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Independence Polynomials of Molecular Graphs

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INDEPENDENCE POLYNOMIALS OF MOLECULAR GRAPHS

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ABSTRACT

In the 1980's, it was noticed by molecular chemists that the stability and boiling point of certain molecules were related to the number of independent vertex sets in the molecular graphs of those chemicals. This led to the definition of the Merrifield-Simmons index of a graph G as the number of independent vertex sets in G. This parameter was extended by graph theorists, who counted independent sets of different sizes and defined the independence polynomial $F_G(x)$ of a graph G to be $\sum_k F_k(G)x^k$ where for each k, $F_k(G)$ is the number of independent sets of k vertices.

This thesis is an investigation of independence polynomials of several classes of graphs, some directly related to molecules of hydrocarbons. In particular, for the graphs of alkanes, alkenes, and cycloalkanes, we have determined the Merrifield-Simmons index, the independence polynomial, and, in some cases, the generating function for the independence polynomial. These parameters are also determined in several classes of graphs which are natural generalizations of the hydrocarbons. The proof techniques used in studying the hydrocarbons have led to some possibly interesting results concerning the coefficients of independence polynomials of regular graphs with large girth.

LIST OF SYMBOLS

$\emptyset$	the empty set; $\{\}$
$\alpha(G)$	the independence number of a graph G; the size of a largest independent set in G
B_n	full binary tree with n levels of vertices
B_n^t	full t-ary tree with n levels of vertices
C_n	a cycle on n vertices
$d(v)$	the degree of a vertex v
$\delta(G)$	the minimum degree of a graph G
$\Delta(G)$	the maximum degree of a graph G
$E(G)$	the edge set of a graph G
$F(G)$	the Fibonacci index of a graph G; the number of independent vertex sets in G
$F_k(G)$	the number of k-element independent sets in a graph G
$F_G(x)$	the independence polynomial of a graph G
$G \cup H$	the disjoint union of the graphs G and H
I_n	the independent graph on n vertices that has no edges
K_n	the complete graph on n vertices that has an edge between every pair of vertices

$K_{m,n}$	the complete bipartite graph with partite sets of size m and n
$n!$	n factorial; $n! = n(n-1)\cdots(2)(1)$
$\binom{n}{k}$	"n choose k;" the binomial coefficient calculated by $\dfrac{n!}{k!(n-k)!}$
$N(u)$	the neighborhood of a vertex u; the set of all vertices that are adjacent to u
$N[u]$	the closed neighborhood of a vertex u; $N[u] = N(u) \cup \{u\}$
$N_G(H)$	the number of distinct subgraphs of a graph G isomorphic to H
P_n	the graph of a path on n vertices
S_n	a sequence of graphs defined by deleting a vertex from T_n; see Figure 8
S_n^m	a sequence of graphs generalizing S_n; see Figure 16
T_n	a sequence of graphs associated with the structure of alkanes; see Figure 7
T_n^m	a sequence of graphs generalizing T_n; see Figure 15
U_n	a sequence of graphs associated with the structure of alkenes; see Figure 9
U_n^m	a sequence of graphs generalizing U_n; see Figure 17
$u \sim v$	vertex u is adjacent to vertex v; $\{u, v\} \in E$
$V(G)$	the vertex set of a graph G
V_n	a sequence of graphs associated with the structure of cycloalkanes; see Figure 10
V_n^m	a sequence of graphs generalizing V_n; see Figure 18
W_n	a wheel on n vertices

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1 INTRODUCTION

Modern mathematics places far more emphasis on abstraction than mathematics in earlier times. Graph theory, even if one considers Euler as its founding father, is a relatively modern field of mathematics, and it is perhaps more honest to credit the 20th century for its development. Graphs can be viewed as abstractions of any situation where relationships are important. For instance, cities are or are not connected by a highway. Pairs of people in a group either know each other or do not. Certain professors are available to teach only in certain time slots. And, when Euler first solved the famous Seven Bridges of Königsberg problem in 1736, certain pieces of land were connected by those bridges. All of these situations can be abstractly modeled by graphs.

Often, there are graph-theoretical parameters such as the connectivity number, the chromatic number, or the independence number which are directly related to practical problems. For example, a desirable feature of a secure computer network would be a high connectivity number, making it difficult for an "enemy" to prevent communication by knocking out relatively few nodes. In another application, coding is often done with sequences of characters as vertices in a graph with edges between similar words. A set of code words is an independent set in that graph, and a high independence number allows for a larger set of code words [10].

The particular application motivating this thesis comes from molecular chemistry. It has been found empirically that the stability and boiling point of certain molecules are related to the number of independent sets in the molecular graph, the graph whose vertices are the atoms of the molecules with two atoms joined by an edge if they share a bond. In the 1980's, the Merrifield-Simmons index was defined by chemists to describe precisely this parameter [2], [4], [6], [12]. This same parameter is better known in graph theory as the Fibonacci index. Graph theorists refined this concept to the independence polynomial of a graph, which counts independent sets of every size.

These parameters have been widely studied in chemical graph theory and in extremal graph theory. Merrifield and Simmons [12] observed a correlation between the number of indendent vertex sets and the boiling point of certain hydrocarbons. Fajtlowicz and Larson [4] noted that the independence number is a predictor of the stability of fullerenes, a conjecture of the computer program Graffiti. From their results, Henry, Pepper, and Sexton [7] inferred that certain stable hydrocarbons also minimize their independence numbers. Many investigations have examined the extremal cases of the Merrifield-Simmons index and a survey of these results is given by Gutman and Wagner [6].

For many classes of graphs, the Fibonacci index and independence polynomial have been determined exactly, and this has even led to some graph-theoretic proofs of combinatorial identities [8], [9]. In general, the following problem is known to be NP-complete [10]: For a graph G on n vertices and an integer k, determine whether or not G contains an independent set of k vertices. Since knowledge of the independence polynomial answers this question, it follows that the determination of the polynomial is a difficult problem (in a technical sense).

This thesis will be an investigation of independence polynomials in several classes of graphs, some directly related to the molecules of hydrocarbons. Since the independence polynomial refines the Merrifield-Simmons index, this parameter is also determined in these graphs. The results concerning hydrocarbons have also been extended to more general classes of graphs. Finally, the proof techniques used in this project have led to some possibly interesting results concering the determination of the coefficients of independence polynomials of regular graphs with large girth.

2 PRELIMINARIES

2.1 Graphs

We define a *graph* G to be an ordered pair $G = (V, E)$ where V is a finite set of elements called *vertices* and E is a set of *edges*, or two-element subsets of V. We may also denote the vertex set of a graph G by $V(G)$ and the edge set by $E(G)$. We say that two vertices u and v are *adjacent* if $\{u, v\} \in E$ and we denote this by $u \sim v$.

Graphs are typically depicted by assigning a point for each vertex and a line between points to represent an edge between those vertices. Figure 1 represents the graph with the vertex set $V = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$ and the edge set $E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 9\}, \{1, 4\}, \{1, 5\}, \{4, 5\}, \{4, 6\}, \{6, 7\}, \{7, 8\}, \{4, 8\}\}$. Note that the physical placement of the points and lines does not matter in an embedding of a graph. The information that determines the graph is the presence or absence of an edge between two vertices.

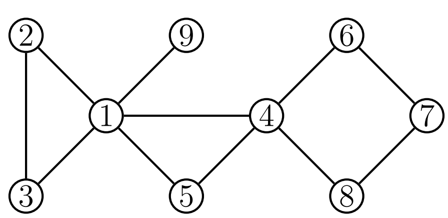


Figure 1: An Example of a Graph $G = (V, E)$

Suppose that $G = (V, E)$ is a graph and $u, v \in V$ are adjacent vertices. We say that u and v are *neighbors*. The *neighborhood* of a vertex u is the set $N(u) = \{v \in V : v \sim u\}$, and the size of this set is called the *degree* of u, denoted by $d(u)$. A vertex with degree 1 is called a *leaf*. For example, in Figure 1 vertex 9 is a leaf. We also have the *closed neighborhood* $N[u] = N(u) \cup \{u\}$, which includes u and its neighbors.

The *degree sequence* of a graph refers to the list of the degrees of the vertices in descending order. We use the symbol $\delta(G)$ to denote the minimum vertex degree in a graph G. Similarly, we use $\Delta(G)$ to denote the maximum vertex degree. A graph is called k-*regular* if every vertex has degree k. For the graph in Figure 1, the degree sequence is $(5, 4, 2, 2, 2, 2, 2, 2, 1)$, $\delta(G) = 1$, and $\Delta(G) = 5$.

If G and H are graphs, we say that H is a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Given a subset of vertices $N \subseteq V(G)$, the *induced subgraph* on N is the graph G' defined by $V(G') = N$ and $E(G') = \{\{u, v\} \in E(G) : u, v \in N\}$. For the graph in Figure 1, the induced subgraph on $\{1, 2, 3, 4\}$ has the edge set $\{\{1, 2\}, \{1, 3\}, \{1, 4\}, \{2, 3\}\}$. If $N \subseteq V(G)$, then $G - N$ is the subgraph induced by the vertex set $V(G) - N = \{v \in V(G) : v \notin N\}$. For a graph G, the *complement graph* is the graph $\bar{G}$ with vertex set $V(G)$ and an edge set defined by $E(\bar{G}) = \{\{x, y\} : x, y \in V(G) \text{ and } \{x, y\} \notin E(G)\}$.

A subset S of the vertices of a graph is said to be *independent* if no two vertices in S are adjacent. For instance, in Figure 1, the set $\{3, 6, 8, 9\}$ is an independent set. The *independence number* of a graph, denoted by $\alpha(G)$, is the size of a largest independent set. The independent graph I_n is the graph consisting of n vertices and no edges. The complement of I_n is the complete graph K_n, the graph consisting of n vertices with an edge between every pair of vertices. The complete bipartite graph, $K_{m,n}$, consists of $m + n$ vertices divided into two sets, one of size m and one of size n, with edges between two vertices if and only if they are in different sets. If G and H are graphs with $V(G) \cap V(H) = \emptyset$, then $G \cup H$ refers to the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

A sequence of vertices in which each vertex is adjacent to the next is called a *walk*, and the *length* of a walk W is one less than the number of vertices in W. We can think of this as the number of edges we would traverse if tracing the sequence of vertices in the graph. A *path* is a walk in which no vertex is repeated, and P_n denotes a path on n vertices. We say that a graph G is *connected* if there is a path between each pair of vertices, and a *component* of G is a maximal connected subgraph. A *cycle* is a walk in which the only repeated vertices in the sequence are the first and the last, and C_n denotes a cycle on n vertices. The wheel, W_n, is a cycle C_n with an additional vertex that is adjacent to all other vertices. In Figure 1, we have the cycle $(4, 6, 7, 8, 4)$. The *girth* of a graph is the length of its shortest cycle, if it has one. A graph G which contains no cycles is called *acyclic* and has infinite girth. A *forest* is an acyclic graph, and if a graph is both acyclic and connected, then it is a *tree*.

2.2 Combinatorics

Combinatorics is a branch of mathematics which studies construction and enumeration problems of discrete mathematical objects. The study of graphs falls under combinatorics. In this thesis, a number of tools and concepts from the more general field will be used, so we will take the opportunity to mention those here.

In the study of counting problems, binomial coefficients arise frequently. The binomial coefficient $\binom{n}{k}$ refers to the number of different ways to choose k objects from a set of n objects. This number can be calculated quite easily as $\binom{n}{k} = \dfrac{n!}{k!(n-k)!}$.

The Principle of Inclusion/Exclusion is another useful tool in counting problems. It can be stated as follows: If $A_1, A_2, ..., A_n$ are finite sets, then

$$\begin{aligned} |\cup_{i=1}^{n} A_i| &= \sum_{i=1}^{n} |A_i| - \sum_{i,j:1 \le i < j \le n} |A_i \cap A_j| + \sum_{i,j,k:1 \le i < j < k \le n} |A_i \cap A_j \cap A_k| - ... \\ &\quad +(-1)^{n-1}|A_1 \cap A_2 \cap ... \cap A_n|. \end{aligned}$$

A special sequence of numbers which arises often in combinatorics is the Fibonacci sequence. The sequence begins 0,1,1,2,3,5,8,13,21,... and can be defined by the following:

$$\begin{aligned} F_0 &= 0 \\ F_1 &= 1 \\ F_n &= F_{n-1} + F_{n-2} \text{ for } n \ge 2 \end{aligned}$$

This last equation is known as a *recurrence relation*, a formula for finding terms of a sequence from earlier terms. The values of the first few terms which are necessary to find the entire sequence are called *initial conditions*. Solving a recurrence relation refers to the process of finding a formula for the nth term of the sequence which does not depend on finding the previous terms first.

One method of solving a recurrence relation involves finding the roots of the characteristic equation. For a recurrence relation of the form $a_n = k_1 a_{n-1} + k_2 a_{n-2} + ... + k_m a_{n-m}$, the characteristic equation is $r^m - k_1 r^{m-1} - k_2 r^{m-2} - ... - k_m = 0$. Each of the roots of this equation raised to the nth power satisfy our recurrence, and in fact, any linear combination of these will also satisfy the recurrence. If $r_1, r_2, ..., r_m$ are distinct roots of the characteristic equation, the general solution for the recurrence relation is given by $a_n = c_1 r_1^n + c_2 r_2^n + ... + c_m r_m^n$ where $c_1, c_2, ..., c_m$ are constants. We can simply solve for the constants which meet the initial conditions to find a formula for a_n in terms of n.

Let's consider the Fibonacci sequence. The characteristic equation for the recurrence relation is $r^2 - r - 1 = 0$. Using the quadratic formula, the roots of this equation are $r_1 = \frac{1+\sqrt{5}}{2}$ and $r_2 = \frac{1-\sqrt{5}}{2}$. So the general solution is given by $F_n = c_1 \left(\frac{1+\sqrt{5}}{2}\right)^n + c_2 \left(\frac{1-\sqrt{5}}{2}\right)^n$. It remains to solve for the constants which meet the initial conditions when $n = 0$ and $n = 1$:

$$0 = F_0 = c_1 + c_2$$

$$1 = F_1 = c_1 \left(\frac{1+\sqrt{5}}{2}\right) + c_2 \left(\frac{1-\sqrt{5}}{2}\right)$$

Solving for c_1 and c_2, we see that

$$F_n = \frac{1}{\sqrt{5}} \left(\frac{1+\sqrt{5}}{2}\right)^n - \frac{1}{\sqrt{5}} \left(\frac{1-\sqrt{5}}{2}\right)^n .$$

Another sequence which occurs often in counting problems is the Lucas sequence. This sequence has the same recurrence relation as the Fibonacci sequence, but with different initial conditions, to produce the sequence 1,3,4,7,11,18,29,... .

Generating functions are yet another common tool in combinatorial problems. The generating function for the sequence $a_0, a_1, a_2, ...$ is the formal power series $a_0 + a_1 x + a_2 x^2 + ... = \sum_{n\geq 0} a_n x^n$. As described by Herbert Wilf [18], "A generating function is a clothesline on which we hang up a sequence of numbers for display." Knowing a generating function for a sequence can be useful for finding an exact formula for the sequence, finding a new recurrence formula, finding statistical properties, finding asymptotic formulas, and proving identities.

Let's revisit the Fibonacci sequence to see how a generating function might be useful for solving a recurrence relation. Let $F(x) = \sum_{n\geq 0} F_n x^n$ be the generating function for the Fibonacci numbers. If we multiply the recurrence relation $F_n = F_{n-1} + F_{n-2}$ by x^n and sum over $n \geq 2$, we can solve for the closed form for $F(x)$.

$$\begin{aligned}
\sum_{n\geq 2} F_n x^n &= \sum_{n\geq 2} F_{n-1} x^n + \sum_{n\geq 2} F_{n-2} x^n \\
F(x) - F_1 x - F_0 &= x(F(x) - F_0) + x^2 F(x) \\
F(x) - x &= xF(x) + x^2 F(x) \\
F(x) &= \frac{x}{1 - x - x^2}
\end{aligned}$$

Using the method of partial fractions and expanding this closed form, we can find that the coefficient of x^n in the expansion is $\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^n - \frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^n$, which was the same formula we obtained for the nth Fibonacci number before.

A common generating function is that of the geometric series: $\sum_{n\geq 0} x^n = \frac{1}{1-x}$. The derivative of the geometric series will also be useful for us: $\sum_{n\geq 1} n x^{n-1} = \frac{1}{(1-x)^2}$.

2.3 Independent Sets

Recall that an independent set in a graph, sometimes known as a *stable set*, refers to a set of vertices with no edges between them. The *Fibonacci index* of a graph G, denoted by $F(G)$, is defined to be the total number of independent sets in G. This concept was introduced in 1982 by Prodinger and Tichy [14]. If k is a non-negative integer, then the number of k-element independent sets in G is denoted by $F_k(G)$. This concept was extended to the *independence polynomial* of G, denoted by $F_G(x)$, to be the polynomial in x such that the coefficient of x^k in $F_G(x)$ is the number of k-element independent sets in G. The independence polynomial has also been refered to as the *Fibonacci polynomial*, and the Fibonacci index is often called the *Merrifield-Simmons index*, as it was introduced by chemists in 1989 [12]. It follows directly from the definitions that $F(G) = \sum_{k\geq 0} F_k(G)$ and that $F_G(x) = \sum_{k\geq 0} F_k(G)x^k$. Hence, $F_G(1) = F(G)$. In other words, evaluating the Fibonacci polynomial of a graph G at $x = 1$ yields the Fibonacci index of G.

