding the following corollary.

Corollary 5.2.3 *For any graph G with r vertices and a path on $n \geq 4$ vertices then*

$$D_{-v_0}(P_n \diamond G, x) = \beta_1 \cdot D_{-v_0}(P_{n-1} \diamond G, x) + \beta_2 \cdot D_{-v_0}(P_{n-2} \diamond G, x),$$
$$D_{+v_0}(P_n \diamond G, x) = \beta_1 \cdot D_{+v_0}(P_{n-1} \diamond G, x) + \beta_2 \cdot D_{+v_0}(P_{n-2} \diamond G, x),$$

where v_0 is labelled in Figure 5.2 and

$$\beta_1 = x(1+x)^r + D(G, x)$$
$$\beta_2 = ((1+x)^r - D(G, x)) \cdot x(1+x)^r.$$

□

Note in Theorem 5.2.2, β_1 and β_2 do not depend on n. This allows for the following useful lemma.

Lemma 5.2.4 *For a graph G and integers $n, k > 0$ such that $n - k \geq 4$ let $f_n(x)$ be*

$$f_n(x) = \sum_{i=0}^{k} c_{1,i} \cdot D(P_{n-i} \diamond G, x) + \sum_{i=0}^{k} c_{2,i} \cdot D_{-v_0}(P_{n-i} \diamond G, x) + \sum_{i=0}^{k} c_{3,i} \cdot D_{+v_0}(P_{n-i} \diamond G, x)$$

where each $c_{j,i} = c_{j,i}(x)$ is a function that does not depend on n and v_0 is as labelled in Figure 5.2. Then $f_n(x)$ satisfies the same recurrence as $D(P_{n-k} \diamond G, x)$. That is,

$$f_n(x) = \beta_1 \cdot f_{n-1}(x) + \beta_2 \cdot f_{n-2}(x),$$

where

$$\beta_1 = x(1+x)^r + D(G, x)$$
$$\beta_2 = ((1+x)^r - D(G, x)) \cdot x(1+x)^r$$

□

Proof. By Theorem 5.2.2 and Corollary 5.2.3 for each $0 \leq i \leq k$ we have

$$D(P_{n-i} \diamond G, x) = \beta_1 \cdot D(P_{n-1-i} \diamond G, x) + \beta_2 \cdot D(P_{n-2-i} \diamond G, x),$$
$$D_{-v_0}(P_{n-i} \diamond G, x) = \beta_1 \cdot D_{-v_0}(P_{n-1-i} \diamond G, x) + \beta_2 \cdot D_{-v_0}(P_{n-2-i} \diamond G, x),$$
$$D_{+v_0}(P_{n-i} \diamond G, x) = \beta_1 \cdot D_{+v_0}(P_{n-1-i} \diamond G, x) + \beta_2 \cdot D_{+v_0}(P_{n-2-i} \diamond G, x).$$

Therefore

$$\begin{aligned} f_n(x) &= \sum_{i=0}^{k} c_{1,i}(x) D(P_{n-i} \diamond G, x) + \sum_{i=0}^{k} c_{2,i}(x) D_{-v_0}(P_{n-i} \diamond G, x) \\ &\quad + \sum_{i=0}^{k} c_{3,i}(x) D_{+v_0}(P_{n-i} \diamond G, x) \\ &= \sum_{i=0}^{k} c_{1,i}(x) \cdot (\beta_1 \cdot D(P_{n-1-i} \diamond G, x) + \beta_2 \cdot D(P_{n-2-i} \diamond G, x)) \end{aligned}$$

$$
\begin{aligned}
&+\sum_{i=0}^{k} c_{2,i}(x)\cdot(\beta_1\cdot D_{-v_0}(P_{n-1-i}\diamond G,x)+\beta_2\cdot D_{-v_0}(P_{n-2-i}\diamond G,x))\\
&+\sum_{i=0}^{k} c_{3,i}(x)\cdot(\beta_1\cdot D_{+v_0}(P_{n-1-i}\diamond G,x)+\beta_2\cdot D_{+v_0}(P_{n-2-i}\diamond G,x))\\
=&\beta_1\sum_{i=0}^{k} c_{1,i}(x)\cdot D(P_{n-1-i}\diamond G,x)+\beta_2\sum_{i=0}^{k} c_{1,i}(x)\cdot D(P_{n-2-i}\diamond G,x))\\
&+\beta_1\sum_{i=0}^{k} c_{2,i}(x)\cdot D_{-v_0}(P_{n-1-i}\diamond G,x)+\beta_2\sum_{i=0}^{k} c_{2,i}(x)\cdot D_{-v_0}(P_{n-2-i}\diamond G,x))\\
&+\beta_1\sum_{i=0}^{k} c_{3,i}(x)\cdot D_{+v_0}(P_{n-1-i}\diamond G,x)+\beta_2\sum_{i=0}^{k} c_{3,i}(x)\cdot D_{+v_0}(P_{n-2-i}\diamond G,x))\\
=&\beta_1\cdot f_{n-1}(x)+\beta_2\cdot f_{n-2}(x).
\end{aligned}
$$

Therefore our assertion is true. □

Kotek et. al. [67] defined an *irrelevant edge* of graph G to be an edge e such that $D(G,x)=D(G-e,x)$, and completely classified all such edges as follows.

Theorem 5.2.5 ([67]) *Let G be a graph. An edge $e=\{u,v\}$ is an irrelevant edge in G if and only if u and v are domination-covered in $G-e$.*

We are now ready to show $D(C_n\diamond G,x)$ follows the same recursion as $D(P_n\diamond G,x)$.

Theorem 5.2.6 *For any graph G with r vertices and a cycle on $n\geq 5$ vertices then*

$$D(C_n\diamond G,x)=\beta_1\cdot D(C_{n-1}\diamond G,x)+\beta_2\cdot D(C_{n-2}\diamond G,x),$$

where

$$
\begin{aligned}
\beta_1&=x(1+x)^r+D(G,x)\\
\beta_2&=((1+x)^r-D(G,x))\cdot x(1+x)^r
\end{aligned}
$$

Proof. A labelling of $D(C_n\diamond G,x)$ is shown in Figure 5.3, where $G_i\cong G$ for all $0\leq i\leq n-1$.

Consider the edge $e=\{v_0,v_{n-1}\}$. Both $N[v_0]$ and $N[v_{n-1}]$ contain the closed neighbourhoods of each vertex in G_1 and G_{n-1} respectively. Therefore they are both domination-covered in $(C_n\diamond G)-e$ and hence by Theorem 5.2.5 e is an irrelevant edge.

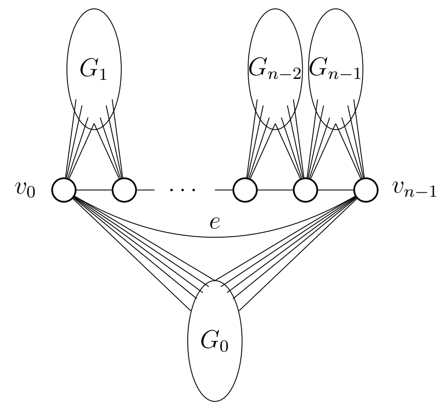


Figure 5.3: $C_n \diamond G$

For simplicity let CG_n denote the graph $(C_n \diamond G) - e$. Note $D(CG_n, x) = D(C_n \diamond G, x)$ as e is an irrelevant edge.

Now $CG_n - G_0 \cong P_n \diamond G$ so let PG_n denote $CG_n - G_0$. For a dominating subset of vertices $S \subseteq V$ let $S[G_0]$ and $S[PG_n]$ be the subsets of S restricted to the vertices of G_0 and PG_n respectively. Similar to the proof of Theorem 5.2.2 we will now determine a generating function for all such dominating sets S. To do so we will consider whether or not $S[G_0]$ dominates G_0. If $S[G_0]$ dominates G_0 we will show all such dominating sets S are enumerated by

$$D(G, x) \cdot D(P_n \diamond G, x). \tag{5.3}$$

If $S[G_0]$ does not dominate G_0, we will show all such dominating sets S are enumerated by

$$((1+x)^r - D(G, x)) \cdot (x(1+x)^r D_{+v_0}(P_{n-1} \diamond G, x) + 2x(1+x)^r D_{-v_0}(P_{n-1} \diamond G, x)), \tag{5.4}$$

Then together with equations (5.3) and (5.4), $D(C_n \diamond G, x)$ can be written in terms of $D(P_n \diamond G, x)$, $D_{-v_0}(P_{n-1} \diamond G, x)$, and $D_{+v_0}(P_{n-1} \diamond G, x)$. Therefore by Lemma 5.2.4 it will follow that our recursion is satisfied for $n \geq 5$. We conclude this proof with these two cases.

Case 1: $S[G_0]$ is a dominating set of G_0

If $S[G_0]$ is a dominating set of G_0 then $S[G_0]$ is non-empty and also dominates v_0 and v_{n-1}. Note v_0 and v_{n-1} are both domination-covered vertices. It follows for the same argument of case 1 in the proof of Theorem 5.2.2 that S is a dominating set if and only if $S[PG_n]$ is a dominating set of PG_n. The dominating sets of G_0 are enumerated by $D(G,x)$ and the dominating sets of PG_n are enumerated by $D(P_n \diamond G, x)$. Therefore all dominating sets of CG_n for this case can be enumerated by equation (5.3).

Case 2: $S[G_0]$ is not a dominating set of G_0

If $S[G_0]$ is not a dominating set of G_0 then at least one of v_0 or v_{n-1} must be in S in order for S to dominate CG_n. Additionally $S[PG_n]$ must also be a dominating set of PG_n which contain at least one of v_0 or v_{n-1}. The non-dominating sets of G_0 are enumerated by $(1+x)^r - D(G,x)$. Therefore it suffices to show the dominating sets of PG_n which contains at least one of v_0 or v_{n-1} are enumerated by

$$x(1+x)^r D_{+v_0}(P_{n-1} \diamond G, x) + 2x(1+x)^r D_{-v_0}(P_{n-1} \diamond G, x).$$

We will show the dominating sets of PG_n with contain both v_0 and v_{n-1} are enumerated by

$$x(1+x)^r D_{+v_0}(P_{n-1} \diamond G, x)$$

and the dominating sets of $CG_n - G_0$ with contain exactly one of v_0 or v_{n-1} are enumerated by

$$2x(1+x)^r D_{-v_0}(P_{n-1} \diamond G, x).$$

Similar to the proof of Theorem 5.2.2, let H_{n-1} be the subgraph of $P_n \diamond G$ induced by v_{n-1} and G_{n-1}. Furthermore let $S[H_{n-1}]$ and $S[V - H_{n-1}]$ be the subset of S restricted to the vertices of H_{n-1} and $PG_n - H_{n-1}$.

