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Dendrimer Growth Based on Algebraic Multiplicity

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Abstract:-Matching Theory is one of the important concepts of Graph Theory. The matching theory concept has been studied in many areas. In this paper, the growth of Dendrimer through the maximum matching of an undirected sparse graph based on algebraic multiplicity of its eigenvalues is studied. The matrix adjacency of an undirected Dendrimer is a sparse graph and it is related to the exact controllability network for finding the maximum matched nodes and the corresponding match edges using the largest algebraic multiplicity of eigenvalues. The growth of the Dendrimer is expanded to nth- generation and the molecular formula is calculated. The process of finding the maximum matching starts initially from the core molecule and extended by adding branch molecule to the end groups at each stage of its growth forms the generation.

Keywords*:Dendrimer, Molecules, Dendrimer Nanostar, Generation Polyaryl ether*

1. Introduction

Matching theory is used not only to study the structure of a graph, it also has a relation with molecular graph which is an important branch of chemistry [3], [4]. In this graph theory, it deal with molecular graph constructed by molecules and molecular compounds where the nodes correspond to the atoms and lines correspond to the chemical bond between the atoms [5], [11]. All the molecules are added in layers to the molecule branch from the core molecule and it forms a spherical shape known as Dendrimers. The added layers are known as generation.

Dendrimers are hyperbranched with multivalent functional end groups and it is used in exploring drug delivery like anticancer, antiviral, antimalarial etc [7]. There are many different types of Dendrimers containing different core molecules for drug delivery. In this paper, we have consider Polyaryl ether Dendrimer Nanostar which is one of the fundamental objects of nanobiotechnology characterized in subatomic topology. It is a hyperbranched macromolecules. Nanostar Dendrimer has an extraordinary applications in gathering another piece of Nanostar Dendrimer [9]. Basically, it has two strategy to synthesis and control they are, divergent and convergent. Here we have considered divergent that start building from a central core out to the periphery in each step the monomer reacts with the endgroups to add a new layer. Then by each successive increase in layer increases the reactions. This work can be extended to some nanostar Dendrimer also to obtain the molecular weight at certain generation or the number of molecules used to react.

In an undirected graph the largest set of edges without common nodes is known as maximum matching [2]. Maximum matched nodes can be obtained using the largest algebraic multiplicity of its eigen values. The maximum matching of an undirected sparse graph is discussed under this topic separately. The basic idea of this method is obtained from the exact controllability for Sparse Network. The Definitions and working rules are discussed before proving it by theorem.

2. Preliminaries

2.1. Definition (Sparse graph)

A graph is called sparse if the total edges is very less than the actual number of edges. An undirected graph can have at most $\frac{n(n-1)}{2}$ edges.

2.2. Largest Algebraic Multiplicity

The minimum number of driver's node N_D of an undirected graph is obtained by the largest algebraic multiplicity $\delta(\lambda_j)$ of the Eigen value λ_j

$$N_D = \max\{\delta(\lambda_j)\}.$$

3. Maximum matching of an undirected Graph based on largest Algebraic Multiplicity

If $\delta(\lambda_j)$ is the algebraic multiplicity of the eigen values λ_j of A [1] which is the maximum number of identical eigen values and the sum of algebraic multiplicity $\delta(\lambda_j)$ of all identical eigen values is N

(i.e.) $\sum_{j=1}^{l} \delta(\lambda_j) = N$

For an undirected sparse graph the adjacency matrix will be symmetric and by performing fundamental column transformation the matrix can be reduced to a diagonal matrix or a triangular matrix. Then the maximum matching of the graph is obtained through the algebraic multiplicity of the eigen values λ_j of A .

3.1 Theorem

For all $n \geq 0$ the molecular formula $C_{C_n}O_{O_n}H_{H_n}$ of Polyaryl ether Dendrimer Nanostar sparse graph is obtained at each stage of its growth through maximum matching using largest algebraic multiplicity of its Eigen values.

Proof: A Polyaryl ether Dendrimer Nanostar [6] consist of three dimensional structure constructed by a core molecule denoted by G(0) figure.1. The core molecule of Polyaryl ether dendrimer Nanostar consist of four OH end group. The core molecule is considered as a molecular graph. The molecular graph is a sparse graph with 40 vertices and 43 edges.

