ON THE NEIGHBOURHOOD POLYNOMIAL

by

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Abstract

The neighbourhood polynomial of a graph G is the polynomial neigh $_G(x) = \sum x^{|S|}$ where the sum is taken over all sets of vertices $S \subset V(G)$ which have a common neighbour in G. We begin with some formulas for computing the neighbourhood polynomial for common families of graphs and graph operations. We then show the neighbourhood polynomial and domination polynomial $D_G(x)$ are linked by the equation $\operatorname{neigh}_G(x) + D_{\overline{G}}(x) = (1+x)^n$, and prove that computing the neighbourhood polynomial is NP-hard. Concerning the roots of the neighbourhood polynomial, we consider when all the roots are real and what bounds we can place on them. We show that the possible rational roots of neighbourhood polynomials are exactly those numbers of the form -1/2n with $n \in \mathbb{N}$. We also answer the question of the closure of the neighbourhood roots, which is $(-\infty, 0]$ for the real roots and all of \mathbb{C} for the complex roots. Finally, we use random graphs to show that almost all neighbourhood polynomials do not have all real roots.

List of Abbreviations and Symbols Used

C_n	Cycle graph on n vertices
$\deg(v)$	Degree of a vertex v
$D_G(x)$	Domination polynomial of a graph G
E(G)	Edge set of a graph G
G[H]	Lexicographic product of graphs G and H
\overline{G}	Complement of a graph G
$G \cup H$	Disjoint union of graphs G and H
i(G,x)	Independence polynomial of a graph ${\cal G}$
K_n	Complete graph on n vertices
$K_{m,n}$	Complete bipartite graph
$\mu(G,x)$	Matching polynomial of a graph G
$\mathcal{N}(G)$	Neighbourhood complex of a graph ${\cal G}$
N(v)	Neighbourhood of a vertex v
$\mathrm{neigh}_G(x)$	Neighbourhood polynomial of a graph ${\cal G}$

 $\pi(G,x)$ Chromatic polynomial of a graph G

 P_n Path graph on n vertices

TP Tadpole Graph

V(G) Vertex set of a graph G

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Chapter 1

Introduction

1.1 Background

Since Birkhoff first defined the chromatic polynomial of a graph in his 1912 paper [2], several graph polynomials have been defined and studied, including the neighbour-hood polynomial. Before we can examine these graph polynomials, we must first discuss a number of graph theory terms and establish the notation we will use. We will begin with a definition of a graph.

Definition 1.1.1. A graph G = (V(G), E(G)) consists of a vertex set V(G) and an edge set E(G) containing unordered pairs of vertices.

Each of the two vertices associated with an edge are called the **endpoints** of the edge. If the two endpoints of an edge are the same, the edge is called a **loop**. **Multiple edges** are edges which have the same pair of endpoints. A **simple graph** has no loops or multiple edges, so each edge has a unique pair of distinct endpoints.

We call a graph **finite** if |V(G)| and |E(G)| are both finite. Every graph we consider will be finite and simple.

Example 1.1.1. Let G be a graph with $V(G) = \{a, b, c, d, e\}$ and $E(G) = \{ab, ac, bd, be, cd, de\}$. Then G is a finite and simple graph. See Figure 1.1 for a visual representation of G.

For any two vertices $u, v \in V(G)$, we say that u and v are **adjacent** and write $u \sim v$ if $uv \in E(G)$.

Definition 1.1.2. Let G be a graph. The **(open) neighbourhood** of a vertex $u \in V(G)$ is the set of all vertices in G adjacent to u, denoted $N_G(u) = \{v \in V(G) \mid u \sim v\}$, or just N(u) when the corresponding graph is made obvious through context. We call the elements of N(u) the **neighbours** of u. The closed neighbourhood $N_G[u] = N_G(u) \cup \{u\}$ includes u as well. For a set of vertices $U \subseteq V(G)$, we define the

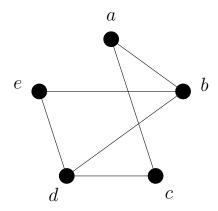


Figure 1.1: Example of a Graph

common neighbourhood N(U) to be the intersection of the neighbourhoods of the vertices contained in U, that is $N(U) = \bigcap_{u \in U} N(u)$. The elements of N(U) are the common neighbours of the set U.

Example 1.1.2. Let G be the graph in Example 1.1.1 and consider vertex a. Since b and c are the only vertices adjacent to a, we can write $a \sim b$ and $a \sim c$. We can also say the neighbourhood of vertex a contains b and c and write $N(a) = \{b, c\}$. Similarly, $N(e) = \{b, d\}$. If we let $U = \{a, e\}$, then their common neighbourhood is $N(U) = \{b\}$, so the only common neighbour of a and e is b.

The **degree** of a vertex v is the size of its neighbourhood, and we say deg(v) = |N(v)|. The **degree sequence** of a graph G is the sequence of the degrees of every vertex of G, written in nonincreasing order.

Example 1.1.3. For the graph G in Example 1.1.1, vertex a has two neighbours, so deg(a) = 2. The degree sequence of G is 3, 3, 2, 2, 2.

The **complement** of a graph G, denoted \overline{G} , is the graph with vertex set $V(\overline{G}) = V(G)$ and edge set $E(\overline{G}) = \{uv \mid u, v \in V(G) \text{ and } uv \notin E(G)\}.$

There are a few families of graphs which arise regularly due to their simplicity, so we will define them here (see Figure 1.2 for some examples of these). The **complete graph** (on n **vertices**), K_n , is the graph with n vertices and all possible edges. The **empty graph** (on n **vertices**), its complement, is denoted $\overline{K_n}$ and has n vertices and no edges. The **path** graph on n vertices, P_n , consists of n vertices $V(P_n) = \{v_1, v_2, \ldots, v_n\}$ and n-1 edges $E(P_n) = \{v_1, v_2, \ldots, v_{n-1}v_n\}$. The

cycle graph on n vertices, C_n , consists of n vertices $V(C_n) = \{v_1, v_2, \dots, v_n\}$ and n edges $E(C_n) = \{v_1v_2, v_2v_3, \dots, v_{n-1}v_n, v_nv_1\}$.

A subgraph H of a graph G has vertex set $V(H) \subseteq V(G)$ and edge set $E(H) \subseteq E(G)$. A subgraph is an **induced subgraph** if $u, v \in V(H)$ and $uv \in E(G)$ implies $uv \in E(H)$. Two vertices u and v are **connected** if G contains as a subgraph a path which starts at u and ends at v. A graph G is **connected** if every pair of vertices $u, v \in V(G)$ is connected. Otherwise, the graph is **disconnected**. The **(connected) components** of a graph are the connected induced subgraphs which are maximal in size.

A tree is a graph which is connected and does not contain a cycle (*i.e.* it is **acyclic**). If a tree T has n vertices, it must have n-1 edges [30]. A **forest** is a (not necessarily connected) graph, all of whose components are trees. A **leaf** is a vertex v of degree deg(v) = 1, so named because every tree other than K_1 has at least one leaf.

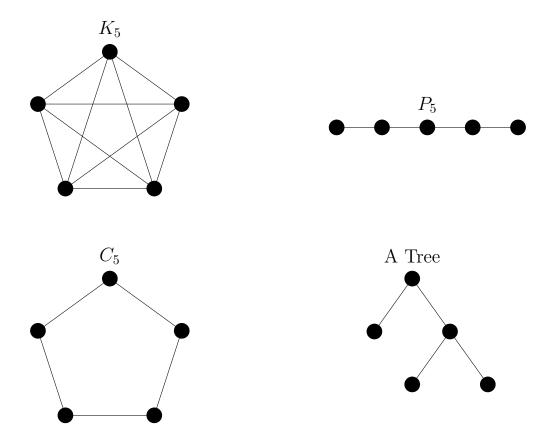


Figure 1.2: Examples of Common Families of Graphs

1.2 Graph Polynomials

A graph polynomial is essentially just a way of assigning a polynomial to a graph, typically defined in such a way that the polynomial encodes useful information from the graph. Many graph polynomials, including the neighbourhood polynomial, can be defined based on an underlying structure called a simplicial complex. Given a finite set X, a simplicial complex or complex on X is a collection \mathcal{C} of subsets of X which is closed under containment. The vertices of the complex are the elements of X and the faces of the complex are the elements of \mathcal{C} . We call the maximal faces with respect to containment the facets or bases of the complex, and the cardinality of the largest face or faces the dimension of the complex.

The **f-vector** or **face-vector** for a complex of dimension d is the vector (f_0, f_1, \ldots, f_d) , where f_i is the number of faces of C with i elements. From this we can define the **f-polynomial**, which is just the generating function of the f-vector,

$$f_{\mathcal{C}}(x) = \sum_{i=0}^{d} f_i x^i.$$

Several different graph polynomials have been studied besides neighbourhood polynomials. One of the first to be defined is the **chromatic polynomial** $\pi(G, x)$, which is a function which maps x to the number of valid colourings of the vertices of G with x colours (a valid **colouring** is one which assigns different colours to adjacent vertices). Initially defined by Birkhoff [2], they have been widely studied [4, 6, 27], including investigations into the behaviour of their roots [8, 10].

As an example, consider the complete graph K_n . For any integer $x \geq n$ we can form a valid colouring by choosing any of x colours for one vertex, then any of the remaining x-1 colours for the next, and by continuing in this manner arrive at $x(x-1)(x-2)\cdots(x-n+1)$ distinct colourings. This process includes every valid colouring of K_n , and so we can conclude that

$$\pi(K_n, x) = x(x-1)(x-2)\cdots(x-n+1).$$

Note that if $0 \le x < n$ then $\pi(K_n, x) = 0$, which correctly encodes the fact that we cannot colour K_n with fewer than n colours. Also, $\pi(K_n, x)$ happens to be a polynomial in x, which was not explicitly guaranteed by our definition, but does in fact happen for any graph [1].

Another example of a graph polynomial is the **independence polynomial**, which is the generating function for the number of independent sets of a graph of various sizes (an **independent set** is a set of vertices which contains no edges). Independence polynomials [11, 14, 19–21, 25, 26, 28] and their roots [9, 12, 13] have attracted considerable interest. Let i_k be the number of independence sets of size k in a graph G with n = |V(G)|. The independence polynomial of G is,

$$i(G, x) = \sum_{k=0}^{n} i_k x^k.$$

Similarly, if we let m_k be the number of matchings with k edges of a graph G with n vertices, then we can use this to define the **matching polynomial** $\mu(G, x)$, where a **matching** is a set of edges of G with no endpoints in common. We assume $m_0 = 1$ since the empty set is a matching with no edges, and let

$$\mu(G, x) = \sum_{k=0}^{n} (-1)^k m_k x^{n-2k}.$$

The matching polynomial has also been the subject of several studies, such as [20–22].

Chapter 2

Neighbourhood Polynomials

The **neighbourhood complex** $\mathcal{N}(G)$ of a graph G with vertex set V is the collection of subsets $S \subset V$ for which every element of S has a common neighbour in G. That is, any face $S \in \mathcal{N}(G)$ is a subset of the neighbourhood of one of the vertices of G. Since any subset of $S \in \mathcal{N}(G)$ will still have the same common neighbour as S, this collection is closed under containment, as required to be a complex.

Definition 2.0.1. The **neighbourhood polynomial** of a graph G with neighbourhood complex $\mathcal{N}(G)$ is the f-polynomial of $\mathcal{N}(G)$, that is,

$$\operatorname{neigh}_G(x) = \sum_{S \in \mathcal{N}(G)} x^{|S|}.$$

We note that the degree of the neighbourhood polynomial is just the maximum degree of the graph.

2.1 Known Formulas for Families of Graphs

In their paper on neighbourhood polynomials, Brown and Nowakowski [15] calculate the neighbourhood polynomials for a number of families of graphs which will be useful to us and which we summarize in Table 2.1. The first of these is the complete graph K_n , for which any set of vertices has a common neighbour, except of course the entire set. Thus the coefficient of x^k in neigh $K_n(x)$ is $\binom{n}{k}$ for all $0 \le k \le n-1$, which can be written more succinctly as

$$neigh_{K_n}(x) = (1+x)^n - x^n.$$

In the case of the path P_n on $n \ge 2$ vertices, every vertex except the two endpoints has a unique pair of neighbours (contributing an x^2 term) and every vertex has a common neighbour (contributing an x term) since there are no isolated vertices.