First consider the dominating sets S of PG_n with contain both v_0 and v_{n-1}. As v_{n-1} is a universal vertex of H_{n-1} then $S[H_{n-1}]$ dominates H_{n-1}. Thus by a similar argument used in case 1 of the proof of Theorem 5.2.2, S is a dominating set of PG_n (which contains v_0) if and only if $S[PG_n - H_{n-1}]$ is a dominating set of $PG_n - H_{n-1}$ (which contains v_0). Note the subsets of H_{n-1} which contain v_{n-1} are enumerated by $x(1+x)^r$ and the dominating sets of $PG_n - H_{n-1} \cong PG_{n-1}$ which contain v_0 are enumerated by $D_{+v_0}(P_{n-1} \diamond G, x)$. Therefore all dominating sets of PG_n for this case can be enumerated by equation $x(1+x)^r D_{+v_0}(P_{n-1} \diamond G, x)$.

Now consider the dominating sets S of PG_n with contain exactly one of v_0 or v_{n-1}. Without loss of generality suppose $v_0 \notin S$ and $v_{n-1} \in S$. Again as v_{n-1} is a universal vertex of H_{n-1} then $S[H_{n-1}]$ dominates H_{n-1}. Thus by a similar argument used in case 1 of the proof of Theorem 5.2.2, S is a dominating set of PG_n (which does not contains v_0) if and only if $S[PG_n - H_{n-1}]$ is a dominating set of $PG_n - H_{n-1}$ (which does not contains v_0). Note the subsets of H_{n-1} which contain v_{n-1} are enumerated by $x(1+x)^r$ and the dominating sets of $PG_n - H_{n-1} \cong PG_{n-1}$ which do not contain v_0 are enumerated by $D({}_{-v_0}P_{n-1} \diamond G, x)$. Therefore all dominating sets of PG_n for this case can be enumerated by equation $2x(1+x)^r D_{-v_0}(P_{n-1} \diamond G, x)$. $\square$

We are now ready to derive the closed form of $D(C_n \diamond G, x)$. We will do so by solving for the general solutions of the recursion from Theorem 5.2.6 and then show $D(C_n \diamond G, x)$ always has the same specific solution for any graph G.

Theorem 5.2.7 *For any graph G with r vertices and a cycle on $n \geq 3$ vertices,*

$$D(C_n \diamond G, x) = \left(\frac{\beta_1 + \sqrt{\beta_1^2 + 4\beta_2}}{2}\right)^n + \left(\frac{\beta_1 - \sqrt{\beta_1^2 + 4\beta_2}}{2}\right)^n$$

where

$$\beta_1 = x(1+x)^r + D(G, x)$$
$$\beta_2 = ((1+x)^r - D(G, x)) \cdot x(1+x)^r$$

Proof. For $n \geq 5$ we know from Theorem 5.2.6 that $D(C_n \diamond G, x)$ follows this homogeneous linear recursive relation

$$D(C_n \diamond G, x) = \beta_1 \cdot D(C_{n-1} \diamond G, x) + \beta_2 \cdot D(C_{n-2} \diamond G, x). \tag{5.5}$$

Therefore $D(C_n \diamond G, x) = s_1 \cdot \lambda_1^n + s_2 \cdot \lambda_2^n$ where each $\lambda_i = \lambda_i(x)$ satisfy

$$\lambda_i^2 - \beta_1 \lambda_i - \beta_2 = 0.$$

The solutions of this quadratic equation are

$$\lambda_1 = \frac{\beta_1 + \sqrt{\beta_1^2 + 4\beta_2}}{2} \text{ and } \lambda_2 = \frac{\beta_1 - \sqrt{\beta_1^2 + 4\beta_2}}{2}.$$

It suffices to show $D(C_n \diamond G, x) = \lambda_1^n + \lambda_2^n$ for $n = 3$ and $n = 4$ as all other cases will follow from the recursion in equation (5.5). Let S be a dominating set of $C_n \diamond G$. We will now determine the generating function of S for $n = 3$ and $n = 4$. In each case we will partition the generating function of S by considering the number of copies of G which are dominated by the vertices in C_n which are contained in S. Let $S[C_n]$ denote the vertices of S restricted to the vertices of C_n.

First consider $n = 3$. For any dominating set S of $C_3 \diamond G$ consider how many vertices are in $S[C_3]$:

- If S contains 2 or 3 vertices of the C_3, then all three copies of G are dominated by these vertices. Therefore S could contain any subset of the vertices of each copy of G and the generating function for these dominating sets is given by $(x^3 + 3x^2)(1 + x)^{3r}$.

- If S contains exactly one vertex of C_3, then two of the copies of G will be dominated by these vertices and one will not. Therefore S could contain any subset of the vertices of the two dominated copies of G and must contain a dominating set in the other copy of G. The generating function for these dominating sets is given by $3x(1 + x)^{2r}D(G, x)$.

- If S does not contain any vertices of C_3 then S must contain a dominating set in each copy of G. The generating function for these dominating sets is given by $(D(G, x))^3$.

Therefore

$$D(C_3 \diamond G, x) = (x^3 + 3x^2)(1 + x)^{3r} + 3x(1 + x)^{2r}D(G, x) + (D(G, x))^3.$$

Furthermore

$$\begin{aligned}\lambda_1^3 + \lambda_2^3 =& \beta_1^3 + 3\beta_1\beta_2\\ =&(x^3 + 3x^2)(1 + x)^{3r} + 3x(1 + x)^{2r}D(G, x) + D(G, x)^3\\ =&D(C_3 \diamond G, x).\end{aligned}$$

Now consider where $n = 4$. For any dominating set S of $C_3 \diamond G$ again consider how many vertices are in $S[C_4]$.

- If S contains 4 or 3 vertices of the C_4, then all four copies of G are dominated by these vertices. In each case S could contain any subset of the vertices of each copy of G and the generating function for these dominating sets is given by $(x^4 + 4x^3)(1 + x)^{4r}$.

- If S contains two non-adjacent vertices of the C_4, then all four copies of G are dominated by these vertices. In each case S could contain any subset of the vertices of each copy of G and the generating function for these dominating sets is given by $2x^2(1 + x)^{4r}$.

- If S contains two adjacent vertices of the C_4, then three copies of G are dominated by these vertices and one is not. Therefore S could contain any subset of the vertices of the three dominated copies of G and must contain a dominating set in the other copy of G. The generating function for these dominating sets is given by $4x^2(1 + x)^{3r}D(G, x)$.

- If S contains exactly one vertex of C_4, then two of the copies of G will be dominated by these vertices and the other two will not. Therefore S could contain any subset of the vertices of the two dominated copies of G and must contain a dominating set in the other two copies of G. The generating function for these dominating sets is given by $4x(1 + x)^{2r}(D(G, x))^2$.

- If S does not contain any vertices of C_4 then S must contain a dominating set in each copy of G. The generating function for these dominating sets is given by $(D(G, x))^4$.

Therefore

$$\begin{aligned} D(C_4 \diamond G, x) =&(x^4 + 4x^3 + 2x^2)(1 + x)^{4r} + 4x^2(1 + x)^{3r}D(G, x) \\ &+ 4x(1 + x)^{2r}(D(G, x))^2 + (D(G, x))^4. \end{aligned}$$

Furthermore

$$\lambda_1^4 + \lambda_2^4 =\beta_1^4 + 4\beta_1^2\beta_2 + 2\beta_2^2$$

$$
\begin{aligned}
=&(x^4+4x^3+2x^2)(1+x)^{4r}+4x^2(1+x)^{3r}D(G,x)\\
&+4x(1+x)^{2r}(D(G,x))^2+(D(G,x))^4.\\
=&D(C_4\diamond G,x).
\end{aligned}
$$

Therefore $D(C_n \diamond G, x) = \lambda_1^n + \lambda_2^n$ for all $n \geq 3$. □

We will now show $D(C_n \diamond K_1, x)$ is log-concave by bounding the location of its roots. In Chapter 4 we primarily discussed combinatorial arguments to show a polynomial was log-concave. However it is possible to show a polynomial is log-concave simply by the location of its roots. We will now call on a Theorem from Brenti et al. [30].

Theorem 5.2.8 ([30]) *If all the roots z of a polynomial $f(x)$ with positive coefficients are in the region*

$$\left\{ z \in \mathbb{C} : \frac{2\pi}{3} < |\arg(z)| < \frac{4\pi}{3} \right\}$$

then the sequence of coefficients of $f(x)$ is strictly log-concave.

We will now bound the roots of $D(C_n \diamond K_1, x)$ to the two blue curves shown in Figure 5.4 (appears on page 91). It will then follow from Theorem 5.2.8 that $D(C_n \diamond K_1, x)$ is log-concave.

Theorem 5.2.9 *For $n \geq 3$, $D(C_n \diamond K_1, x)$ is log-concave.*

Proof. Using Theorem 5.2.7 with $r = 1$ and $D(K_1, x) = x$ we have $\beta_1 = x^2 + 2x$, $\beta_2 = x^2 + x$ and

$$D(C_n \diamond K_1, x) = (\lambda_1(x))^n + (\lambda_2(x))^n,$$

where

- $\lambda_1(x) = \frac{x^2+2x+\sqrt{x^4+4x^3+8x^2+4x}}{2}$
- $\lambda_2(x) = \frac{x^2+2x-\sqrt{x^4+4x^3+8x^2+4x}}{2}$.

For $z \in \mathbb{C}$, if $D(C_n \diamond K_1, z) = 0$ then $|\lambda_1(z)| = |\lambda_2(z)|$, that is,

$$\left|z^2 + 2z + \sqrt{z^4 + 4z^3 + 8z^2 + 4z}\right| = \left|z^2 + 2z - \sqrt{z^4 + 4z^3 + 8z^2 + 4z}\right|.$$

Clearly this is satisfied for $z = 0$ and $z = -2$ as $z^2 + 2z = 0$. Thus suppose $z \neq 0, -2$. Divide both sides by $|z^2 + 2z|$ and multiply the right hand side by $|-1|$ to obtain

$$\left|1 + \frac{\sqrt{z^4 + 4z^3 + 8z^2 + 4z}}{z^2 + 2z}\right| = \left|-1 + \frac{\sqrt{z^4 + 4z^3 + 8z^2 + 4z}}{z^2 + 2z}\right|.$$

This implies that $\frac{\sqrt{z^4+4z^3+8z^2+4z}}{z^2+2z}$ must be purely imaginary, and hence

$$\left(\frac{\sqrt{z^4 + 4z^3 + 8z^2 + 4z}}{z^2 + 2z}\right)^2 = \frac{z^4 + 4z^3 + 8z^2 + 4z}{z^4 + 4z^3 + 4z^2} \tag{5.6}$$

must be real and negative. As $z \neq 0$ then be can factor out a z from the numerator and denominator. Furthermore if we multiple the numerator and denominator of (5.6) by the conjugate of $z^3 + 4z^2 + 4z$ the resultant fraction would have a positive denominator and it would suffice to show the resultant numerator is real and negative. Let $f(z) = z^3 + 4z^2 + 8z + 4$, $g(z) = z^3 + 4z^2 + 4z$, and $z = a + bi$ for $a, b \in \mathbb{R}$. Then

$$\begin{aligned} f(a+bi) =& a^3 - 3ab^2 + 4a^2 - 4b^2 + 8a + 4 + (3a^2b - b^3 + 8ab + 8b)i \\ g(a+bi) =& a^3 - 3ab^2 + 4a^2 - 4b^2 + 4a + (3a^2b - b^3 + 8ab + 4b)i \end{aligned}$$