For any graph G with n vertices and e edges, $F_0(G) = 1$ since the empty set is the unique independent set of size zero. The number of independent sets of size one is the size of the set of vertices, so $F_1(G) = n$. A two-element independent set is a pair of vertices that are not adjacent, and hence, $F_2(G) = \binom{n}{2} - e$. For K_3-free graphs, the following characterization is known for $F_3(G)$.

Lemma 1 *[19] For a triangle-free graph G with n vertices and e edges,*

$$F_3(G) = \binom{n}{3} - e(n-2) + \sum_{v\in V(G)} \binom{d(v)}{2}.$$

Proof: Since G is triangle-free, there are at most two edges between any set of three vertices in the graph. Using the Principle of Inclusion/Exclusion, we can count the number of 3-element independent sets by counting the total number of subsets of size 3, subtracting the number of sets with at least one edge, and adding the number of sets with two edges which were subtracted twice. We can pick an edge and any of the other $n-2$ vertices to get a subset of size three with one edge. For each vertex, we can choose two of its neighbors to get three vertices with two edges. Note that $\binom{d(v)}{2}$ is zero if $d(v) < 2$. Hence, $F_3(G) = \binom{n}{3} - e(n-2) + \sum_{v \in V(G)} \binom{d(v)}{2}$. □

In general, the degree sequence of G does not determine $F_4(G)$, even in acyclic graphs. The counterexample in Figure 2 appears in Wingard [19]. Graphs G_1 and G_2 have the same degree sequence, but $F_4(G_1) = 1$ and $F_4(G_0) = 0$.

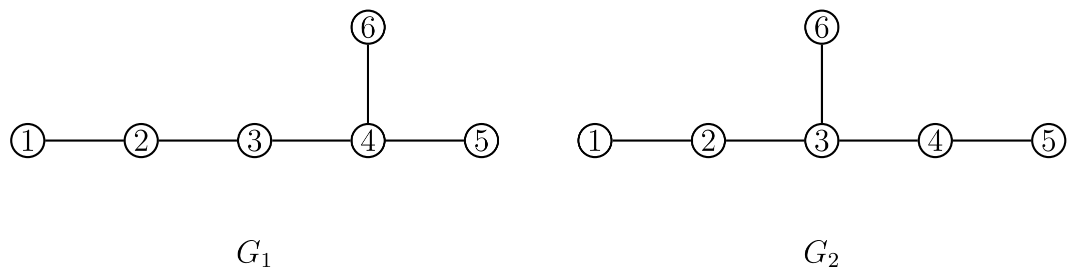


Figure 2: Graphs G_1 and G_2 with the same degree sequence, but $F_4(G_1) \neq F_4(G_2)$

When counting the number of independent sets in a graph G, we can reduce the problem by counting the number of sets that do and do not include a particular vertex $v \in V(G)$. The following reduction formulas are useful for enumerating independent sets.

Lemma 2 *[14] Let $v \in V(G)$. Then $F(G) = F(G-v) + F(G-N[v])$.*

Proof: If S is an independent set in G, then either $v \in S$ or $v \notin S$. There are $F(G-v)$ independent sets in G that do not include v. If such a set includes v, the other elements must come from $V(G) - N[v]$ and hence, there are $F(G - N[v])$ of these sets. So $F(G) = F(G-v) + F(G-N[v])$. □

Lemma 3 *[19] For any $v \in V(G)$ and $k \geq 1$, $F_k(G) = F_k(G-v) + F_{k-1}(G-N[v])$.*

Proof: Each k-element independent set in G either contains v or it does not. If it does not, then it is a k-element independent set in $G - v$. If it does, then the other $k-1$ elements are an independent set in $G - N[v]$. □

In other words, we can count the number of k-element independent sets in G by adding the number of k-element independent sets in $G-v$ and the number of $(k-1)$-element independent sets after the deletion of the closed neighborhood of v for any $v \in V(G)$. The following lemma gives us a reduction formula for the independence polynomial of a graph based on the same idea.

Lemma 4 *[19] For $v \in V(G)$, $F_G(x) = F_{G-v}(x) + xF_{G-N[v]}(x)$.*

Proof: By using the definition of the independence polynomial and Lemma 3,

$$\begin{aligned}
F_{G-v}(x) + xF_{G-N[v]}(x) &= \sum_{k\geq 0} F_k(G-v)x^k + x\sum_{k\geq 0} F_k(G-N[v])x^k \\
&= \sum_{k\geq 0} F_k(G-v)x^k + \sum_{k\geq 1} F_{k-1}(G-N[v])x^k \\
&= F_0(G-v) + \sum_{k\geq 1} \left(F_k(G-v) + F_{k-1}(G-N[v])\right) x^k \\
&= 1 + \sum_{k\geq 1} F_k(G)x^k \\
&= \sum_{k\geq 0} F_k(G)x^k \\
&= F_G(x). \qquad \square
\end{aligned}$$

In a graph with more than one component, note that an independent set will be the union of independent sets in each of the components. Hence, the independence polynomial will result from the product of the polynomials of each of the components as shown in the following lemma.

Lemma 5 *[19] Suppose that a graph $G = \bigcup_{i=1}^{n} G_i$ where each graph G_i is a component of G. Then $F_G(x) = \prod_{i=1}^{n} F_{G_i}(x)$.*

Proof: A k-element independent set in G is the union of independent sets of size $j_1, j_2, ..., j_n$ from the components $G_1, G_2, ..., G_n$, respectively, where $j_1 + j_2 + ... + j_n = k$. So, after multiplying the independence polynomials of the components, the coefficient of x^k will be $F_k(G)$. □

Similarly, the Fibonacci index will be the product of the indices of each of the components.

Lemma 6 *Suppose that a graph* $G = \bigcup_{i=1}^{n} G_i$ *where each graph* G_i *is a disjoint component of* G*. Then* $F(G) = \prod_{i=1}^{n} F(G_i)$*.*

Proof: By the previous lemma, $F_G(x) = \prod_{i=1}^{n} F_{G_i}(x)$. Letting $x = 1$ to count the Fibonacci index, $F(G) = F_G(1) = \prod_{i=1}^{n} F_{G_i}(1) = \prod_{i=1}^{n} F(G_i)$. □

The Fibonacci index received its name because the number of independent sets in the graph P_n is actually the Fibonacci number F_{n+2} [14]. To see this, consider a vertex reduction on a leaf of a path with n vertices. By Lemma 2,

$$\begin{aligned} F(P_n) &= F(P_n - v) + F(P_n - N[v]) \\ &= F(P_{n-1}) + F(P_{n-2}) \end{aligned}$$

and we have the initial conditions $F(P_0) = 1$ and $F(P_1) = 2$. Similarly, it can be shown that the sequence of Fibonacci indices of cycles is essentially the Lucas sequence [14].

The following simple examples of independence polynomials appear in Wingard [19]. In the complete graph K_n, every two vertices are adjacent, so there are no independent sets with size larger than one. Hence,

$$F_{K_n}(x) = 1 + nx.$$

The independent graph I_n is the union of n individual vertices, so

$$F_{I_n}(x) = \prod_{i=1}^{n}(1 + x) = (1 + x)^n.$$

An independent set in the complete bipartite graph $K_{m,n}$ cannot have vertices in both partite sets. So it must come entirely from only one set, either I_m or I_n. After accounting for the empty set being counted twice, we see that

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

Other classes of graphs for which the Fibonacci index or independence polynomials have been determined include stars, wheels, various lattices, Möbius ladders, combs, and some classes of regular and almost-regular graphs [1], [3], [8], [9], [14], [19].

In this thesis, we will investigate full binary and t-ary trees, graphs of molecular hydrocarbons, and generalizations of these graphs.

3 FULL t-ARY TREES

A *binary tree* is a tree with a root of degree at most two in which every vertex is adjacent to at most two "children" vertices. A *full binary tree* is one in which every vertex other than the leaves has exactly two children and each level is as full as possible. Let B_n represent a full binary tree with n levels of vertices. Then B_0 is the empty graph, B_1 is a single vertex, and for $n \geq 2$, B_n is obtained from B_{n-1} by adding two "children" to each leaf of the tree. We can see that each tree B_n has $2^n - 1$ vertices and $2^n - 2$ edges. As an example, B_3 is shown in Figure 3 with 7 vertices and 6 edges.

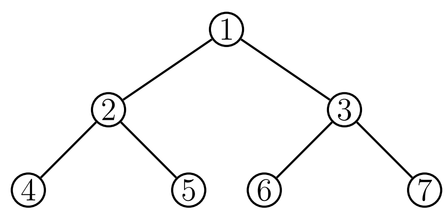


Figure 3: A Full Binary Tree with 3 Levels of Vertices

Full binary trees can be generalized to full t-ary trees in which each non-leaf vertex has t children. Let B_n^t represent a full t-ary tree with n levels of vertices. Then B_n^1 is just a path, and $B_n^2 = B_n$. Prodinger and Tichy investigated the Fibonacci index of full t-ary trees and the following lemma is their result. In addition, they developed asympototic formulas for $F(B_n^t)$ [11].

Lemma 7 *[11] Let $t \geq 1$. Then $F(B_0^t) = 1$, $F(B_1^t) = 2$, and for $n \geq 2$,*

$$F(B_n^t) = F(B_{n-1}^t)^t + F(B_{n-2}^t)^{t^2}.$$

Proof: We can determine that $F(B_0^t) = 1$ and $F(B_1^t) = 2$ for any values of t. Let $n \geq 2$ and let v be the root vertex in a full t-ary tree B_n^t. By Lemma 2,

$$\begin{aligned} F(B_n^t) &= F(B_n^t - v) + F(B_n^t - N[v]) \\ &= F\left(\bigcup_{i=1}^{t} B_{n-1}^t\right) + F\left(\bigcup_{i=1}^{t^2} B_{n-2}^t\right) \\ &= F(B_{n-1}^t)^t + F(B_{n-2}^t)^{t^2}. \end{aligned}$$

□

In the case of full binary trees, $F(B_n) = F(B_{n-1})^2 + F(B_{n-2})^4$ for $n \geq 2$. Table 1 shows values for $F(B_n)$ for small n.

n	$F(B_n)$
0	1
1	2
2	5
3	41
4	2,306
5	8,143,397

Table 1: $F(B_n)$ for $n \leq 5$

We can also recursively count the number of k-element independent sets in B_n.

Proposition 1 *For $n \geq 2$, $k \geq 1$, we have*

$$F_k(B_n) = F_k\left(\bigcup_{i=1}^{2} B_{n-1}\right) + F_{k-1}\left(\bigcup_{i=1}^{4} B_{n-2}\right).$$

Proof: If a k-element independent set in B_n does not include the root vertex, then it is contained entirely in the two subtrees with $n-1$ levels of vertices. If a k-element independent set in B_n does contain the root, then the other $k-1$ vertices must come from four subtrees with $n-2$ levels of vertices. By Lemma 2, $F_k(B_n) = F_k\left(\bigcup_{i=1}^{2} B_{n-1}\right) + F_{k-1}\left(\bigcup_{i=1}^{4} B_{n-2}\right)$. □

As with any graph, $F_0(B_n) = 1$. Since the graph B_n has $2^n - 1$ vertices, we know that $F_1(B_n) = |V(B_n)| = 2^n - 1$. Also, $F_2(B_n) = \binom{|V(B_n)|}{2} - |E(B_n)| = \binom{2^n - 1}{2} - (2^n - 2)$. In the following two propositions, we obtain a formula for the number of independent sets of size three in B_n. Note that a formula also could be obtained by using Lemma 1, but we will find the method of using generating functions used here to be useful later.

Proposition 2 *For $n \geq 3$, we have $F_3(B_n) = 2F_3(B_{n-1}) - 4^n + 8^{n-1} + 12$.*

Proof: Let $n \geq 3$. By Proposition 1, $F_3(B_n) = F_3\left(\bigcup_{i=1}^{2} B_{n-1}\right) + F_2\left(\bigcup_{i=1}^{4} B_{n-2}\right)$. To count $F_3\left(\bigcup_{i=1}^{2} B_{n-1}\right)$, note that each 3-element independent set either comes entirely from the first subtree B_{n-1}, entirely from the second subtree, has two vertices in first subtree and one in the second, or has two vertices in the second and one in the first. Hence, $F_3\left(\bigcup_{i=1}^{2} B_{n-1}\right) = 2F_3(B_{n-1}) + 2F_2(B_{n-1})F_1(B_{n-1})$. To count $F_2\left(\bigcup_{i=1}^{4} B_{n-2}\right)$, note that the two vertices in each independent set either come from the same subtree or from two different ones. So $F_2\left(\bigcup_{i=1}^{2} B_{n-2}\right) = 4F_2(B_{n-2}) + \binom{4}{2}(F_1(B_{n-1}))^2$. Hence,

$$
\begin{aligned}
F_3(B_n) &= F_3\left(\bigcup_{i=1}^{2} B_{n-1}\right) + F_2\left(\bigcup_{i=1}^{4} B_{n-2}\right) \\
&= 2F_3(B_{n-1}) + 2F_2(B_{n-1})F_1(B_{n-1}) + 4F_2(B_{n-2}) + \binom{4}{2}(F_1(B_{n-1}))^2 \\
&= 2F_3(B_{n-1}) + 2\left(\binom{2^{n-1} - 1}{2} - (2^{n-1} - 2)\right)(2^{n-1} - 1) \\
&\quad +4\left(\binom{2^{n-2} - 1}{2} - (2^{n-2} - 2)\right) + 6(2^{n-2} - 1)^2 \\
&= 2F_3(B_{n-1}) - 4^n + 8^{n-1} + 12. \qquad \square
\end{aligned}
$$

Proposition 3 *For $n \geq 2$, $F_3(B_n) = -12 - 2^{2n+1} + \frac{1}{3}2^{3n-1} + \frac{25}{3}2^n$.*

Proof: Note that for $n = 2$, $F_3(B_2) = 0 = -12 - 2^1 + \frac{1}{3} \cdot 2^5 + \frac{25}{3} \cdot 2^2$. Now, let $n \geq 3$. By Proposition 2, $F_3(B_n) = 2F_3(B_{n-1}) - 4^n + 8^{n-1} + 12$. We can define a generating function for $F_3(B_n)$ by $f(x) = \sum_{n=0}^{\infty} F_3(B_n)x^n$. Note that $F_3(B_n) = 0$ for $n < 3$, so

$$\begin{aligned}
f(x) &= \sum_{n=3}^{\infty} F_3(B_n)x^n \\
&= \sum_{n=3}^{\infty} \left(2F_3(B_{n-1}) - 4^n + 8^{n-1} + 12\right) x^n \\
&= 2x\sum_{n=3}^{\infty} F_3(B_{n-1})x^{n-1} - \sum_{n=3}^{\infty}(4x)^n + x\sum_{n=3}^{\infty}(8x)^{n-1} + 12\sum_{n=3}^{\infty} x^n \\
&= 2x\sum_{n=2}^{\infty} F_3(B_n)x^n - \sum_{n=3}^{\infty}(4x)^n + x\sum_{n=3}^{\infty}(8x)^{n-1} + 12\sum_{n=3}^{\infty} x^n \\
&= 2xf(x) - \frac{64x^3}{1-4x} + \frac{64x^3}{1-8x} + \frac{12x^3}{1-x}.
\end{aligned}$$

Hence,

$$\begin{aligned}
f(x) &= \frac{-64x^3}{(1-2x)(1-4x)} + \frac{64x^3}{(1-2x)(1-8x)} + \frac{12x^3}{(1-2x)(1-x)} \\
&= 4x^3\left(\frac{-3}{1-x} - \frac{32}{1-4x} + \frac{\frac{64}{3}}{1-8x} + \frac{\frac{50}{3}}{1-2x}\right) \\
&= 4x^3\left(-3\sum_{n=0}^{\infty} x^n - 32\sum_{n=0}^{\infty}(4x)^n + \frac{64}{3}\sum_{n=0}^{\infty}(8x)^n + \frac{50}{3}\sum_{n=0}^{\infty}(2x)^n\right) \\
&= 4x^3\sum_{n=0}^{\infty}\left(-3 - 32\cdot 4^n + \frac{64}{3}\cdot 8^n + \frac{50}{3}\cdot 2^n\right)x^n \\
&= \sum_{n=0}^{\infty}\left(-12 - 32\cdot 4^{n+1} + \frac{256}{3}\cdot 8^n + \frac{50}{3}\cdot 2^{n+2}\right)x^{n+3} \\
&= \sum_{n=3}^{\infty}\left(-12 - 2^{2n+1} + \frac{1}{3}\cdot 2^{3n-1} + \frac{25}{3}\cdot 2^n\right)x^n.
\end{aligned}$$

So for $n \geq 3$, $F_3(B_n) = -12 - 2^{2n+1} + \frac{1}{3}\cdot 2^{3n-1} + \frac{25}{3}\cdot 2^n$. □

Table 2 shows values of $F_3(B_n)$ for small n. We can also find the independence polynomial for B_n recursively as shown in the following proposition.