Family	Neighbourhood Polynomial
Complete Graphs K_n	$\frac{1+x)^n - x^n}{(1+x)^n - x^n}$
Paths P_n	$1 + nx + (n-2)x^2$
Cycles $C_n, n \neq 4$	$1 + nx + nx^2$
Cycles C_n , $n=4$	$1 + 4x + 2x^2$
Complete Bipartite Graphs $K_{m,n}$	$(1+x)^m + (1+x)^n - 1$

Table 2.1: Formulas for the Neighbourhood Polynomial of Common Graph Families

These along with the empty set are the only sets which share a common neighbour, so

$$\operatorname{neigh}_{P_n}(x) = 1 + nx + (n-2)x^2.$$

The cycle graph C_n is very similar to the path, as it can be formed by adding an edge to P_n connecting the two endpoints. With the exception of n = 4, the only effect of this new edge is to add two new pairs of vertices with common neighbours, and so for n = 3 and $n \ge 5$ we have $1 + nx + nx^2$. However, in the case of C_4 , the two newly created pairs are precisely the pairs we started with, and so $\operatorname{neigh}_{C_4}(x) = \operatorname{neigh}_{P_4}(x)$. Overall, this means

$$\operatorname{neigh}_{C_n}(x) = \begin{cases} 1 + nx + nx^2, & n \neq 4\\ 1 + 4x + 2x^2, & n = 4. \end{cases}$$

For the complete bipartite graph $K_{m,n}$, we simply note that any subset of the first partite set has a common neighbour (namely anything in the second partite set), and similarly for subsets of the second partite set. This counts the empty set twice, so after accounting for this we are left with

$$neigh_{K_{m,n}}(x) = (1+x)^m + (1+x)^n - 1.$$

Finally, given the degree sequence of the graph, which can be found in polynomial time, we can roughly approximate the neighbourhood polynomial by counting every possible subset of the neighbourhoods of each vertex, that is,

$$\operatorname{neigh}_{G}(x) \approx \sum_{v \in V(G)} (1+x)^{\operatorname{deg}(v)}.$$

Of course, this overcounts any sets of vertices with multiple common neighbours. For the empty set and individual vertices, it is not too difficult to account for this overcounting, and so a first order approximation was found for a graph G with n vertices and m edges.

$$\operatorname{neigh}_{G}(x) = \sum_{v \in V(G)} (1+x)^{\operatorname{deg}(v)} - (2m-n)x - (n-1). \tag{2.1}$$

This still overcounts sets of size two or larger which have multiple common neighbours, but if such a set exists then G must have C_4 as a subgraph, although not necessarily an induced one. If we call graphs which do not have C_4 as a subgraph C_4 -free, then the above approximation is exact for the family of C_4 -free graphs.

Theorem 2.1.1. [15] For a C_4 -free graph G with n vertices and m edges, equation 2.1 holds.

This implies that for C_4 -free graphs, the neighbourhood polynomial depends only on the degree sequence of the graph.

2.2 Graph Operations

One graph operation whose effect on the neighbourhood polynomial is simple to track is that of adding a leaf to a graph. If G is a graph with a leaf u, then u has exactly one neighbour, say v. Then any set of vertices in G-u with a common neighbour will also have a common neighbour in G. In addition, any subset of the neighbourhood of v in G-u along with the vertex u will form a set of vertices in G that has v as a common neighbour. As long as v has another neighbour, these are the only new elements of the neighbourhood complex formed by adding a leaf, so we can relate the neighbourhood polynomials of G and G-u.

Proposition 2.2.1. Let G be a graph with a vertex u of degree 1 (i.e. a leaf), where the only neighbour of u is v of degree $\deg(v) \geq 2$. Then,

$$\operatorname{neigh}_{G}(x) = \operatorname{neigh}_{G-u}(x) + x(1+x)^{\deg(v)-1}.$$

Proof. The result follows immediately from the preceding discussion by noting that v has deg(v) - 1 neighbours in G - u.

Note that the condition that $deg(v) \geq 2$ is required, or else adding the leaf u will add $\{v\}$ to the neighbourhood complex by giving v a neighbour. This does not happen in any other case and so will not be counted correctly by the formula.

Leaves are of special interest in the study of one particular family of graphs of course, trees. Since every tree except K_1 and K_2 has a leaf which satisfies the condition for Proposition 2.2.1, we can use the proposition as a reduction formula for the neighbourhood polynomials of trees. This gives us another way to write the neighbourhood polynomial of a tree.

Theorem 2.2.2. Let T be a tree with $n = |V(T)| \ge 2$, and define,

$$L = \{ v \in V(T) \mid \deg(v) = 1 \},$$

the set of leaves of T. Then,

$$\operatorname{neigh}_{T}(x) = 1 + 2x + \sum_{v \in V(G) \setminus L} \sum_{k=1}^{\deg(v)-1} x(1+x)^{k}.$$
 (2.2)

Proof. Starting with the tree T, we can remove leaves one by one until we are left with only a single edge, the graph K_2 . Alternatively, starting with the graph K_2 , for which $\operatorname{neigh}_{K_2}(x) = 1 + 2x$, we can construct T by iteratively adding a leaf n-2 times. We can track the effect of this process on the neighbourhood polynomial by using Proposition 2.2.1.

If $v \in L$, then v is a leaf in the final graph T so we never add a leaf to it. Otherwise, $\deg(v) \geq 2$, so at some point in our construction of T we added $\deg(v) - 1$ leaves to v.

The first of these was added when v was a leaf itself, the second when v had 2 neighbours, and in general when we add the k^{th} leaf to v in this process it has k neighbours, so adding leaves to v adds

$$\sum_{k=1}^{\deg(v)-1} x (1+x)^k$$

to the neighbourhood polynomial of the tree. Summing this over every non-leaf of T gives us the total effect of this construction on the neighbourhood polynomial. Since we start with $\operatorname{neigh}_{K_2}(x) = 1 + 2x$, we are left with our result.

Corollary 2.2.3. If T is a tree with $n \geq 3$ vertices, then,

•
$$\operatorname{neigh}_{T}(-1) = -1$$
, and,

- $\operatorname{neigh}_{T}(-1/2) < 0$, and,
- $\operatorname{neigh}_{T}(x) = 0 \text{ for some } x \in (-1/2, 0).$

Proof. If we let x = -1 in (2.2), then every term involving a power of 1 + x vanishes and we are left with $\operatorname{neigh}_T(-1) = 1 + 2(-1) = -1$. If instead we let x = -1/2, the first two terms sum to zero and we note that every term in the double sum will be negative, as they are the product of -1/2 and a power of 1/2. Since $n \geq 3$, there is at least one term in the double sum, so $\operatorname{neigh}_T(-1/2) < 0$. Finally, we know $\operatorname{neigh}_T(0) = 1$ because this is true for any neighbourhood polynomial, and since this is positive we must have a root in the interval (-1/2,0) by the Intermediate Value Theorem.

Note that this says the neighbourhood polynomial of every tree on three or more vertices has a real root in the interval (-1/2,0). This is interesting to us, as many graphs have neighbourhood polynomials without any real roots.

Another graph operation which interacts well with the neighbourhood polynomial is the lexicographic product of a graph G with the empty graph $\overline{K_n}$, as shown by Brown and Nowakowski [15].

Proposition 2.2.4. [15] For any graph G with neighbourhood polynomial $\operatorname{neigh}_G(x)$, the neighbourhood polynomial of the lexicographic product $G[\overline{K_n}]$ is,

$$\operatorname{neigh}_{G[\overline{K_n}]}(x) = \operatorname{neigh}_G((1+x)^n - 1).$$

Proof. For any set S of vertices with a common neighbour in G, we can replace each vertex in S with a nonempty subset of the n corresponding vertices in $G[\overline{K_n}]$ to get a set of vertices in $G[\overline{K_n}]$ with a common neighbour. This is accounted for by substituting $(1+x)^n-1$ into the original generating function $\operatorname{neigh}_G(x)$. Since the vertices of G were replaced with empty graphs, every set of vertices with a common neighbour in $G[\overline{K_n}]$ has the above form, so we are done.

2.3 Relationship with the Domination Polynomial

The neighbourhood polynomial of a graph G is directly related to the domination polynomial of the complement graph \overline{G} . To draw the connection, we need a pair of definitions.

Definition 2.3.1. For a graph G with vertex set V(G), a set $S \subset V(G)$ is a **dominating set** if every vertex $v \notin S$ is adjacent to a vertex in S.

Definition 2.3.2. For a graph G with d_k dominating sets of size k, the **domination** polynomial of G, denoted $D_G(x)$, is

$$\sum_{k=1}^{n} d_k x^k = \sum_{S} x^{|S|},$$

where the second sum is taken over all dominating sets S.

We can now relate this to the neighbourhood polynomial.

Theorem 2.3.1. For any graph G on n vertices, the following equation holds.

$$\operatorname{neigh}_{G}(x) + D_{\overline{G}}(x) = (1+x)^{n}$$

Proof. The theorem relies on the fact that a set of vertices S with a common neighbour in G corresponds directly to a non-dominating set in \overline{G} and vice versa, as first noted in [5].

If S has a common neighbour $v \notin S$ in G, then there are no edges between v and any element of S in \overline{G} . Thus, S is not a dominating set of \overline{G} since v is not in S nor is it adjacent to any element of S.

If S is a non-dominating set of \overline{G} , then there exists a vertex $v \notin S$ which is not adjacent to any element of S in \overline{G} . Therefore v is adjacent to every element of S in G, so S has a common neighbour in G, namely v.

This tells us that the neighbourhood polynomial of G is equal to the generating function for the non-dominating sets of \overline{G} . Since every subset of the vertices of G is either dominating or not (and not both), and because the generating function for any subset of the n vertices is $(1+x)^n$, the generating function for the non-dominating polynomial of \overline{G} is simply $(1+x)^n - D_{\overline{G}}(x)$. Setting this equal to neigh_G(x) and rearranging yields the result.

This result allows us to extend knowledge about the neighbourhood polynomial to the domination polynomial. Each of the formulas in Section 2.1 can be used to find the dominating polynomial of the complementary graph. For example,

$$D_{\overline{K_n}}(x) = (1+x)^n - \operatorname{neigh}_{K_n}(x) = x^n,$$

though this is more easily derived by noting that the entire vertex set is the only dominating set of the empty graph.

2.4 Complexity

The formulas and relationships mentioned throughout this chapter are useful for computing the neighbourhood polynomials of specific graphs, but there is no known efficient method for computing the neighbourhood polynomial of an arbitrary graph. In order to clarify what we consider efficient and ultimately show that computing the neighbourhood polynomial is difficult in general, we must discuss some complexity theory.

In their book [17] on the subject, Garey and Johnson define a number of terms useful to us and for which we will give an informal overview. A **decision problem** is a problem which, for each given input, can only have a "yes" or "no" answer. If an algorithm runs for at most $O(n^k)$ simple operations (e.g. addition, multiplication) for any input of size n and some fixed natural number k, then we say that the algorithm requires **polynomial time** to run. If a polynomial time algorithm exists which will solve a decision problem, we say that the decision problem belongs to class \mathbf{P} .

If it is possible to verify that the answer to a decision problem is "yes," given some additional information (called a **certificate**), then we say that the decision problem belongs to class \mathbf{NP} . For example, while determining if a large number can be factored may be difficult, only one division operation is required to verify a number can be factored if we are given a factor, so the decision problem "can N be factored?" is in NP.

The class **NP-complete** contains decision problems in NP which any member of NP can be reduced to in polynomial time. In other words, we mean that if an algorithm A exists to solve a NP-complete problem X, then for any problem Y in NP there exists a polynomial time algorithm to convert an input for Y into an input for X such that algorithm A with this input will correctly answer problem Y. The utility of this class is that if a polynomial time algorithm exists for any member of NP-complete, then a polynomial time algorithm exists for every problem in NP. This would prove that P=NP, which is generally thought to be false.

Finally, if a problem can be reduced to an NP-complete problem in polynomial

time but is not necessarily in NP, we say the problem is **NP-hard**. The problems in NP-hard do not need to be decision problems, they can be of arbitrary form. Similar to NP-complete, the problems in NP-hard likely can not be solved in polynomial time, since the existence of a polynomial time algorithm would imply the existence of a polynomial time algorithm for every problem in NP.