Now multiple the numerator and denominator of (5.6) by the conjugate of $g(a + bi)$. The resultant numerator has real part

$$\begin{aligned} R(a,b) =& (a^3 - 3ab^2 + 4a^2 - 4b^2 + 8a + 4)(a^3 - 3ab^2 + 4a^2 - 4b^2 + 4a) \\ & + (3a^2b - b^3 + 8ab + 8b)(3a^2b - b^3 + 8ab + 4b) \\ =& a^6 + 8a^5 + (3b^2 + 28)a^4 + (16b^2 + 52)a^3 + (3b^4 + 32b^2 + 48)a^2 \\ & + (8b^4 + 36b^2 + 16)a + b^6 + 4b^4 + 16b^2, \end{aligned}$$

and imaginary part

$$\begin{aligned}I(a,b) =& -(a^3 - 3ab^2 + 4a^2 - 4b^2 + 8a + 4)(3a^2b - b^3 + 8ab + 4b)\\&+ (a^3 - 3ab^2 + 4a^2 - 4b^2 + 4a)(3a^2b - b^3 + 8ab + 8b)\\=& -4b(2a^3 + 2ab^2 + 7a^2 + 3b^2 + 8a + 4).\end{aligned}$$

Therefore if $z = a + bi$ is a root of $D(C_n \diamond K_1, x)$ with $z \neq 0, -2$ it must satisfy $R(a,b) < 0$ and $I(a,b) = 0$. Note that $I(a,b)$ is the product of b and a quadratic of b. Therefore $I(a,b) = 0$ if and only if $b = 0$ or $b = \pm\frac{\sqrt{-(2a+3)(2a^3+7a^2+8a+4)}}{2a+3}$. In each case we substituted these values into $R(a,b)$.

- If $b = 0$, then $R(a,b) = a(a^3 + 4a^2 + 8a + 4)(a + 2)^2$. Again using Maple we solve that $R(a,b) < 0$ when

$$a \in \left(\frac{\sqrt[3]{26 + 3\sqrt{33}}}{3} - \frac{8}{3\sqrt[3]{26 + 3\sqrt{33}}} - \frac{4}{3}, 0\right) \approx (-0.7044022572, 0).$$

- As $R(a,b)$ is an even function of b, without loss of generality suppose

$$b = \frac{\sqrt{-(2a+3)(2a^3 + 7a^2 + 8a + 4)}}{2a + 3}.$$

  By assumption b is real and the case where $b = 0$ was covered previously. Therefore $b^2 > 0$ and more specifically $-(2a + 3)(2a^3 + 7a^2 + 8a + 4) > 0$. With the use of Maple we can show $2a^3 + 7a^2 + 8a + 4$ has exactly one real root at $a = -2$ and is positive for $a > -2$ and negative for $a < -2$. Therefore $-(2a + 3)(2a^3 + 7a^2 + 8a + 4) > 0$ when $a \in \left(-2, -\frac{3}{2}\right)$. Again using Maple we substituted b into $R(a,b)$ and solved for when $R(a,b) < 0$ and $a \in \left(-2, -\frac{3}{2}\right)$. We obtain

$$a \in \left(-2, -\frac{\sqrt[3]{26 + 3\sqrt{33}}}{6} + \frac{4}{3\sqrt[3]{26 + 3\sqrt{33}}} - \frac{4}{3}\right) \approx (-2, -1.647798871).$$

The curves defined by each case, as well as $z = 0, -2$ are shown in blue in Figure 5.4. Note for any $n \geq 3$, the roots of $D(C_n \diamond G, x)$ are contained within one of these

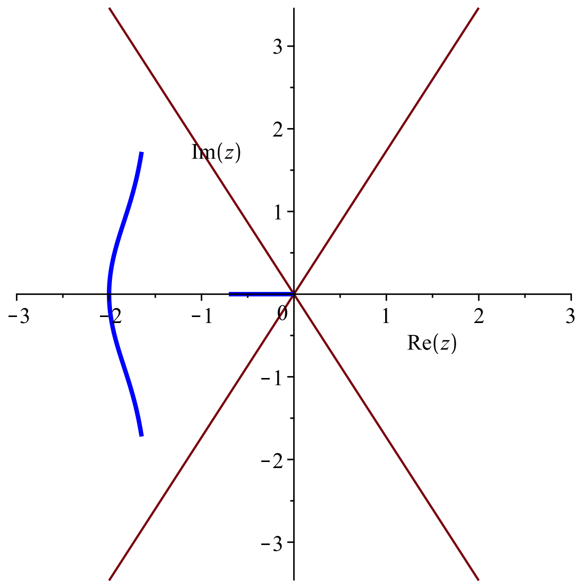


Figure 5.4: Limit of the roots of $D(C_n \diamond K_1, x)$

curves. Also in Figure 5.4 we provide the lines which border the region $\{z \in \mathbb{C} : \frac{2\pi}{3} < |\arg(z)| < \frac{4\pi}{3}\}$ from Theorem 5.2.8 in red.

We will show that all of the non-real roots are contained in the box $\mathcal{B} = \{a + ib : a \in (-2, -\frac{13}{8}), b \in (-2, 2)\}$. Note that $\mathcal{B}$ is contained within the region of Theorem 5.2.8 and therefore as $D(C_n \diamond G, x)$ has all positive coefficients then $D(C_n \diamond G, x)$ is log-concave. As we have already shown $a \in (-2, -1.647798871)$ (note $-\frac{13}{8} = -1.625$) it suffices to show $|b| < 2$. Recall

$$b = \frac{\pm\sqrt{-(2a+3)(2a^3+7a^2+8a+4)}}{2a+3} = \pm\sqrt{-\frac{2a^3+7a^2+8a+4}{2a+3}}.$$

We can simplify b via polynomial division to

$$|b| = \sqrt{-\frac{(2a+3)(a^2+2a+1)+1}{2a+3}} = \sqrt{-(a+1)^2 - \frac{1}{2a+3}}.$$

Note that $-1 < -(a+1)^2 < 0$ for $a \in (-2, -1.625)$ and $-\frac{1}{2a+3} > 1$ for $a \in (-2, -1.625)$. Therefore $|b| < \sqrt{-\frac{1}{2a+3}}$. Furthermore the $-\frac{1}{2a+3}$ is decreasing on the interval $(-2, -1.625)$ and therefore largest at $a = -1.625$. Finally

$$|b| < \sqrt{-\frac{1}{2\frac{-13}{8}+3}} = \sqrt{-\frac{8}{-26+24}} = \sqrt{\frac{8}{2}} = 2.$$

All non-roots of $D(C_n \diamond G, x)$ are contained in $\mathcal{B}$ which itself is contained in the region of Theorem 5.2.8. Therefore, as $D(C_n \diamond G, x)$ has all positive coefficients, $D(C_n \diamond G, x)$ is log-concave. $\square$

In $C_n \diamond K_1$ every vertex in the copy of C_n is domination-covered. By Theorem 5.2.5 any additional edge between these vertices would be an irrelevant edge. This gives us the following simple corollary.

Corollary 5.2.10 *For $n \geq 1$, consider $C_n \diamond K_1$ and let E be the collection of all edges in $\overline{C_n}$. For any subset $S \subseteq E$, let $(C_n \diamond K_1) + S$ denote the graph formed by adding the edges in S to $C_n \diamond K_1$. Then $C_n \diamond K_1 + S$ is log-concave.*

The proof of Theorem 5.2.9 shows the roots of $D(C_n \diamond K_1, x)$ are all on one of the blue curves in Figure 5.4. The following result from Beraha, Kahane, and Weiss shows that as n gets large the limit set of the roots of $D(C_n \diamond K_1, x)$ is *exactly* the blue curves in Figure 5.4.

Theorem 5.2.11 ([76]) *Suppose functions $f_n(x)$ satisfy*

$$f_n(x) = \alpha_1(x)(\lambda_1(x))^n + \alpha_2(x)(\lambda_2(x))^n + \cdots + \alpha_k(x)(\lambda_k(x))^n,$$

where $\alpha_i(x)$ and $\lambda_i(x)$ are fixed non-zero analytic functions, such that no $\alpha_i(x)$ is identically zero and that for no pair $i \neq j$ it is true that $\lambda_i(x) \equiv \omega\lambda_j(x)$ for some complex number ω of unit modulus. Then $z \in \mathbb{C}$ is a limit of the roots of $f_n(z)$ if and only if either

(i) two or more of the $\lambda_i(z)$ are of equal modulus, and strictly greater (in modulus) than the others; or

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

The proof of Theorem 5.2.9 shows the blue curves in Figure 5.4 are the exact curves satisfying condition (i) of Theorem 5.2.11. Note condition (ii) of Theorem 5.2.11 cannot be satisfied as $\alpha_1(x) = \alpha_2(x) = 1 \neq 0$. Therefore by Theorem 5.2.11 the collection of roots of $D(C_n \diamond K_1, x)$ for all $n \geq 3$ are dense on those blue curves in Figure 5.4.

5.3 Closure of Real Domination Roots

For our investigation, we now turn to real domination roots, and in particular, their closure. While Brown and Tufts [37] showed each real number is the limit of domination roots, not all real numbers are domination roots. For example any positive real number can not be a domination root as the domination polynomial has all positive coefficients.

To find the closure of the real domination roots, we will need a graph operation, *graph substitution*. Let G and H be graphs. The graph $G[H]$, formed by substituting a copy of H for every vertex of G, is constructed by taking a disjoint copy of H, H_v, for each vertex v of G, and joining every vertex in H_u to every vertex in H_v if and only if u is adjacent to v in G. For example, the complete bipartite graph graph $K_{n,n}$ is the same as $K_2[\overline{K}_n]$. Domination polynomials are well-behaved with regards to graph substitution of complete graphs .

Lemma 5.3.1 ([37]) *Let G be any graph and let K_n be the complete graph on n vertices. Then*

$$D(G[K_n], x) = D(G, (x + 1)^n - 1).$$

We now proceed to prove that real domination roots are dense in the negative real axis.

Theorem 5.3.2 *The closure of the real domination roots is* $(-\infty, 0]$.

