The Neighbourhood Polynomial of some Nanostructures

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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. In other word

$$N(G,x) = \sum_{U \in N(G)} x^{|U|},$$

where $N(G)$ 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. In this paper we compute this polynomial for some nanostructures.

Keywords: Neighbourhood polynomial, Dendrimer nanostar.

1. INTRODUCTION

A (simplicial) complex on a finite set $X$ is a collection $C$ of subsets of $X$, closed under containment. Each set in $C$ 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 $C$ is the maximum cardinality of a face.

The $f$–vector (or face–vector) of a $d$–dimensional complex $C$ is $(f_0, f_1, ..., f_d)$, where $f_i$ is the number of faces of cardinality $i$ in $C$. The $f$–polynomial of a $d$–dimensional complex $C$ is the generating function $f(C,x) = \sum_i f_i x^i$ for the $f$–vector $(f_0, f_1, ..., f_d)$ of the complex. For each graph polynomials, 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 independent sets of $G$. The independence polynomial is merely the $f$–polynomial of the independence 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 $N(G)$ of a graph, whose vertices are the vertices of the graph and

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whose faces are subsets of vertices that have a common neighbour.

We consider a univariate polynomial, which called the \textit{neighbourhood polynomial} of graph \( G \). 
\[ N(G, x) = \sum_{U \in N(G)} x^{|U|} \] 
where \( N(G) \) 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.

\textbf{Example 1.} For a cycle with four vertices \{a,b,c,d\} we have \( N(C_4, x) = 1 + 4x + 2x^2 \).

Because the empty set trivially has a common neighbour (as the graph has at least one vertex) while each of the single vertices has a neighbour. Each set \{a, c\} and \{b, d\} has two common neighbours, but one suffices, and there is no subset of three vertices that have a common neighbour. Thus the neighbourhood complex is
\[
\{\emptyset, \{a\}, \{b\}, \{c\}, \{d\}, \{a, b\}, \{b, d\}\}
\]
and so we have the result.

\textbf{Example 2:} For a complete graph \( K_n \) we have \( N(K_n, x) = (1 + x)^n - x^n \). Since every subset of the vertices of a complete graph except the entire vertex set has a common neighbour.

The nanostar dendrimer is a part of a new group of macromolecules that seem photon 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]).

In this paper we consider some specific graphs and nanostructures and study their neighborhood polynomials.

\section{Main Results}

In this section we compute the neighbourhood polynomial for some graphs and nanostructures. First we state some properties of neighbourhood polynomial. We say \( G \) is \( C_4 \)-\textit{free} if \( G \) does not contain \( C_4 \) as a sub-graph (not necessarily induced). The following theorem gives the neighborhood polynomial of \( C_4 \)-free graph.

\textbf{Theorem 1 ([3])} Let \( G \) be \( C_4 \)-free with \( n \) vertices and \( m \) edges. Then
\[ N(G, x) = \sum_{v \in V} (1 + x)^{\deg v} - x(2m - n) - (n - 1). \]

\textbf{Proof:} Let \( N_1, \ldots, N_k \) be the maximal (with respect to containment) neighbourhoods of the vertices of a graph \( G \) with \( n \) vertices and \( m \) edges. Note that in general, \( k \leq n \) as some vertices may have the same neighbours, or one might be a subset of the other. A set belongs to the neighbourhood complex of \( G \) if and only if it is a subset of one of the \( N_i \)'s.
By assuming that \( G \) has no isolated vertices and is \( C_4 \)-free, a first order approximation for the neighbourhood polynomial is
\[
N(G, x) = \sum_{v \in V} (1 + x)^{\deg v} - x \sum_{v \in V} (\deg v - 1) - (n - 1) = \sum_{v \in V} (1 + x)^{\deg v} - x(2m - n) - (n - 1),
\]
Proving the result.

Using Theorem 1 we have the neighbourhood polynomials for many graphs.