We now return to the neighbourhood polynomial, starting with a result on the complexity of computing the value of the polynomial at a given location.

Theorem 2.4.1. Computing the value of neigh(t) for a real number $t \notin \{-2, -1, 0\}$ is NP-hard.

Proof. Assume there exists a real number $t \notin \{-2, -1, 0\}$, such that for any graph, computing the value of neigh(x) at x = t is possible in polynomial time.

Now we will consider a graph G and its complement $H \cong \overline{G}$. If they have n vertices, the degree of the neighbourhood polynomial of H is at most n-1, so there exist coefficients $a_0, a_1, \ldots, a_{n-1}$ such that $\operatorname{neigh}_H(x) = a_0 + a_1x + \cdots + a_{n-1}x^{n-1}$. Now recall that, by Proposition 2.2.4,

$$\operatorname{neigh}_{H[\overline{K_m}]}(t) = \operatorname{neigh}_G((1+t)^m - 1),$$

and so we can find the value of $\operatorname{neigh}_{H[\overline{K_m}]}(x)$ at $x=(1+t)^m-1$ for $2\leq m\leq n$ by computing the value of $\operatorname{neigh}_{H[\overline{K_m}]}(t)$ for each m. Constructing the graph $H[\overline{K_m}]$ involves creating $mn\leq n^2$ vertices and deciding whether or not the edge between each of the at most $\binom{n^2}{2}=O(n^4)$ pairs of vertices exists, so this can be done in polynomial time. Then by assumption we can compute the value of $\operatorname{neigh}_{H[\overline{K_m}]}(x)$ at x=t in polynomial time as well. This gives us the following system of equations

with the variables a_i .

$$a_0 + a_1 t + \dots + a_{n-1} t^{n-1} = \text{neigh}_H(t)$$

$$a_0 + a_1((1+t)^2 - 1) + \dots + a_{n-1}((1+t)^2 - 1)^{n-1} = \operatorname{neigh}_H((1+t)^2 - 1)$$

= $\operatorname{neigh}_{H[\overline{K_2}]}(x)$

:

$$a_0 + a_1((1+t)^n - 1) + \dots + a_{n-1}((1+t)^n - 1)^{n-1} = \operatorname{neigh}_H((1+t)^n - 1)$$

= $\operatorname{neigh}_{H[\overline{K_n}]}(x)$

This system has n equations and n unknowns, so it has a solution if and only if the determinant of the following matrix has a nonzero determinant.

$$M = \begin{pmatrix} 1 & t & t^2 & \cdots & t^{n-1} \\ 1 & (1+t)^2 - 1 & ((1+t)^2 - 1)^2 & \cdots & ((1+t)^2 - 1)^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & (1+t)^n - 1 & ((1+t)^n - 1)^2 & \cdots & ((1+t)^n - 1)^{n-1} \end{pmatrix}$$

This matrix is a Vandermonde matrix [24], that is, each row of the matrix is composed entirely of consecutive powers of a number, namely $M_{i,2}$ in the i^{th} row. If we let $c_i = M_{i,2} = (1+t)^i - 1$, then the determinant of M can be found from the following well-known formula [24],

$$\det(M) = \prod_{1 \le i < j \le n} (c_j - c_i)$$

$$= \prod_{1 \le i < j \le n} ((1+t)^j - (1+t)^i)$$

$$= \prod_{1 \le i < j \le n} (1+t)^i ((1+t)^{j-i} - 1).$$

Thus $\det(M) = 0$ if and only if $(1+t)^i = 0$ or $(1+t)^{j-i} = 1$ for some i and j. Since t is real, the only solutions to either of the above equations are t = -2, t = -1, and t = 0, all of which do not occur by assumption. Thus $\det(M) \neq 0$, so the system of equations has a unique solution. Computing the values of the coefficients a_i is possible in $O(n^3)$ time (via Gauss-Jordan elimination), and so we can compute the neighbourhood polynomial of H in polynomial time.

By Theorem 2.3.1,

$$neigh_H(x) + D_G(x) = (1+x)^n,$$

where $D_G(x)$ is the dominating polynomial of G. So we can subtract $\operatorname{neigh}_H(x)$ from $(1+x)^n$ to get the dominating polynomial of G in polynomial time. Then we can easily find the smallest k such that x^k has a nonzero coefficient in $D_G(x)$, which is the domination number of G (the cardinality of a smallest dominating set of G). Thus we have a polynomial time algorithm to determine the domination number of an arbitrary graph G, which is known to be NP-hard [17]. This reduction allows us to conclude that for all real numbers t other than possibly -2, -1, or 0, it is NP-hard to compute the value of $\operatorname{neigh}(t)$.

In particular, this implies that computing the value of neigh(1), which is the cardinality of the neighbourhood complex, is NP-hard. This provides an answer to Problem 6 in [15].

We can expand this result to complex t by noting that the proof only requires t does not satisfy $(1+t)^i=0$ nor $(1+t)^{j-i}=1$ for all integers $1 \leq i < j$. The first equation only has the solution t=-1. The second equation can be satisfied whenever 1+t is a root of unity ω (that is, $\omega \in \mathbb{C}$ satisfies $\omega^n=1$ for some natural number n). This proves the following corollary.

Corollary 2.4.2. Computing neigh(t) for any complex number t which is not -1 or $\omega - 1$ for some root of unity ω is NP-hard.

Note that computing neigh(0) is trivially possible in polynomial time, since it is always equal to 1. It is not clear how difficult it is to compute neigh(t) at the remaining values of t, namely -1 and the set $\{\omega - 1 \mid \omega^n = 1, \omega \neq 1, n \in \mathbb{N}\}$.

If we can compute the entire neighbourhood polynomial in polynomial time then we can compute its value anywhere in polynomial time, so we also get the following result which provides an answer to Problem 5 in [15].

Corollary 2.4.3. Computing all of the coefficients of the neighbourhood polynomial is NP-hard.

Keep in mind that computing the coefficients of the highest and lowest degree terms is often easy. For example, the coefficient of x^d in a neighbourhood polynomial of degree d can be found by considering the vertices of the graph with degree d and eliminating vertices of this class that have the same neighbourhood as one of their classmates until the only vertices left have distinct neighbourhoods, which can be done fairly quickly. On the lower end, the constant term is again always 1, and the coefficient of x is the number of vertices of degree at least one. Thus it is the middle terms of the polynomial which are difficult to calculate, and so while we can often compute a handful of the coefficients of the neighbourhood polynomial in polynomial time, it is difficult to compute the entire polynomial.

The results in this section have corresponding results for the domination polynomial. In particular, computing the domination polynomial is difficult in general.

Corollary 2.4.4. Computing all of the coefficients of the domination polynomial is NP-hard.

Proof. Theorem 2.3.1 allows us to compute the coefficients of the neighbourhood polynomial in polynomial time given the domination polynomial of the complimentary graph. By Corollary 2.4.3, computing the coefficients of the neighbourhood polynomial is NP-hard, so computing the coefficients of the domination polynomial must be at least as difficult.

2.5 Additional Formulas for Families of Graphs

In addition to the formulas presented in Section 2.1, there are a few more families of graphs for which we would like to have the general form of their neighbourhood polynomials, as they will be mentioned again in Chapter 3 on the roots of neighbourhood polynomials.

To construct the first of these families, consider the cycle C_n with vertices $U = \{u_1, u_2, \ldots, u_n\}$ and the path P_k with vertices $V = \{v_1, v_2, \ldots, v_k\}$. Let TP be their disjoint union plus an edge e between u_1 and v_1 . Such a graph is sometimes called a **tadpole graph**. Any subset of U or V which had a common neighbour before adding e will still have a common neighbour, though the empty set is counted twice by this argument. The only new elements of the neighbourhood complex after adding e will

be $\{u_1, v_2\}, \{u_2, v_1\}, \{u_n, v_1\}$, and $\{u_2, u_n, v_1\}$. Thus the neighbourhood polynomial for TP is,

$$\operatorname{neigh}_{TP}(x) = \operatorname{neigh}_{C_n}(x) + \operatorname{neigh}_{P_k}(x) - 1 + 3x^2 + x^3$$

$$= \begin{cases} 1 + (n+k)x + (n+k+1)x^2 + x^3, & n \neq 4\\ 1 + (k+4)x + (k+3)x^2 + x^3, & n = 4 \end{cases}$$

Note that for $n \neq 4$ this depends only on the total number of vertices n+k of TP and not on the relative size of the cycle and path. We will occasionally write TP_N to refer to the tadpole graphs of size N = n + k and for which $n \neq 4$ since they conveniently share the same neighbourhood polynomial.

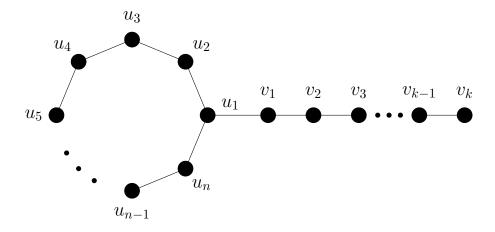


Figure 2.1: Tadpole Graph

Similarly, consider the disjoint union of K_k and P_n , which has neighbourhood polynomial $\operatorname{neigh}_{K_k}(x) + \operatorname{neigh}_{P_n}(x) - 1$. If we let G be the result of adding an edge between a vertex u in K_k and an endpoint v of P_n , then any nonempty subset of the vertices of $K_k \setminus \{u\}$ along with v will form a unique element of the neighbourhood complex of G that was not in the neighbourhood complex of the disjoint union. In addition, if w is the lone neighbour of v in P_n then $\{u, w\}$ has the common neighbour v. This accounts for all the new elements of the neighbourhood complex created by the addition of the edge, so,

$$\operatorname{neigh}_{G}(x) = \operatorname{neigh}_{K_{k}}(x) + \operatorname{neigh}_{P_{n}}(x) - 1 + x((1+x)^{k-1} - 1) + x^{2}$$
$$= (1+x)^{k} - x^{k} + x(1+x)^{k-1} + (n-1)x + (n-1)x^{2}$$

Of course, this only applies to nontrivial paths, which have at least two vertices. However, it is easy to see that we get a similar formula for a graph which consists of a complete graph K_n with an added leaf. This is our third and final family we will consider in this section, and its neighbourhood polynomial is

$$(1+x)^n - x^n + x(1+x)^{n-1} = (1+x)^{n-1}(1+2x) - x^n.$$

Chapter 3

Roots of Neighbourhood Polynomials

One of the most natural questions to consider, given a family of polynomials, is the nature of the roots of these polynomials, which leads us to study the behaviour of the roots of neighbourhood polynomials. Indeed, the roots of every graph polynomial mentioned in Section 1.2 have been widely studied.

Birkhoff, who first defined the chromatic polynomial [2], later showed along with Lewis in a 1946 paper [3] that the chromatic polynomial of a plane triangulation can have no roots in any of the intervals $(-\infty, 0)$, (0, 1), (1, 2), or $[5, \infty)$. Later, Tutte drew a connection between the roots of the chromatic polynomials of certain graphs and the golden ratio [29]. Even more recently, Brown showed that all connected graphs with n vertices and m edges have a chromatic root of modulus at least (m-1)/(n-2) [6].

In many areas of combinatorics, the concept of unimodality appears. A sequence of real numbers a_0, a_1, \ldots, a_n is said to be **unimodal** if there is a $k \in \{0, 1, \ldots, n\}$ such that

$$a_0 \le a_1 \le \dots \ge a_{k-1} \le a_k \ge a_{k+1} \ge \dots \ge a_{n-1} \ge a_n$$
.

Newton showed (see [16], for example) that if a polynomial $\sum_{j=0}^{n} a_j x^j$ has all positive coefficients and all real roots, then the sequence a_0, a_1, \ldots, a_n is unimodal. Thus we are often interested in finding out when graph polynomials have all real roots. In [18], Godsil and Gutman show that the roots of the matching polynomial are always real, and that the roots of $\mu(G)$ are interlaced by the roots of $\mu(G-v)$ for any vertex v of G. We consider the neighbourhood polynomials with all real roots in Section 3.1.

Alternatively, the closure of the roots of all the graph polynomials of a particular kind can be considered, or one can find areas where the roots are dense. In [12], Brown, Hickman, and Nowakowski show that the real independence roots are dense in the interval $(-\infty, 0]$. We show that the same is true for neighbourhood roots in Section 3.4. We also find the closure of the complex neighbourhood roots in Section 3.5.