Proof. Fix $z \in (-\infty, 0]$ and $\varepsilon > 0$; we need to show that there is a domination root z' in the interval $(z - \varepsilon, z + \varepsilon)$. Without loss, we can assume that $z \neq -2, 0$. Our proof will essentially be in two parts – for $z \in (-2, 0)$ and for $z \in (-\infty, -2)$. In either case, note that from Lemma 5.3.1, if z_1 is a domination root of some graph G, then any solution of $(z' + 1)^m - 1 = z_1$ is a domination root (of the graph $G[K_m]$). If m is an odd integer and $z_1 < 0$ is a domination root, then $(z_1 + 1)^{1/m} - 1$ will be a real domination root as well. Finally, $z' = (z_1 + 1)^{1/m} - 1 \in (z - \varepsilon, z + \varepsilon)$ iff $z_1 \in ((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1)$, so it suffices to show that for some odd $m \geq 1$, the interval $((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1)$ contains a domination root.

Case 1: $z \in (-2, 0)$

We shall consider two subcases that are similar in approach, splitting at $z = -1$.

Subcase 1.1: $z \in (-2, -1)$

We can assume that $z - \varepsilon > -2$ and $z + \varepsilon < -1$ by decreasing ε, so that both $(z - \varepsilon + 1)^m - 1$ and $(z + \varepsilon + 1)^m - 1$ are in $(-2, -1)$. Observe that if we set $b = -(z - \varepsilon + 1)$ and $a = -(z + \varepsilon + 1)$, then $1 > b > a > 0$. Note that for odd m the intervals $((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1) = (-b^m - 1, -a^m - 1)$ approach -1 from the left, that is, the intervals all lie to the left of -1, and both end points approach -1 as m increases. Moreover, as

$$-b^{m+1} - 1 < -a^m - 1 \leftrightarrow b\left(\frac{b}{a}\right)^m > 1,$$

we conclude that if m is odd and large enough, the left end point of the next interval $(-b^{m+1} - 1, -a^{m+1} - 1)$ lies inside the previous interval $(-b^m - 1, -a^m - 1)$. It follows that the union of all the intervals,

$$\bigcup_m ((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1),$$

will contain an interval $(w, -1)$, with $w \in (-2, -1)$.

Now consider the domination polynomial of the complete bipartite graph $K_{k,\ell}$, which is clearly given by

$$D(K_{k,\ell}, x) = ((x + 1)^k - 1)((x + 1)^\ell - 1) + x^k + x^\ell,$$

so that

$$D(K_{2,\ell}, x) = (x + 1)^\ell (x^2 + 2x) + x^\ell - 2x.$$

Now let ℓ be odd. Then $D(K_{2,\ell}, -1) = (-1)^\ell + 2 = 1 > 0$. For any $\delta \in (0, 1)$,

$$D(K_{2,\ell}, -1 - \delta) \quad = \quad -\delta^\ell(\delta^2 - 1) - (1 + \delta)^\ell + 2\delta + 2,$$

which is negative for ℓ sufficiently large. Thus for ℓ large enough, there will be a real domination root in the interval $(-1 - \delta, -1)$. By choosing $\delta = -w - 1$ then there is a root in the interval $(w, -1) \subseteq \bigcup_m ((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1)$, so some interval $((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1)$ contains a real domination root.

Subcase 1.2: $z \in (-1, 0)$

The proof of this subcase follows along that of the previous one. We can assume that $z-\varepsilon > -1$ and $z+\varepsilon < 0$, so that both $(z-\varepsilon+1)^m - 1$ and $(z+\varepsilon+1)^m - 1$ are in $(-1, 0)$. Observe that if we set $b = (z-\varepsilon+1)$ and $a = (z+\varepsilon+1)$, then $1 > a > b > 0$. Note that the intervals $((z-\varepsilon+1)^m - 1, (z+\varepsilon+1)^m - 1) = (b^m - 1, a^m - 1)$ approach -1 from the right, that is, the intervals all lie to the right of -1, and both end points approach -1 monotonically as m increases. Moreover, as

$$b^m - 1 < a^{m+1} - 1 \leftrightarrow 1 < a\left(\frac{a}{b}\right)^m,$$

we conclude that if m is large enough, the right end point of the next interval $(b^{m+1} - 1, a^{m+1} - 1)$ lies inside the previous interval $(b^m - 1, a^m - 1)$. It follows that the union of all the intervals,

$$\bigcup_m ((z-\varepsilon+1)^m - 1, (z+\varepsilon+1)^m - 1),$$

contains an interval $(-1, w)$, with $w \in (-1, 0)$.

We again consider the domination polynomial of the complete bipartite graphs $K_{k,\ell}$, but with equal parts:

$$D(K_{k,k}, x) = (x+1)^{2k} - 2(x+1)^k + 2x^k + 1.$$

Then for k odd, $D(K_{k,k}, -1) = 1 + 2(-1)^k = -1 < 0$. For any $\delta \in (0, 1)$,

$$D(K_{k,k}, -1+\delta) \quad = \quad \delta^{2k} - 2\delta^k + 1 + 2(-1+\delta)^k,$$

which is positive for k sufficiently large. Thus for k large enough, there will be a real domination root in the interval $(-1, -1+\delta)$. By choosing $\delta = w+1$ then there is a root in the interval $(-1, w) \subseteq \bigcup_m ((z-\varepsilon+1)^m - 1, (z+\varepsilon+1)^m - 1)$, so some interval $((z-\varepsilon+1)^m - 1, (z+\varepsilon+1)^m - 1)$ contains a real domination root.

Case 2: $z \in (-\infty, -2)$

We can assume that $z+\varepsilon < -2$. Again, set $a = -(z+\varepsilon+1)$ and $b = -(z-\varepsilon+1)$; note that $b > a > 1$. Note that for odd m the interval $((z-\varepsilon+1)^m - 1, (z+\varepsilon+1)^m - 1) = (-b^m - 1, -a^m - 1)$ has width

$$\begin{aligned}(z+\varepsilon+1)^m - 1 - ((z-\varepsilon+1)^m - 1) \quad &= \quad b^m - a^m \\ &= \quad (b-a)\left(b^{m-1} + b^{m-2}a + \cdots + a^{m-1}\right)\end{aligned}$$

$$\geq \quad 2\varepsilon m a^m,$$

which is unbounded. Thus the width of the interval $((z-\varepsilon+1)^m-1,(z+\varepsilon+1)^m-1)$ can be arbitrarily large. We are seeking a domination root in this interval. If we can show that there is a sequence of real domination roots that tends to $-\infty$ such that the distance between successive roots is bounded, then if m is odd and large enough, there will be a domination root in the interval $((z-\varepsilon+1)^m-1,(z+\varepsilon+1)^m-1)$ and we are done.

Now the domination polynomial of the star $K_{1,k}$ (yet another complete bipartite graph!) is, as noted earlier,

$$D(K_{1,k},x) = x(x+1)^k + x^k.$$

Note that if we set $x = -R$, then

$$-R(1-R)^k + (-R)^k = (-1)^{k+1}(R(R-1)^k - R^k).$$

Thus, setting $g_k(R) = R(R-1)^k - R^k$, we see that R is a root of g_k iff $-R$ is a root of $D(K_{1,k},x)$, so we turn our attention to g_k for the time being. Note that $g_k(R) = 0$ iff

$$\left(\frac{R}{R-1}\right)^k \quad = \quad R \tag{5.7}$$

Clearly on $(1,\infty)$, the left side of (5.7), $\left(\frac{R}{R-1}\right)^k$, is a decreasing function of R while the right side, R is obviously increasing. So there is exactly one solution to (5.7), and hence exactly one root, say r_k, of g_k, in $(1,\infty)$ (it is the unique place where g_k changes sign from negative to positive). Moreover, $r_{k+1} > r_k$, as

$$\begin{aligned} g_{k+1}(r_k) &= r_k(r_k-1)^{k+1} - r_k^{k+1} \\ &= (r_k-1)r_k(r_k-1)^k - r_k^{k+1} \\ &= (r_k-1)r_k^k - r_k^{k+1} \\ &= -r_k^k \\ &< 0. \end{aligned}$$

What about the differences between successive roots r_k? First of all, the derivative of $g_{k+1}(x) = x(x-1)^{k+1} - x^{k+1}$ is

$$g'_{k+1}(x) \quad = \quad (x-1)^{k+1} + (k+1)x(x-1)^k - (k+1)x^k$$

$$= (x-1)^{k+1} + (k+1)g_k(x),$$

and so

$$\begin{aligned} g''_{k+1}(x) &= (k+1)(x-1)^k + (k+1)g'_k(x) \\ &= (k+1)(x-1)^k + (k+1)((x-1)^k + kg_{k-1}(x)). \end{aligned}$$

As $r_{k-1} > 1$, the second derivative of $g_{k+1}(x)$ is clearly non-negative on the interval $[r_{k-1}, \infty)$. Noting from above that $g_{k+1}(r_k) = -r_k^k$, it follows that

$$\begin{aligned} r_k^k &= g_{k+1}(r_{k+1}) - g_{k+1}(r_k) \\ &= \int_{r_k}^{r_{k+1}} g'_{k+1}(x)\ dx \\ &\geq (r_{k+1} - r_k)g'_{k+1}(r_k) \\ &= (r_{k+1} - r_k)(r_k - 1)^{k+1}. \end{aligned}$$

Since $(r_k - 1)^{k+1} = (r_k - 1)(r_k - 1)^k = (r_k - 1)r_k^{k-1}$, we find that

$$r_{k+1} - r_k \leq \frac{r_k}{r_k - 1} \leq \frac{r_1}{r_1 - 1} = 2.$$

Thus, returning back to the domination polynomial of stars, it follows that $-r_i, -r_2, \ldots,$ is a decreasing sequence of negative domination roots (of stars) that tend to $-\infty$, and that have distance bounded between successive terms. It follows that *any* sufficiently large subinterval of the negative real axis will contain such a term, and thus we see that for large enough m, the interval $((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1)$ will contain (at least) one of these, and we have completed this case as well.

In all cases, there is always a real domination root in an interval $((z - \varepsilon + 1)^m - 1, (z + \varepsilon + 1)^m - 1)$, so we conclude that the real domination roots are dense in the interval $(-\infty, 0]$. $\square$

While showing the closure of the real domination roots, the proof of Theorem 5.3.2 omitted $z = 0$, -1, and -2 (although these "holes" are filled in the closure). It should be noted 0 and -2 are both domination roots of $D(K_2, x)$. However, Oboudi [73] showed that -1 (and all other odd integers) are not domination roots. Moreover 0 and -2 are conjectured [2] to be the only rational domination roots.

Chapter 6

Conclusion

In this thesis we have discussed four different problems related in some way to the domination polynomial. In this final chapter, we will focus on what open problems and conjectures arise from our work.

