The neighbourhood polynomial of some families of dendrimers

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Abstract. The neighbourhood polynomial $N(G, x)$ is generating function for the number of faces of each cardinality in the neighbourhood complex of a graph and it is defined as $N(G, x) = \sum_{U \in \mathcal{N}(G)} x^{|U|}$, where $\mathcal{N}(G)$ is neighbourhood complex of a graph, whose vertices of the graph and faces are subsets of vertices that have a common neighbour. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, we compute this polynomial for some families of dendrimer.

1. Introduction

A (simplicial) complex on a finite set $X$ is a collection $\mathcal{C}$ of a subsets of $X$, closed under containment. Each set in $\mathcal{C}$ is called a face of the complex, and the maximal faces (with respect to containment) are called facets or bases. The dimension of a complex $\mathcal{C}$ is the maximum cardinality of a face. The $f$-vector (or face-vector) of a d-dimensional complex $\mathcal{C}$ is $(f_0, f_1, ..., f_d)$, where $f_i$ is the number of faces of cardinality $i$ in $\mathcal{C}$. The $f$– polynomial of a d-dimensional complex $\mathcal{C}$ is the generating function $f(\mathcal{C}, x) = \sum_{i} f_i x^i$ for the $f$-vector $(f_0, f_1, ..., f_d)$ of the complex. For each graph polynomial, there is a complex for which the graph polynomial is a simple evaluation of the $f$– polynomial. For instance, the independence complex $I(G)$ of graph $G$ is the complex on the vertex set $V$ of $G$ whose faces are the independence set of $G$. The independence polynomial is merely the $f$– polynomial of the independent complex. One of the applications of simplicial complexes to graph theory is undoubtedly Lovasz’s proof [4] of the chromatic number of Kneser graphs. His argument centers on the neighbourhood complex $\mathcal{N}(G)$ of a graph, whose vertices are the vertices of the graph and whose faces are subsets of vertices that have common neighbour.

We consider a univariate polynomial, which called the neighbourhood polynomial of graph $G$, $N(G, x) = \sum_{U \in \mathcal{N}(G)} x^{|U|}$ (see [3]), where $\mathcal{N}(G)$ is neighbourhood complex of a graph, whose vertices are the vertices of the graph and faces are subsets of vertices that have a common neighbour.

The nanostars dendrimer is a part of a new group of macromolecules that seem photo funnels just like artificial antennas and also is a great resistant of photo bleaching. Recently some people investigated the mathematical properties of these nanostructures (see for example [1,2,5,7,8]).

Brown and Nowakowski [3] examined the neighbourhood polynomial for hypercube, for graphs not containing a four-cycle and for the graphs resulting from joins and Cartesian products.
Alikhani and Mahmoudi [6] studied some specific graphs and nanostructures and study their neighbourhood polynomial. So far not many results known on this polynomial. In this paper, we will consider some families of dendrimers and compute their neighbourhood polynomial.

2. Discussion and Main Results

In this section, we shall determine the neighbourhood polynomial of three families of dendrimers. We first state some properties of neighbourhood polynomial.

**Theorem 1** [3] Let $G$ be a free graph with $n$ vertices and $m$ edges. Then

$$N(G, x) = \sum_{v \in V} (1 + x)^{\deg v} - x(2m - n) - (n - 1)$$

An immediate observation is the following.

**Corollary 1** [3] The neighbourhood polynomial for a $C_4$ - free graph depends only on the degree sequence of the graph and can be calculated in polynomial time.

Theorem 1 gives us the neighbourhood polynomial for many graphs, including:

- If $G = C_n$ is a cycle of length $n > 4$, then $N(C_n, x) = 1 + nx + nx^2$;
- If $G$ is an $r$ - regular graph of girth at least 5, then $N(G, x) = n(1 + x)^r + n(r - 1)x - (n - 1)$. In particular, if $G$ is Petersen graph, $N(G, x) = 1 + 10x + 30x^2 + 10x^3$;
- 3) If $G$ is a tree, then $N(G, x) = \sum_{v \in V} (1 + x)^{\deg v} - x(n - 1) - (n - 1)$.
- 4) Let $F_n$ be a friendship graph, then $N(F_n, x) = 2n(1 + x)^2 + (1 + x)^{2n} - (4n - 1)x - 2n$.