Another method to gain insight on the nature of the roots is to attempt to bound them. It has been shown [13], for example, that the roots of independence polynomials for graphs with independence number β and number of vertices n have modulus at most $(n/\beta)^{\beta-1} + O(n^{\beta-2})$. In Section 3.2, we consider what bounds may be placed on the roots of neighbourhood polynomials.

3.1 Neighbourhood Polynomials with All Real Roots

As mentioned in the preceding section, it can be useful to consider when a graph polynomial has all real roots. This is particularly true in the case of neighbourhood polynomials, as an empirical analysis of the neighbourhood polynomial for small graphs reveals the polynomial often has unimodal coefficients, and a result by Newton [16] states that polynomials with all positive coefficients and all real roots must have unimodal coefficients. Indeed, as shown in Appendices A and B, every graph on four or five vertices has a neighbourhood polynomial with unimodal coefficients. There are neighbourhood polynomials which are not unimodal, as shown in [15], but they do not appear to be common. The appendices also reveal that many neighbourhood polynomials have nonreal roots, an idea we will expand on in Section 3.6, but some neighbourhood polynomials have all real roots and we desire a way to characterize them.

The neighbourhood polynomial never has nonnegative real roots, as its coefficients are all positive, but it can have negative real roots or complex roots. Two families of graphs in particular always have all real roots: nontrivial paths, and cycles of size at least 4.

It can be readily verified that $\operatorname{neigh}_{C_4}(x) = 1 + 4x + 2x^2$ has all real roots. For cycles C_n with n > 4, the neighbourhood polynomial is $\operatorname{neigh}_{C_n}(x) = 1 + nx + nx^2$, which has two roots.

$$x = \frac{-n \pm \sqrt{n^2 - 4n}}{2n} = -\frac{1}{2} \pm \frac{\sqrt{n^2 - 4n}}{2n}$$

These two roots are real (and centred at -1/2) for all n > 4.

Similarly, the path P_n has neighbourhood polynomial $\operatorname{neigh}_{P_n}(x) = 1 + nx + (n - 2)x^2$ as long as $n \geq 2$. The trivial case of a lone vertex gives rise to the constant polynomial 1, which has no roots. For nontrivial paths, the neighbourhood polynomial

has two roots,

$$x = \frac{-n \pm \sqrt{n^2 - 4n + 8}}{2n - 4},$$

which are always real as $n^2 - 4n + 8 > 0$ for all n.

Cycles and paths are the only connected graphs with maximum degree 2, and this relationship will allow us to obtain the following.

Theorem 3.1.1. If G is a graph with degree at most 2, its neighbourhood polynomial has no nonreal roots, unless G is the disjoint union of K_3 and isolated vertices.

Proof. If G is the disjoint union of K_3 and isolated vertices, it is easy to verify neigh_G has two nonreal roots. Otherwise, we first note that the only connected graphs of degree at most 2 are the cycles and paths. So G is the disjoint union of cycles, paths of length at least 2, and isolated vertices.

Note that C_4 is unique among cycles in that its neighbourhood polynomial does not follow the pattern $\operatorname{neigh}_{C_n} = 1 + nx + nx^2$. To simplify our computations, we will take advantage of the fact that $\operatorname{neigh}_{C_4}(x) = \operatorname{neigh}_{P_4}(x)$. This and the form of the neighbourhood polynomial of a disjoint union allows us to replace each copy of C_4 in G with a copy of P_4 without changing the neighbourhood polynomial. We call this new graph H and note that since $\operatorname{neigh}_H(x) = \operatorname{neigh}_G(x)$ the roots of each polynomial will be the same.

Let M_1 be the size of the largest cycle in H and M_2 the size of the largest path. Let c_i be the number of copies of C_i in H for $3 \le i \le M_1$, and let p_j be the number of copies of P_j for $2 \le j \le M_2$. Then,

$$\operatorname{neigh}_{H}(x) = 1 + \sum_{i=3}^{M_{1}} c_{i}(\operatorname{neigh}_{C_{i}}(x) - 1) + \sum_{j=2}^{M_{2}} p_{j}(\operatorname{neigh}_{P_{j}}(x) - 1).$$

By the construction of H, $c_4 = 0$, so,

$$\operatorname{neigh}_{H}(x) = 1 + \sum_{i=3}^{M_{1}} c_{i}(ix + ix^{2}) + \sum_{j=2}^{M_{2}} p_{j}(jx + (j-2)x^{2})$$

$$= 1 + x \sum_{i=3}^{M_{1}} c_{i}i + x^{2} \sum_{i=3}^{M_{1}} c_{i}i + x \sum_{j=2}^{M_{2}} p_{j}j + x^{2} \sum_{j=2}^{M_{2}} p_{j}(j-2).$$

Now, let $N_1 = \sum_{i=3}^{M_1} c_i i$, which is the total number of vertices of H contained in a cycle. Also, let $N_2 = \sum_{j=2}^{M_2} p_j j$, the total number of vertices of H contained in a

path. Finally, let $N_3 = \sum_{j=2}^{M_2} p_j \ge 0$, the number of path components of H. These definitions allow us to simplify our expression for neigh_H,

Let $N = N_1 + N_2$, which is the number of vertices of H contained in any cycle or path, or the number of nonisolated vertices of H. Equivalently, N is the number of nonisolated vertices of G. Thus $\operatorname{neigh}_H(x) = \operatorname{neigh}_G(x) = 1 + Nx + (N - 2N_3)x^2$. The roots of this quadratic are real whenever the discriminant $N^2 - 4N + 8N_3$ is nonnegative. Since $N_3 \geq 0$, the discriminant is clearly nonnegative if $N \geq 4$. We will handle the remaining cases individually.

If N = 0, then all vertices of G are isolated, so neigh_G(x) = 1 which has no roots at all.

The case N=1 is not possible, as N only counts vertices in paths of length at least 2 and vertices in cycles, and so we cannot have just 1.

If N=2, then G must be the disjoint union of P_2 and some number of isolated vertices, since there is no cycle of length 2. Then $\operatorname{neigh}_G(x)=1+2x$ which has x=-1/2 as its only root, which is of course real.

Finally, if N=3, then either G contains a copy of $C_3\cong K_3$ along with some isolated vertices (which is the graph excluded in the theorem statement), or else it consists of P_3 along with some isolated vertices and so $\operatorname{neigh}_G(x)=1+3x+x^2$, which has two real roots.

There are families of graphs whose neighbourhood polynomials have all real roots and which have maximum degree greater than 2, however. For example, consider the graphs formed by attaching a leaf to any vertex of P_{n-1} other than one of its endpoints (so as not to simply construct P_n). All of them have the same neighbourhood polynomial, namely,

$$1 + nx + (n-1)x^2 + x^3.$$

This formula holds because there are n vertices, all of which have a neighbour, so the coefficient of x is n. There are n-3 pairs of vertices with a common neighbour along the path, and in addition 2 pairs created by attaching the leaf v to vertex

u (each pair consists of v and one of the neighbours of u in the path). Thus the coefficient of x^2 is n-1. Finally there is a single set of three vertices with a common neighbour, these are the neighbourhood of u, and so we have a lone x^3 term.

We claim the following.

Proposition 3.1.2. Let $p(x) = 1 + nx + (n-1)x^2 + x^3$, the neighbourhood polynomial of any graph consisting of P_{n-1} plus a leaf attached at a non-endpoint vertex. Then if $n \ge 6$, the polynomial p(x) has all real roots, and the leftmost of these roots lies in the interval (-(n-2), -(n-3)).

Proof. We will calculate the polynomial at the following locations,

$$p(0) = 1$$

$$p(-1) = -1$$

$$p(-2) = 2n - 11 > 0$$

$$p(-(n-3)) = n^2 - 9n + 19$$

$$p(-(n-2)) = -2n + 5 < 0$$

We find that $n^2 - 9n + 19 = 0$ when $n = 9/2 \pm \sqrt{5}/2$, or roughly $n \approx 3.38$ and $n \approx 5.62$, so p(-(n-3)) > 0 for all $n \geq 6$. The sign changes above give us the location of all three roots of p(x): the polynomial has a root in the intervals (-1,0) and (-2,-1), and in particular the leftmost root lies in (-(n-2),-(n-3)). Since p(x) is a cubic with three real roots, it must have all real roots. Note that if n < 6, there are only two permissible cases, n = 4 and n = 5 (otherwise the path is too short to have a non-endpoint vertex). It can be directly verified that p(x) does not have all real roots in these two cases.

These are not the only graphs with all real roots. As discussed in Section 3.2 on bounding the roots of the neighbourhood polynomial, the tadpole graphs have all real roots as long as the total number of vertices is at least five. Other graphs yield neighbourhood polynomials with all real roots as well, such as the cycle C_5 with any one of the missing edges added in (*i.e.*, the graph formed by adding an edge between a pair of non-adjacent vertices in C_5). Its neighbourhood polynomial,

 $\operatorname{neigh}_{C_5+e}(x) = 1 + 5x + 7x^2 + 2x^3$, has three real roots, but it does not fit into any of the families mentioned above.

Many other examples of graphs whose neighbourhood polynomials have all real roots exist as well. Many of the smaller ones have similarities to the families mentioned, such as cycles with more than one path attached to different vertices, graphs that are nearly cycles except for a small number of added edges, or complete graphs with a small number of removed edges. Beyond seven or so vertices, the structures of graphs with this property become harder to characterise.

It is not clear if there is a maximum degree of a neighbourhood polynomial with all real roots either. So far we have presented neighbourhood polynomials up to degree 3 with all real roots. Due to Theorem 2.1.1, the neighbourhood polynomial of C_4 -free graphs depends only on the degree sequence of the graph. Using this and the fact that trees are always C_4 -free, we have found trees of maximum degree 4 and 5 which have neighbourhood polynomials with all real roots through brute force calculation, which leads us to conjecture neighbourhood polynomials with all real roots can have arbitrarily large degree.

The smallest trees whose neighbourhood polynomial have degree 4 and all real roots have 13 vertices and degree sequence 1, 1, 1, 1, 1, 1, 1, 1, 3, 3, 3, 3, 4. Their neighbourhood polynomial is neigh_T $(x) = x^4 + 8x^3 + 18x^2 + 13x + 1$. An example of one of these trees is shown in Figure 3.1.

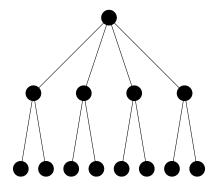


Figure 3.1: A Tree with Max Degree 4 and All Real Neighbourhood Roots

For degree 5, the smallest such trees have 75 vertices. Their degree sequence consists of forty-four 1's, zero 2's, twenty-one 3's, nine 4's and a single 5, and they all have the neighbourhood polynomial $\operatorname{neigh}_T(x) = x^5 + 14x^4 + 67x^3 + 127x^2 + 75x + 1$.

The sum of the degree sequence, 148, correctly implies such a tree would have 74 edges, which is sufficient to show such a tree exists [15].

For some C_4 -free graphs, it is possible to determine the neighbourhood polynomial has a pair of nonreal roots by examining the degree sequence of the graph.

Theorem 3.1.3. For a graph G, let $\Delta = \max_{v \in V(G)} \deg(v)$. If G is C_4 -free, has at least one vertex of degree 2, and there exists $k \in \mathbb{N}$ with $3 \le k \le \Delta$ such that $\deg(v) \ne k$ for all $v \in V(G)$, then $\operatorname{neigh}_G(x)$ has at least two nonreal roots.

Proof. By Theorem 2.1.1, the neighbourhood polynomial of a C_4 -free graph with n vertices and m edges is,

$$\operatorname{neigh}_{G}(x) = \sum_{v \in V(G)} (1+x)^{\deg(v)} - (2m-n)x - (n-1).$$

Making the substitution y = 1 + x yields,

$$p(y) = \sum_{v \in V(G)} y^{\deg(v)} - (2m - n)y - (2n - 2m - 1).$$

By Descartes' Law of Signs, the number of positive real roots of p(y) is at most the number of sign changes in the list of its coefficients. Similarly, the number of negative real roots of p(y) is at most the number of sign changes in the list of the coefficients of p(-y). Thus, the number of real roots is at most the total number of sign changes in the two lists.

By assumption, the coefficient of y^k is zero. Thus there are at most Δ nonzero coefficients in each polynomial p(y) and p(-y), which means at most $\Delta - 1$ adjacent pairs of coefficients of $2\Delta - 2$ pairs total. So the total number of sign changes is at most $2\Delta - 2$.