6.1 Optimal Domination Polynomials

In Chapter 2 we completely characterized the existence of (n, m)-optimal graphs. Recall $\mathcal{S}_{n,m}$ is the collection of all simple graphs with n vertices and m edges. Furthermore a graph $G \in \mathcal{S}_{n,m}$ is (n, m)-optimal if for all $H \in \mathcal{S}_{n,m}$ we have $D(G, x) \geq D(H, x)$ for all $x \geq 0$. A natural next step is to consider (n, m)-least optimal graphs. That is, does there exist a graph $G \in \mathcal{S}_{n,m}$ such for all $H \in \mathcal{S}_{n,m}$ we have $D(G, x) \leq D(H, x)$ for all $x \geq 0$? With Observation 2.2.1 and Lemma 2.2.6 we are easily able to make the following progress to completely characterize (n, m)-least optimal graphs.

Theorem 6.1.1 *Let G be a graph on $n \geq 7$ vertices and $m = \binom{n}{2} - k$, $2 \leq k \leq n-2$ edges. Then an (n, m)-least optimal graph does not exist.*

Proof. By Observation 2.2.1 and Lemma 2.2.6 we know that the graph in $\mathcal{S}_{n,m}$ which minimizes the domination polynomial for values of x as x approaches infinity, will have the smallest minimum degree amongst all graphs in $\mathcal{S}_{n,m}$.

Let G_k be K_n with k edges, each incident to the same vertex, are removed. This is the unique graph of order n and size $m = \binom{n}{2} - k$, $2 \leq k \leq n-2$ that has minimum degree $n - k$. That is, G_k minimizes the domination polynomial for values of x as x approaches infinity. Therefore if an (n, m)-least optimal graph exists, it must necessarily be G_k. Note that the number of universal vertices in this case is $n - k - 1$ and by Lemma 2.2.10, $d_1(G_k) = n - k - 1$. By Observation 2.2.1, it is sufficient to show there exists another graph of order n and size $m = \binom{n}{2} - k$ with fewer universal vertices. If $k > \frac{n}{2}$, then enough edges can be removed such that no vertex is universal - all you need to do is to insure you choose a maximum matching and possibly one other edge so that every vertex was an endpoint of at least one removed edge. If $k \leq \frac{n}{2}$ let G'_k be K_n with the edges of a matching of size k removed. Note G'_k has $n-2k$ universal vertices. As $n-2k < n-k-1$ for $k \geq 2$ then an (n,m)-least optimal graph does not exist. $\square$

Corollary 6.1.2 *If G is an (n,m)-least optimal graph then $G \cong \overline{K_r} \cup H$ where $H \in \{K_{n-r}, K_{n-r} - e\}$ for some $0 \leq r \leq n-1$.*

Proof. Let G be an (n,m)-least optimal graph. By Observation 2.2.1 and Lemma 2.2.7 we know that the graph in $\mathcal{S}$ which minimizes the domination polynomial for values of x as x approaches infinity will have the largest number of isolated vertices. Therefore for some $0 \leq r \leq n$ and least optimal graph H of order $n-r$, we have $G \cong \overline{K_r} \cup H$. In order for G to have the maximum number of isolated vertices, H must contain at least $\binom{n-r-1}{2} + 1$ edges. As all of the edges of G are contained in H, we have that $m = \binom{n-r}{2} - k$, where $0 \leq k \leq n-r-2$. By Theorem 6.1.1, no least optimal graphs exist for $2 \leq k \leq n-r-2$ therefore $k \in \{0,1\}$ and we obtain our result. $\square$

It remains an open problem to characterize the values of n and m such that (n,m)-least optimal graphs exist. Appendix A gives all (n,m)-least optimal and (n,m)-optimal graphs up to order 7.

6.2 The Average Order of Dominating Sets of a Graph

In Chapter 3 we discussed the average order of dominating sets of a graph. The most salient open problem is that in Conjecture 3.3.9, namely, $\text{avd}(G) \leq \frac{2n}{3}$ among all connected graphs G of order n. Theorem 3.3.10 showed that $\text{avd}(G) \leq \frac{2n}{3}$ for every quasi-regularizable graph G of order n. Additionally, it follows from Corollary 3.3.8 that if a graph G of order n has minimum degree $\delta \geq 4$, then $\text{avd}(G) \leq \frac{19n}{30}$ and hence the $\frac{2n}{3}$ conjecture holds for almost all graphs. In a recent paper by Erey [46], Conjecture 3.3.9 has been shown to hold for forests.

Another avenue of research is investigating the monotonicity of avd(G) with respect to vertex or edge deletion. For example, the removal of any edge or vertex in a graph does not increase the number of dominating sets. However, this is not necessarily the case for avd(G). Let G be the graph pictured in Figure 6.1.

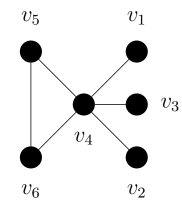


Figure 6.1: A vertex labelled graph

We can conclude that $D(G,x) = x^6 + 6x^5 + 12x^4 + 10x^3 + 5x^2 + x$ and therefore $\text{avd}(G) = 25/7$. However,

- $\text{avd}(G - v_1) = \frac{58}{19} < \text{avd}(G) < \frac{13}{3} = \text{avd}(G - v_4)$,
- $\text{avd}(G - v_5v_6) = \frac{39}{11} < \text{avd}(G) < \frac{78}{19} = \text{avd}(G - v_1v_4)$.

Despite this example, the following conjecture holds for all graphs on up to 7 vertices.

Conjecture 6.2.1 *For every nonempty graph G there exists a vertex v and an edge e such that*

$$\text{avd}(G - v) < \text{avd}(G) < \text{avd}(G - e).$$

6.3 On the Unimodality of Domination Polynomials

Chapter 4 discusses the unimodality of the domination polynomial. There are two conjectures which remain open. We first discuss Conjecture 4.1.1, which posits that every domination polynomial is unimodal. Theorem 4.3.2 shows Conjecture 4.1.1 is true for graphs with sufficiently high minimum degree ($\delta > 2\ln_2(n)$). However, the conjecture remains elusive for graphs with low minimum degree, and in particular for trees. Another interesting family of graphs to investigate are graphs with universal vertices. We verified using Maple that all graphs of order up to 10 which have universal vertices are unimodal, with mode at either $\lceil \frac{n}{2} \rceil$ or $\lceil \frac{n}{2} \rceil + 1$. It may be possible that a technique similar to the one used in Theorem 4.3.2 can yield some results for this class. Recall that for a graph G of order n, we write $r_i(G)$ for the proportion of subsets of vertices of G with cardinality i which are dominating. That is,

$$r_i(G) = \frac{d_i(G)}{\binom{n}{i}}.$$

We showed that if $r_i(G)$ is sufficiently close to one then $D(G,x)$ is unimodal with mode $\lceil \frac{n}{2} \rceil$. If a graph G with n vertices has a universal vertex then $d_i(G) \geq \binom{n-1}{i-1}$ and hence $r_i(G) \geq \frac{i}{n}$.

The second conjecture, Conjecture 4.4.3, claims the coefficients of the domination polynomial are non-increasing after the two-thirds mark. Theorem 4.4.2 shows that if a graph has no isolated vertices, then $d_i(G) \leq d_{i-1}(G)$ for $i \geq \frac{3n+1}{4}$. It would certainly be worthwhile to investigate further the last half of the coefficients sequence for graphs with isolated vertices, and the third quarter for those without.

There are many parallels between the results in Chapter 3 and Chapter 4. In particular Theorem 4.3.2 and Theorem 3.2.4 which together show that if a graph has minimum degree $\delta > 2\ln_2(n)$, it is unimodal with mode and mean size at roughly half the number of vertices. This brings two question to the forefront: Can the mean and mode be far apart? And what is the *median* size of dominating sets?

For the former, we observed all graphs up to nine vertices are unimodal with a mode within one of both the mean and median size of dominating sets. For the median size, we have the following two results which together parallel the results in Theorem 4.3.2 and Theorem 3.2.4.

Theorem 6.3.1 *For any graph G on n vertices, the median size of dominating sets in G is at least $\frac{n}{2}$.*

Proof. Proposition 3.2.3 states that for any graph G on n vertices and all $k \leq \frac{n}{2}$, we have $d_{n-k}(G) \geq d_k(G)$. Therefore

$$\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} d_i(G) \leq \sum_{i=\lceil \frac{n}{2} \rceil}^{n} d_i(G),$$

and hence the median size of dominating sets in G is at least $\frac{n}{2}$. $\square$

Theorem 6.3.2 *If G is a graph with $n \geq 2$ vertices with minimum degree $\delta(G) \geq 2\log_2(n)$ then the median size of dominating sets in G is $\lceil \frac{n}{2} \rceil$.*

Proof. Let G be a graph of order n with minimum degree $\delta \geq 2\log_2(n)$. For now let n be even; the proof when n is odd will follow from the even case. From Theorem 6.3.1, the median size of dominating sets in G is at least $\frac{n}{2}$. Therefore it suffices to show that the median size of dominating sets in G is at most $\frac{n}{2}$. From Proposition 3.2.3, we have $d_{n-i}(G) \geq d_i(G)$ for all $i \leq \frac{n}{2}$. Therefore it is sufficient to show that

$$\sum_{i=0}^{\frac{n}{2}-1}(d_{n-i}(G) - d_i(G)) \leq d_{\frac{n}{2}}(G).$$

Recall from the proof of Theorem 4.3.2 that

$$r_i(G) = \frac{d_i(G)}{\binom{n}{i}} \leq 1$$

and

$$r_i(G) \geq 1 - \frac{n\binom{n-\delta-1}{i}}{\binom{n}{i}} \geq 1 - (n-i)\left(\frac{n-i}{n}\right)^{\delta}.$$

We can now obtain

$$r_{\frac{n}{2}}(G) \geq 1 - \left(n - \frac{n}{2}\right)\left(\frac{1}{2}\right)^{2\log_2(n)} = 1 - \frac{n}{2}\left(\frac{1}{n^2}\right) = \frac{2n-1}{2n},$$

and

$$\begin{aligned}
\sum_{i=0}^{\frac{n}{2}-1}(d_{n-i}(G) - d_i(G)) &= \sum_{i=0}^{\frac{n}{2}-1}\left(r_{n-i}(G)\cdot\binom{n}{n-i} - r_i(G)\cdot\binom{n}{i}\right)\\
&= \sum_{i=0}^{\frac{n}{2}-1}\binom{n}{i}\cdot(r_{n-i}(G) - r_i(G))\\
&\leq \sum_{i=0}^{\frac{n}{2}-1}\binom{n}{i}\cdot\left(1 - \left(1 - \frac{n\binom{n-\delta-1}{i}}{\binom{n}{i}}\right)\right)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=0}^{\frac{n}{2}-1} n\binom{n-\delta-1}{i} \\
&\leq n2^{n-\delta-1} \\
&\leq n2^{n-2\log_2(n)-1} \\
&= \frac{n2^{n-1}}{n^2} \\
&= \frac{2^{n-1}}{n}.
\end{aligned}
$$

Finally note that $\binom{n}{\frac{n}{2}}$ is the largest binomial coefficient of the form $\binom{n}{i}$ and is hence larger than the average of all such binomial coefficients. That is

$$\binom{n}{\frac{n}{2}} \geq \frac{2^n}{n+1}.$$

Therefore

$$
\begin{aligned}
d_{\frac{n}{2}}(G) =& r_{\frac{n}{2}}(G)\binom{n}{\frac{n}{2}} \\
\geq& \left(\frac{2n-1}{2n}\right)\left(\frac{2^n}{n+1}\right) \\
=& \frac{(2n-1)2^{n-1}}{n(n+1)} \\
\geq& \frac{2^{n-1}}{n} \\
\geq& \sum_{i=0}^{\frac{n}{2}-1}(d_{n-i}(G) - d_i(G)).
\end{aligned}
$$

Therefore when n is even, the median size of dominating sets in G is exactly $\frac{n}{2} = \lceil \frac{n}{2} \rceil$.