Proposition 4 *For $n \geq 2$, $F_{B_n}(x) = (F_{B_{n-1}}(x))^2 + x(F_{B_{n-2}}(x))^4$.*

n	$F_3(B_n)$
0	0
1	0
2	0
3	12
4	292
5	3,668
6	36,020
7	317,812
8	2,667,252
9	21,849,588
10	176,868,340

Table 2: $F_3(B_n)$ for $n \leq 10$

Proof: Let v_0 be the root vertex of B_n. By Lemma 4 and Lemma 5,

$$\begin{aligned} F_{B_n}(x) &= F_{B_n - v_0}(x) + xF_{B_n - N[v_0]}(x) \\ &= F_{\cup_{i=1}^{2} B_{n-1}}(x) + xF_{\cup_{i=1}^{4} B_{n-2}}(x) \\ &= (F_{B_{n-1}}(x))^2 + x(F_{B_{n-2}}(x))^4. \end{aligned}$$

$\square$

The independence polynomials of B_n for small n are listed in Table 3.

n	$F_{B_n}(x)$
0	1
1	$1+x$
2	$1+3x+x^2$
3	$1+7x+15x^2+12x^3+5x^4+x^5$
4	$1+15x+91x^2+292x^3+547x^4+627x^5+452x^6+208x^7+61x^8$ $+11x^9+x^{10}$
5	$1+31x+435x^2+3668x^3+20815x^4+84407x^5+253652x^6+578680x^7$ $+1019787x^8+1407161x^9+1537951x^{10}+1345112x^{11}+950028x^{12}$ $+545940x^{13}+256560x^{14}+98704x^{15}+30925x^{16}+7775x^{17}$ $+1523x^{18}+220x^{19}+21x^{20}+x^{21}$

Table 3: Independence Polynomials $F_{B_n}(x)$ for $n \leq 5$

4 GRAPHS OF HYDROCARBONS

The Fibonacci index, $F(G)$, is more commonly known as the Merrifield-Simmons index among chemists. It is one of the many graph parameters known as topological indices that are studied because of their chemical properties. In particular, the Fibonacci index of a molecular graph is known to correlate with the stability of the substance and with its boiling point ([2], [4], [6], [7], [12]).

A hydrocarbon, a chemical compound consisting of carbon and hydrogen, is an important class of molecules in organic chemistry, including such common substances as methane, propane, and octane. Hydrocarbons provide us with petroleum products such as gasoline, oil, asphalt, and plastic. There are several subclasses of hydrocarbons, defined by the saturation and the structure of the carbon atoms. In this thesis, we will study the molecular graphs of three of these subclasses.

Alkanes are the first type that we want to consider. A normal alkane is a saturated hydrocarbon in which the carbons form a chain. So every atom is bonded to the maximum number of other atoms; the vertices representing carbon atoms have degree four, and those representing hydrogen atoms have degree one. The chemical formula for an alkane is of the form C_nH_{2n+2}. The structure of an alkane is shown for the case where $n = 3$ in Figure 4.

$$
\begin{array}{ccccccccc}
 & & \mathrm{H} & & \mathrm{H} & & \mathrm{H} & & \\
 & & | & & | & & | & & \\
\mathrm{H} & - & \mathrm{C} & - & \mathrm{C} & - & \mathrm{C} & - & \mathrm{H} \\
 & & | & & | & & | & & \\
 & & \mathrm{H} & & \mathrm{H} & & \mathrm{H} & &
\end{array}
$$

Figure 4: Molecular Structure of an Alkane

Another subclass of hydrocarbons is the alkenes. These are unsaturated hydrocarbons which are missing two of the hydrogen atoms found in an alkane. The chemical formula is of the form C_nH_{2n}, and Figure 5 shows an example for $n = 3$.

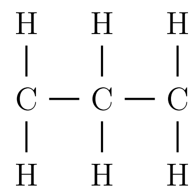


Figure 5: Molecular Structure of an Alkene

It is also possible for the carbon atoms to be arranged in cycles. Cycloalkanes refer to saturated hydrocarbons with a single cycle of carbon atoms. They also have the chemical formula C_nH_{2n}, and Figure 6 shows an example for $n = 4$ [13].

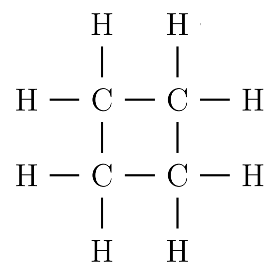


Figure 6: Molecular Structure of a Cycloalkane

The nomenclature for these subclasses of hydrocarbons is demonstrated in Table 4.

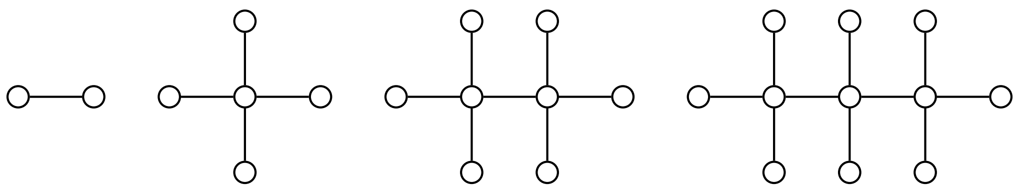
In addition to these normal molecular layouts of hydrocarbons, each chemical may have a number of isomers with the same numbers of atoms, but a slightly different molecular graph. See Figure 23 for the isomers of butane. For now, we will only study the normal structure of these chemicals.

We can associate the sequence of graphs T_n shown in Figure 7 with the molecular structure of alkanes. We will consider the vertex shown on the far left in each picture as the root vertex of each tree. If we let T_0 be two vertices and a single edge as shown, we can define T_n recursively by adjoining three vertices to the root of T_{n-1}. Note that the leaves of each

Number of Carbons	Alkane	Alkene	Cycloalkane
1	Methane	–	–
2	Ethane	Ethene	–
3	Propane	Propene	Cyclopropane
4	Butane	Butene	Cyclobutane
5	Pentane	Pentene	Cyclopentane
6	Hexane	Hexene	Cyclohexane
7	Heptane	Heptene	Cycloheptane
8	Octane	Octene	Cyclooctane
9	Nonane	Nonene	Cyclononane
10	Decane	Decene	Cyclodecane

Table 4: A Table of Hydrocarbons

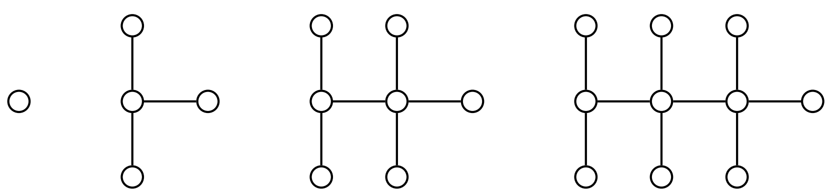
graph T_n correspond to the $2n+2$ hydrogen atoms and the vertices of degree 4 represent the carbons.



T_0 T_1 T_2 T_3

Figure 7: The Sequence of Graphs T_n

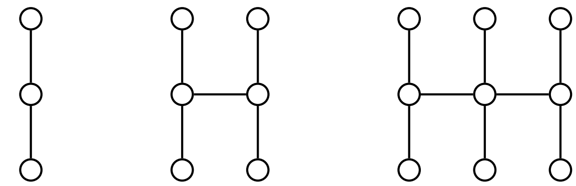
To aid us in studying the structure of these graphs, we can define another sequence of graphs S_n as shown in Figure 8. Each graph S_n is the graph T_n after the deletion of the root vertex.



S_0 S_1 S_2 S_3

Figure 8: The Sequence of Graphs S_n

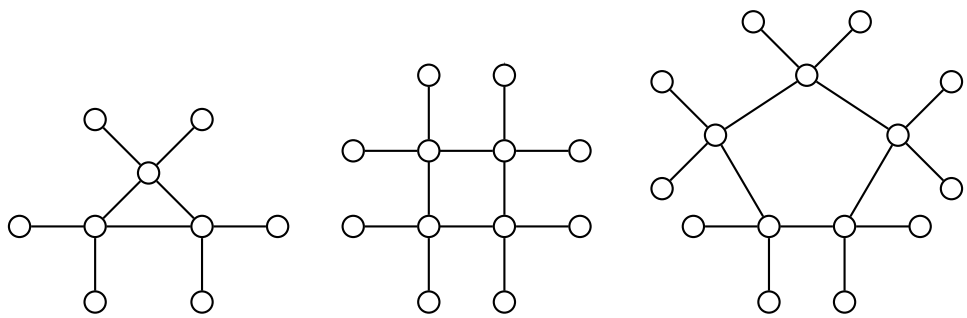
Similarly, we can define a sequence of graphs U_n that model the structure of alkenes as pictured in Figure 9. Each graph U_n is formed by adjoining n paths of length two at their center vertices to form a chain.



U_0 U_1 U_2 U_3

Figure 9: The Sequence of Graphs U_n

For the cycloalkanes, we can define the sequence of graphs V_n for $n \geq 3$ in Figure 10 which are formed by adjoining the two vertices of degree three in U_n.



V_3 V_4 V_5

Figure 10: The Sequence of Graphs V_n

We can establish recurrence relations to count the number of independent sets in these graphs, and we can use these to find explicit formulas for the Merrifield-Simmons index and the independence polynomial.

4.1 Fibonacci Indices of Hydrocarbons

First, we will consider the sequence of graphs S_n.

Proposition 5 *We have $F(S_0) = 2$, $F(S_1) = 9$, and for $n \geq 2$, we have the recurrence relation*

$$F(S_n) = 4F(S_{n-1}) + 4F(S_{n-2}).$$

Proof: The number of independent sets in S_0 is two, namely the empty set and the set with the single vertex. Enumerating the number of independent sets in S_1 yields the empty set, four single vertices, three independent sets of size two, and one set of size three.

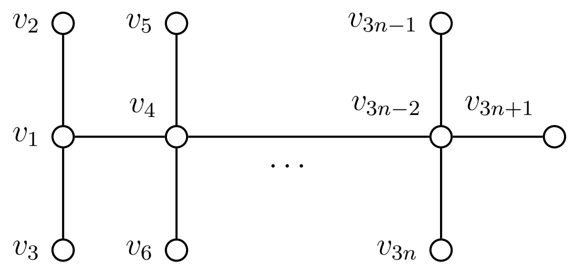


Figure 11: Independent Sets in S_n

To count the number of independent sets in S_n for $n \geq 2$, we can use a reduction formula with vertex v_1 in Figure 11. By Lemma 2 and Lemma 6,

$$\begin{aligned} F(S_n) &= F(S_n - v_1) + F(S_n - N[v_1]) \\ &= F(S_{n-1} \cup I_2) + F(S_{n-2} \cup I_2) \\ &= F(S_{n-1})F(I_2) + F(S_{n-2})F(I_2) \\ &= 4F(S_{n-1}) + 4F(S_{n-2}). \end{aligned}$$

$\square$

Now that we have a recurrence relation for $F(S_n)$, solving for an explicit formula is routine. The formulas in Propositions 6 and 7 also appear in the text by Merrifield and Simmons [12].

Proposition 6 *[12] For $n \geq 0$, the Fibonacci index of S_n is given by*

$$F(S_n) = \left(\frac{8+5\sqrt{2}}{8}\right)(2+2\sqrt{2})^n + \left(\frac{8-5\sqrt{2}}{8}\right)(2-2\sqrt{2})^n.$$

Proof: Note that $F(S_0) = 2 = \frac{8+5\sqrt{2}}{8} + \frac{8-5\sqrt{2}}{8}$ and $F(S_1) = 9 = \left(\frac{8+5\sqrt{2}}{8}\right)(2+2\sqrt{2}) + \left(\frac{8-5\sqrt{2}}{8}\right)(2-2\sqrt{2})$.

Now, suppose that $n \geq 2$. By Proposition 5, $F(S_n) = 4F(S_{n-1}) + 4F(S_{n-2})$. This recurrence relation yields the characteristic equation $r^2 - 4r - 4 = 0$, and hence the characteristic roots $r = 2 \pm 2\sqrt{2}$. So the general solution is $F(S_n) = c_1(2+2\sqrt{2})^n + c_2(2-2\sqrt{2})^n$ for some constants c_1 and c_2. Solving for these constants with the initial conditions when $n = 0, 1$ gives us the desired formula. □

Using the previous propositions for counting the independent sets of S_n, we can derive the following formula for the Fibonacci index of T_n.

Proposition 7 *[12] We have $F(T_0) = 3$, and for $n \geq 1$, the Fibonacci index of T_n is*

$$F(T_n) = \left(\frac{34+23\sqrt{2}}{4}\right)(2+2\sqrt{2})^{n-1} + \left(\frac{34-23\sqrt{2}}{4}\right)(2-2\sqrt{2})^{n-1}.$$

Proof: There are three independent sets in T_0, namely the empty set and two sets which consist of a single vertex. Now let $n \geq 1$. Then we can use a reduction formula on vertex v_1 in Figure 12.

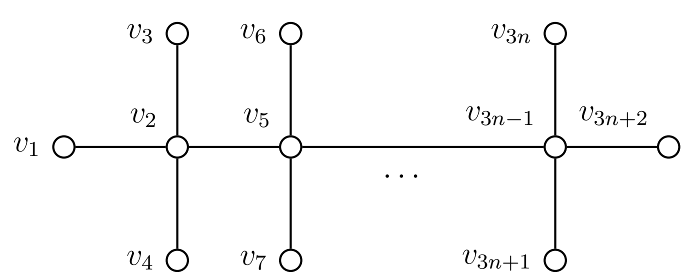


Figure 12: Independent Sets in T_n

By Lemma 2 and Lemma 6,

$$\begin{aligned} F(T_n) &= F(T_n - v_1) + F(T_n - N[v_1]) \\ &= F(S_n) + F(S_{n-1} \cup I_2) \\ &= F(S_n) + F(S_{n-1})F(I_2) \\ &= F(S_n) + 4F(S_{n-1}) \end{aligned}$$

$$\begin{aligned} &= \left(\frac{8+5\sqrt{2}}{8}\right)(2+2\sqrt{2})^n + \left(\frac{8-5\sqrt{2}}{8}\right)(2-2\sqrt{2})^n \\ &\quad +4\left(\frac{8+5\sqrt{2}}{8}\right)(2+2\sqrt{2})^{n-1} + 4\left(\frac{8-5\sqrt{2}}{8}\right)(2-2\sqrt{2})^{n-1} \\ &= \left(\frac{34+23\sqrt{2}}{4}\right)(2+2\sqrt{2})^{n-1} + \left(\frac{34-23\sqrt{2}}{4}\right)(2-2\sqrt{2})^{n-1}. \ \Box \end{aligned}$$

Proposition 8 *For $n \geq 0$, the Fibonacci index for U_n is given by*

$$F(U_n) = \left(\frac{4+3\sqrt{2}}{8}\right)(2+2\sqrt{2})^n + \left(\frac{4-3\sqrt{2}}{8}\right)(2-2\sqrt{2})^n.$$

Proof: Note that $F(U_0) = 1 = \left(\frac{4+3\sqrt{2}}{8}\right) + \left(\frac{4-3\sqrt{2}}{8}\right)$ and that $F(U_1) = 5 = \left(\frac{4+3\sqrt{2}}{8}\right)(2+2\sqrt{2}) + \left(\frac{4-3\sqrt{2}}{8}\right)(2-2\sqrt{2})$.

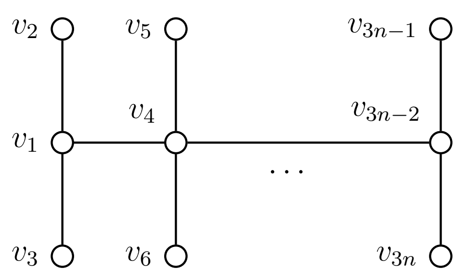


Figure 13: Independent Sets in U_n

Let $n \geq 2$. Then we can establish a recurrence relation for the Fibonacci index of U_n using reduction on vertex v_1 in Figure 13. By Lemma 2 and Lemma 6,

$$\begin{aligned} F(U_n) &= F(U_n - v_1) + F(U_{n-1} - N[v_1]) \\ &= F(U_{n-1} \cup I_2) + F(U_{n-2} \cup I_2) \\ &= F(U_{n-1})F(I_2) + F(U_{n-2})F(I_2) \\ &= 4F(U_{n-1}) + 4F(U_{n-2}). \end{aligned}$$

Since this relation is the same as the recurrence for S_n, the general solution is the same. So $F(U_n) = c_1(2+2\sqrt{2})^n + c_2(2-2\sqrt{2})^n$ for some constants c_1 and c_2. Solving to meet the initial conditions yields the formula. $\square$

The following proposition establishes a formula for $F(V_n)$, the Merrifield-Simmons index of a cycloalkane.

Proposition 9 *For $n \geq 3$, the Fibonacci index for V_n is given by*

$$F(V_n) = (2+2\sqrt{2})^n + (2-2\sqrt{2})^n.$$

Proof: We can use a reduction formula on vertex v_1 in V_n as shown in Figure 14 to count the number of independent sets in V_n.