However, the coefficients of y^j for $2 \le j \le \Delta$ and $j \ne k$ are all positive or zero in p(y), which eliminates $\Delta - 3$ potential sign changes.

If 2m - n = 0, the coefficient of y is zero in both polynomials which eliminates another 4 potential sign changes. Or, if 2n - 2m - 1 = 0, the constant coefficient is zero in both polynomials which eliminates 2 potential sign changes. Otherwise, both of these coefficients are nonzero. Since the constant coefficient has the same sign in both polynomials and the coefficient of y has opposite sign in the two polynomials, the sign of these two coefficients matches in one of the polynomials, eliminating 1

potential sign change. The coefficient of y will also be positive in one of the two polynomials, matching the sign of the coefficient of y^2 , eliminating 1 more potential sign change. In all of these scenarios, at least 2 potential sign changes are eliminated.

Thus, at least $\Delta - 1$ of the $2\Delta - 2$ potential sign changes do not occur, so there are at most $\Delta - 1$ sign changes. This implies there are at most $\Delta - 1$ real roots of p(y), which is a polynomial of degree Δ , so p(y) has a nonreal root. In fact, it has a pair of nonreal roots, since it has all real coefficients so nonreal roots occur only in conjugate pairs. Finally, if y = x + 1 is a root of p(y) then x = y - 1 is a root of neigh_G(x), so the neighbourhood polynomial has a pair of nonreal roots as well. \square

3.2 Bounding Neighbourhood Roots

We would like to find some bounds on the set of roots of neighbourhood polynomials. This set is unbounded if we consider all neighbourhood polynomials [15], but if we restrict the graphs we consider, this may also restrict the possible roots. For example, the roots of neighbourhood polynomials of graphs of order n certainly have some maximum modulus (this set is finite for fixed n), so perhaps a relationship exists between this maximum modulus and n. For small n, we can calculate and plot every neighbourhood root for graphs on n vertices; see Figures 3.2 through 3.5.

Looking at these plots, a few patterns are evident. The first is that the majority of the roots, particularly the nonreal roots, tend to cluster around the negative real axis and have relatively small modulus. This clustering is most obvious near -1/2. In addition, there are a number of real roots, and at least for small graphs the roots of largest modulus are always real. We conjecture that this pattern continues for all n.

We wonder just how large the root of maximum modulus can be for a fixed n. To that end, we will consider two families of graphs which have some of the largest roots in modulus for the small graphs. These are the tadpole graphs and the graphs formed by adding a leaf to a complete graph. In particular, we conjecture that the second family have the roots of largest moduli for a fixed number of vertices, and that their root of largest modulus happens to be a (negative) real number.

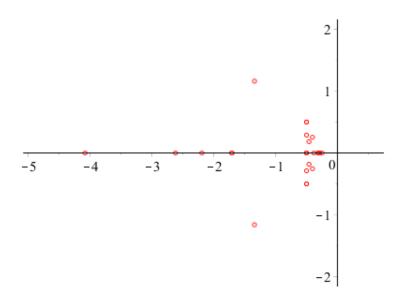


Figure 3.2: Neighbourhood Roots of all Graphs on 4 Vertices

For the tadpole graphs, which consist of a cycle connected to a path by a single edge attached to an endpoint of the path, the neighbourhood polynomial is $\operatorname{neigh}_{TP_n}(x) = 1 + nx + (n+1)x^2 + x^3$, where $n \geq 5$ is the total number of vertices of the entire graph. For large enough n, this polynomial's three roots appear to be real and lie near -n, -1, and 0. To show this, note that $\operatorname{neigh}_{TP_n}(0) = \operatorname{neigh}_{TP_n}(-1) = 1$ and consider the value of the polynomial in the following places:

$$\operatorname{neigh}_{TP_n}\left(\frac{-1}{n-2}\right) = 1 - \frac{n}{n-2} + \frac{n+1}{(n-2)^2} - \frac{1}{(n-2)^3}$$
$$= \frac{-n^2 + 7n - 11}{(n-2)^3}$$
$$< 0$$

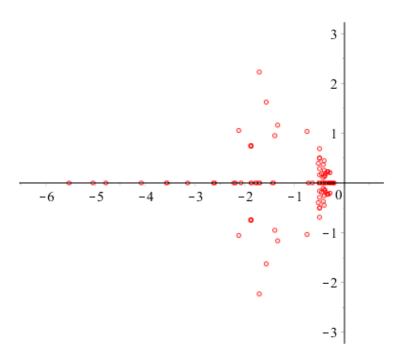


Figure 3.3: Neighbourhood Roots of all Graphs on 5 Vertices

for all $n \geq 5$, and

$$\operatorname{neigh}_{TP_n}\left(-1 + \frac{1}{n-3}\right) = \frac{-1}{n-3} + \frac{1}{(n-3)^2} + \frac{1}{(n-3)^3}$$
$$= \frac{-n^2 + 7n - 11}{(n-3)^3}$$
$$< 0$$

again for $n \geq 5$. The smallest nontrivial cycle and path have 3 and 2 vertices, respectively, so requiring at least 5 total vertices is no restriction. Since $\operatorname{neigh}_{TP_n}$ changes sign at these locations, it has a real root in each of the intervals (-1, -1 + 1/(n-3)) and (-1/(n-2), 0). Also, $\operatorname{neigh}_{TP_n}$ is a cubic polynomial with two real roots, so the final root must be real, and because the sum of the roots of a monic cubic is the negative of the coefficient of x^2 , the third root must add to the first two to yield -n-1. This implies that the third root lies in (-n-1/(n-3), -n+1/(n-2)).

Since $\operatorname{neigh}_{TP_n}(-1) = 1$ and $\operatorname{neigh}_{TP_n}(-n) = 1$ are both positive, there exists an even number of roots (counting multiplicities) in the interval [-n, -1]. We have already determined two of the three roots do not lie in this interval, so there is also at

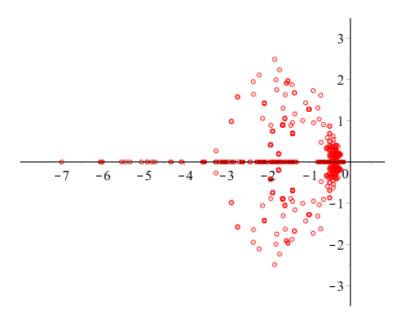


Figure 3.4: Neighbourhood Roots of all Graphs on 6 Vertices

most one root in [-n, -1]. Therefore there are exactly zero roots in [-n, -1], which allows us to trim the interval in which our third root lies from (-n - 1/(n - 3), -n + 1/(n - 2)) to (-n - 1/(n - 3), -n). In summary, for $n \ge 5$, one root of neigh_{TP_n}(x) lies in each of the following intervals,

$$\left(-n - \frac{1}{n-3}, -n\right), \quad \left(-1, -1 + \frac{1}{n-3}\right), \quad \left(-\frac{1}{n-2}, 0\right).$$

Next, we consider graphs formed by adding a leaf to a complete graph. More precisely, start with the disjoint union of K_n and K_1 and add an edge between any vertex of K_n and the lone vertex of K_1 . We shall call this graph G_n for this section. This graph has as its neighbourhood polynomial,

$$\operatorname{neigh}_{G_n}(x) = (1+x)^{n-1}(1+2x) - x^n,$$

as shown in Section 2.5. It can be verified directly that this graph on n+1 vertices has the root of largest modulus, and that this root is a negative number, for $2 \le n \le 6$. We conjecture that this is the case for larger n as well.

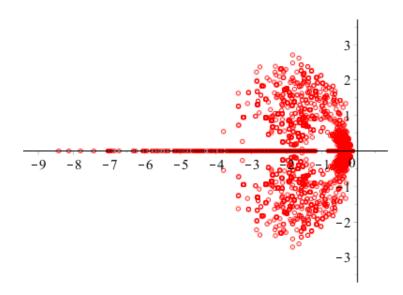


Figure 3.5: Neighbourhood Roots of all Graphs on 7 Vertices

We can show that $\operatorname{neigh}_{G_n}(x)$ has a root which tends toward $-n/\ln(2) \approx -1.4427n$ as $n \to \infty$. To show this, we compute $\operatorname{neigh}_{G_n}(kn)$ for some real constant k,

$$neigh_{G_n}(kn) = (1+kn)^{n-1}(1+2kn) - (kn)^n$$
$$= (kn)^n \left[\left(\frac{1+kn}{kn} \right)^n \left(\frac{1+2kn}{1+kn} \right) - 1 \right].$$

We are interested in real k < 0 since any roots of the neighbourhood polynomial are negative, so with that assumption, the sign of the $(kn)^n$ factor alternates based on the parity of n. So, consider the limit of the factor in the square brackets,

$$\lim_{n \to \infty} \left(\frac{1 + kn}{kn} \right)^n \left(\frac{1 + 2kn}{1 + kn} \right) - 1 = \lim_{n \to \infty} \left(1 + \frac{1/k}{n} \right)^n \left(\frac{1 + 2kn}{1 + kn} \right) - 1$$
$$= 2e^{1/k} - 1,$$

since $\lim_{n\to\infty} (1+x/n)^n = e^x$. The expression $2e^{1/k} - 1$ changes sign at $k = -1/\ln(2)$, so for any large and fixed n, the sign of $\operatorname{neigh}_{G_n}(x)$ will also change near $x = kn = -n/\ln(2)$, implying it has a root near that value.

3.3 Integral and Rational Neighbourhood Roots

It is natural to wonder what integers or rational numbers, if any, can be roots of neighbourhood polynomials. Before we answer this question, we must first show that $\operatorname{neigh}_G(1)$ is always odd.

Theorem 3.3.1. For any graph G, the number $\operatorname{neigh}_G(1)$ is odd.

Proof. This follows from the fact that the number of dominating sets of a graph is odd [5], and from Theorem 2.3.1, which states,

$$\operatorname{neigh}_{G}(x) + D_{\overline{G}}(x) = (1+x)^{n}.$$

Substituting x = 1, we get $D_{\overline{G}}(1)$ (the number of dominating sets) which is odd, and 2^n which is even, so $\operatorname{neigh}_G(1)$ must be odd.

Note that $\operatorname{neigh}_G(1)$ is just the sum of the coefficients of $\operatorname{neigh}_G(x)$, which is the cardinality of the neighbourhood complex, so we have the following corollary.

Corollary 3.3.2. For any graph G, the cardinality of the neighbourhood complex, $|\mathcal{N}(G)|$, is odd.

Theorem 3.3.1 and the fact that $\operatorname{neigh}_G(0) = 1$ is also always odd, gives us the following result.

Corollary 3.3.3. For any graph G, the neighbourhood polynomial $\operatorname{neigh}_G(x)$ has no integral roots.

Proof. Let G be a graph and $a \in \mathbb{Z}$. If $a \equiv 0 \pmod{2}$, then $\operatorname{neigh}_{G}(a) \equiv \operatorname{neigh}_{G}(0) \equiv 1 \pmod{2}$, and since zero is even this implies a is not a root. Otherwise, $a \equiv 1 \pmod{2}$, so $\operatorname{neigh}_{G}(a) \equiv \operatorname{neigh}_{G}(1) \equiv 1 \pmod{2}$, and again a is not a root. \square

We now turn to the subject of rational roots. By the Rational Root Theorem, if the leading coefficient of $\operatorname{neigh}_G(x)$ is a, then the only possible rational roots are $\pm 1/b$ where b divides a, as the constant term is always 1. It turns out that 1/b is a root of a neighbourhood polynomial if and only if b is even.

Theorem 3.3.4. The numbers -1/2n for $n \in \mathbb{N}$ are all roots of neighbourhood polynomials, and are the only rational numbers which are roots of neighbourhood polynomials.

Proof. For any $n \in \mathbb{N}$, let $G = \bigcup_{k=1}^{n} K_2$, the disjoint union of n copies of K_2 . Then $\operatorname{neigh}_{G}(x) = 2nx + 1$, which has a root at -1/2n.

Since the neighbourhood polynomial has no nonnegative roots, and by our previous discussion involving the Rational Root Theorem, the only other possible rational roots are of the form -1/(2n+1) for $n \in \mathbb{N}$.