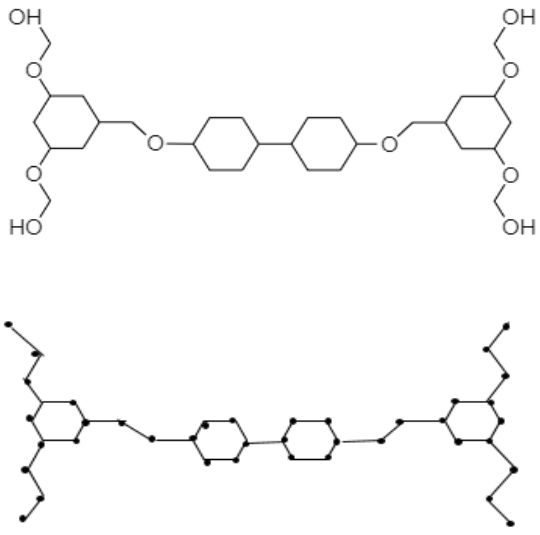

Figure.1. Core Molecule

The adjacency matrix of the sparse graph A ∈ R_{NXN} with V vertices and E edges is given by,

$$a_{ij} = \begin{cases} 1, & if\ (v_i, v_j) \in E \\ 0, & otherwise \end{cases}$$

By performing column transformation the adjacency matrix of the sparse graph with 40 columns and 40 rows will be reduced to triangular matrix. Then the eigen values $\lambda_1 = 1$ (34 times) and $\lambda_2 = 0$ (6 times) of the matrix is the leading diagonal elements of the triangular matrix.

3.1.1. Maximum Matching based on Largest Algebraic multiplicity

The algebraic multiplicity $\delta(\lambda_j)$ of the eigen values $\lambda_j$of A is the maximum number of identical eigen values. For $\lambda_1 = 1$, the algebraic multiplicity is $\delta(\lambda_1) = 34$ and for $\lambda_2 = 0$, the algebraic multiplicity is $\delta(\lambda_2) = 6$

Therefore, the maximum matching of the graph based on largest algebraic multiplicity is $\delta(\lambda_1) = 34$ and molecular formula is $C_{30}O_{10}H_4$.

3.1.2. Maximum matched edges

Maximum matched edges for the 34 matched vertices are 17 given in red lines. It is given in a way that no two edges share a node. Fig.2 shows the maximum matched graph for an undirected sparse graph with 40 vertices and 43 edges.

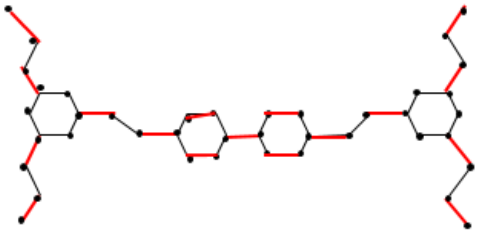

Figure.2. Maximum matched Core molecule

The branches which are added is denoted as H figure.3 reacts with OH of the core molecule to form first Generation Dendrimer [8].

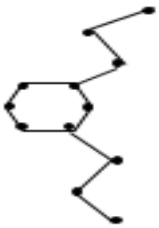

Figure.3. Added Branch (H)

Case (i): First Generation Dendrimer (G(1)- Polyaryl ether Dendrimer Nanostar)