By Lemma 2 and Lemma 6,

$$\begin{aligned} F(V_n) &= F(V_n - v_1) + F(V_n - N[v_1]) \\ &= F(U_{n-1} \cup I_2) + F(U_{n-3} \cup I_4) \\ &= F(U_{n-1})F(I_2) + F(U_{n-3})F(I_4) \\ &= 4F(U_{n-1}) + 16F(U_{n-3}) \end{aligned}$$

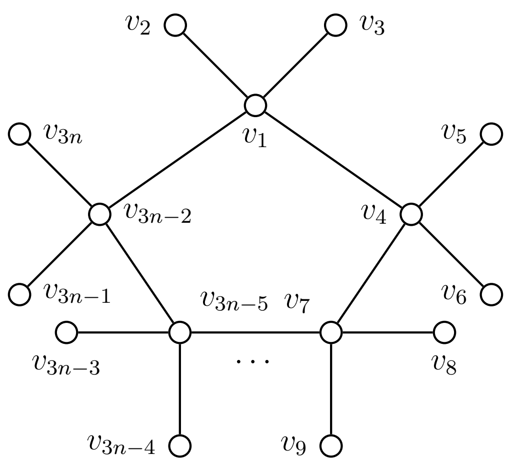


Figure 14: Independent Sets in V_n

$$\begin{aligned}
&= 4\left[\left(\frac{4+3\sqrt{2}}{8}\right)(2+2\sqrt{2})^{n-1}+\left(\frac{4-3\sqrt{2}}{8}\right)(2-2\sqrt{2})^{n-1}\right] \\
&\quad +16\left[\left(\frac{4+3\sqrt{2}}{8}\right)(2+2\sqrt{2})^{n-3}+\left(\frac{4-3\sqrt{2}}{8}\right)(2-2\sqrt{2})^{n-3}\right] \\
&= (2+2\sqrt{2})^{n}+(2-2\sqrt{2})^{n}.
\end{aligned}$$

$\square$

The values for $F(S_n)$, $F(T_n)$, $F(U_n)$, and $F(V_n)$ when $n \leq 10$ are shown in Table 5.

n	$F(S_n)$	$F(T_n)$	$F(U_n)$	$F(V_n)$
0	2	3	1	–
1	9	17	5	–
2	44	80	24	–
3	212	388	116	112
4	1,024	1,872	560	544
5	4,944	9,040	2,704	2,624
6	23,872	43,648	13,056	12,672
7	115,264	210,752	63,040	61,184
8	556,544	1,017,600	304,384	295,424
9	2,687,232	4,913,408	1,469,696	1,426,432
10	12,975,104	23,724,032	7,096,320	6,887,424

Table 5: Fibonacci Indices for the Graphs S_n, T_n, U_n, and V_n for $n \leq 10$

4.2 Independence Polynomials of Hydrocarbons

We are interested in obtaining formulas for the independence polynomials of our sequences of graphs that we have associated with the structure of hydrocarbons. First, we will investigate $F_{S_n}(x)$.

Proposition 10 *We have* $F_{S_0}(x) = 1 + x$, $F_{S_1}(x) = 1 + 4x + 3x^2 + x^3$, *and for* $n \geq 2$, *we have the recurrence relation*

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

Proof: In the graph S_0 which consists of a single vertex, the only independent sets are the empty set and the set consisting of the single vertex. So $F_{S_0}(x) = 1 + x$. Listing the independent sets in S_1 reveals that $F_{S_1}(x) = 1 + 4x + 3x^2 + x^3$.

Now, suppose $n \geq 2$. We can use vertex reduction on vertex v_1 in Figure 11 to establish a recurrence relation. By Lemma 4 and Lemma 5,

$$\begin{aligned}
F_{S_n}(x) &= F_{S_n - v_1}(x) + xF_{S_n - N[v_1]}(x) \\
&= F_{S_{n-1} \cup I_2}(x) + xF_{S_{n-2} \cup I_2}(x) \\
&= F_{S_{n-1}}(x)F_{I_2}(x) + xF_{S_{n-2}}(x)F_{I_2}(x) \\
&= (1 + x)^2 F_{S_{n-1}}(x) + x(1 + x)^2 F_{S_{n-2}}(x).
\end{aligned}$$

□

Recall that $F_k(S_n)$ represents the number of k-element independent sets in S_n and is the coefficient of x^k in $F_{S_n}(x)$. Regardless of the value of n, $F_0(S_n) = 1$. Since each graph S_n has $3n + 1$ vertices, $F_1(S_n) = 3n + 1$. Since S_n is a tree with $3n + 1$ vertices, it has $3n$ edges. So $F_2(S_n) = \binom{3n+1}{2} - 3n = \binom{3n}{2}$. We are interested in finding a formula for $F_3(S_n)$. Again, this formula could be found by Lemma 1, but we will employ the method of generating functions. By the previous proposition,

$$\begin{aligned} F_{S_n}(x) &= (1+x)^2(F_{S_{n-1}}(x)) + x(1+x)^2(F_{S_{n-2}}(x)) \\ &= F_{S_{n-1}}(x) + 2xF_{S_{n-1}}(x) + x^2F_{S_{n-1}}(x) + xF_{S_{n-2}}(x) \\ &\quad +2x^2F_{S_{n-2}}(x) + x^3F_{S_{n-2}}(x). \end{aligned}$$

It follows that the recurrence relation for the number of k-element independent sets for $n \geq 2, k \geq 3$ in S_n is given by

$$F_k(S_n) = F_k(S_{n-1}) + 2F_{k-1}(S_{n-1}) + F_{k-2}(S_{n-1}) + F_{k-1}(S_{n-2}) + 2F_{k-2}(S_{n-2}) + F_{k-3}(S_{n-2}).$$

Proposition 11 *For $n \geq 1$, $F_3(S_n) = \frac{9}{2}n^3 - 9n^2 + \frac{17}{2}n - 3$.*

Proof: If $n = 1$, there is only one independent set of size three, so $F_3(S_1) = 1 = \frac{9}{2}(1^3) - 9(1^2) + \frac{17}{2}(1) - 3$. Now, suppose that $n \geq 2$. It follows from the previous proposition that $F_3(S_n) = F_3(S_{n-1}) + 2F_2(S_{n-1}) + F_1(S_{n-1}) + F_2(S_{n-2}) + 2F_1(S_{n-2}) + F_0(S_{n-2})$. Recall that $F_0(S_n) = 1$, $F_1(S_n) = 3n+1$, and $F_2(S_n) = \binom{3n}{2}$ for all n. Hence,

$$\begin{aligned} F_3(S_n) &= F_3(S_{n-1}) + 2\binom{3(n-1)}{2} + (3(n-1)+1) + \binom{3(n-2)}{2} \\ &\quad +2(3(n-2)+1) + 1 \\ &= F_3(S_{n-1}) + \frac{27}{2}n^2 - \frac{63}{2}n + 22. \end{aligned}$$

To solve this recurrence relation, we can define the following generating function for $F_3(S_n)$:

$$f(x) = \sum_{n=0}^{\infty} F_3(S_n)x^n$$

Solving, this yields

$$\begin{aligned}
f(x) &= F_3(S_0) + F_3(S_1)x + \sum_{n=2}^{\infty} F_3(S_n)x^n \\
&= x + \sum_{n=2}^{\infty} \left(F_3(S_{n-1}) + \frac{27}{2}n^2 - \frac{63}{2}n + 22 \right) x^n \\
&= x + \sum_{n=2}^{\infty} F_3(S_{n-1})x^n + \frac{27}{2}\sum_{n=2}^{\infty} n^2x^n - \frac{63}{2}\sum_{n=2}^{\infty} nx^n + 22\sum_{n=2}^{\infty} x^n \\
&= xf(x) + \frac{27x^2}{(1-x)^3} - \frac{18x}{(1-x)^2} + \frac{22x^2}{1-x} + 19x.
\end{aligned}$$

Hence,

$$\begin{aligned}
f(x) &= \frac{27x^2}{(1-x)^4} - \frac{18x}{(1-x)^3} + \frac{22x^2}{1-x} + \frac{19x}{1-x} \\
&= \frac{3x^4 + 13x^3 + 10x^2 + x}{(1-x)^4}
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{6}(3x^4 + 13x^3 + 10x^2 + x)\sum_{n=0}^{\infty} (x^n)''' \\
&= \frac{1}{6}(3x^4 + 13x^3 + 10x^2 + x)\sum_{n=0}^{\infty} n(n-1)(n-2)x^{n-3} \\
&= \sum_{n=0}^{\infty} \left(\frac{1}{2}n^3 - \frac{3}{2}n^2 + n\right)x^{n+1} + \left(\frac{13}{6}n^3 - \frac{13}{2}n^2 + \frac{13}{3}n\right)x^n \\
&\quad + \left(\frac{5}{3}n^3 - 5n^2 + \frac{10}{3}n\right)x^{n-1} + \left(\frac{1}{6}n^3 - \frac{1}{2}n^2 + \frac{1}{3}n\right)x^{n-2}.
\end{aligned}$$

Thus, in $f(x)$, the coefficient of x^n is $(\frac{1}{2}(n-1)^3 - \frac{3}{2}(n-1)^2 + (n-1)) + (\frac{13}{6}n^3 - \frac{13}{2}n^2 + \frac{13}{3}n) + (\frac{5}{3}(n+1)^3 - 5(n+1)^2 + \frac{13}{3}(n+1)) + (\frac{1}{6}(n+2)^3 - \frac{1}{2}(n+2)^2 + \frac{1}{3}(n+2))$ $= \frac{9}{2}n^3 - 9n^2 + \frac{17}{2}n - 3$. So for $n \geq 2$, $F_3(S_n) = \frac{9}{2}n^3 - 9n^2 + \frac{17}{2}n - 3$. $\square$

Proposition 12 *For $n \geq 0$, $F_{S_n}(x) =$*

$$\left(\frac{1+x}{2} + \frac{x^3+3x^2+5x+1}{2\sqrt{x^4+8x^3+14x^2+8x+1}}\right)\left(\frac{(1+x)^2+\sqrt{x^4+8x^3+14x+8x+1}}{2}\right)^n$$

$$+\left(\frac{1+x}{2} - \frac{x^3+3x^2+5x+1}{2\sqrt{x^4+8x^3+14x^2+8x+1}}\right)\left(\frac{(1+x)^2-\sqrt{x^4+8x^3+14x+8x+1}}{2}\right)^n.$$

Proof: By Proposition 10, the following recurrence relation holds for $n \geq 2$:

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

This yields the characteristic equation $r^2 - (1+x)^2 r - x(1+x)^2 = 0$. So the characteristic roots are

$$r = \frac{1+2x+x^2 \pm \sqrt{x^4+8x^3+14x^2+8x+1}}{2}.$$

Thus, the general solution for this recurrence relation is

$$F_{S_n}(x) = c_1(x)\left(\frac{1+2x+x^2+\sqrt{x^4+8x^3+14x^2+8x+1}}{2}\right)^n$$

$$+c_2(x)\left(\frac{1+2x+x^2-\sqrt{x^4+8x^3+14x^2+8x+1}}{2}\right)^n$$

for some polynomials $c_1(x)$ and $c_2(x)$. By Proposition 10, we also know that the solution must meet the initial conditions that $F_{S_0}(x) = 1+x$ and $F_{S_1}(x) = 1+4x+3x^2+x^3$. After solving for $c_1(x)$ and $c_2(x)$, we obtain the formula given in the proposition. □

Proposition 13 *We have $F_{T_0}(x) = 1+2x$, and for $n \geq 1$, $F_{T_n}(x) =$*

$$\left(\frac{1+5x+6x^2+4x^3+x^4}{2} + \frac{1+8x+17x^2+14x^3+5x^4+x^5}{2\sqrt{1+6x+x^2}}\right)$$

$$\left(\frac{(1+x)(1+x+\sqrt{1+6x+x^2}}{2}\right)^{n-1}$$

$$+\left(\frac{1+5x+6x^2+4x^3+x^4}{2}-\frac{1+8x+17x^2+14x^3+5x^4+x^5}{2\sqrt{1+6x+x^2}}\right)$$

$$\left(\frac{(1+x)(1+x-\sqrt{1+6x+x^2}}{2}\right)^{n-1}.$$

Proof: Since the graph T_0 consists of two vertices joined by a single edge, the independent sets are the empty set and the two sets which consist of a single vertex each. So $F_{T_0}(x) = 1 + 2x$. Now, suppose that $n \geq 1$. We can use vertex reduction on v_1 in Figure 12 with Lemma 4 and Lemma 5, and hence,

$$\begin{aligned}
F_{T_n}(x) &= F_{T_n - v_1}(x) + xF_{T_n - N[v_1]}(x) \\
&= F_{S_n}(x) + xF_{S_{n-1} \cup I_2}(x) \\
&= F_{S_n}(x) + xF_{S_{n-1}}(x)F_{I_2}(x) \\
&= F_{S_n}(x) + x(1+x)^2(F_{S_{n-1}}(x)).
\end{aligned}$$

The result is obtained by substituting the closed form for $F_{S_n}(x)$ from Proposition 12 and simplifying. □

By the previous proposition,

$$\begin{aligned}
F_{T_n}(x) &= F_{S_n}(x) + x(1+x)^2(F_{S_{n-1}}(x)) \\
&= F_{S_n}(x) + xF_{S_{n-1}}(x) + 2x^2F_{S_{n-1}}(x) + x^3F_{S_{n-1}}(x).
\end{aligned}$$

The coefficient of x^k in the polynomial $F_{T_n}(x)$ is $F_k(T_n)$, so we can see that for $n \geq 1, k \geq 3$,

$$F_k(T_n) = F_k(S_n) + F_{k-1}(S_{n-1}) + 2F_{k-2}(S_{n-1}) + F_{k-3}(S_{n-1}).$$

Proposition 14 *For $n \geq 0$, the independence polynomial for U_n is given by*

$$\begin{aligned} F_{U_n}(x) &= \left(\frac{1}{2} + \frac{1+4x+x^2}{2\sqrt{(1+x)^2(1+6x+x^2)}}\right)\left(\frac{(1+x)^2 + \sqrt{(1+x)^2(1+6x+x^2)}}{2}\right)^n \\ &\quad + \left(\frac{1}{2} - \frac{1+4x+x^2}{2\sqrt{(1+x)^2(1+6x+x^2)}}\right)\left(\frac{(1+x)^2 - \sqrt{(1+x)^2(1+6x+x^2)}}{2}\right)^n \end{aligned}$$

Proof: Using vertex reduction on v_1 in Figure 13 with Lemma 4 and Lemma 5,

$$\begin{aligned} F_{U_n}(x) &= F_{U_n - v_1}(x) + xF_{U_n - N[v_1]}(x) \\ &= F_{U_{n-1} \cup I_2}(x) + xF_{U_{n-2} \cup I_2}(x) \\ &= F_{U_{n-1}}(x)F_{I_2}(x) + xF_{U_{n-2}}(x)F_{I_2}(x) \\ &= (1+x)^2 F_{U_{n-1}}(x) + x(1+x)^2 F_{U_{n-2}}(x). \end{aligned}$$

Since this is the same relation as the recurrence for $F_{S_n}(x)$ in Proposition 12, the general solution is also the same. Hence,

$$\begin{aligned} F_{U_n}(x) &= c_1(x)\left(\frac{1+2x+x^2+\sqrt{x^4+8x^3+14x^2+8x+1}}{2}\right)^n \\ &\quad + c_2(x)\left(\frac{1+2x+x^2-\sqrt{x^4+8x^3+14x^2+8x+1}}{2}\right)^n \end{aligned}$$

for some polynomials $c_1(x)$ and $c_2(x)$. Note that $F_{U_0}(x) = 1$ and $F_{U_1}(x) = 1 + 3x + x^2$. Solving for the initial conditions, we obtain the result. □

It follows from this last proposition that for $n \geq 2, k \geq 3$, the number of k-element independent sets in U_n is given by the recurrence relation

$$F_k(U_n) = F_k(U_{n-1}) + 2F_{k-1}(U_{n-1}) + F_{k-2}(U_{n-1}) + F_{k-1}(U_{n-2}) + 2F_{k-2}(U_{n-2}) + F_{k-3}(U_{n-2}).$$

We can also find the independence polynomial for the molecular graph of the cycloalkanes as shown in the next proposition.