We now determine the neighbourhood polynomial of some families of dendrimers. First, we compute the neighbourhood polynomial of PAMAM dendrimer which denoted by $PD_4[3]$ as depicted in Figure 1.

**Figure 1.** PAMAM dendrimer of generations $G_n$ with growth stages, $PD_4[3]$

| Degree of Vertex | Number of Vertex |
|-----------------|-----------------|
| 1               | $9 \times 2^n - 3$ |
| 2               | $15 \times 2^{n+1} - 15$ |
**Theorem 2**  Let \( n \) be the number of growth stages in \( PD_1[n] \) and \( n \in N_0 \). Then the neighbourhood polynomial of \( PD_1[n] \) for \( n = 0,1,2,3 \ldots \) is given by

\[
N(PD_1[n], x) = (9 \times 2^n - 5)(1 + x)^3 + (30 \times 2^n - 15)(1 + x)^2 + (9 \times 2^n - 3)(1 + x) - x(12 \times 2^{n+2} - 25) - (12 \times 2^{n+2} - 24)
\]

**Proof.** Let \( G \) be the PAMAM dendrimer \( PD_1[n] \). The number vertices and edges in PAMAM dendrimer \( PD_1[n] \) are \( |V(PD_1[n])| = 12 \times 2^{n+2} - 23 \) and \( |E(PD_1[n])| = 12 \times 2^{n+2} - 24 \). We find the vertex partition of the form 1, 2 and 3 for PAMAM dendrimer \( PD_1[n] \) based on the number degree of vertex. Table 1 explain such partition for \( PD_1[n] \). Now by using the partition given in Table 1, we can compute the neighbourhood polynomial for \( PD_1[n] \). Since (1), this implies that

\[
N(PD_1[n], x) = (9 \times 2^n - 3)(1 + x) + (15 \times 2^{n+1} - 15)(1 + x)^2 + (9 \times 2^n - 5)(1 + x)^3 - x(24 \times 2^{n+2} - 48 - 12 \times 2^{n+2} + 23) - (12 \times 2^{n+2} - 23 - 1)
\]

By simple calculation, we get

\[
N(PD_1[n], x) = (9 \times 2^n - 5)(1 + x)^3 + (30 \times 2^n - 15)(1 + x)^2 + (9 \times 2^n - 3)(1 + x) - x(12 \times 2^{n+2} - 25) - (12 \times 2^{n+2} - 24)
\]

This completes the proof. 

The following theorem computes the neighbourhood polynomial for tetrathiafulvalene dendrimer \( TD_2[n] \). The graph \( TD_2[n] \) is depicted in Figure 2.

![Figure 2. Tetrathiafulvalene dendrimer with 2-growth stages, \( TD_2[2] \)](image)

**Table 2.** Vertex partition of Tetrathiafulvalene dendrimer \( TD_2[n] \) based on the number degree of vertex

| Degree of Vertex | Number of Vertex |
|-----------------|-----------------|
| 1               | 8 \times 2^n - 4 |
Theorem 3 Let $n$ be the number of growth stages in $TD_2[n]$ and $n \in N_0$. Then the neighbourhood polynomial of $TD_2[n]$ for $n = 0,1,2,3 \ldots$ is given by

$$N(TD_2[n],x) = (40 \times 2^n - 26)(1 + x)^3 + (76 \times 2^n - 44)(1 + x)^2 + (8 \times 2^n - 4)(1 + x)$$
$$- x(39 \times 2^{n+2} - 96) - (31 \times 2^{n+2} - 75)$$