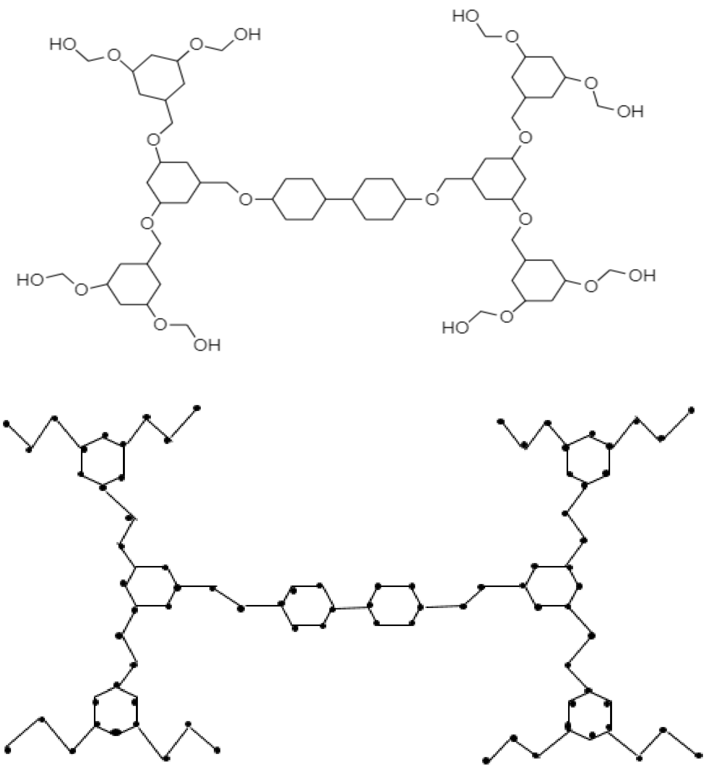

Figure.4. First Generation Polyaryl ether Dendrimer Nanostar

First generation Polyaryl (ether) Dendrimer Nanostar is constructed by the first additional branch from the core molecule. From figure.4 it is known that first generation Dendrimer has 8 endgroups (OH). Considering the Dendrimer as molecular graph (sparse graph) with 84 vertices and 91 edges.

Then by performing column transformation in the adjacency matrix of the sparse graph with 84 columns and 84 rows will reduce to a triangular matrix. Then the eigen values $\lambda_1 = 1$ (66 times) and $\lambda_2 = 0$ (18 times) of the matrix is the leading diagonal elements of the triangular matrix.

3.1.3. Maximum Matching based on Largest Algebraic multiplicity

The algebraic multiplicity $\delta(\lambda_j)$ of the eigen values $\lambda_j$of A is the maximum number of identical eigen values. For $\lambda_1 = 1$, the algebraic multiplicity is $\delta(\lambda_1) = 66$ and for $\lambda_2 = 0$, the algebraic multiplicity is $\delta(\lambda_2) = 18$

Therefore, the maximum matching of the graph based on largest algebraic multiplicity is $\delta(\lambda_1) = 66$ and the molecular formula is $C_{62}O_{22}H_{8}$.

3.1.4. Maximum matched edges

Maximum matched edges for the 66 matched vertices are 33 given in red lines. It is given in a way that no two edges share a node figure.5 shows the maximum matched graph for an undirected sparse graph with 84 vertices and 91

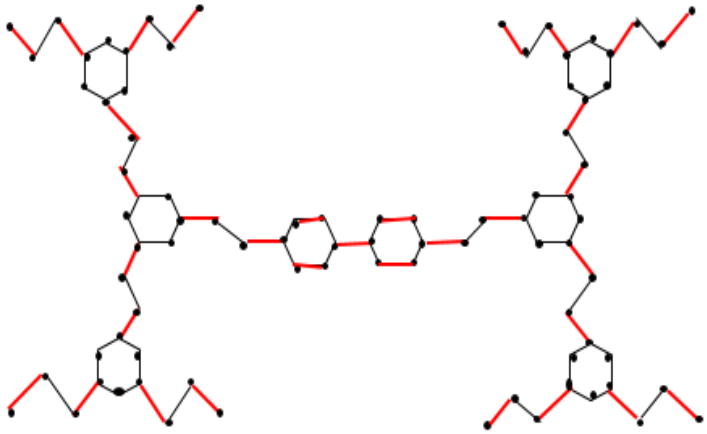

Figure.5. Maximum matched First generation Dendrimer

The added branches reacts with 8 endgroups (OH) of the first Generation to form second Generation Dendrimer.

Case (ii): Second Generation Dendrimer (G(2)- Polyaryl ether Dendrimer Nanostar)