Proposition 15 *For $n \geq 3$, the independence polynomial for V_n is*

$$F_{V_n}(x) = \left(\frac{(1+x)^2 + \sqrt{(1+x)^2(1+6x+x^2)}}{2}\right)^n + \left(\frac{(1+x)^2 - \sqrt{(1+x)^2(1+6x+x^2)}}{2}\right)^n.$$

Proof: Let $n \geq 3$. By reduction on v_1 in Figure 14 with Lemma 4 and Lemma 5,

$$\begin{aligned} F_{V_n}(x) &= F_{V_n - v_1}(x) + xF_{V_n - N[v_1]}(x) \\ &= F_{U_{n-1}\cup I_2}(x) + xF_{U_{n-3}\cup I_4}(x) \\ &= F_{U_{n-1}}(x)F_{I_2}(x) + xF_{U_{n-3}}(x)F_{I_4}(x) \\ &= (1+x)^2F_{U_{n-1}}(x) + x(1+x)^4F_{U_{n-3}}(x). \end{aligned}$$

By inserting the formula for $F_{U_n}(x)$ from Proposition 14 and simplifying, we see that the formula for $F_{V_n}(x)$ holds. □

From this proposition, we can determine that the number of k-element independent sets in V_n for $n \geq 3, k \geq 5$ is

$$F_k(V_n) = F_k(U_{n-1}) + 2F_{k-1}(U_{n-1}) + F_{k-2}(U_{n-1}) + F_{k-1}(U_{n-3})$$

$$+4F_{k-2}(U_{n-3}) + 6F_{k-3}(U_{n-3}) + 4F_{k-4}(U_{n-3}) + F_{k-5}(U_{n-3}).$$

The first few independence polynomials of S_n, T_n, U_n, and V_n are shown in Table 6.

4.3 Generating Functions for the Independence Polynomials of Hydrocarbons

Let us consider the independence polynomials of S_n and define the following two-variable generating function $S(x, y)$ in which the coefficient of $x^k y^n$ is the number of independent sets of size k in S_n:

n	Independence Polynomials
0	$F_{S_0}(x) = 1 + x$ $F_{T_0}(x) = 1 + 2x$ $F_{U_0}(x) = 1$
1	$F_{S_1}(x) = 1 + 4x + 3x^2 + x^3$ $F_{T_1}(x) = 1 + 5x + 6x^2 + 4x^3 + x^4$ $F_{U_1}(x) = 1 + 3x + x^2$
2	$F_{S_2}(x) = 1 + 7x + 15x^2 + 14x^3 + 6x^4 + x^5$ $F_{T_2}(x) = 1 + 8x + 21x^2 + 26x^3 + 17x^4 + 6x^5 + x^6$ $F_{U_2}(x) = 1 + 6x + 10x^2 + 6x^3 + x^4$
3	$F_{S_3}(x) = 1 + 10x + 36x^2 + 63x^3 + 60x^4 + 32x^5 + 9x^6 + x^7$ $F_{T_3}(x) = 1 + 11x + 45x^2 + 93x^3 + 111x^4 + 81x^5 + 36x^6 + 9x^7 + x^8$ $F_{U_3}(x) = 1 + 9x + 28x^2 + 40x^3 + 28x^4 + 9x^5 + x^6$ $F_{V_3}(x) = 1 + 9x + 27x^2 + 38x^3 + 27x^4 + 9x^5 + x^6$
4	$F_{S_4}(x) = 1 + 13x + 66x^2 + 175x^3 + 273x^4 + 264x^5 + 160x^6 + 59x^7 + 12x^8 + x^9$ $F_{T_4}(x) = 1 + 14x + 78x^2 + 232x^3 + 418x^4 + 486x^5 + 375x^6 + 192x^7 + 63x^8 + 12x^9$ $+x^{10}$ $F_{U_4}(x) = 1 + 12x + 55x^2 + 128x^3 + 168x^4 + 128x^5 + 55x^6 + 12x^7 + x^8$ $F_{V_4}(x) = 1 + 12x + 54x^2 + 124x^3 + 162x^4 + 124x^5 + 54x^6 + 12x^7 + x^8$

Table 6: Fibonacci Polynomials for the Graphs S_n, T_n, U_n, and V_n for $n \leq 4$

$$S(x,y) := \sum_{n=0}^{\infty} F_{S_n}(x) y^n = \sum_{n=0}^{\infty} \sum_{k=0}^{2n+1} F_k(S_n) x^k y^n.$$

Note that we can end the summation over k at $2n+1$ since that is the size of the largest independent set in S_n. So $F_k(S_n) = 0$ for $k > 2n+1$.

Theorem 1 *The following is the closed form solution for the generating function $S(x,y)$:*

$$S(x,y) = \frac{1 + x + xy}{1 - y - 2xy - x^2y - xy^2 - 2x^2y^2 - x^3y^2}.$$

Proof: Recall that $S(x,y) = \sum_{n=0}^{\infty} \sum_{k=0}^{2n+1} F_k(S_n) x^k y^n$. By separating the first few terms, we have

$$\begin{aligned}
S(x,y) &= [1+x]+[1+4x+3x^2+x^3]y+\sum_{n=2}^{\infty}\sum_{k=0}^{2n+1}F_k(S_n)x^ky^n \\
&= [1+x]+[1+4x+3x^2+x^3]y+\sum_{n=2}^{\infty}y^n+\sum_{n=2}^{\infty}(3n+1)xy^n \\
&\quad +\sum_{n=2}^{\infty}\left(\binom{3n+1}{2}-3n\right)x^2y^n+\sum_{n=2}^{\infty}\sum_{k=3}^{2n+1}F_k(S_n)x^ky^n
\end{aligned}$$

By finding the closed form for the sums over just n, we have $\sum_{n=2}^{\infty} y^n = \frac{y^2}{1-y}$ and

$$\begin{aligned}
\sum_{n=2}^{\infty}(3n+1)xy^n &= 3xy\sum_{n=2}^{\infty}ny^{n-1}+xy^2\sum_{n=0}^{\infty}y^n \\
&= 3xy\left(\frac{1}{(1-y)^2}-1\right)+\frac{xy^2}{1-y} \\
&= \frac{3xy}{(1-y)^2}-3xy+\frac{xy^2}{1-y}
\end{aligned}$$

and

$$\begin{aligned}
\sum_{n=2}^{\infty}\left(\binom{3n+1}{2}-3n\right)x^2y^n &= \sum_{n=2}^{\infty}\frac{9n^2-3n}{2}x^2y^n \\
&= \frac{9}{2}x^2\sum_{n=2}^{\infty}(n(n-1)+n)y^n-\frac{3}{2}x^2y\sum_{n=2}^{\infty}ny^{n-1} \\
&= \frac{9}{2}x^2y^2\sum_{n=2}^{\infty}n(n-1)y^{n-2}+3x^2y\sum_{n=2}^{\infty}ny^{n-1} \\
&= \frac{9x^2y^2}{(1-y)^3}+\frac{3x^2y}{(1-y)^2}-3x^2y
\end{aligned}$$

It remains to solve for the closed form of $\sum_{n=2}^{\infty}\sum_{k=3}^{2n+1}F_k(S_n)x^ky^n$. We have already seen that $F_k(S_n)=F_k(S_{n-1})+2F_{k-1}(S_{n-1})+F_{k-2}(S_{n-1})+F_{k-1}(S_{n-2})+2F_{k-2}(S_{n-2})+F_{k-3}(S_{n-2})$.

So we can divide this last summation into six parts:

$$\sum_{n=3}^{\infty}\sum_{k=3}^{2n+1} F_k(S_n)x^ky^n = \sum_{n=3}^{\infty}\sum_{k=3}^{2n+1} F_k(S_{n-1})x^ky^n + 2F_{k-1}(S_{n-1})x^ky^n$$

$$+F_{k-2}(S_{n-1})x^ky^n + F_{k-1}(S_{n-2})x^ky^n + 2F_{k-2}(S_{n-2})x^ky^n + F_{k-3}(S_{n-2})x^ky^n$$

We will consider each of these sums separately:

$$\begin{aligned}
1. \sum_{n=2}^{\infty}\sum_{k=3}^{2n+1} F_k(S_{n-1})x^ky^n &= y\sum_{n=1}^{\infty}\sum_{k=3}^{2n+1} F_k(S_n)x^ky^n \\
&= y\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1} F_k(S_n)x^ky^n - y(1+x) - y\sum_{n=1}^{\infty}\sum_{k=0}^{2} F_k(S_n)x^ky^n \\
&= yS(x,y) - y(1+x) - y\sum_{n=1}^{\infty} y^n + y\sum_{n=1}^{\infty}(3n+1)xy^n \\
&\quad +y\sum_{n=1}^{\infty}\left(\frac{9}{2}n^2 - \frac{3}{2}n\right)x^2y^n \\
&= yS(x,y) - y(1+x) - \frac{y^2}{1-y} - \frac{3xy^2}{(1-y)^2} - \frac{xy^2}{1-y} \\
&\quad -\frac{9}{2}x^2y^3\sum_{n=1}^{\infty} n(n-1)y^{n-2} - 3x^2y^2\sum_{n=1}^{\infty} ny^{n-1} \\
&= yS(x,y) - y(1+x) - \frac{y^2}{1-y} - \frac{3xy^2}{(1-y)^2} - \frac{xy^2}{1-y} \\
&\quad -\frac{9x^2y^3}{(1-y)^3} - \frac{3x^2y^2}{(1-y)^2}
\end{aligned}$$

$$\begin{aligned}
2. \sum_{n=2}^{\infty}\sum_{k=3}^{2n+1} 2F_{k-1}(S_{n-1})x^ky^n &= 2xy\sum_{n=1}^{\infty}\sum_{k=2}^{2n+1} F_k(S_n)x^ky^n \\
&= 2xy\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1} F_k(S_n)x^ky^n - 2xy(1+x) \\
&\quad -2xy\sum_{n=1}^{\infty}(y^n + (3n+1)xy^n) \\
&= 2xyS(x,y) - 2xy(1+x) - \frac{2xy^2}{1-y} - \frac{6x^2y^2}{(1-y)^2} - \frac{2x^2y^2}{1-y}
\end{aligned}$$

$$3.\sum_{n=2}^{\infty}\sum_{k=3}^{2n+1} F_{k-2}(S_{n-1})x^k y^n = x^2y\sum_{n=1}^{\infty}\sum_{k=1}^{2n+1} F_k(S_n)x^k y^n$$
$$= x^2y\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1} F_k(S_n)x^k y^n - x^2y(1+x) - x^2y\sum_{n=1}^{\infty} y^n$$
$$= x^2yS(x,y) - x^2y(1+x) - \frac{x^2y^2}{1-y}$$

$$4.\sum_{n=2}^{\infty}\sum_{k=3}^{2n+1} F_{k-1}(S_{n-2})x^k y^n = xy^2\sum_{n=0}^{\infty}\sum_{k=2}^{2n+1} F_k(S_n)x^k y^n$$
$$= xy^2\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1} F_k(S_n)x^k y^n - xy^2\sum_{n=0}^{\infty}(y^n + (3n+1)xy^n)$$
$$= xy^2S(x,y) - \frac{xy^2}{1-y} - \frac{3x^2y^3}{(1-y)^2} - \frac{x^2y^2}{1-y}$$

$$5.\sum_{n=2}^{\infty}\sum_{k=3}^{2n+1} 2F_{k-2}(S_{n-2})x^k y^n = 2x^2y^2\sum_{n=0}^{\infty}\sum_{k=1}^{2n+1} F_k(S_n)x^k y^n$$
$$= 2x^2y^2\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1} F_k(S_n)x^k y^n - 2x^2y^2\sum_{n=0}^{\infty} y^n$$
$$= 2x^2y^2S(x,y) - \frac{2x^2y^2}{1-y}$$

$$6.\sum_{n=2}^{\infty}\sum_{k=3}^{2n+1} F_{k-3}(S_{n-2})x^k y^n = x^3y^2\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1} F_k(S_n)x^k y^n$$
$$= x^3y^2S(x,y)$$

By combining the initial terms with these six series and solving for $S(x,y)$, we see that $S(x,y) = \dfrac{1+x+xy}{1-y-2xy-x^2y-xy^2-2x^2y^2-x^3y^2}$. □

Using $S(x,y)$, we can solve for the closed form of the generating function for $F_{T_n}(x)$.

Let

$$T(x,y) = \sum_{n=0}^{\infty} F_{T_n}(x) y^n = \sum_{n=0}^{\infty} \sum_{k=0}^{2n+2} F_k(T_n) x^k y^n.$$

Theorem 2 *The following is the closed form solution for the generating function $T(x,y)$:*

$$T(x,y) = \frac{1 + 2x + xy + x^2y + 2x^3y + x^4y}{1 - y - 2xy - x^2y - xy^2 - 2x^2y^2 - x^3y^2}.$$

Proof: By separating the first few terms of $T(x,y)$, we have

$$\begin{aligned} T(x,y) &= \sum_{n=0}^{\infty} \sum_{k=0}^{2n+2} F_k(T_n) x^k y^n \\ &= \sum_{n=0}^{\infty} y^n + \sum_{n=0}^{\infty} (3n+2) x y^n + \sum_{n=0}^{\infty} \left(\binom{3n+2}{2} - (3n+1) \right) x^2 y^n \\ &\quad + \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_k(T_n) x^k y^n \\ &= \frac{1+2x}{1-y} + \frac{3xy + 6x^2y}{(1-y)^2} + \frac{9x^2y^2}{(1-y)^3} + \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_k(T_n) x^k y^n. \end{aligned}$$

It remains to solve for the last term. It will be helpful to recall that $F_k(T_n) = F_k(S_n) + F_{k-1}(S_{n-1}) + 2F_{k-2}(S_{n-1}) + F_{k-3}(S_{n-1})$. So

$$\begin{aligned} \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_k(T_n) x^k y^n &= \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_k(S_n) x^k y^n + \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_{k-1}(S_{n-1}) x^k y^n \\ &\quad + 2 \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_{k-2}(S_{n-1}) x^k y^n + \sum_{n=1}^{\infty} \sum_{k=3}^{2n+2} F_{k-3}(S_{n-1}) x^k y^n \end{aligned}$$

We will need to find a closed form for each of these series using the generating function $S(x,y)$.

$$1. \sum_{n=1}^{\infty}\sum_{k=3}^{2n+2} F_k(S_n)x^k y^n = S(x,y) - \sum_{n=0}^{\infty} y^n - \sum_{n=0}^{\infty}(3n+1)xy^n - \sum_{n=0}^{\infty}\left(\binom{3n+1}{2} - 3n\right)x^2y^n$$
$$= S(x,y) - \frac{1}{1-y} - \frac{3xy}{(1-y)^2} - \frac{x}{1-y} + \frac{9x^2y^2}{(1-y)^3} - \frac{\frac{9}{2}x^2y}{(1-y)^2} + \frac{3x^2y}{(1-y)^2}$$

$$2. \sum_{n=1}^{\infty}\sum_{k=3}^{2n+2} F_{k-1}(S_{n-1})x^k y^n = xyS(x,y) - xy\sum_{n=0}^{\infty} y^n - xy\sum_{n=0}^{\infty}(3n+1)xy^n$$
$$= xyS(x,y) - \frac{xy}{1-y} - \frac{3x^2y^2}{(1-y)^2} - \frac{x^2y}{1-y}$$

$$3. \quad 2\sum_{n=1}^{\infty}\sum_{k=3}^{2n+2} F_{k-2}(S_{n-1})x^k y^n = 2x^2yS(x,y) - 2x^2y\sum_{n=0}^{\infty} y^n$$
$$= 2x^2yS(x,y) - \frac{2x^2y}{1-y}$$

$$4. \sum_{n=1}^{\infty}\sum_{k=3}^{2n+2} F_{k-3}(S_{n-1})x^k y^n = x^3yS(x,y)$$

By combining the initial terms with the closed form for these last four series and substituting the closed form for $S(x,y)$ from Theorem 1, we see that

$$T(x,y) = \frac{1+2x+xy+x^2y+2x^3y+x^4y}{1-y-2xy-x^2y-xy^2-2x^2y^2-x^3y^2}.$$

□

By the same method, we can find a closed form for the generating function for the k-element independent sets in the sequence of graphs U_n. Let

$$U(x,y) = \sum_{n=0}^{\infty} F_{U_n}(x) y^n = \sum_{n=0}^{\infty} \sum_{k=0}^{2n} F_k(U_n) x^k y^n.$$

Theorem 3 *The following is the closed form solution for the generating function $U(x,y)$:*

$$U(x,y) = \frac{1+xy}{1-y-2xy-x^2y-xy^2-2x^2y^2-x^3y^2}.$$

Proof: By separating the first few terms of $U(x,y)$, we have

$$\begin{aligned} U(x,y) &= \sum_{n=0}^{\infty} \sum_{k=0}^{2n} F_k(U_n) x^k y^n \\ &= (1) + (1+3x+x^2)y + \sum_{n=2}^{\infty} y^n + \sum_{n=2}^{\infty} 3nxy^n \\ &\quad + \sum_{n=2}^{\infty} \left(\binom{3n}{2} - (3n-1) \right) x^2 y^n + \sum_{n=2}^{\infty} \sum_{k=3}^{2n} F_k(U_n) x^k y^n. \end{aligned}$$

By solving for the closed forms of the sums over just n, we have $\displaystyle\sum_{n=2}^{\infty} y^n = \frac{y^2}{1-y}$ and

$$\begin{aligned} \sum_{n=2}^{\infty} 3nxy^n &= 3xy \sum_{n=2}^{\infty} ny^{n-1} \\ &= \frac{3xy}{(1-y)^2} - 3xy \end{aligned}$$

and

$$\begin{aligned} \sum_{n=2}^{\infty} \left(\binom{3n}{2} - (3n-1) \right) x^2 y^n &= \sum_{n=2}^{\infty} \left(\frac{9}{2}n^2 - \frac{9}{2}n + 1 \right) x^2 y^n \\ &= \frac{9}{2}x^2 \sum_{n=2}^{\infty} (n(n-1)+n) y^n - \frac{9}{2}x^2 y \sum_{n=2}^{\infty} ny^{n-1} + x^2 \sum_{n=2}^{\infty} y^n \end{aligned}$$

$$= \frac{9x^2y^2}{(1-y)^3} + \frac{x^2y^2}{1-y}.$$

It remains to solve for the closed form of the double sum. Recall that $F_k(U_n) = F_k(U_{n-1}) + 2F_{k-1}(U_{n-1}) + F_{k-2}(U_{n-1}) + F_{k-1}(U_{n-2}) + 2F_{k-2}(U_{n-2}) + F_{k-3}(U_{n-2})$. So we can divide the double sum into six pieces and solve for each separately.