Suppose a graph G and a natural number n exist such that -1/(2n+1) is a root of $\operatorname{neigh}_G(x)$. Let d be the degree of $\operatorname{neigh}_G(x)$, and let $p(x) = x^d \operatorname{neigh}_G(1/x)$, a polynomial with the same coefficients as $\operatorname{neigh}_G(x)$ but with their order reversed. Since -1/(2n+1) is a root of $\operatorname{neigh}_G(x)$, we must have that -(2n+1) is a root of p(x).

However, by Theorem 3.3.1, neigh_G(1) is odd, so

$$p(1) = 1^d \operatorname{neigh}_G(1/1) = \operatorname{neigh}_G(1)$$

is odd too. Since $-(2n+1) \equiv 1 \pmod 2$, we have $p(-(2n+1)) \equiv p(1) \equiv 1 \pmod 2$, which contradicts -(2n+1) being a root of p(x). Thus -1/(2n+1) is not a root of any neighbourhood polynomial for any natural number n, so the only possible rational roots are of the form -1/2n.

3.4 Closure of the Real Neighbourhood Roots

The closure of the real neighbourhood roots is at most $(-\infty, 0]$, since any real roots of a neighbourhood polynomial are negative. We know from the discussion of tadpole graphs in Section 3.2 that there is a sequence of roots that approach 0 and -1, so they are both included at the very least.

Proposition 3.4.1. The closure of the set of real roots of neighbourhood polynomials contains the interval $(-\infty, -1]$.

Proof. Let $U_k = \bigcup_{i=1}^k K_2$ be the disjoint union of k complete graphs on two vertices each, so U_k has 2k vertices and k edges. Let $G_{k,n} = U_k \cup C_{2n}$, the disjoint union of U_k with an even cycle on 2n vertices. Then, for $k \geq 1$ and $n \geq 3$,

$$\operatorname{neigh}_{G_{k,n}}(x) = 2kx + (1 + 2nx + 2nx^2) = 1 + 2(n+k)x + 2nx^2,$$

which we claim has a root in the following interval,

$$I(k,n) := \left(-1 - \frac{k}{n}, -1 - \frac{k-1}{n}\right).$$

To confirm this, we calculate,

$$\operatorname{neigh}_{G_{k,n}}\left(-1 - \frac{k}{n}\right) = 1 > 0,$$

and,

$$\operatorname{neigh}_{G_{k,n}}\left(-1 - \frac{k-1}{n}\right) = -\frac{n+2k-2}{n} < 0.$$

These have opposite sign, and so $\operatorname{neigh}_{G_{k,n}}(x)$ has at least one real root in the interval I(k,n) by the Intermediate Value Theorem.

Finally, for any real number r < -1 and $\epsilon > 0$, we can choose an $n > 1/\epsilon$ so that width $(I(k, n)) = 1/n < \epsilon$. Keeping n fixed, let $k = \lceil -n(r+1) \rceil$, which is the ceiling of a positive number and so $k \ge 1$ and $k \in \mathbb{N}$. Thus

$$k-1 < -n(r+1) \le k$$
$$-1 - \frac{k-1}{n} > r \ge -1 - \frac{k}{n},$$

and so both r and a root of $\operatorname{neigh}_{G_{k,n}}(x)$ are in the closed interval $\overline{I(k,n)}$. Since this interval also has width $1/n < \epsilon$, this yields a root of a neighbourhood polynomial within ϵ of r, as desired.

Note that this proof relies on the disconnected graphs $G_{k,n}$ to work, which leaves open the question of the density of the real roots for connected graphs only.

It is also worth noting that only graphs of maximum degree two are required to obtain this result. Graphs with maximum degree zero have no edges, and thus no vertices have common neighbours, so their neighbourhood polynomial is the constant neigh(x) = 1 which has no roots. Graphs with minimum degree one are essentially disjoint copies of K_2 and have neighbourhood polynomial neigh $_m(x) = 2mx+1$, where m is the number of edges. This is because each endpoint of each edge is a unique vertex which has a common neighbour with itself, namely the other endpoint of the edge, and there are 2m endpoints. Each of these polynomials has exactly one root at x = -1/2m, which are real and approach zero.

Even connected graphs of maximum degree two are insufficient; these graphs are characterised by paths and cycles. Other than the special case of C_4 , their neighbourhood polynomials are,

$$\operatorname{neigh}_{C_n}(x) = 1 + nx + nx^2, \ n \ge 5,$$

 $\operatorname{neigh}_{P_n}(x) = 1 + nx + (n-2)x^2, \ n \ge 2,$

from which we can use the quadratic formula to show both of these have roots which approach -1 and 0 as $n \to \infty$. Thus, the roots of these polynomials are not dense in the nonpostive real numbers.

Proposition 3.4.1 does not tell us if the real roots of neighbourhood polynomials are dense or not in the interval (-1,0). Many roots lie in this interval, so we suspect the real roots may be dense there as well and thus on the entire negative real axis. To show this, we will first need the following lemma.

Lemma 3.4.2. For all $x \in (0,1)$ and $\epsilon > 0$ such that $0 < x - \epsilon < x + \epsilon < 1$, there exists $\delta > 0$ such that the following union of intervals,

$$S = \bigcup_{n=0}^{\infty} ((x - \epsilon)^n, (x + \epsilon)^n),$$

contains the interval $(0, \delta)$.

Proof. The proof will hinge on the fact that the intervals that form S are not disjoint, instead for large enough n they begin to overlap. To that end, let $N \in \mathbb{N}$ be such that for all $n \geq N$,

$$\frac{n+1}{n} < \frac{\ln(x-\epsilon)}{\ln(x+\epsilon)}.$$

Since $0 < x - \epsilon < x + \epsilon < 1$, we have $\ln(x - \epsilon) < \ln(x + \epsilon) < 0$, and so the right hand side of the above equation is greater than 1. The left hand side monotonically approaches 1 from the right as $n \to \infty$, so such an N exists.

Thus, for all $n \geq N$,

$$(n+1)\ln(x+\epsilon) > n\ln(x-\epsilon)$$
$$\ln\left[(x+\epsilon)^{n+1}\right] > \ln\left[(x-\epsilon)^n\right]$$
$$(x+\epsilon)^{n+1} > (x-\epsilon)^n,$$

which implies that the right endpoint of the $(n+1)^{th}$ interval lies to the right of the left endpoint of the n^{th} interval; that is, the two intervals have a nonempty intersection.

Therefore, for all $N' \geq N$,

$$S \supset \bigcup_{n=N}^{N'} ((x-\epsilon)^n, (x+\epsilon)^n) = \left((x-\epsilon)^{N'}, (x+\epsilon)^N \right),$$

because in this union all the intervals intersect with their neighbours, and so the union contains everything from the left endpoint of the last interval to the right endpoint of the first interval. Let $\delta = (x + \epsilon)^N > 0$ and note that if we take the limit as $N' \to \infty$ the left endpoint will approach zero since $0 < x - \epsilon < 1$. This gives us our result,

$$S \supset \lim_{N' \to \infty} \bigcup_{n=N}^{N'} ((x - \epsilon)^n, (x + \epsilon)^n) = (0, \delta).$$

We can now provide an answer to Problem 2 in [15].

Theorem 3.4.3. The closure of the real roots of neighbourhood polynomials is the negative real numbers $(-\infty, 0]$.

Proof. From Proposition 3.4.1 and the discussion that preceded it, the closure of the real roots of neighbourhood polynomials contains zero and $(-\infty, -1]$, so all that remains to be shown is (-1, 0).

Let $x' \in (-1,0)$ and let $\epsilon > 0$ be small enough such that $x' - \epsilon$ and $x' + \epsilon$ are both in (-1,0) as well. To show the real roots of neighbourhood polynomials are dense in the interval (-1,0), we seek a real root of a neighbourhood polynomial in the interval $(x' - \epsilon, x' + \epsilon)$.

Let x = x' + 1 so $0 < x - \epsilon < x + \epsilon < 1$. By Lemma 3.4.2, there exists $\delta > 0$ such that,

$$(0,\delta) \subset \bigcup_{n=0}^{\infty} ((x-\epsilon)^n, (x+\epsilon)^n).$$

From the discussion of tadpole graphs in Section 3.2, there exists a sequence of roots of neighbourhood polynomials which approaches -1 from the right. So, there exists a graph G whose neighbourhood polynomial has a root $\rho' \in (-1, -1 + \delta)$, and if we

let $\rho = \rho' + 1$ then $\rho \in (0, \delta)$. This means $\rho \in ((x - \epsilon)^n, (x + \epsilon)^n)$ for some $n \in \mathbb{N}$, so if we fix n to this value then,

$$(x - \epsilon)^n < \rho < (x + \epsilon)^n. \tag{3.1}$$

Similar to the proof of Corollary 3.5.1, we can use the lexicographic product $G[\overline{K_m}]$, which has neighbourhood polynomial $\operatorname{neigh}_{G[\overline{K_m}]}(x) = \operatorname{neigh}_G((1+x)^m - 1)$, to find more roots of neighbourhood polynomials from the roots of $\operatorname{neigh}_G(x)$. Since ρ' is a root of $\operatorname{neigh}_G(x)$, the real number $(\rho' + 1)^{1/m} - 1 = \rho^{1/m} - 1$ is a root of $\operatorname{neigh}_{G[\overline{K_m}]}(x)$ for all $m \in \mathbb{N}$ (ρ has a real m^{th} root because $\rho > 0$).

In particular, $\rho^{1/n} - 1$ is a real root of a neighbourhood polynomial, and by Equation (3.1),

$$(x - \epsilon) - 1 < \rho^{1/n} - 1 < (x + \epsilon) - 1$$

 $(x' - \epsilon) < \rho^{1/n} - 1 < (x' + \epsilon)$

so this real root of a neighbourhood polynomial lies in the interval $(x' - \epsilon, x' + \epsilon)$, as desired.

3.5 Closure of the Complex Neighbourhood Roots

In [15], Brown and Nowakowski showed that the closure of the set of roots of neighbourhood polynomials contains all of \mathbb{C} except for possibly the unit disk centred at z = -1. We can use Proposition 3.4.1 to show the closure is in fact the entire complex plane, which solves Problem 1 of their paper.

Corollary 3.5.1. The closure of the set of roots of neighbourhood polynomials is all of \mathbb{C} .

Proof. Similar to the proof of Theorem 8 in [15], we can extend a line in \mathbb{C} where the roots of neighbourhood polynomials are dense to a larger region by replacing the vertices of the graphs used above with independent sets of size m. That is, we consider the lexicographic products $G_{k,n}[\overline{K_m}]$.

The neighbourhood polynomial of $G_{k,n}[\overline{K_m}]$ is,

$$\operatorname{neigh}_{G_{k,n}[\overline{K_m}]}(x) = \operatorname{neigh}_{G_{k,n}}((1+x)^m - 1),$$

by Proposition 2.2.4.

Thus, if ρ is a root of neigh_{$G_{k,n}$}(x), then the m complex solutions of $(1+x)^m-1=\rho$ are roots of neighbourhood polynomials as well. We can rearrange this to $(1+x)^m=\rho+1$, and note that the set

$$S = \left\{ \rho + 1 \mid \rho \text{ is a root of } \operatorname{neigh}_{G_{k,n}}(x) \right\}$$

is dense in the entire negative real axis. We claim that the set of m-th roots of elements of S are dense in the entire complex plane. If so, then the same goes for the set of possible values of 1 + x, and so the set of roots of $G_{k,n}[\overline{K_m}]$ are dense in the plane as well since a translation of \mathbb{C} is still \mathbb{C} .

To verify our claim, let $c \in \mathbb{C}$ be any nonzero complex number and $\epsilon > 0$. We seek a root of a neighbourhood polynomial within a distance of ϵ of c. There exists δ with $0 < \delta < |c|$ such that if the argument and modulus of a complex number c' are within δ of the argument and modulus of c, then c' is within ϵ of c.

Now there exists an $m \in \mathbb{N}$ sufficiently large that every nonzero complex number has an m-th root with argument within δ of the argument of c. For this fixed value of m, consider the interval $J = ((|c| - \delta)^m, (|c| + \delta)^m)$, which is a nonempty subset of the positive real numbers. By the density of S in the negative reals, there exists $\rho + 1 \in S$ such that ρ is the root of a neighbourhood polynomial and $|\rho + 1|$ is in the interval J. Then any m-th root of $\rho + 1$ will have modulus within δ of c, and one of these m-th roots will have argument within δ of c as well, and so an m-th root of $\rho + 1 \in S$ lies within ϵ of c. Thus the closure of the set of m-th roots of elements of S contains all of C except possibly zero, but since the closure of a set must be closed it must contain zero as well, and so the closure of the m-th roots of the elements of S is \mathbb{C} as claimed.