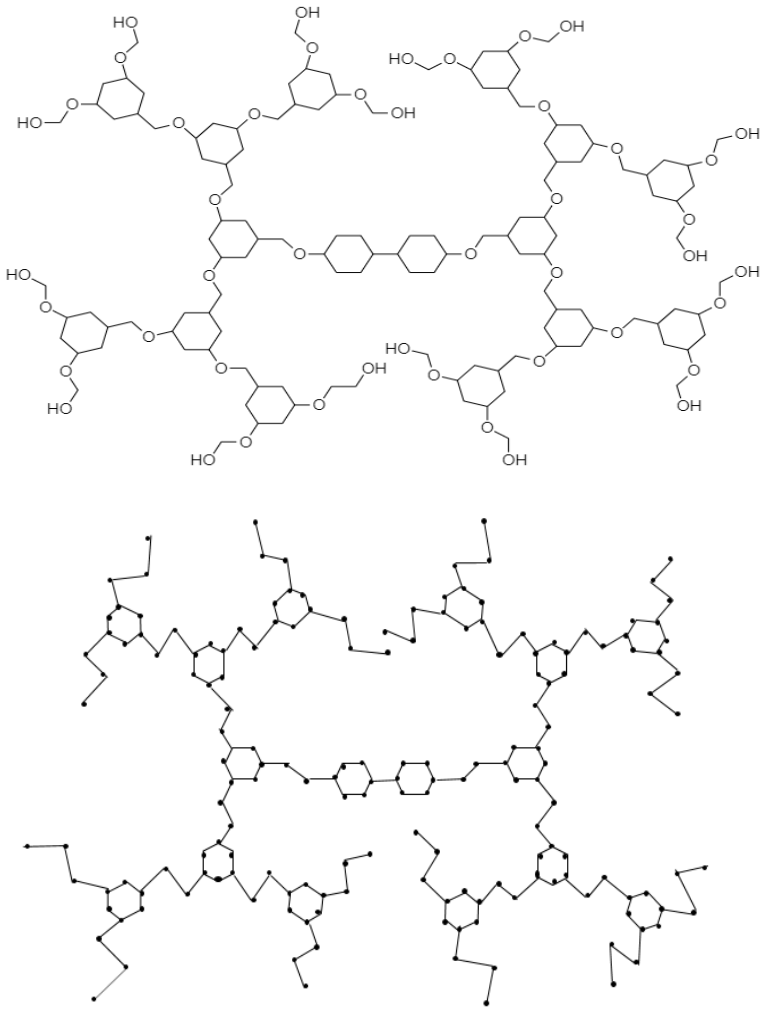

Figure.6. Second Generation Dendrimer

The second generation Polyaryl ether Dendrimer Nanostar is grown out of the first generation Dendrimer by the reaction of added branch with the 8 endgroups. From fig.5 it is known that second generation Dendrimer has 16 endgroups (OH)

Considering the Dendrimer as molecular graph (sparse graph) with 172 vertices and 187 edges. Then by performing column transformation in the adjacency matrix of the sparse graph with 172 columns and 172 rows it will reduce to a triangular matrix. Then the eigen values $\lambda_1 = 1$ (130 times) and $\lambda_2 = 0$ (42 times) of the matrix is the leading diagonal elements of the triangular matrix.

3.1.5. Maximum Matching based on Largest Algebraic multiplicity

The Algebraic multiplicity $\delta(\lambda_j)$ of the eigen values $\lambda_j$of A is the maximum number of identical eigen values. For $\lambda_1 = 1$, the Algebraic multiplicity is $\delta(\lambda_1) = 130$ and for $\lambda_2 = 0$, the algebraic multiplicity is $\delta(\lambda_2) = 42$

Therefore, the maximum matching of the graph based on largest algebraic multiplicity is $\delta(\lambda_1) = 130$ and the molecular formula is $C_{126}O_{46}H_{16}$.

3.1.6. Maximum matched edges

Maximum matched edges for the 130 matched vertices are 65 given in red lines. It is given in a way that no two edges share a node figure.7 shows the maximum matched graph for an undirected sparse graph with 172 vertices and 187 edges.

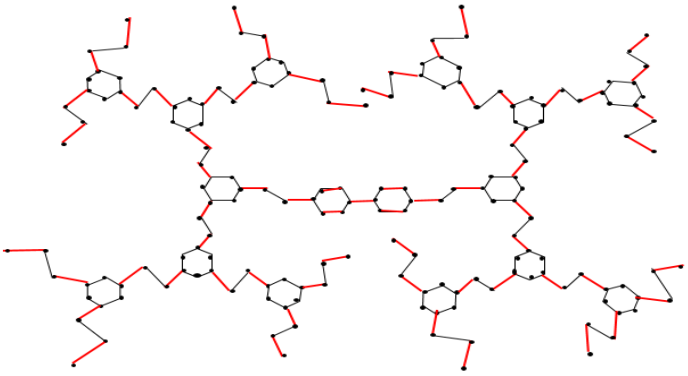

Figure.7. Maximum matched Second generation Dendrimer

Case (iii) In general, the n[th] Generation Polyaryl ether Dendrimer Nanostar (G(n)) is constructed from the core molecule G(0) by the added branch reacting with end groups $(OH)_n$ =4, 8, 16,32, . . .4$(2)^n$ for all $n \geq 0$ at each stage of its growth. Thus, the Polyaryl ether Dendrimer Nanostar forms a spherical shape with $n$added branches.