$$
\begin{aligned}
1. \sum_{n=2}^{\infty}\sum_{k=3}^{2n} F_k(U_{n-1})x^k y^n &= y\sum_{n=1}^{\infty}\sum_{k=3}^{2n} F_k(U_n)x^k y^n \\
&= y\sum_{n=0}^{\infty}\sum_{k=0}^{2n} F_k(U_n)x^k y^n - y(1) - y\sum_{n=1}^{\infty} y^n \\
&\quad -y\sum_{n=1}^{\infty} 3nxy^n - y\sum_{n=1}^{\infty}\left(\frac{9}{2}n^2 - \frac{9}{2}n + 1\right)x^2y^n \\
&= yU(x,y) - y - \frac{y^2}{y-1} - 3xy^2\sum_{n=1}^{\infty} ny^{n-1} \\
&\quad -\frac{9}{2}x^2y\sum_{n=1}^{\infty} n^2y^n + \frac{9}{2}x^2y^2\sum_{n=1}^{\infty} ny^{n-1} - x^2y\sum_{n=1}^{\infty} y^n \\
&= yU(x,y) - y - \frac{y^2}{1-y} - \frac{3xy^2}{(1-y)^2} - \frac{9x^2y^3}{(1-y)^3} - \frac{x^2y^2}{1-y}
\end{aligned}
$$

$$
\begin{aligned}
2. \sum_{n=2}^{\infty}\sum_{k=3}^{2n} 2F_{k-1}(U_{n-1})x^k y^n &= 2xy\sum_{n=1}^{\infty}\sum_{k=2}^{2n} F_k(U_n)x^k y^n \\
&= 2xy\sum_{n=0}^{\infty}\sum_{k=0}^{2n} F_k(U_n)x^k y^n - 2xy(1) - 2xy\sum_{n=1}^{\infty}(y^n + 3nxy^n) \\
&= 2xyU(x,y) - 2xy - \frac{2xy^2}{1-y} - \frac{6x^2y^2}{(1-y)^2}
\end{aligned}
$$

$$
\begin{aligned}
3. \sum_{n=2}^{\infty}\sum_{k=3}^{2n} F_{k-2}(U_{n-1})x^k y^n &= x^2 y \sum_{n=1}^{\infty}\sum_{k=1}^{2n} F_k(U_n)x^k y^n \\
&= x^2 y \sum_{n=0}^{\infty}\sum_{k=0}^{2n} F_k(U_n)x^k y^n - x^2y(1) - x^2y\sum_{n=1}^{\infty} y^n \\
&= x^2 y U(x,y) - x^2 y - \frac{x^2y^2}{1-y}
\end{aligned}
$$

$$
\begin{aligned}
4. \sum_{n=2}^{\infty}\sum_{k=3}^{2n} F_{k-1}(U_{n-2})x^k y^n &= xy^2 \sum_{n=0}^{\infty}\sum_{k=2}^{2n} F_k(U_n)x^k y^n \\
&= xy^2 \sum_{n=0}^{\infty}\sum_{k=0}^{2n} F_k(U_n)x^k y^n - xy^2\sum_{n=0}^{\infty}(y^n + 3nxy^n) \\
&= xy^2 U(x,y) - \frac{xy^2}{1-y} - \frac{3x^2y^3}{(1-y)^2}
\end{aligned}
$$

$$
\begin{aligned}
5. \sum_{n=2}^{\infty}\sum_{k=3}^{2n} 2F_{k-2}(U_{n-2})x^k y^n &= 2x^2y^2 \sum_{n=0}^{\infty}\sum_{k=1}^{2n} F_k(U_n)x^k y^n \\
&= 2x^2y^2 \sum_{n=0}^{\infty}\sum_{k=0}^{2n} F_k(U_n)x^k y^n - 2x^2y^2\sum_{n=0}^{\infty} y^n \\
&= 2x^2y^2 U(x,y) - \frac{2x^2y^2}{1-y}
\end{aligned}
$$

$$
\begin{aligned}
6. \sum_{n=2}^{\infty}\sum_{k=3}^{2n} F_{k-3}(U_{n-2})x^k y^n &= x^3y^2 \sum_{n=0}^{\infty}\sum_{k=0}^{2n} F_k(U_n)x^k y^n \\
&= x^3y^2 U(x,y)
\end{aligned}
$$

By combining the initial terms with each of these series and solving for $U(x,y)$, we obtain the desired formula. □

5 GENERALIZED HYDROCARBON GRAPHS

The sequences of graphs discussed in the last section are associated with the structure of various hydrocarbons. We can generalize these graphs to define new sequences S_n^m, T_n^m, U_n^m, and V_n^m. In the sequence T_n^m, $T_0^m = T_0$ for all $m \geq 0$ and for $n \geq 1$, T_n^m is obtained by adding $m+1$ leaves to the root vertex of T_{n-1}^m. Just as before, S_n^m is the graph T_n^m after deleting the root vertex.

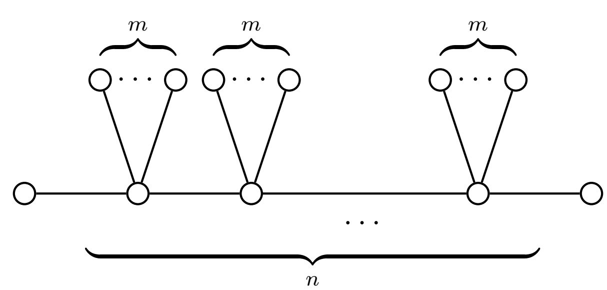


Figure 15: The Graph T_n^m

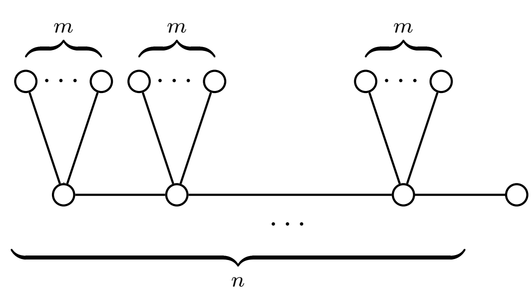


Figure 16: The Graph S_n^m

We can extend this generalization to the graphs U_n as well. Let U_n^m be the graph formed by adjoining n star graphs with m leaves each by their central vertices. Then we get the sequence of graphs pictured in Figure 17.

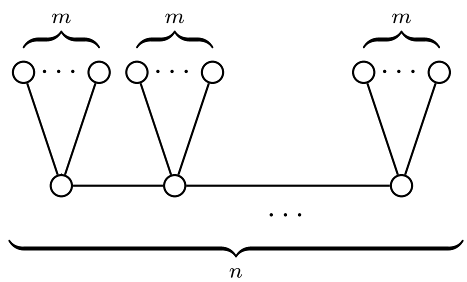


Figure 17: The Graph U_n^m

In the same way, we can extend this generalization to the graphs V_n. Let V_n^m be the sequence of graphs picture in Figure 18.

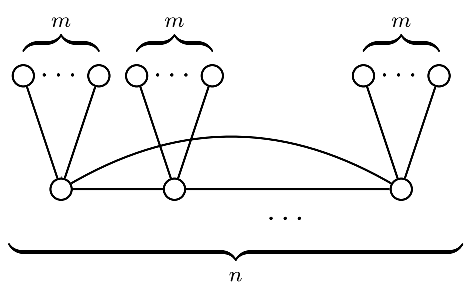


Figure 18: The Graph V_n^m

Note that in this generalization, each central vertex is adjacent to m leaves instead of just two. So $T_n = T_n^2$, $S_n = S_n^2$, $U_n = U_n^2$, and $V_n = V_n^2$. If we let $m = 0$, then the resulting graphs are paths and cycles so that $T_n^0 = P_{n+2}$, S_n^0=P_{n+1}, $U_n^0 = P_n$, and $V_n^0 = C_n$. When $m = 1$, these graphs are generalizations of combs.

5.1 Fibonacci Indices of Generalized Hydrocarbons

Proposition 16 *Let $m \geq 0$. Then $F(S_0^m) = 2$, $F(S_1^m) = 1 + 2^{m+1}$, and for $n \geq 2$, we have the recurrence relation*

$$F(S_n^m) = 2^m F(S_{n-1}^m) + 2^m F(S_{n-2}^m).$$

Proof: Since the graph S_0^m consists of a single vertex, the only independent sets are the empty set and the set consisting of a single vertex. Recall that the graph S_1^m is a star with $m+1$ leaves. Using vertex reduction, we see that $F(S_1^m) = 1 + 2^{m+1}$. Now, suppose that $n \geq 2$. Then we can use a vertex reduction formula on v_1 in Figure 19.

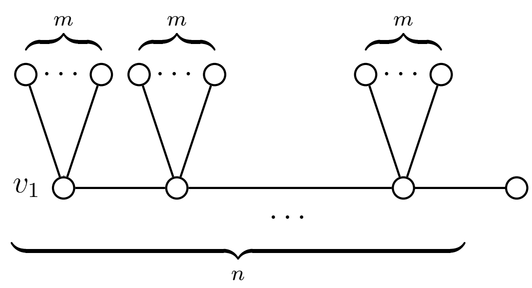


Figure 19: Independent Sets in S_n^m

By Lemma 2 and Lemma 6,

$$\begin{aligned} F(S_n^m) &= F(S_n^m - v_1) + F(S_n^m - N[v_1]) \\ &= F(S_{n-1}^m \cup I_m) + F(S_{n-2}^m \cup I_m) \\ &= F(S_{n-1}^m)F(I_m) + F(S_{n-2}^m)F(I_m) \\ &= 2^m F(S_{n-1}^m) + 2^m F(S_{n-2}^m). \end{aligned}$$

□

Proposition 17 *For $m \geq 0$ and $n \geq 0$,*

$$\begin{aligned} F(S_n^m) &= \left(1 + \frac{1+2^m}{\sqrt{2^{2m}+2^{m+2}}}\right)\left(2^{m-1} + \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n \\ &\quad + \left(1 - \frac{1+2^m}{\sqrt{2^{2m}+2^{m+2}}}\right)\left(2^{m-1} - \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n \end{aligned}$$

Proof: By Proposition 16, we have the recurrence relation $F(S_n^m) = 2^m F(S_{n-1}^m) + 2^m F(S_{n-2}^m)$ for $m \geq 0, n \geq 2$. This yields the characteristic polynomial $r^2 - 2^m r - 2^m = 0$ which has roots $r = 2^{m-1} \pm \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}$. So the general solution to this recurrence relation is

$$F(S_n^m) = c_1(m)\left(2^{m-1} + \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n + c_2(m)\left(2^{m-1} - \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n$$

for some $c_1(m)$ and $c_2(m)$. Our initial conditions are also given by Proposition 16, and solving, we obtain the result. $\square$

We can now use the results for S_n^m to find a formula for the Fibonacci index of T_n^m.

Proposition 18 *Let $m \geq 0$. We have $F(T_0^m) = 3$, and for $n \geq 1$, the Fibonacci index is given by*

$$\begin{aligned} F(T_n^m) &= \left(\frac{1+2^{m+2}}{2} + \frac{2^{2m}+13\cdot 2^m}{2\sqrt{2^{2m}+2^{m+2}}}\right)\left(2^{m-1}+\frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^{n-1} \\ &\quad + \left(\frac{1+2^{m+2}}{2} - \frac{2^{2m}+13\cdot 2^m}{2\sqrt{2^{2m}+2^{m+2}}}\right)\left(2^{m-1}-\frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^{n-1}. \end{aligned}$$

Proof: Since T_0^m consists of two vertices joined by a single edge, it has three independent sets. Hence, $F(T_0^m) = 3$.

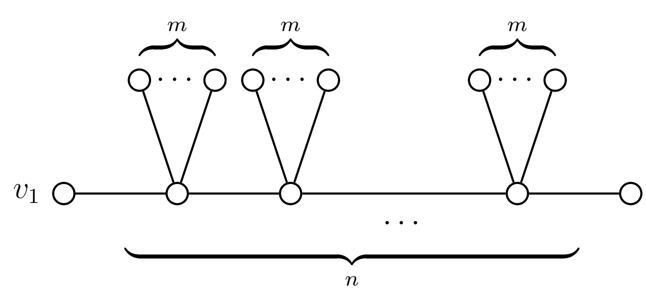


Figure 20: Independent Sets in T_n^m

Suppose that $n \geq 1$. By reduction on the root vertex v_1 in Figure 20,

$$\begin{aligned} F(T_n^m) &= F(T_n^m - v_1) + F(T_n^m - N[v_1]) \\ &= F(S_n^m) + F(S_{n-1}^m \cup I_m) \\ &= F(S_n^m) + F(S_{n-1}^m)F(I_m) \\ &= F(S_n^m) + 2^m F(S_{n-1}^m). \end{aligned}$$

By substituting the closed formula for $F(S_n^m)$ from Proposition 17 and simplifying, we obtain the result. $\square$

Proposition 19 *For $m, n \geq 0$, the Fibonacci index of U_n^m is given by*

$$\begin{aligned} F(U_n^m) &= \left(\frac{1}{2} + \frac{1+2^{m-1}}{\sqrt{2^{2m}+2^{m+2}}}\right)\left(2^{m-1} + \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n \\ &\quad + \left(\frac{1}{2} - \frac{1+2^{m-1}}{\sqrt{2^{2m}+2^{m+2}}}\right)\left(2^{m-1} - \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n. \end{aligned}$$

Proof: Since U_0^m is the empty graph for all m, $F(U_0^m) = 1$. The total number of independent sets in U_1^m is the same as in a star with m leaves, so $F(U_1^m) = 1 + 2^m$.

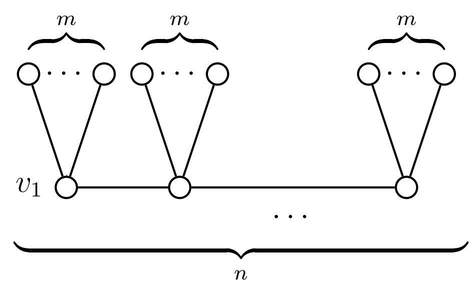


Figure 21: Independent Sets in U_n^m

Let $n \geq 2$. By vertex reduction on v_1 in Figure 21,

$$\begin{aligned} F(U_n^m) &= F(U_n^m - v_1) + F(U_n^m - N[v_1]) \\ &= F(U_{n-1}^m \cup I_m) + F(U_{n-2}^m \cup I_m) \\ &= F(U_{n-1}^m)F(I_m) + F(U_{n-2}^m)F(I_m) \\ &= 2^m F(U_{n-1}^m) + 2^m F(U_{n-2}^m). \end{aligned}$$

Since the recurrence is the same as for $F(S_n^m)$, the general solution is the same. Hence,

$$F(U_n^m) = c_1(m)\left(2^{m-1} + \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n + c_2(m)\left(2^{m-1} - \frac{1}{2}\sqrt{2^{2m}+2^{m+2}}\right)^n$$

for some $c_1(m)$ and $c_2(m)$. The formula is obtained by solving to meet our initial conditions.

$\square$

Proposition 20 *For $n \geq 3, m \geq 0$, the Fibonacci index for V_n^m is*

$$F(V_n^m) = 2^{-n}\left(\left(2^m + \sqrt{2^m(4+2^m)}\right)^n + \left(2^m - \sqrt{2^m(4+2^m)}\right)^n\right).$$

Proof: Let $n \geq 3$. We can use vertex reduction on v_1 in Figure 22.