In the case where n is odd, a similar argument will show

$$\sum_{i=0}^{\frac{n-1}{2}-1}(d_{n-i}(G) - d_i(G)) \leq d_{\frac{n-1}{2}}(G) + d_{\frac{n+1}{2}}(G).$$

This implies the median is at either $\frac{n-1}{2}$ or $\frac{n+1}{2}$. However from Theorem 6.3.1, the median is at least $\frac{n}{2}$, and thus in the case when n is odd the median of G must be $\frac{n+1}{2} = \lceil \frac{n}{2} \rceil$ □

One could consider the order of dominating sets in G as a discrete probability distribution. Let X_G be a discrete random variable which represents the order of a randomly selected dominating set in a graph G. Then $Pr_G(X_G = i)$ denotes the probability that $X_G = i$ and

$$Pr(X_G = i) = \frac{d_i(G)}{D(G,1)}.$$

For a graph G on n vertices with minimum degree $\delta \geq 2\log_2(n)$, Theorem 4.3.2, Theorem 3.2.4, and Theorem 6.3.2 imply that the distribution of X_G is unimodal with mean, median, and mode each close to $\frac{n}{2}$. Is it possible that for these graphs, or even *all* graphs G, X_G is approximately normally distributed? In the case where $G = K_n$, X_{K_n} is one dominating set (the empty set) away from being a binomial distribution with $p = \frac{1}{2}$. Therefore, as n gets large, the distribution of X_{K_n} will approach a normal distribution. But what about other graphs? To estimate a normal distribution for X_G we must find the *standard deviation* of X_G. To do so we will determine $E[X_G^2]$, the expected value of X_G^2. Let $d_i = d_i(G)$. Note

$$D''(G,1) + D'(G,1) = \sum_{i=2}^{n} i(i-1)d_i + \sum_{i=0}^{n} id_i = \sum_{i=2}^{n} i^2 d_i - \sum_{i=2}^{n} id_i + \sum_{i=0}^{n} id_i = \sum_{i=0}^{n} i^2 d_i.$$

Therefore,

$$E[X_G^2] = \sum_{i=0}^{n} i^2 Pr(X_G = i) = \sum_{i=0}^{n} \frac{i^2 d_i}{D(G,1)} = \frac{D''(G,x) + D'(G,x)}{D(G,1)},$$

and X_G has standard deviation

$$\sqrt{\frac{D''(G,1) + D'(G,1)}{D(G,1)} - \left(\frac{D'(G,1)}{D(G,1)}\right)^2}.$$

As an example consider the path graph P_{100}. With the use of Excel, we have calculated the mean and standard deviation of $X_{P_{100}}$ to be 62.0013 and 3.6273 respectively, and the median and mode $X_{P_{100}}$ are both 62. In Figure 6.2 we have plotted the exact distribution of $X_{P_{100}}$ as a histogram in blue accompanied by the red line which plots the normal distribution $N(62.0013, 3.6273)$.

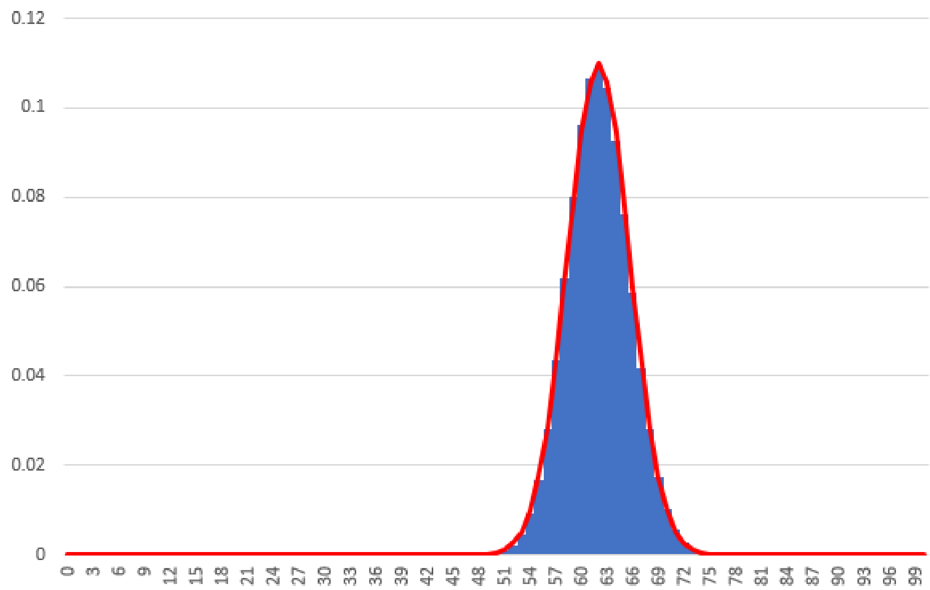


Figure 6.2: The distribution of $X_{P_{100}}$

6.4 The Roots of Domination Polynomials

In Chapter 5 we discussed the roots of the domination polynomial. Theorem 5.3.2 showed the closure of the set of real domination roots is $(-\infty, 0]$. Additionally we showed the family of graphs $C_n \diamond K_1$ is log-concave by determining the location of its domination roots. It may be interesting to further study the location of domination roots for various families of graphs. In particular, are the real domination roots of trees dense in $(-\infty, 0]$? We have already seen in the proof of our main theorem that there are real domination roots of trees (namely stars) that are unbounded, but we do not know if the closure is the entire nonpositive real axis.

Beyond the closure of domination roots, for each order n it is natural to ask which graph has the smallest real domination root? It appears (see Table 6.1) that stars, which we used in case 2, have the extremal roots (and indeed the roots of largest modulus).

Table B.1 in Appendix B gives plots of the domination roots for all graphs up to order 9. The values in Table 6.1 are also the roots of maximum modulus for each order n. There are currently two degree-dependent upper bounds on the modulus of domination roots.

n	Smallest real domination root (and root of maximum modulus)	Graph
1	0	K_1
2	2	$K_{1,1}$
3	-2.618033989	$K_{1,2}$
4	-3.147899036	$K_{1,3}$
5	-3.629658127	$K_{1,4}$
6	-4.079595623	$K_{1,5}$
7	-4.506323246	$K_{1,6}$
8	-4.915076186	$K_{1,7}$
9	-5.309330065	$K_{1,8}$

Table 6.1: Smallest Domination Roots for $n \leq 9$

Theorem 6.4.1 ([73]) *Let G be a graph of order n. Then all roots of $D(G,x)$ lie in the circle with center $(-1,0)$ and the radius $(2^n-1)^{\frac{1}{\delta(G)+1}}$. That is, if $D(G,z)=0$ then $|z+1| \leq (2^n-1)^{\frac{1}{\delta(G)+1}}$.*

Theorem 6.4.2 ([23]) *Let G be a graph without isolated vertices and with maximum degree Δ. If $D(G,z)=0$ then $|z| \leq 2^{\Delta+1}$.*

These results provides a nice bound for graphs with high minimum degree or low maximum degree. In particular if $\delta(G) \geq \frac{n}{2}$ then it follows from Theorem 6.4.1 that the domination roots of G are in the disc $|z+1| < 4$. From this it is not hard to see that the domination roots of almost all graphs are bounded in a disc of fixed radius. Additionally, it follows from Theorem 6.4.2 that the domination roots of P_n and C_n are in the disc $|z| \leq 8$.

We will now give a uniform bound for all graphs which improves each bound for most graphs. We will do so using the *Eneström-Kakeya Theorem* which bounds the roots of a polynomial f in an annulus determined by the ratio of consecutive coefficients or f.

Theorem 6.4.3 (*Eneström-Kakeya* [45,65]) *If $f(x) = a_0 + a_1x + \cdots + a_nx^n$ has positive real coefficients, then all complex roots of f lie in the annulus $r < |z| \leq R$ where*

$$r = \min\left(\frac{a_i}{a_{i+1}} : 0 \leq i \leq n-1\right) \text{ and } R = \max\left(\frac{a_i}{a_{i+1}} : 0 \leq i \leq n-1\right).$$

□

Any dominating set on i vertices can be formed by removing one vertex from a dominating set on $i+1$ vertices. Therefore for any graph G, $(i+1)d(G, i+1) \geq d(G, i)$.

Theorem 6.4.4 *Let G be a graph on n vertices. If z is a root of G then $|z| \leq n$.* □

Each problem discussed in this thesis built upon the work already done for domination polynomials. The open problems raised here will likely fuel further study of the domination polynomial.

Bibliography

[1] G. Aalipour-Hafshejani, S. Akbari, and Z. Ebrahimi. On D-equivalence class of complete bipartite graphs. *Ars Comb.*, 117:275–288, 2014.

[2] S. Akbari, S. Alikhani, M. Oboudi, and Y.-h. Peng. On the zeros of domination polynomial of a graph. *Comb. graphs*, 531:109–115, 2010.

[3] S. Akbari, S. Alikhani, and Y. H. Peng. Characterization of graphs using domination polynomials. *Eur. J. Comb.*, 31:1714–1724, 2010.

[4] S. Akbari and M. R. Oboudi. Cycles are determined by their domination polynomials. *Ars Comb.*, 116:353–358, 2014.

[5] S. Alikhani. On the graphs with four distinct domination roots. *Int. J. Comput. Math.*, 88(13):2717–2720, 2011.

[6] S. Alikhani. *Dominating sets and domination polynomials of graphs*. Lambert Academic Publishing, first edition, 2012.

[7] S. Alikhani. On the D-equivalence Class of a Graph. *Kragujev. J. Math.*, 36:315–321, 2012.

[8] S. Alikhani. On the domination polynomials of non \$P_4\$-free graphs. *Iran. J. Math. Sci. Inform.*, 8(2):49–55, 2013.

[9] S. Alikhani. The Domination Polynomial of a Graph at -1. *Graphs Comb.*, 29:1175–1181, 2013.

[10] S. Alikhani and S. Jahari. Some families of graphs whose domination polynomials are unimodal. *Iran. J. Math. Sci. Informatics*, 12(1):69–80, 2014.