The molecular graph of n[th]- Generation Polyaryl ether Dendrimer Nanostar is considered as a sparse graph with vertices at each stage $V_n = 40, 84, 172, \ldots$ forms a recurrence relation

$V_n - 2V_{n-1} = 4$ with initial value $V_0 = 40$ for all $n \geq 0$ (1)

To find homogeneous solution, put $V_n = r^n$

$$r^n - 2(r^{n-1}) = 0$$

$$r^{n-1}(r-2) = 0$$

$$r^{n-1} \neq 0, \quad r = 2$$

The Homogeneous solution is given by, $V_n^{(h)} = k_1(2)^n$ (2)

To find Particular solution, consider $f(n) = 4(1)^n$ then $V_n^{(p)} = A_0(1)^n$ (3)

The General solution is, $V_n = V_n^{(h)} + V_n^{(p)} = k_1(2)^n + A_0(1)^n$ (4)

Substituting (4) in (1) and equating the like coefficients on both sides gives,

$$k_1(2)^n + A_0(1)^n - 2(k_1(2)^{n-1} + A_0(1)^{n-1}) = 4(1)^n$$

$$A_0 = -4$$

$V_n = k_1(2)^n - 4(1)^n$ (5)

Given $V_0 = 40$

(i.e.) for n=0, $V_0 = k_1(2)^0 - 4(1)^0$

$$40 = k_1 - 4$$

$$k_1 = 44$$

Therefore, in general the number of vertices is, $V_n = 44(2)^n - 4(1)^n$ for all $n \geq 0$.

Similarly, the number of edges of the graph at each stage $E_n = 43, 91, 187, \ldots$ is formed as a recurrence relation, $E_n - 2E_{n-1} = 5$ with initial value $E_0 = 43$ for all $n \geq 0$ (6)

Solving the recurrence relation (6) gives, the number of edges in general as $E_n = 48(2)^n - 5(1)^n$ for all $n \geq 0$

Also the growth of the Dendrimer at each stage is obtained by maximum matching based on largest algebraic multiplicity $\delta_n(\lambda_1) = 34, 66, 130, \ldots$ formed as a recurrence relation

$\delta_n(\lambda_1) - 2\delta_{n-1}(\lambda_1) = -2$ with initial value $\delta_0(\lambda_1) = 34$ for all $n \geq 0$ (7)

Solving the recurrence relation (7) gives, the number of matched nodes in general as,

$\delta_n(\lambda_1) = 32(2)^n + 2(1)^n$. The unmatched nodes is, $\delta_n(\lambda_2) = V_n - \delta_n(\lambda_1)$ for all $n \geq 0$.

Therefore, the molecular formula at n[th]- Generation Dendrimer is $C_{C_n}O_{O_n}H_{H_n}$, $n \geq 0$

$$C_n = \delta_n(\lambda_1) - 4$$

$$O_n = \delta_n(\lambda_1) - C_n + \delta_n(\lambda_2)$$

$$H_n = (OH)_n$$

4. Conclusion

In this topic the new method is for obtaining maximum matched nodes of an undirected Dendrimer sparse graph using largest algebraic multiplicity of eigen values which has a relation with exact controllability network is proved through adjacency matrix of its molecular graph. The new method is proved by a theorem for constructing n[th] - Generation Polyaryl ether Dendrimer Nanostar through matching based on largest algebraic multiplicity of its eigen values. The algebraic multiplicity of core molecule, first and second generation is explained with the number of end groups (OH), Carbon(C) and Oxygen (O) presented and it is extended to n[th] – Generation by forming a recurrence relation. From the solution of recurrence relation the number of vertices, edges, matched nodes etc. can be calculated for all $n \geq 0$ and the maximum matched nodes at each generation is obtained from the largest Algebraic multiplicity of its eigen values also the molecular formula is calculated. In future, this concept can be expanded for some other Dendrimer graph.

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