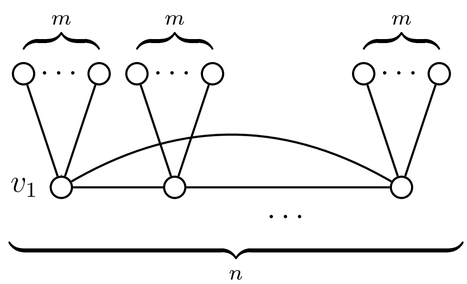


Figure 22: Independent Sets in V_n^m

$$\begin{aligned}
F(V_n^m) &= F(V_n^m - v_1) + F(V_n^m - N[v_1]) \\
&= F(U_{n-1}^m \cup I_m) + F(U_{n-3}^m \cup I_{2m}) \\
&= F(U_{n-1}^m)F(I_m) + F(U_{n-3})F(I_{2m}) \\
&= 2^m F(U_{n-1}^m) + 2^{2m} F(U_{n-3}^m).
\end{aligned}$$

By substituting the formula for $F(U_n^m)$ from Proposition 19, we obtain the formula for $F(V_n^m)$. □

Expressions for the Fibonacci indices of S_n^m, T_n^m, U_n^m, V_n^m for small n are shown in Table 7. Note that when $m = 0$, the Fibonacci indices correspond to those of the graph of a path, and when $m = 2$ the indices correspond to those of S_n and T_n shown in Table 5.

n	Fibonacci index
0	$F(S_0^m) = 2$ $F(T_0^m) = 3$ $F(U_0^m) = 1$
1	$F(S_1^m) = 1 + 2^{m+1}$ $F(T_1^m) = 1 + 2^{m+2}$ $F(U_1^m) = 1 + 2^m$
2	$F(S_2^m) = 3(2^m) + 2^{2m+1}$ $F(T_2^m) = 2^{m+2} + 4^{m+1}$ $F(U_2^m) = 2^{m+1} + 4^m$
3	$F(S_3^m) = 2^m + 5(2^{2m}) + 2^{3m+1}$ $F(T_3^m) = 2^m + 2^{2m+3} + 2^{3m+2}$ $F(U_3^m) = 2^m + 3(4^m) + 8^m$ $F(V_3^m) = 3(4^m) + 8^m$
4	$F(S_4^m) = 2^{4m+1} + 4^{m+1} + 7(8^m)$ $F(T_4^m) = 3(2^{3m+2}) + 5(4^m) + 4^{2m+1}$ $F(U_4^m) = 2^{3m+2} + 3(4^m) + 4^{2m}$ $F(V_4^m) = 2^{2m+1} + 2^{3m+2} + 4^{2m}$

Table 7: Fibonacci Indices for the Graphs S_n^m, T_n^m, U_n^m, and V_n^m for $n \leq 4$

5.2 Independence Polynomials of S_n^m, T_n^m, U_n^m, and V_n^m

Proposition 21 *Let $m \geq 0$. Then $F_{S_0^m}(x) = 1+x$, $F_{S_1^m}(x) = x+(1+x)^{m+1}$, and for $n \geq 2$, we have the recurrence relation*

$$F_{S_n^m}(x) = (1+x)^m F_{S_{n-1}^m}(x) + x(1+x)^m F_{S_{n-2}^m}(x).$$

Proof: Since S_0^m consists of a single vertex, the Fibonacci polynomial is $F_{S_0^m} = 1+x$. The graph S_1^m is a star with $m+1$ leaves. By using vertex reduction on the center vertex, we see that $F_{S_1^m}(x) = x+(1+x)^{m+1}$. Now, suppose that $n \geq 2$. Then using vertex reduction on v_1 in Figure 19,

$$\begin{aligned} F_{S_n^m}(x) &= F_{S_n^m - v_1}(x) + xF_{S_n^m - N[v_1]}(x) \\ &= F_{S_{n-1}^m \cup I_m}(x) + xF_{S_{n-2}^m \cup I_m}(x) \\ &= F_{S_{n-1}^m}(x)F_{I_m}(x) + xF_{S_{n-2}^m}(x)F_{I_m}(x) \end{aligned}$$

$$= \quad (1+x)^m F_{S^m_{n-1}}(x) + x(1+x)^m F_{S^m_{n-2}}(x). \quad \square$$

Proposition 22 *For $m \geq 0$ and $n \geq 0$, $F_{S^m_n}(x) =$*

$$\left(\frac{1+x}{2} + \frac{2x+(1+x)^{m+1}}{2\sqrt{(1+x)^m(4x+(1+x)^m)}}\right)\left(\frac{(1+x)^m + \sqrt{(1+x)^{2m}+4x(1+x)^m}}{2}\right)^n$$
$$+\left(\frac{1+x}{2} - \frac{2x+(1+x)^{m+1}}{2\sqrt{(1+x)^m(4x+(1+x)^m)}}\right)\left(\frac{(1+x)^m - \sqrt{(1+x)^{2m}+4x(1+x)^m}}{2}\right)^n.$$

Proof: By Proposition 21, $F_{S^m_n}(x) = (1+x)^m(F_{S^m_{n-1}}(x)) + x(1+x)^m(F_{S^m_{n-2}}(x))$ for $n \geq 2$. This recurrence relation has the characteristic equation $r^2 - (1+x)^m r - x(1+x)^m = 0$ with roots $r = \dfrac{(1+x)^m \pm \sqrt{(1+x)^{2m}+4x(1+x)^m}}{2}$. Hence, the general solution is given by

$$\begin{aligned} F_{S^m_n}(x) &= c_1(x)\left(\frac{(1+x)^m + \sqrt{(1+x)^{2m}+4x(1+x)^m}}{2}\right)^n \\ &\quad + c_2(x)\left(\frac{(1+x)^m - \sqrt{(1+x)^{2m}+4x(1+x)^m}}{2}\right)^n \end{aligned}$$

for some polynomials $c_1(x)$ and $c_2(x)$. Solving for $c_1(x)$ and $c_2(x)$ to meet our initial conditions given in Proposition 21, we obtain the result. $\square$

Proposition 23 *For $m \geq 0$, $F_{T^m_0}(x) = 1+2x$ and for $n \geq 1$, the independence polynomial is $F_{T^m_n}(x) =$*

$$\left(\frac{1}{2}\right)^{n+1}\left((1+x)^m + \sqrt{(1+x)^m(4x+(1+x)^m)}\right)^{n-1} *$$
$$\left(1+x+\frac{2x+(1+x)^{m+1}}{\sqrt{(1+x)^m(4x+(1+x)^m)}}\right)\left((1+2x)(1+x)^m + \sqrt{(1+x)^m(4x+(1+x)^m)}\right)$$
$$+\left(\frac{1}{2}\right)^{n+1}\left((1+x)^m - \sqrt{(1+x)^m(4x+(1+x)^m)}\right)^{n-1} *$$
$$\left(1+x-\frac{2x+(1+x)^{m+1}}{\sqrt{(1+x)^m(4x+(1+x)^m)}}\right)\left((1+2x)(1+x)^m - \sqrt{(1+x)^m(4x+(1+x)^m)}\right)$$

Proof: Since T_0^m is two adjacent vertices, $F_{T_0^m}(x) = 1 + 2x$. Suppose $n \geq 1$. Then by vertex reduction on v_1 in Figure 20,

$$\begin{aligned} F_{T_n^m}(x) &= F_{T_n^m - v_1}(x) + xF_{T_n^m - N[v_1]}(x) \\ &= F_{S_n^m}(x) + xF_{S_{n-1}^m \cup I_m}(x) \\ &= F_{S_n^m}(x) + xF_{S_{n-1}^m}(x)F_{I_m}(x) \\ &= F_{S_n^m}(x) + x(1+x)^m(F_{S_{n-1}^m}(x)). \end{aligned}$$

By substituting in the closed formula for the independence polynomial $F_{S_n^m}(x)$ from Proposition 22 and simplifying, the result is obtained. □

We can find a similar formula for U_n^m as shown in the following proposition.

Proposition 24 *For $m \geq 0$, $n \geq 0$, the independence polynomial for U_n^m is*

$$\begin{aligned} F_{U_n^m} &= \left(\frac{2x + (1+x)^m + \sqrt{(1+x)^m(4x + (1+x)^m)}}{2\sqrt{(1+x)^m(4x+(1+x)^m)}} \right) \\ &\quad * \left(\frac{(1+x)^m + \sqrt{(1+x)^m(4x+(1+x)^m)}}{2} \right)^n \\ &\quad + \left(\frac{-2x - (1+x)^m + \sqrt{(1+x)^m(4x+(1+x)^m)}}{2\sqrt{(1+x)^m(4x+(1+x)^m)}} \right) \\ &\quad * \left(\frac{(1+x)^m - \sqrt{(1+x)^m(4x+(1+x)^m)}}{2} \right)^n . \end{aligned}$$

Proof: Since U_0^m is the empty graph, $F_{U_0^m}(x) = 1$. Note that U_1^m is a star with m leaves, so $F_{U_1^m}(x) = x + (1+x)^m$.

Now, let $n \geq 2$. Then by vertex reduction on v_1 in Figure 21,

$$\begin{aligned}
F_{U_n^m}(x) &= F_{U_n^m - v_1}(x) + xF_{U_n^m - N[v_1]}(x) \\
&= F_{U_{n-1}^m \cup I_m}(x) + xF_{U_{n-2}^m \cup I_m}(x) \\
&= F_{U_{n-1}^m}(x)F_{I_m}(x) + xF_{U_{n-2}^m}(x)F_{I_m}(x) \\
&= (1+x)^m F_{U_{n-1}^m}(x) + x(1+x)^m F_{U_{n-2}^m}(x).
\end{aligned}$$

Since this recurrence relation is the same as for S_n^m, the general solution is the same. So

$$\begin{aligned}
F_{U_n^m}(x) &= c_1(x)\left(\frac{(1+x)^m + \sqrt{(1+x)^m(4x+(1+x)^m)}}{2}\right)^n \\
&\quad + c_2(x)\left(\frac{(1+x)^m - \sqrt{(1+x)^m(4x+(1+x)^m)}}{2}\right)^n
\end{aligned}$$

for some polynomials $c_1(x)$ and $c_2(x)$. Solving for the initial conditions when $n = 0, 1$, we obtain the result. □

Proposition 25 *For $n \geq 3, m \geq 0$, the independence polynomial for V_n^m is given by*

$$\begin{aligned}
F_{V_n^m}(x) &= \left(\frac{(1+x)^m + \sqrt{(1+x)^m(4x+(1+x)^m)}}{2}\right)^n \\
&\quad + \left(\frac{(1+x)^m - \sqrt{(1+x)^m(4x+(1+x)^m)}}{2}\right)^n.
\end{aligned}$$

Proof: By using vertex reduction on v_1 in Figure 22,

$$\begin{aligned}
F_{V_n^m}(x) &= F_{V_n^m - v_1}(x) + xF_{V_n^m - N[v_1]}(x) \\
&= F_{U_{n-1}^m \cup I_m}(x) + xF_{U_{n-3}^m \cup I_{2m}}(x) \\
&= F_{U_{n-1}^m}(x)F_{I_m}(x) + xF_{U_{n-3}^m}(x)F_{I_{2m}}(x) \\
&= (1+x)^m F_{U_{n-1}^m}(x) + x(1+x)^{2m} F_{U_{n-3}^m}(x).
\end{aligned}$$

The closed formula is obtained by using the previous proposition to subsititute for $F_{U_n^m}(x)$.

$\square$

Note that the constants in our formulas for the Fibonacci index and the independence polynomial of both V_n and V_n^m are 1, which leads to formulas more elegant than those of our other sequences of graphs.

Expressions for some of the independence polynomials of S_n^m, T_n^m, U_n^m, and V_n^m for small n are given in Table 8. Note that when $m = 0$, the polynomials correspond to those of paths, and when $m = 2$, the polynomials are the same as those found for S_n, T_n, U_n, and V_n.

n	Independence Polynomials
0	$F_{S_0^m}(x) = 1 + x$ $F_{T_0^m}(x) = 1 + 2x$ $F_{U_0^m}(x) = 1$
1	$F_{S_1^m}(x) = x + (1 + x)^{m+1}$ $F_{T_1^m}(x) = x + (1 + x)^{m+2}$ $F_{U_1^m}(x) = x + (1 + x)^m$
2	$F_{S_2^m}(x) = (1 + x)^m(2x + x^2 + (1 + x)^{m+1})$ $F_{T_2^m}(x) = (1 + x)^{m+1}(2x + (1 + x)^{m+1})$ $F_{U_2^m}(x) = (1 + x)^m(2x + (1 + x)^m)$
3	$F_{S_3^m}(x) = (1 + x)^m(x^2 + (3x + 2x^2)(1 + x)^m + (1 + x)^{1+2m})$ $F_{T_3^m}(x) = (1 + x)^m(x^2 + (3x + 4x^2 + x^3)(1 + x)^m + (1 + x)^{2+2m})$ $F_{U_3^m}(x) = (1 + x)^m(x^2 + 3x(1 + x)^m + (1 + x)^{2m})$ $F_{V_3^m}(x) = (1 + x)^{2m}(3x + (1 + x)^m)$

Table 8: Independence Polynomials for the Graphs S_n^m, T_n^m, U_n^m and V_n^m for $n \leq 3$

6 EXAMINATION OF $F_k(G)$

For any graph G, the factors that determine independent sets of size at most two are well known. If $|V(G)| = n$ and $|E(G)| = e$, then the following hold:

$$\begin{aligned} F_0(G) &= 1 \\ F_1(G) &= n \\ F_2(G) &= \binom{n}{2} - e \end{aligned}$$

By Lemma 1, the number of three-element independent sets when G is triangle-free is

$$F_3(G) = \binom{n}{3} - e(n-2) + \sum_{v \in V(G)} \binom{d(v)}{2}.$$

Figure 2 shows that, in general, four-element independent sets are not determined by the degree sequence. However, under certain circumstances, $F_4(G)$ can be calculated from the degree sequence.

Figure 23 shows the two isomers of the hydrocarbon C_4H_{10}, normal butane and isobutane. If we consider the molecular graphs of these chemicals, the independence polynomial of normal butane is

$$F_{T_4}(x) = 1 + 14x + 78x^2 + 232x^3 + 418x^4 + 486x^5 + 375x^6 + 192x^7 + 63x^8 + 12x^9 + x^{10}$$

and the independence polynomial of isobutane is

$$1 + 14x + 78x^2 + 232x^3 + 418x^4 + 495x^5 + 402x^6 + 225x^7 + 84x^8 + 19x^9 + 2x^{10}.$$

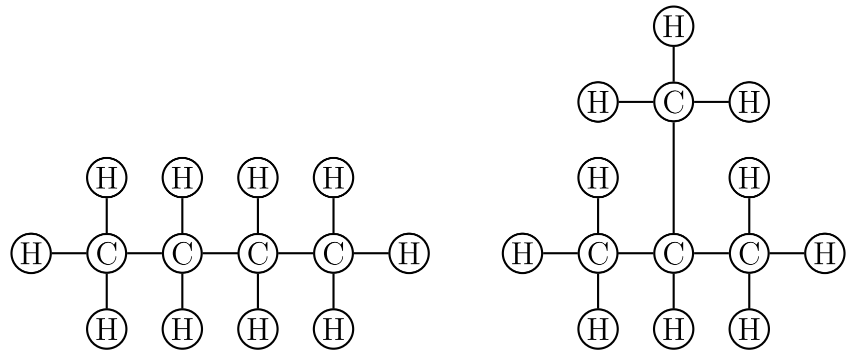


Figure 23: The Isomers of Butane: Normal Butane and Isobutane

These polynomials have the same coefficients up to x^4 indicating that the molecular graphs have the same number of independent sets of each size less than five. It is also the case that every vertex in both of these trees has degree 1 or 4. As shown by the following proposition, this can be generalized using the Principle of Inclusion/Exclusion.

Proposition 26 *Let G be an n-vertex graph with e edges and girth at least 5. If G has c vertices of degree Δ and $n-c$ of degree 1, then*

$$F_4(G) = -c + \frac{11}{3}c\Delta - \frac{5}{2}c\Delta^2 - \frac{1}{6}c\Delta^3 - \frac{9}{2}e + 2\Delta e - \Delta^2 e + \frac{1}{2}e^2 + \frac{3}{4}n - 2\Delta n$$

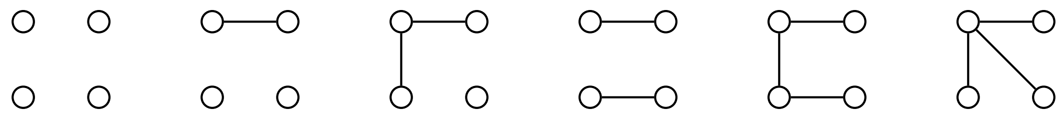
$$-\frac{1}{2}c\Delta n + \Delta^2 n + \frac{1}{2}c\Delta^2 n + \frac{5}{2}en + \frac{11}{24}n^2 - \frac{1}{2}en^2 - \frac{1}{4}n^3 + \frac{1}{24}n^4.$$

Proof: Since the girth of G is at least 5, then there are at most three edges between any set of four vertices in the graph. Using the Principle of Inclusion/Exclusion, we can count the number of 4-element independent sets of size 4 by counting the total number of sets of size four, subtracting sets with one edge, adding sets with two edges, and subtracting sets with three edges.

There are $\binom{n}{4}$ total sets. Each of the cases containing edges can be counted as shown in Figure 24.

Hence,

$$F_4(G) = \binom{n}{4} - e\binom{n-2}{2} + c\binom{\Delta}{2}(n-3) + \binom{e}{2} - c\binom{\Delta}{2} - (\Delta-1)^2(e+c-n) - c\binom{\Delta}{3}.$$



$\binom{n}{4}$ $e\binom{n-2}{2}$ $c\binom{\Delta}{2}(n-3)$ $\binom{e}{2}-c\binom{\Delta}{2}(\Delta-1)^2(e+c-n)$ $c\binom{\Delta}{3}$

Figure 24: Counting Small Forests in a Graph with Vertices of Degree Δ or 1

Expanding and simplifying yields the result. $\square$

This result applies not only to the sequence of graphs T_n, but also to the generalized hydrocarbon sequence T_n^m which consists of trees in which all vertices have degree 1 or $m+2$.