[11] S. Alikhani and S. Jahari. On D-equivalence class of friendship graphs. *Filomat*, 30(1):169–178, 2016.

[12] S. Alikhani, S. Jahari, and R. Hasni. Counting the number of dominating sets of cactus chains. *Optoelectron. Adv. Mater. - Commun.*, 8(9-10):955–960, 2014.

[13] S. Alikhani and Y. H. Peng. Dominating sets and domination polynomials of Cycles. *Glob. J. Pure Appl. Math.*, 4:151–162, 2008.

[14] S. Alikhani and Y. H. Peng. Dominating sets and domination polynomials of paths. *Int. J. Math. Math. Sci.*, 10:1–10, 2009.

[15] S. Alikhani and Y. H. Peng. Dominating sets and domination polynomials of certain graphs. II. *Opusc. Math.*, 30:37–51, 2010.

[16] S. Alikhani and Y. H. Peng. Domination polynomials of cubic graphs of order 10. *Turkish J. Math.*, 35:355–366, 2011.

[17] S. Alikhani and Y. H. Peng. Introduction to domination polynomial of a graph. *Ars Comb.*, 114:257–266, 2014.

[18] E. O. Andriantiana, V. R. Misanantenaina, and S. Wagner. The average size of independent sets of graphs. *Eur. J. Math.*, 6(2):561–576, 2020.

[19] E. O. Andriantiana, V. R. Misanantenaina, and S. Wagner. The Average Size of Matchings in Graphs. *Graphs Comb.*, 36(3):539–560, 2020.

[20] B. M. Anthony and M. E. Picollelli. Complete r-partite Graphs Determined by their Domination Polynomial. *Graphs Comb.*, 31:1993–2002, 2015.

[21] J. L. Arocha and B. Llano. Mean Value for the Matching and Dominating Polynomial. *Discuss. Math.*, 20:57–69, 2000.

[22] Y. Ath and M. Sobel. Some conjectured uniformly optimal reliable networks. *Probab. Engrg. Inform. Sci.*, 14:375–383, 2011.

[23] F. Bencs, G. Regts, and P. Csikvári. Some applications of wagner's weighted subgraph counting polynomial. *Pre-print*, 2020.

[24] C. Berge. *Some common properties for regularizable graphs, edge-critical graphs and B-graphs*, volume 108. Springer-Verlag, Berlin, 1980.

[25] G. Birkhoff. A Determinant Formula for the Number of Ways of Coloring a Map. *Ann. Math.*, 14:42–46, 1912.

[26] M. Blidia, M. Chellali, T. W. Haynes, and M. A. Henning. Independent and double domination in trees. *Util. Math.*, 70, 2006.

[27] F. Boesch, X. Li, and C. Suffel. On the existence of uniformly optimally reliable networks. *Networks*, 21:181–194, 1991.

[28] F. T. Boesch and C. L. Suffel. Least Reliable Networks and the Reliability Domination. *IEEE Trans. Comm.*, 38:2004–2009, 1990.

[29] F. Brenti. Log-concave and unimodal sequences in algebra, combinatorics, and geometry: an update. *Jerusalem Comb.*, 178:71–89, 1994.

[30] F. Brenti, G. F. Royle, and D. G. Wagner. Locations of Zeros of Chromatic and Related Polynomials of Graphs. *Canad. J. Math*, 46:55–80, 1994.

[31] D. Brod and Z. law Skupien. Trees with extremal numbers of dominating sets. *Australas. J. Comb.*, 35:273–290, 2006.

[32] J. Brown and L. Mol. On the roots of all-terminal reliability polynomials. *Discrete Math.*, 340(6)::1287–1299, 2017.

[33] J. I. Brown. *Discrete Structures and Their Interactions*. Chapman and Hall, 2016.

[34] J. I. Brown and C. J. Colbourn. Roots of the Reliability Polynomials. *SIAM J. Discret. Math.*, 5(4):571–585, 1992.

[35] J. I. Brown and D. Cox. Nonexistence of Optimal Graphs for All Terminal Reliability. *Networks*, 63:146–153, 2014.

[36] J. I. Brown and D. Cox. Optimal Graphs for Independence and k -Independence Polynomials. *Graphs Comb.*, 34(6):145–157, 2018.

[37] J. I. Brown and J. Tufts. On the Roots of Domination Polynomials. *Graphs Comb.*, 30(3):527–547, 2014.

[38] M. Chudnovsky and P. Seymour. The roots of the independence polynomial of a clawfree graph. *J. Comb. Theory, Ser. B*, 97:350–357, 2007.

[39] W. E. Clark and S. Suen. An Inequality Related to Vizing ' s Conjecture. *Electron. J. Comb.*, 7(1):2–4, 2000.

[40] C. J. Colbourn. *The Combinatorics of Network Reliability*. Oxford University Press, Oxford and New York, 1987.

[41] J. N. Darroch. On the Distribution of the Number of Successes in Independent Trials. *Ann. Math. Stat.*, 35(3):1317–1321, 1964.

[42] K. Dohmen and P. Tittmann. Domination reliability. *Electron. J. Comb.*, 19:1–14, 2012.

[43] F. Dong, K. Koh, and K. Teo. *Chromatic Polynomials and Chromaticity of Graphs.* World Scientific Publishing, Singapore, 2005.

[44] J. Doyle and J. Graver. Mean Distance in a Graph. *Discrete Math.*, 17:147–154, 1977.

[45] G. Enestrom. Harledning af en allman formel for antalet pensionarer, som vid en godtyeklig tidpunkt forefinnas inom en sluten pensionslcassa. *O fversigt af Vetenskaps-Akademiens Foorhandlingar*, 50:405–415, 1893.

[46] A. Erey. On the average order of a dominating set of a forest. *Pre-print*, 2021.

[47] R. Frucht and F. Harary. On the corona of two graphs. *Aequationes Math*, 4:322–324, 1970.

[48] D. Gross and J. Saccoman. Uniformly optimal reliable graphs. *Networks*, 31:217–225, 1991.

[49] I. Gutman and F. Harary. Generalizations of the matching polynomial. *Util. Math.*, 24:97–106, 1983.

[50] Y. O. Hamidoune. On the Numbers of independent k-Sets in a Claw Free Graph. *J. Comb. Theory, Ser. B*, 50:241–244, 1990.

[51] F. Harary and T. W. Haynes. Double domination in graphs. *Ars Comb.*, 55:201–213, 2000.

[52] J. Haslegrave. Extremal results on average subtree density of series-reduced trees. *J. Comb. Theory, Ser. B*, 107:26–41, 2014.

[53] S. T. Hedetniemi and R. C. Laskar. Bibliography on Domination in Graphs and Some Basic Definitions of Domination Parameters. *Ann. Discret. Math.*, 48:257–277, 1991.

[54] O. Heilmann and E. Lieb. Theory of Monomer-Dimer Systems. *Commun. Math. Phys.*, 25(3):190–232, 1972.

[55] M. Henning. Trees with equal average domination and independent domination numbers. *Ars Comb.*, 71:305–318, 2004.

[56] W. Hoeffding. Probability inequalities for sums of bounded random variables. *J. Am. Stat. Assoc.*, 301(58):13–30, 1963.

[57] T. Honjo, K. i. Kawarabayashi, and Nakamoto A. Dominating sets in triangulations on surfaces. *J. Graph Theory*, 63(1):17–30, 2010.

[58] D. G. C. Horrocks. Note: The Numbers of Dependent k-Sets in a Graph Are Log Concave. *J. Comb. Theory, Ser. B*, 84:180–185, 2002.

[59] Y. Hou and W.-C. Shiu. The Spectrum of the Edge Corona of two Graphs. *Electron. J. Linear Algebr.*, 20:586–594, 2010.

[60] J. Huh. Milnor Numbers of Projective Hypersurfaces and the Chromatic Polynomial of Graphs. *J. Am. Math. Soc.*, 25(3):907–927, 2012.

[61] B. Jackson. A zero-free interval for chromatic polynomials of graphs. *Comb. Probab. Comput.*, 2:325–336, 1993.

[62] S. Jahari and S. Alikhani. On D-equivalence classes of some graphs. *Bull. Georg. Natl. Acad. Sci.*, 10:2016, 2015.

[63] R. E. Jamison. On the Average Number of Nodes in a Subtree of a Tree. *J. Comb. Theory, Ser. B*, 35:207–223, 1983.

[64] R. E. Jamison. Monotonicity of the Mean Order of Subtrees. *J. Comb. Theory, Ser. B*, 37:70–78, 1984.

[65] S. Kakeya. On the limits of the roots of an algebraic equation with positive coefficients. *Tohoku Math. J.*, 2:140–142, 1912.

[66] A. K. Kelmans. On graphs with randomly deleted edge. *Acta Math Acad Sci Hung*, 37:197–214, 1981.

[67] T. Kotek, J. Preen, F. Simon, P. Tittmann, and M. Trinks. Recurrence relations and splitting formulas for the domination polynomial. *Electron. J. Comb.*, 19:1–27, 2012.

[68] C. Krattenthaler. Note Combinatorial Proof of the Log-Concavity of the Sequence of Matching Numbers. *J. Comb. Theory, Ser. A*, 74:351–354, 1996.

[69] F. Lazebnik. On the greatest number of 2 and 3 colorings of a (V,E)-graph. *J. Graph Theory*, 13:203–214, 1989.

[70] V. E. Levit and E. Mandrescu. The independence polynomial of a graph - a survey. *Proc. 1st Int. Conf. Algebr. Informatics*, 5:231–252, 2005.

[71] L. Matheson and Tarjan R.E. Dominating sets in planar graphs. *Eur. J. Comb.*, 17(6):565–568, 1996.

[72] W. Myrvold, K. Cheung, L. Page, and J. Perry. Uniformly most reliable networks do not always exist. *Networks*, 21:417–419, 1991.

[73] M. R. Oboudi. On the roots of domination polynomial of graphs. *Discret. Appl. Math.*, 205:126–131, 2016.

[74] T. Pino, S. Choudhury, and F. Al-turjman. Dominating Set Algorithms for Wireless Sensor Networks Survivability. *IEEE Access*, 6:17527–17532, 2018.

[75] G. Royle and A. D. Sokal. The Brown – Colbourn conjecture on zeros of reliability polynomials is false. *J. Comb. Theory, Ser. B*, 91:345–360, 2004.

[76] N. J. W. S. Beraha, J. Kahane. Limits of zeroes of recursively defined polynomials. *Proc. Natl. Acad. Sci.*, 72(11):4209, 1975.

[77] A. Sakaloglu and A. Satyanarayana. Graphs with the least number of colourings. *J. Graph Theory*, 19:523–533, 1995.

[78] M. Saks and N. Linial. Every poset has a central element. *J. Comb. Theory, Ser. A*, 40(2):195–210, 1985.

[79] C. Shen and T. Li. 23rd International Conference on Computational Linguistics. In *Multi-Document Summ. via Minim. Domin. Set*, pages 984–992, 2010.