Proof. Let $G$ be the Tetrathiafulvalene dendrimer $TD_2[n]$. The number vertices and edges in tetrathiafulvalene dendrimer $TD_2[n]$ are $|V(TD_2[n])| = 31 \times 2^{n+2} - 74$ and $|E(TD_2[n])| = 12 \times 2^{n+2} - 24$. We find the vertex partition of the form 1, 2 and 3 for tetrathiafulvalene dendrimer $TD_2[n]$ based on the number degree of vertex. Table 2 explain such partition for $TD_2[n]$. Now by using the partition given in Table 2, we can compute the neighbourhood polynomial for $TD_2[n]$. Since (1), this implies that

$$N(TD_2[n],x) = (8 \times 2^n - 4)(1 + x) + (76 \times 2^n - 44)(1 + x)^2 + (40 \times 2^n - 26)(1 + x)^3$$
$$- x(70 \times 2^{n+2} - 170 - 31 \times 2^{n+2} + 74) - (31 \times 2^{n+2} - 74 - 1)$$

By simple calculation, we get

$$N(TD_2[n],x) = (40 \times 2^n - 26)(1 + x)^3 + (76 \times 2^n - 44)(1 + x)^2 + (8 \times 2^n - 4)(1 + x)$$
$$- x(39 \times 2^{n+2} - 96) - (31 \times 2^{n+2} - 75)$$

This completes the proof.$ \square$

The following theorem computes the neighbourhood polynomial for POPAM dendrimer $POD_2[n]$. The graph $POD_2[n]$ is depicted in Figure 3.

![Figure 3. POPAM dendrimer of generations $G_n$ with two growth stages, $POD_2[2]$](image)

Table 3. Vertex partition of POPAM dendrimer $POD_2[n]$ based on the number degree of vertex

| Degree of Vertex | Number of Vertex |
|------------------|------------------|
| 1                | $4 \times 2^n$   |
| 2                | $24 \times 2^n - 8$ |
| 3                | $4 \times 2^n - 2$ |
Theorem 4 Let $n$ be the number of growth stages in $POD_2[n]$ and $n \in \mathbb{N}_0$. Then the neighbourhood polynomial of $POD_2[n]$ for $n = 0, 1, 2, 3$ ... is given by

$$N(POD_2[n], x) = (4 \times 2^n - 2)(1 + x)^3 + (24 \times 2^n - 8)(1 + x)^2 + (4 \times 2^n)(1 + x) - x(2^{n+5} - 12) - (2^{n+5} - 11)$$

Proof. Let $G$ be the POPAM dendrimer $POD_2[n]$ with $n$ growth stages. The number vertices and edges in POPAM dendrimer $POD_2[n]$ are $|V(POD_2[n])| = 2^{n+5} - 10$ and $|E(POD_2[n])| = 2^{n+5} - 11$. We find the vertex partition of the form 1, 2 and 3 for POPAM dendrimer $POD_2[n]$ based on the number degree of vertex. Table 5.3 explain such partition for $POD_2[n]$. Now by using the partition given in Table 5.3, we can compute the neighbourhood polynomial for $POD_1[n]$. Since (1), this implies that

$$N(POD_2[n], x) = (4 \times 2^n)(1 + x) + (24 \times 2^n - 8)(1 + x)^2 + (4 \times 2^n - 2)(1 + x)^3 - x(2 \times 2^{n+5} - 22 - 2^{n+5} + 10) - (2^{n+5} - 10 - 1)$$

By simple calculation, we get

$$N(POD_2[n], x) = (4 \times 2^n - 2)(1 + x)^3 + (24 \times 2^n - 8)(1 + x)^2 + (4 \times 2^n)(1 + x) - x(2^{n+5} - 12) - (2^{n+5} - 11)$$

This completes the proof.$\square$

3. Conclusion and Open Problem

The concept of neighborhood polynomial in graph was introduced formally by Brown and Nowakowski [3]. Alikhani and Mahmoodi [6] later considered the neighborhood polynomial for some nanostructures. In this paper, we presented this polynomial for three families of dendrimer graphs namely, PAMAM $PD_1[n]$, tetrathiafulvalene $TD_2[n]$ and POPAM $POD_2[n]$. One may consider the application of this polynomial in QSAR/QSPR researches for future investigation. Another research direction is study the neighborhood polynomial of various nano-structures such as nanotube, nancones and fullerenes.

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