**Corollary 1:**

i. If \( G = C_n \) is a cycle of length \( n > 4 \), then \( N(C_n, x) = 1 + nx + nx^2 \).

ii. If \( G \) is an \( r \)-regular graph of girth at least 5, then
\[
N(G, x) = n(1 + x)^r - n(r - 1)x - (n - 1).
\]

iii. If \( G \) is a tree, then \( N(G, x) = \sum_{v} (1 + x)^{\deg v} - x(n - 1) - (n - 1) \).

iv. Let \( F_n \) be a friendship graph (Figure 1), then
\[
N(F_n, x) = 2n(1 + x)^2 + (1 + x)^{2n} - (4n - 1)x - 2n.
\]

![Figure 1: Friendship Graph F2, F3, F4 and Fn.](image)

Here we shall compute the neighbourhood polynomial of some dendrimers. First we compute the neighbourhood polynomial for the first kind of dendrimer of generation 1-3 has grown \( n \) stages. We denote this graph by \( D_3[n] \). Figure 2 show the first kind of dendrimer of generation 1-3 has grown 3 stages \( (D_3[3]) \).

**Theorem 2.** ([1])

(i) The number of vertices of \( D_3[n] \) is \( |V(D_3[n])| = 45 \times 2^n - 26 \).

(ii) The number of edges of \( D_3[n] \) is \( |E(D_3[n])| = 48 \times 2^n - 24 \).

Using Theorems 1 and 2 we have the following theorem for \( N(D_3[n], x) \).

**Theorem 3.** The neighbourhood polynomial of \( D_3[n] \) is:
\[
N(D_3[n], x) = (15 \times 2^n - 8)(1 + x)^3 + 12(2^{n+1} - 1)(1 + x)^2 + 3 \times 2^n (1 + x) - x(51 \times 2^n - 22) - (45 \times 2^n - 27).
\]
Figure 2: The First Kind of Dendrimer of Generation $1–3$ has Grown $3$ Stages

**Proof.** Let $n_i$ be the number of vertices of degree $i$ in $D_i[n]$, where $i = 1, 2, 3$. It is easy to see that $n_1 = 3 \times 2^n$, $n_2 = 12 \times (2^{n+1} - 1)$ and $n_3 = 15 \times 2^n - 8$. Now by Theorems 1 and 2 we have,

$$N(D_3[n], x) = n_1 (1 + x) + n_2 (1 + x)^2 + n_3 (1 + x)^3$$

$$- x(96 \times 2^n - 48 - 45 \times 2^n + 26) - (45 \times 2^n - 27)$$

$$= (15 \times 2^n - 8)(1 + x)^3 + 12(2^{n+1} - 1)(1 + x)^2 + 3 \times 2^n (1 + x)$$

$$- x(51 \times 2^n - 22) - (45 \times 2^n - 27).$$

This completes our argument.

Here we shall compute the neighbourhood polynomial of the first kind of dendrimer which has grown $n$ steps denoted $D_i[n]$. Figure 3 show $D_i[4]$. Note that there are three edges between each two cycle $C_6$ in this dendrimer.

**Theorem 4.** ([1])

(i) The order of $D_i[n]$ is $2^{n+1} - 9$.

(ii) The size of $D_i[n]$ is $9 \times 2^{n+1} - 12$.

Using Theorems 1 and 4 we have the following theorem for $N(D_i[n], x)$.

**Theorem 5.** The neighbourhood polynomial of $D_i[n]$ is:

$$N(D_i[n], x) = (6 \times 2^{n+1} - 6)(1 + x)^3 + (5 \times 2^{n+1} - 7)(1 + x)^2 + (1 + x)$$

$$- x(5 \times 2^{n+2} - 33) - (2^{n+4} - 10).$$
The neighbourhood polynomial of some nanostructures

Figure 3. The First Kind of Dendrimer of Generation 1–3 has Grown 4 Stages.

Proof. Let $n_i$ be the number of vertices of degree $i$ in $D_3[n]$, where $i = 1, 2, 3$. It is easy to see that $n_1 = 1$, $n_2 = 5 \times 2^{n+1} - 7$ and $n_3 = 6 \times 2^{n+1} - 6$. Now by Theorems 1 and 4 we have,

$$N(D_1[n], x) = n_1(1 + x) + n_2(1 + x)^2 + n_3(1 + x)^3 - x(9 \times 2^{n+2} - 24 - 2^{n+4} - 9)$$

$$- (2^{n+4} - 10)$$

$$= (6 \times 2^{n+1} - 6)(1 + x)^3 + (5 \times 2^{n+1} - 7)(1 + x)^2 + (1 + x) - x(5 \times 2^{n+2} - 33)$$

$$- (2^{n+4} - 10),$$

as desired.

REFERENCES