Corollary 1 *If G is a Δ-regular graph on n vertices with girth at least 5, then*

$$F_4(G) = \frac{-1}{4}n - \frac{7}{12}\Delta n - \frac{1}{2}\Delta^2 n - \frac{2}{3}\Delta^3 n + \frac{11}{24}n^2 + \frac{3}{4}\Delta n^2 + \frac{5}{8}\Delta^2 n^2 - \frac{1}{4}n^3 - \frac{1}{4}\Delta n^3 + \frac{1}{24}n^4.$$

Proof: This follows directly from the previous proposition by noting that $e = \dfrac{n\Delta}{2}$ and that $c = n$. So, in this case,

$$F_4(G) = \binom{n}{4} - \frac{n\Delta}{2}\binom{n-2}{2} + n(n-3)\binom{\Delta}{2} + \binom{\frac{n\Delta}{2}}{2} - n\binom{\Delta}{2} - \frac{n\Delta}{2}(\Delta-1)^2 - n\binom{\Delta}{3}.$$

Expanding and simplifying will yield the formula. $\square$

Proposition 27 *In a full binary tree, B_n, with $n \geq 3$ levels of vertices,*

$$F_4(B_n) = 55 - \frac{391}{3}2^{n-2} + \frac{191}{3}2^{2n-3} - \frac{11}{3}2^{3n-2} + \frac{1}{3}2^{4n-3}.$$

Proof: In a full binary tree with n levels of vertices, there are $v = 2^n - 1$ vertices including 2^{n-1} of degree 1, 1 of degree 2, and $2^{n-1} - 2$ of degree 3, and there are $e = 2^n - 2$ edges. We can count the independent sets of size four by the Principle of Inclusion/Exclusion considering the same cases as before since there are no cycles.

There are $\binom{v}{4} = \binom{2^n-1}{4}$ total sets. Of these, $e\dbinom{v-2}{2} = (2^n-2)\dbinom{2^n-3}{2}$ contain one edge. The number of sets with two edges that share a vertex is $(2^n-4)+(2^{n-1}-2)(3)(2^n-4) =$

$(3(2^{n-1})-5)(2^n-4)$ which comes from selecting the edges incident with the root or selecting two edges incident with a vertex of degree 3. The number of sets with two independent edges is $\binom{2^n-2}{2} - (3(2^{n-1})-5)(2^n-4)$. A path of length 3 could have the center edge incident with the root or incident with two vertices of degree 3, so there are $4+4(2^{n-1}-4)$ of these. And there are $2^{n-1}-2$ copies of $K_{1,3}$. Hence,

$$F_4(B_n) = \binom{2^n-1}{4} - (2^n-2)\binom{2^n-3}{2} + (3(2^{n-1})-5)(2^n-4) + \binom{2^n-2}{2} - (3(2^{n-1})-5)$$
$$-4 - (4(2^{n-1})-16) - (2^{n-1}-2).$$

The formula is obtained from expanding and simplifying. □

Proposition 28 *If G is a Δ-regular graph on n vertices with girth at least 6, then*

$$F_5(G) = \frac{n}{5} + \frac{7\Delta n}{12} + \frac{23\Delta^2 n}{24} + \frac{5\Delta^3 n}{12} + \frac{25\Delta^4 n}{24} - \frac{5n^2}{12} - \Delta n^2 - \Delta^2 n^2 - \frac{11\Delta^3 n^2}{12}$$
$$+\frac{7n^3}{24} + \frac{\Delta n^3}{2} + \frac{3\Delta^2 n^3}{8} - \frac{n^4}{12} - \frac{\Delta n^4}{12} + \frac{n^5}{120}.$$

Proof: Since G has girth at least 6, there are at most 4 edges in any set of 5 vertices. So we can use the Principle of Inclusion/Exclusion to count the independent sets of size 5 by removing the forests with at most four edges. We can count these by considering the cases shown in Figure 25.

Hence,

$$\begin{aligned} F_5(G) &= \binom{n}{5} - e\binom{n-2}{3} + n\binom{\Delta}{2}\binom{n-3}{2} + \left(\binom{e}{2} - n\binom{\Delta}{2}\right)(n-4) \\ &\quad -e(\Delta-1)^2(n-4) - n\binom{\Delta}{3}(n-4) - n\binom{\Delta}{2}(e-3\Delta+2) + n\binom{\Delta}{2}(\Delta-1)^2 \\ &\quad +3n\binom{\Delta}{3}(\Delta-1) + n\binom{\Delta}{4} \end{aligned}$$

By substituting $e = \frac{\Delta n}{2}$ and simplifying, the formula is obtained. □

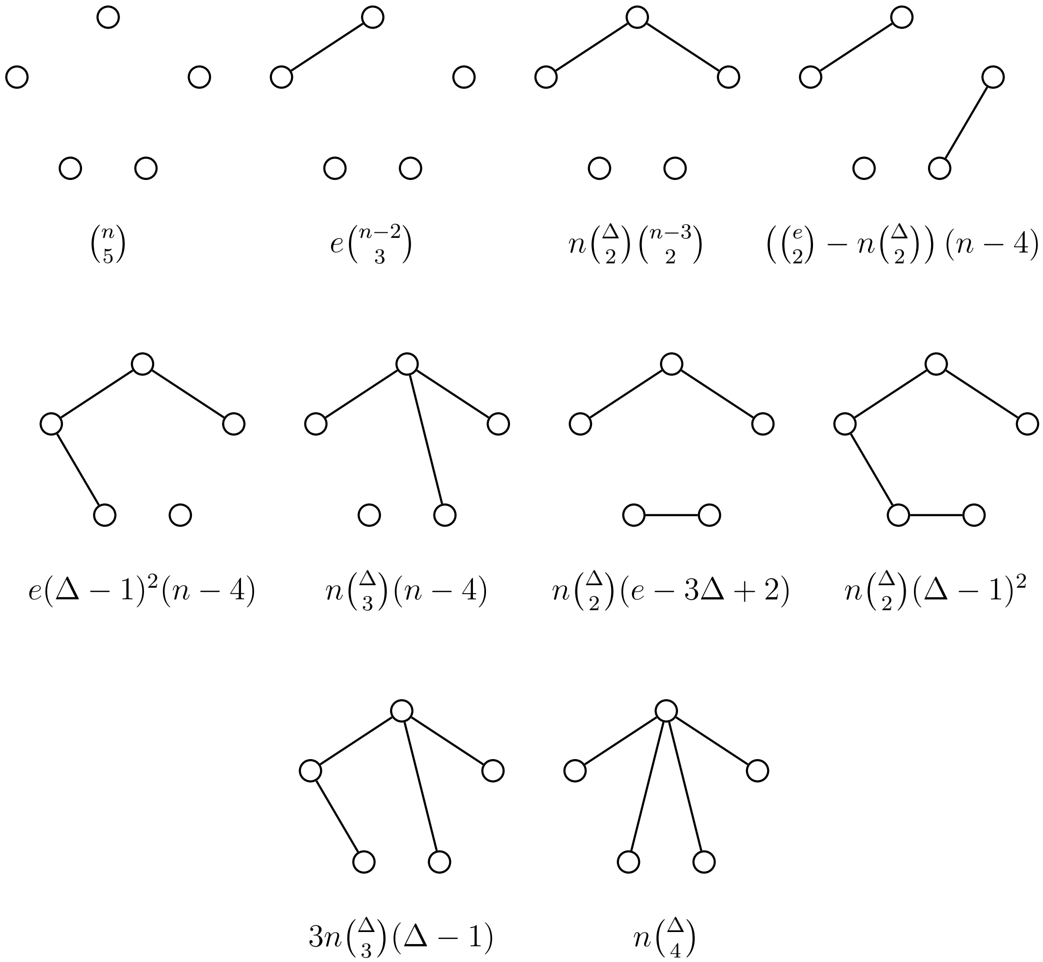


Figure 25: Counting Small Forests in a Δ-Regular Graph

If we consider the Petersen graph, which is 3-regular but only has girth 5, this formula yields 12, which happens to be the number of 5-cycles in the graph (since it has no independent sets of size five).

This method of deriving a formula for the number of k-element independent sets in a regular graph by removing small forests using inclusion/exclusion does not rely on the girth being any particular size, as long as that size is greater than the size of the sets we are investigating. Our goal is to generalize this method to show that regular graphs with girth g have the same number of k-element independent sets for all $k < g$. The notation given in the following definition will aid us in proving this.

Definition 1 *Let $N_G(H)$ represent the number of distinct subgraphs of a graph G isomorphic to H.*

Lemma 8 *Let G_1 and G_2 be Δ-regular graphs on n vertices with girth g. Let T be a tree with at most $g-1$ vertices. Then G_1 and G_2 contain the same number of subgraphs isomorphic to T.*

Proof: We will proceed by induction on $|V(T)|$. If $|V(T)| = 1$, then T is a single vertex. So the number of copies of T in G_1 and G_2 is the same, namely n.

Suppose that the lemma is true for any tree with $w < g-1$ vertices. Let T be a tree with $|V(T)| = w+1$, and let $x \in V(T)$ be a leaf. Then $|V(T-x)| = w$, so by the induction hypothesis, $N_{G_1}(T-x) = N_{G_2}(T-x)$.

Suppose we are given a copy of $T-x$ in any Δ-regular graph G with girth g. We can form a copy of T by choosing any of the q vertices $y \in V(T-x)$ such that adjoining x to y yields a copy of T. We can choose any of the other $\Delta - d_{T-x}(y)$ neighbors in G for x without creating a cycle since the graph has girth g. By using this method, we generate each distinct copy of T in G exactly $N_T(T-x)$ times. Hence,

$$N_G(T) = \frac{N_G(T-x) \cdot q \cdot (\Delta - d_{T-x}(y))}{N_T(T-x)}.$$

Since the only part of this formula that is not independent of the choice of the graph is $N_G(T-x)$ and this number is the same for the graphs G_1 and G_2, we have that $N_{G_1}(T) = N_{G_2}(T)$. Hence, the lemma holds by induction. $\square$

Lemma 9 *Let G_1 and G_2 be Δ-regular graphs on n vertices with girth g. Let F be a forest with at most $g-1$ vertices. Then G_1 and G_2 have the same number of subgraphs isomorphic to F.*

Proof: Let the components of F be $T_1, T_2, ..., T_r$. Note that each component of F is a tree on at most $g-1$ vertices. We will proceed by induction on r. If $r = 1$, then $F = T_1$ and by the previous lemma, $N_{G_1}(F) = N_{G_2}(F)$.

Suppose the lemma is true for any forest with less than g vertices and less than r components. Let F be a forest with at most $g-1$ vertices and components $T_1, T_2, ..., T_r$. If F' is the forest consisting of $T_1, T_2, ...T_{r-1}$, then by the induction hypothesis, $N_{G_1}(F') = N_{G_2}(F')$. By the previous lemma, $N_{G_1}(T_r) = N_{G_2}(T_r)$.

Each subgraph isomorphic to F is the union of disjoint copies of F' and T_r. There is a finite number of ways to overlap the graphs F' and T_r. If an overlap creates a cycle, then the cycle is on less than g vertices, so there are zero copies of this graph in both G_1 and G_2. Otherwise, the result is a forest F_i with less than r components. By the induction hypothesis, $N_{G_1}(F_i) = N_{G_2}(F_i)$ for each such F_i. Hence,

$$\begin{aligned} N_{G_1}(F) &= N_{G_1}(F') \cdot N_{G_1}(T_r) - \sum_i N_{G_1}(F_i) \\ &= N_{G_2}(F') \cdot N_{G_2}(T_r) - \sum_i N_{G_2}(F_i) \\ &= N_{G_2}(F). \end{aligned}$$

By induction, both graphs contain the same number of copies of any forest with at most $g-1$ vertices. □

Theorem 4 *Let G_1 and G_2 be Δ-regular graphs on n vertices with girth g. Then for $k \leq g-1$, $F_k(G_1) = F_k(G_2)$.*

Proof: Let $f_{G,s,m}$ represent the number of subgraphs in G isomorphic to a forest on s vertices with m edges. For any given forest F such that $|V(F)| \leq g-1$, $N_{G_1}(F) = N_{G_2}(F)$ by the previous lemma. By summing over the finite number of forests on s vertices with m edges, we see that $f_{G_1,s,m} = f_{G_2,s,m}$ for each choice of s and m.

Also, note that for any subset of k vertices in either graph, there are at most $k-1$ edges in the subgraph induced by those vertices since more edges would imply the existence of a cycle of length less than g. So the induced subgraph on any set of k vertices is a forest.

The number of k-element independent sets in a graph G, $F_k(G)$, will be the number of k-element subsets of $V(G)$ that contain no edges. By the Principle of Inclusion/Exclusion, we have

$$\begin{aligned}
F_k(G_1) &= \binom{n}{k} - f_{G_1,k,1} + f_{G_1,k,2} - f_{G_1,k,3} + ... + (-1)^{k-1} f_{G_1,k,k-1} \\
&= \binom{n}{k} - f_{G_2,k,1} + f_{G_2,k,2} - f_{G_2,k,3} + ... + (-1)^{k-1} f_{G_2,k,k-1} \\
&= F_k(G_2).
\end{aligned}$$

$\square$

LIST OF REFERENCES

References

[1] Burstein, A., Kitaev, S., & Mansour, T. (2009). Counting independent sets in some classes of (almost) regular graphs. In *Pure Mathematics and Applications, 19, no. 2-3* 17-26.

[2] Bruyére, V. & Mèlot, H. (2008). Turàn graphs, stability number, and Fibonacci index. In *Lecture Notes in Computer Science, 5165,* 127-138.

[3] Chism, L.M. (2009). *On independence polynomials and independence equivalence in graphs.* (Doctoral dissertation, the University of Mississippi).

[4] Fajtlowicz, S. & Larson, C. (2003). Graph-theoretic independence as a predictor of fullerene stability. In *Chemical Physics Letters, 377, no. 5-6,* 485-490.

[5] Graham, R., Knuth, D., & Patashnik, O. (1994). *Concrete mathematics: A foundation for computer science (2nd ed.).* Upper Saddle River, NJ: Addison-Wesley.

[6] Gutman, I. & Wagner, S. (2010). Maxima and minima of the Hosoya index and the Merrifield-Simmons index: A survey of results and techniques. In *Acta Appl. Math., 12, no 3,* 323-346.

[7] Henry, G., Pepper, R., & Sexton, D. (2006). Cut-edges and the independence number. *Communications in Mathematical and in Computer Chemistry, 56,* 403-408.

[8] Hopkins, G. & Staton, W. (1984). Some identities arising from the Fibonacci numbers of certain graphs. In *Fibonnaci Quarterly, 22,* 255-258.

[9] Hopkins, G. & Staton, W. (1984). An identity arising from counting independent sets. In *Congressus Numerantium, 44,* 5-10.

[10] Johnsonbaugh, R. & Schaefer, M. (2004). *Algorithms.* New Jersey: Pearson Education.

[11] Kirschenhofer, P., Prodinger, H., & Tichy, R.F. (1983). Fibonacci numbers of graphs: II. In *Fibonnaci Quarterly, 21,* 219-229.

[12] Merrifield, R.E., and Simmons, H.E. (1989). *Topological Methods in Chemistry.* Wiley, New York.

[13] Molnár, Á., and Olah, G. (1995). *Hydrocarbon Chemistry.* Wiley-Interscience, New York.

[14] Prodinger, H. & Tichy, R.F. (1982). Fibonacci numbers of graphs. In *Fibonnaci Quarterly, 20,* 16-21.

[15] Scheinerman, E. (2006). *Mathematics: A discrete introduction.* Belmont, CA: Thomson Brooks/Cole.

[16] Song, L. (2009). *On the independence polynomials of k-tree related and well-covered graphs.* (Doctoral dissertation, the University of Mississippi).

[17] West, D. (2001). *Introduction to graph theory (2nd ed.).* Upper Saddle River, NJ: Prentice Hall.

[18] Wilf, H. (1994). *Generatingfunctionology (2nd ed.).* Academic Press, Inc. http://www.math.upenn.edu/ wilf/DownldGF.html.

[19] Wingard, G.C. (1995). *Properties and applications of the Fibonacci polynomial of a graph.* (Doctoral dissertation, the University of Mississippi).

VITA

Born August 19, 1987 in Memphis, Tennessee, Cameron Byrum graduated as Valedictorian and Star Student from Hernando High School in 2005. Cameron then attended the University of Mississippi where she studied Mathematics, her major, and Computer Science. She had several opportunites to participate in research as an undergraduate, including the completion of an honors thesis for the Sally McDonnell Barksdale Honors College and two research papers as part of a Research Experience for Undergraduates program at the University of North Carolina at Greensboro. During her undergraduate career, she traveled to Hungary and Spain, among other locations, for the presentation of research results.

In May 2009, Cameron graduated Summa Cum Laude, as a Taylor Medalist, and as an Honors Scholar from the University of Mississippi with a Bachelor's of Science degree. She continued her studies in Mathematics at Ole Miss in the graduate program where she completed this thesis under the direction of Dr. William Staton. Cameron hopes to continue in a career path involving mathematical research, to use her skills to serve the community, and to grow in her Christian faith.