[80] I. Simonelli. Optimal graphs for chromatic polynomials. *Discrete Math.*, 308(11):2228–2239, 2008.

[81] A. D. Sokal. Bounds on the Complex Zeros of (Di) Chromatic Polynomials and Potts-Model Partition Functions. *Comb. Probab. Comput.*, 10:41–77, 2001.

[82] S. Spacapan. The domination number of plane triangulations. *J. Comb. Theory, Ser. B*, 143:42–64, 2020.

[83] B. O. Stjan, B. R. E. Sar, P. Dorbec, W. Goddard, B. L. Hartnell, M. A. Henning, S. K. Zar, and D. F. Rall. Vizing's conjecture: a survey and recent results. *J. Graph Theory*, 69(1):46–76, 2012.

[84] C. Thomassen. The zero-free intervals for chromatic polynomials of graphs. *Comb. Probab. Comput.*, 6:497–506, 1997.

[85] A. Vince. The average size of a connected vertex set of a graph-Explicit formulas and open problems. *J. Graph Theory*, 97:82–103, 2021.

[86] A. Vince and H. Wang. The average order of a subtree of a tree. *J. Comb. Theory, Ser. B*, 100(2):161–170, 2010.

[87] V. G. Vizing. Some unsolved problems in graph theory. *Usp. Mat. Nauk*, 23(6):117–134, 1968.

[88] S. Wagner and H. Wang. On the Local and Global Means of Subtree Orders. *J. Graph Theory*, 70560:154–166, 2015.

[89] D. B. West. *Introduction to Graph Theory.* Prentice Hall, Upper Saddle River, 1996.

Appendix A

Optimal Graphs of Small Order

Table A.1 gives all (n,m)-least optimal and (n,m)-optimal graphs up to order 7. A dash $-$ represents when an optimal graph does not exist for a given order and size.

Order n	Size m	(n,m)-least optimal graph	(n,m)-optimal graph
1	0	K_1	K_1
2	0	$\overline{K_2}$	$\overline{K_2}$
2	1	K_2	K_2
3	0	$\overline{K_3}$	$\overline{K_3}$
3	1	$K_1 \cup K_2$	$K_1 \cup K_2$
3	2	$K_{1,2}$	$K_{1,2}$
3	3	K_3	K_3
4	0	$\overline{K_4}$	$\overline{K_4}$
4	1	$\overline{K_2} \cup K_2$	$\overline{K_2} \cup K_2$
4	2	$K_1 \cup K_{1,2}$	$K_2 \cup K_2$
4	3	$K_1 \cup K_3$	$-$
4	4	$-$	$-$
4	5	$K_4 - e$	$K_4 - e$
4	6	K_4	K_4
5	0	$\overline{K_5}$	$\overline{K_5}$
5	1	$\overline{K_3} \cup K_2$	$\overline{K_3} \cup K_2$
5	2	$\overline{K_2} \cup K_{1,2}$	$K_1 \cup 2K_2$
5	3	$\overline{K_2} \cup K_3$	$K_2 \cup K_{1,2}$
5	4	$-$	$-$
5	5	$\overline{K_2} \cup (K_4 - e)$	$-$
5	6	$\overline{K_2} \cup K_4$	$K_1 \vee 2K_2$
5	7	$-$	$-$

Order n	Size m	(n,m)-least optimal graph	(n,m)-optimal graph
5	8	–	–
5	9	$K_5 - e$	$K_5 - e$
5	10	K_5	K_5
6	0	$\overline{K_6}$	$\overline{K_6}$
6	1	$\overline{K_4} \cup K_2$	$\overline{K_4} \cup K_2$
6	2	$\overline{K_3} \cup K_{1,2}$	$\overline{K_2} \cup 2K_2$
6	3	$\overline{K_3} \cup K_3$	$3K_2$
6	4	–	–
6	5	$\overline{K_2} \cup (K_4 - e)$	–
6	6	$\overline{K_2} \cup K_4$	–
6	7	–	–
6	8	–	–
6	9	$\overline{K_1} \cup (K_5 - e)$	–
6	10	$\overline{K_1} \cup K_5$	–
6	11	–	–
6	12	–	–
6	13	–	–
6	14	$K_6 - e$	$K_6 - e$
6	15	K_6	K_6
7	0	$\overline{K_7}$	$\overline{K_7}$
7	1	$\overline{K_5} \cup K_2$	$\overline{K_5} \cup K_2$
7	2	$\overline{K_4} \cup K_{1,2}$	$\overline{K_3} \cup 2K_2$
7	3	$\overline{K_4} \cup K_3$	$2K_2 \cup K_{1,2}$
7	4	–	–
7	5	$\overline{K_3} \cup (K_4 - e)$	–
7	6	$\overline{K_3} \cup K_4$	–
7	7	–	–
7	8	–	–

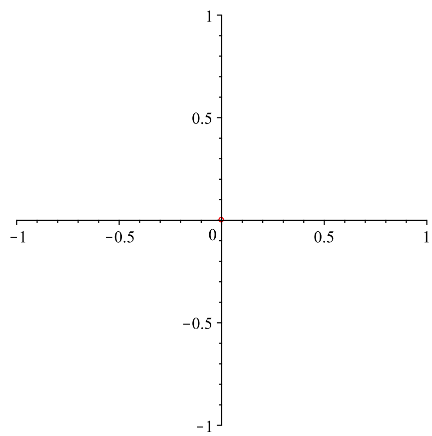
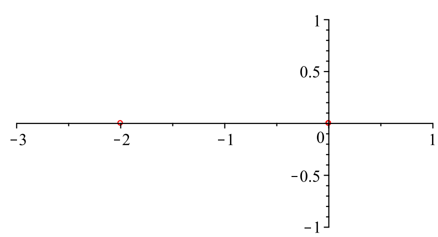
Order n	Size m	(n,m)-least optimal graph	(n,m)-optimal graph
7	9	$\overline{K_2} \cup (K_5 - e)$	–
7	10	$\overline{K_2} \cup K_5$	–
7	11	–	–
7	12	–	–
7	13	–	–
7	14	$\overline{K_1} \cup (K_6 - e)$	–
7	15	$\overline{K_1} \cup K_6$	–
7	16	–	–
7	17	–	–
7	18	–	–
7	19	–	–
7	20	$K_7 - e$	$K_7 - e$
7	21	K_7	K_7

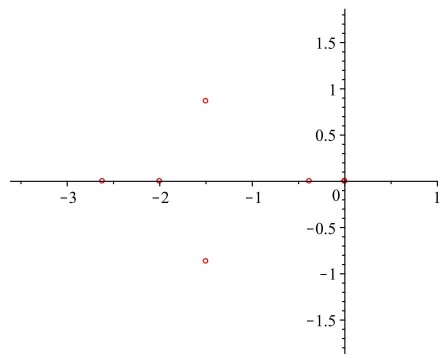
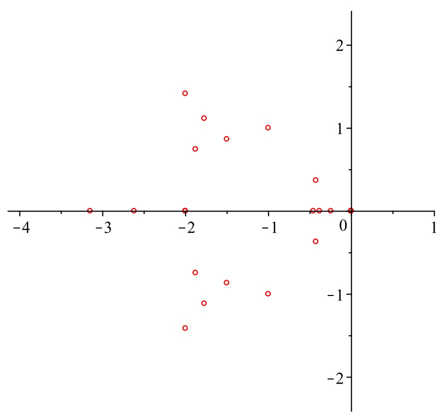
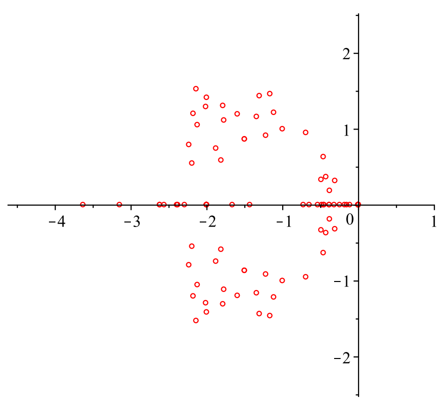
Table A.1: The (n,m)-least optimal and (n,m)-optimal graphs up to order 7

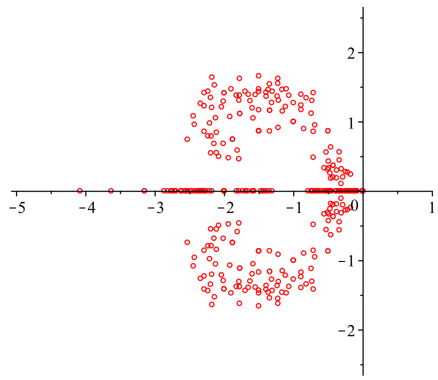
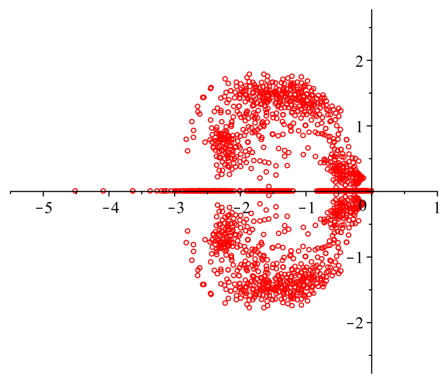
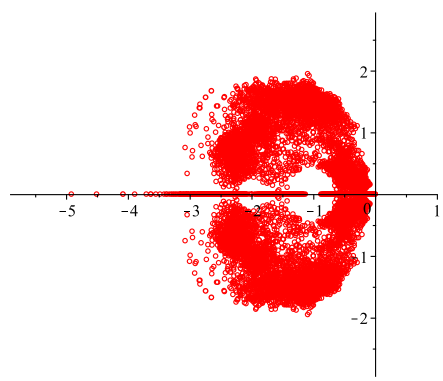
Appendix B

Domination Roots of Small Graphs

Table B.1 gives plots of the domination roots for all graphs up to order 9.

Order n	Domination Roots
1	
2	
Order n	Domination Roots

<table>
<tr><td>3</td><td>
</td></tr>
<tr><td>4</td><td>
</td></tr>
<tr><td>5</td><td>
</td></tr>
<tr><td>Order n</td><td>Domination Roots</td></tr>
</table>

6	
7	
8	
Order n	Domination Roots

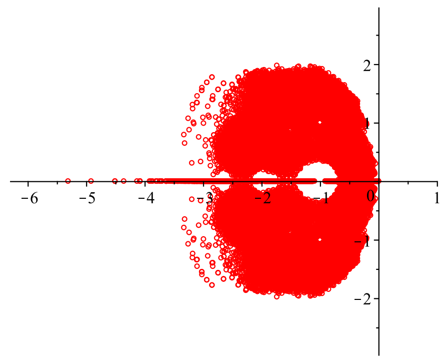
9	

Table B.1: The domination roots for all graphs up to order 9