3.6 Random Graphs

While it is difficult to characterise the families of graphs which have all real roots, we can at least claim that most graphs have a nonreal root, in the sense that randomly generated graphs have neighbourhood polynomials which have a nonreal root with probability approaching 1. By randomly generated, we mean graphs $G_{n,p}$ with n

vertices where each possible edge exists independently with probability $p \in (0,1)$. To show that these graphs usually have a nonreal root, we will use the following lemma on the coefficients of such graphs.

Lemma 3.6.1. Given a randomly generated graph $G_{n,p}$ with n its number of vertices, $p \in (0,1)$ a fixed probability, and a fixed integer $k \geq 0$, the coefficient of x^k in $\operatorname{neigh}_{G_{n,p}}(x)$ is $\binom{n}{k}$ with probability approaching 1 as $n \to \infty$.

Proof. Let $S \subset V(G_{n,p})$ be a subset of the vertices such that |S| = k. Then for any given vertex not in S, the probability that it is a common neighbour to all the vertices in S is p^k , so $1 - p^k$ is the probability that this is not the case. This applies independently to all n - k vertices not in S, so the probability of the event that S has no common neighbour is $(1-p^k)^{n-k}$. Let E_S denote this event so $P(E_S) = (1-p^k)^{n-k}$.

Now, the event that there exists a set $S \subset V(G_{n,p})$ with |S| = k such that E_S occurs (and thus that the coefficient of x^k is not $\binom{n}{k}$) is just the union $\bigcup_S E_S$ taken over all possible subsets of k vertices. This allows us to find an upper bound of the probability of this event, and we can use the fact that there are $\binom{n}{k}$ possible subsets of vertices of size k to get a closed form for this bound.

$$P\left(\bigcup_{S} E_{S}\right) \leq \sum_{S} P(E_{S}) = \binom{n}{k} (1 - p^{k})^{n-k}$$

To facilitate taking the limit of this expression, note that

$$0 \le \binom{n}{k} (1 - p^k)^{n-k} \le n^k (1 - p^k)^{n-k}$$

and so

$$n^{k}(1-p^{k})^{n-k} = \exp\left[\ln\left(n^{k}(1-p^{k})^{n-k}\right)\right]$$
$$= \exp\left[k\ln(n) + n\ln(1-p^{k}) - k\ln(1-p^{k})\right]$$

Now we can take the limit of the expression inside the exponential. Since $1-p^k < 1$, the expression $\ln(1-p^k) < 0$. Thus the second term, $n\ln(1-p^k)$, grows negative linearly with n, while the $k\ln(n)$ term and the constant term become negligibly small relative to the second term. So, the expression inside the exponential approaches $-\infty$, which implies $n^k(1-p^k)^{n-k} \to 0$. Finally, since $0 \le P(\bigcup_S E_S) \le n^k(1-p^k)^{n-k}$, we have that $P(\bigcup_S E_S) \to 0$ as $n \to \infty$. Therefore every set of k vertices of $G_{n,p}$

has a common neighbour with probability approaching 1, so the coefficient of x^k in $\operatorname{neigh}_{G_{n,p}}(x)$ is $\binom{n}{k}$.

The proof of our next two results will require the Gauss-Lucas Theorem, so we will state it below.

Theorem 3.6.2 (Gauss-Lucas). [23] Let R be the set of roots of a polynomial p(x), and let Γ be the smallest convex set containing R (i.e. the convex hull of R). Then all of the roots of the derivative of p(x) will lie in Γ .

Theorem 3.6.3. The neighbourhood polynomial of a randomly generated graph $G_{n,p}$ on n vertices, where each possible edge exists independently with fixed probability 0 , has a nonreal root with probability approaching <math>1 as $n \to \infty$.

Proof. Let Δ be the maximum degree of a vertex of $G_{n,p}$, and thus the maximum degree of $\operatorname{neigh}_{G_{n,p}}(x)$ as well. The constant coefficient of $\operatorname{neigh}_{G_{n,p}}(x)$ is 1, since this is always the constant coefficient for a neighbourhood polynomial.

By the preceding lemma, the coefficient of x is n with probability approaching 1 as $n \to \infty$, and similarly the coefficient of x^2 is almost surely $\binom{n}{2}$. Thus, $\operatorname{neigh}_{G_{n,p}}(x)$ almost always has the following form,

$$\operatorname{neigh}_{G_{n,p}}(x) = a_{\Delta}x^{\Delta} + \dots + \frac{n(n-1)}{2}x^2 + nx + 1,$$

for some constant a_{Δ} and so,

$$x^{\Delta} \operatorname{neigh}_{G_{n,p}}(1/x) = x^{\Delta} + nx^{\Delta-1} + \frac{n(n-1)}{2}x^{\Delta-2} + \dots + a_{\Delta}.$$

Note that $\operatorname{neigh}_{G_{n,p}}(x)$ has all real roots if and only if $x^{\Delta} \operatorname{neigh}_{G_{n,p}}(1/x)$ has all real roots as well. Now by the Gauss-Lucas Theorem, if $x^{\Delta} \operatorname{neigh}_{G_{n,p}}(1/x)$ has all real roots, then the convex hull of its roots is a subset of \mathbb{R} , and thus none of its derivatives has a nonreal root. However,

$$\frac{d^{\Delta-2}}{dx^{\Delta-2}}x^{\Delta} \operatorname{neigh}_{G_{n,p}}(1/x) = (\Delta-2)! \left(\frac{\Delta(\Delta-1)}{2}x^2 + n(\Delta-1)x + \frac{n(n-1)}{2}\right),$$

which is a quadratic with discriminant

$$(n(\Delta-1))^2 - 4\left(\frac{\Delta(\Delta-1)}{2}\right)\left(\frac{n(n-1)}{2}\right),$$

which simplifies to the following,

$$n(\Delta - 1)\left(n(\Delta - 1) - \Delta(n - 1)\right) = n(\Delta - 1)(\Delta - n). \tag{3.2}$$

Clearly n > 0, and for sufficiently large n we have $\Delta - 1 > 0$ with probability approaching 1 as well. This is because otherwise otherwise $\Delta \leq 1$, implying every vertex has at most one neighbour. The probability of a particular vertex having at most one neighbour is $(1-p)^{n-1} + (n-1)p(1-p)^{n-2}$, which approaches zero as $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and so $n \to \infty$, and the probability for sufficiently large $n \to \infty$, and so $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of this occurring for every vertex is even smaller. So $n \to \infty$, and the probability of

Corollary 3.6.4. The following statements about the roots of the neighbourhood polynomial of the random graph $G_{n,p}$ with notation from Theorem 3.6.3 and its proof all hold with probability approaching 1 as $n \to \infty$.

1. There exists a root with modulus at most

$$\sqrt{\frac{\Delta(\Delta-1)}{n(n-1)}} < \frac{\Delta}{n}.$$

- 2. There exists a root with real part at most $-\Delta/n$.
- 3. There exists a root with imaginary part at most

$$\Delta\sqrt{\frac{\Delta-1}{n(n-m)}}$$

in absolute value.

Proof. From the proof of Theorem 3.6.3, the $(\Delta - 2)^{th}$ derivative of x^{Δ} neigh_{$G_{n,p}$} (1/x) has the form,

$$(\Delta - 2)! \left(\frac{\Delta(\Delta - 1)}{2} x^2 + n(\Delta - 1)x + \frac{n(n-1)}{2} \right).$$

Before, we only calculated the discriminant of this quadratic, $n(\Delta - 1)(\Delta - n)$, but we can also explicitly calculate the roots.

$$r_{+}, r_{-} = \frac{-n(\Delta - 1) \pm \sqrt{n(\Delta - 1)(\Delta - n)}}{\Delta(\Delta - 1)}$$

We know the discriminant is negative from before, so after some simplification these roots become,

$$r_+, r_- = \frac{-n}{\Delta} \pm i \frac{\sqrt{n(\Delta - 1)(n - m)}}{\Delta(\Delta - 1)}.$$

Finally we note that both roots have the same modulus, which is,

$$\mu = \sqrt{\frac{n^2}{\Delta^2} + \frac{n(n-m)}{\Delta^2(\Delta-1)}} = \sqrt{\frac{n(n-1)}{\Delta(\Delta-1)}}.$$

Now, by Gauss-Lucas, this pair of roots must be within the convex hull of the roots of x^{Δ} neigh_{$G_{n,p}$} (1/x). So this polynomial must have a root with modulus at least as large as μ , or else all of the roots (and thus their convex hull) would be strictly contained in the circle $|z| = \mu$ which would prevent r_+ or r_- being inside the convex hull. By similar reasoning, there must exist a root with real part at least $-n/\Delta$, and a root with imaginary part at least as large in absolute value as the imaginary parts of r_+ and r_- .

We can relate these roots to roots of the original neighbourhood polynomial, $\operatorname{neigh}_{G_{n,p}}(x)$. The roots of $x^{\Delta}\operatorname{neigh}_{G_{n,p}}(1/x)$ are just reciprocals of the roots of $\operatorname{neigh}_{G_{n,p}}(x)$, so from the conclusions in the last paragraph we can draw the three new conclusions about the roots of the neighbourhood polynomial laid out in the corollary.

First, the modulus of the reciprocal is the reciprocal of the modulus, and taking the reciprocal flips the inequality, so neigh_{$G_{n,p}$}(x) has a root of modulus at most $1/\mu$. Note that we can bound $1/\mu$ by a simpler expression,

$$\frac{1}{\mu} = \sqrt{\frac{\Delta(\Delta - 1)}{n(n - 1)}} < \sqrt{\frac{\Delta^2}{n^2}} = \frac{\Delta}{n},$$

because $\Delta < n$ implies $(\Delta - 1)/(n - 1) < \Delta/n$.

Second, for a complex number z = a + ib, the real part of

$$\frac{1}{z} = \frac{a - ib}{a^2 + b^2}$$

is

$$\frac{a}{a^2 + b^2} \le \frac{1}{a},$$

so the real part of the reciprocal is at most the reciprocal of the real part. So we can conclude that the neighbourhood polynomial $\operatorname{neigh}_{G_{n,p}}(x)$ has a root with real part at most $-\Delta/n$.

Similarly, the absolute value of the imaginary part of 1/z for z = a + ib is $b/(a^2 + b^2) \le 1/b$, so if $x^{\Delta} \operatorname{neigh}_{G_{n,p}}(1/x)$ has a root with imaginary part at least as large as the imaginary part of r_+ in absolute value, then $\operatorname{neigh}_{G_{n,p}}(x)$ has a root with imaginary part at most,

$$\frac{\Delta(\Delta-1)}{\sqrt{n(\Delta-1)(n-m)}} = \Delta\sqrt{\frac{\Delta-1}{n(n-m)}},$$

in absolute value. Note that if this root has nonzero imaginary part (i.e. it is a nonreal root), then its conjugate must exist as well to make two such roots. \Box

As one final observation from calculations on small graphs, the nonreal roots of random graphs tend to line up on a circle around -1. Also, the roots of largest modulus tend to be real. For some examples of this, see Figures 3.6 through 3.10.

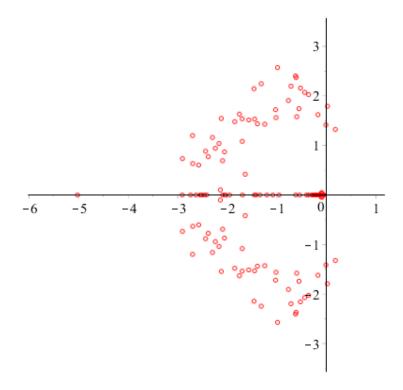


Figure 3.6: Roots of 20 instances of $\operatorname{neigh}_{G_{n,p}}(x), n=20, p=0.2$

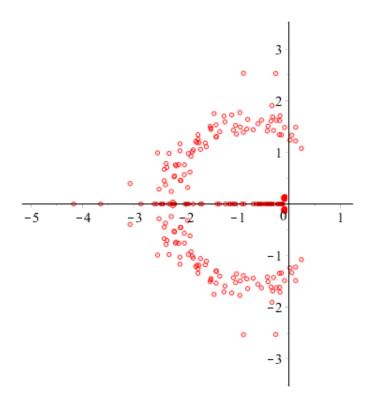


Figure 3.7: Roots of 20 instances of $\operatorname{neigh}_{G_{n,p}}(x), n=20, p=0.5$

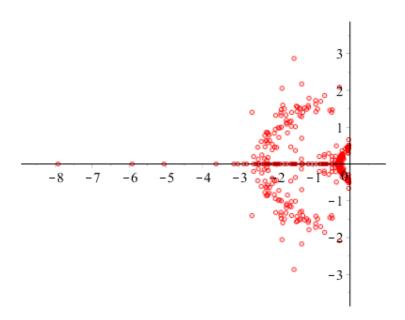


Figure 3.8: Roots of 20 instances of $\operatorname{neigh}_{G_{n,p}}(x), n=20, p=0.8$

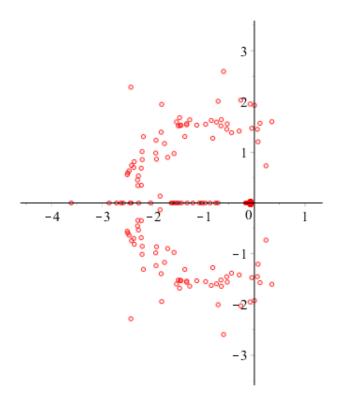


Figure 3.9: Roots of 20 instances of $\operatorname{neigh}_{G_{n,p}}(x), \, n=25, \, p=0.2$

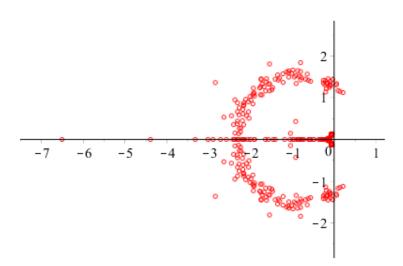


Figure 3.10: Roots of 20 instances of $\operatorname{neigh}_{G_{n,p}}(x), n=25, p=0.5$

Chapter 4

Conclusion

The study of the neighbourhood polynomial is still in its infancy. We have found new ways to compute the polynomial. We found a relationship between the neighbourhood polynomial and the domination polynomial, allowing us to find new results for each polynomial using old results for the other. In particular, this allowed us to conclude that computing the neighbourhood polynomial is NP-hard, motivating us to study the properties of the polynomial in more indirect ways.

We examined the roots of the polynomial, including when these roots are all real and what bounds we can place upon them. We were able to show there are no integral roots, and that the rational roots are restricted to the form $-1/2n, n \in \mathbb{N}$ (and that all such roots occur). We were able to find the closure of the real and complex neighbourhood roots, and we were able to use random graphs to conclude that almost all neighbourhood polynomials do not have all real roots.

Still, many questions remain, which provide plenty of room for further study. To conclude, we will state and discuss a few of these remaining problems.

Problem 1. Which graphs have neighbourhood polynomials with all real roots?

As we discussed in Section 3.1, nontrivial paths and cycles of length at least 4 have all real neighbourhood roots, and there are other families which have all real roots as well. However, empirical analysis reveals several graphs with all real neighbourhood roots and which do not belong to any of the families found thus far, such as the graph in Figure 4.1, which has a neighbourhood polynomial with all real roots, $1 + 6x + 11x^2 + 6x^3 + x^4$.

Problem 2. Do graphs of arbitrarily large maximum degree exist with all real neighbourhood roots?

Since the maximum degree of the graph is the degree of its neighbourhood polynomial, the total number of neighbourhood roots is always equal to the maximum

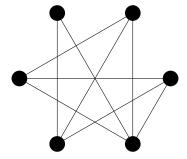


Figure 4.1: Graph with All Real Neighbourhood Roots

degree of the graph. We provided examples in Section 3.1 of graphs with maximum degree $1 \le \Delta \le 5$ and all real neighbourhood roots. We conjecture that the answer to this problem is "yes," in fact it seems likely that trees with arbitrarily large maximum degrees and all real neighbourhood roots exist since we were able to find examples for $\Delta = 4$ and $\Delta = 5$ through an exhaustive search. The tree with $\Delta = 5$ has 75 vertices and was already computationally intensive to find, so finding larger examples will require a less brute force approach, and ultimately one would hope to find a family of graphs with increasing maximum degree and all real neighbourhood roots.

Problem 3. What is the maximum modulus root of the neighbourhood polynomials of graphs on n vertices? Is it real?

For small graphs, it appears that the maximum modulus root is real, and is the most negative root of the graph formed by adding a leaf to a complete graph. At the very least, these graphs always have a large negative root, which approaches $-n/\ln(2)$ as $n \to \infty$. We wonder if this is always the maximum modulus root or if some other family of graphs eventually overtakes this family. If it does, perhaps the maximum modulus root can be nonreal. Even if such a family does not exist, one might consider what bounds can be placed on the modulus of the nonreal roots. We are also interested in the minimum modulus of neighbourhood roots. In general -1/2n is a root of a neighbourhood polynomial for $n \in \mathbb{N}$ so the modulus can be arbitrarily small, but for specific sizes or families of graphs the minimum modulus is likely nontrivial to find.

Problem 4. Which polynomials are the neighbourhood polynomial of some graph? When is a neighbourhood polynomial unique, that is, for which polynomials is there only one graph which has that polynomial as its neighbourhood polynomial?

Neighbourhood polynomials have exclusively nonnegative integer coefficients, their constant term is always 1, and the sum of their coefficients is odd. Beyond these obvious restrictions, it is difficult to say if a particular polynomial is a neighbourhood polynomial. There are certainly more conditions necessary, as for example $p(x) = 1 + 11x + 40x^2 + 121x^3$ is not the neighbourhood polynomial of any graph. This can be verified by using Sperner's Lemma (see for example [7, p. 124]), which states that for a complex on a set of order n, the f-vector of the complex $\{f_0, f_1, \ldots, f_d\}$ satisfies the following inequality for all $i = 1, 2, \ldots, d$:

$$\frac{n-i+1}{i}f_{i-1} \ge f_i.$$

The f-vector of the neighbourhood complex is the coefficients of the neighbourhood polynomial, so the coefficients of any neighbourhood polynomial must also satisfy this inequality. The coefficients of p(x) do not, because when n = 11 and i = 3 we have,

$$\frac{9}{3} \cdot 40 = 120 < 121.$$

Note that n = 11 follows from the coefficient of x being 11 and the fact that we can ignore isolated vertices, as they have no effect on the neighbourhood polynomial.

We note that it is not the case that each graph has a unique neighbourhood polynomial; for example $\operatorname{neigh}_{P_4}(x) = \operatorname{neigh}_{C_4}(x) = 1 + 4x + 2x^2$. Still, one may ask which neighbourhood polynomials do belong to only one graph up to isomorphism, or how many nonisomorphic graphs have a particular neighbourhood polynomial.

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Appendix A

The Neighbourhood Polynomial and its Roots for all Graphs on Four Vertices

Grap	ph	Neighbourhood Roots	Neighbourhood Polynomial
	×	- a 0 a	1
2	3. 4	-1.5 -1 -0.5 0 0.5 -0.5 -1	1+2x
3	2	-3 -2 -1 0 -0.5	$x^2 + 3x + 1$
		2 - 15 -1 -0.5 0 0.5 -1	$x^3 + 3x^2 + 4x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
3	-12 -10 -08 -06 -04 -02 0 02 04 06	1+4x
1	-1.5 -1 -0.5 0 0.5 -0.51.7	$3x^2 + 3x + 1$
	-25 -2 -13 -1 -05 0 05 -05	$2x^2 + 4x + 1$
2	-5 -4 -3 -2 -1 0 0 -0.5	$x^3 + 5x^2 + 4x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
2	-2.5 -2 -1.5 -1 -0.5 0 0.5 -0.5 -0.5 -1.3	$2x^2 + 4x + 1$
7	-3 -2 -1 0 -0.5 -	$2x^3 + 6x^2 + 4x + 1$
	1.5 1.6 0.5 -1.5 -1 -0.5 -0.5 -1 -1.5	$4x^3 + 6x^2 + 4x + 1$

Appendix B

The Neighbourhood Polynomial and its Roots for all Graphs on Five Vertices

	Graph	Neighbourhood Roots	Neighbourhood Polynomial
E	2	- m 0 m	1
×.	2 1	-1.5 -1 -0.5 -0.5 -0.5 -0.5 -1	1+2x
	*	-3 -2 -1 0 -65	$x^2 + 3x + 1$
4	5 5	2 - 15 -1 -05 0 05 -1 - 1 - 2 - 2 - 1	$x^3 + 3x^2 + 4x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
	-3 -1 0 0 -1 -1 -2 -2 -1	$x^4 + 4x^3 + 6x^2 + 5x + 1$
3 3 2	-12 -10 -03 -08 -04 -02 0 02 04 06	1+4x
3 5	-3 -2 -1 00 -05	$x^2 + 5x + 1$
3	0.5 - 0.5 -	$3x^2 + 3x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
3 5	-2.5 -2 -1.5 -1 -0.5 0 0.5 -0.5 -0.5	$2x^2 + 4x + 1$
3	-5 -4 -3 -2 -1 0 0 -0.5 -1 :	$x^3 + 5x^2 + 4x + 1$
3	-25 -2 -15 -1 -05 0 05 -05-	$x^3 + 4x^2 + 5x + 1$
2	2 - 1 - 252 - 15 - 1 - 0 0 05 - 1 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2	$x^4 + 4x^3 + 8x^2 + 5x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
2	03 - 03 - -3 -2 -1 0 -03 -	$2x^3 + 7x^2 + 5x + 1$
2	-2.5 -1.5 -1 -0.5 • 0 0.5 -0.5	$2x^2 + 4x + 1$
J. J	-3 -2 -1 0 -05-	$2x^3 + 6x^2 + 4x + 1$
3	-2.5 -2 -1.5 -1 -0.5 0 0.5 -0.5 -1.5 -1.5	$x^3 + 4x^2 + 5x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
2	-3 -2 -1 0 0	$x^4 + 5x^3 + 9x^2 + 5x + 1$
	-25 -2 -15 -1 -65 0 05 -05 -1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1	$x^3 + 4x^2 + 5x + 1$
2	-2 -1.5 -1 -0.5 0 0.5 -0.5 -1.5	$2x^4 + 7x^3 + 10x^2 + 5x + 1$
	-2 -15 -1 -05 0 -05	$3x^2 + 5x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
3	-2 -1.5 -1 -0.5 -0.5 -0.5 -1.1	$3x^2 + 5x + 1$
2	-6 -6 -6 -6 -6 -6 -6 -6 -6 -6 -6 -6 -6 -	$x^3 + 6x^2 + 5x + 1$
2	2 1 1 -25 -2 -15 -1 -0 • 0 05 -1 -2 -2 -3 -	$x^4 + 4x^3 + 10x^2 + 5x + 1$
3	1.5	$4x^3 + 6x^2 + 4x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
2	-2.5 -2 -1.5 -1 -0.5 0 0.5 -0.5	$3x^3 + 8x^2 + 5x + 1$
2	-6 -5 -4 -3 -2 -1 0 0.05 -1 .	$x^4 + 7x^3 + 9x^2 + 5x + 1$
2	-1.5 -1 -0.5 0 0.5 -0.5 -	$5x^2 + 5x + 1$
2	-3 -2 -1 -0 -03 -	$2x^3 + 7x^2 + 5x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
2	-4 -3 -2 -1 0 -0.5	$x^4 + 6x^3 + 10x^2 + 5x + 1$
2	-4 -3 -2 -1 0 -0.5	$2x^4 + 9x^3 + 10x^2 + 5x + 1$
	-2.5 -2 -1.5 -1 -0.5 0 0.5 -0.5 -1 -1	$3x^3 + 8x^2 + 5x + 1$
2	-4 -3 -2 -1 0 -0.5	$x^4 + 6x^3 + 10x^2 + 5x + 1$

Graph	Neighbourhood Roots	Neighbourhood Polynomial
***	-3 -2 -1 0 -0.5 -1 -1 -1	$3x^4 + 10x^3 + 10x^2 + 5x + 1$
	-1.5 -1 -0 0.5 -0.5 -1.5 -1.5	$5x^4 + 10x^3 + 10x^2 + 5x + 1$