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Distance and Detour Matrices of an Infinite Class of Dendrimer Nanostars

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Abstract

Let G be a graph. The Wiener index of G is defined as the sum of all pairwise distances of vertices of the graph. Suppose DD = [dd_{ij}] is a matrix such that dd_{ij} is the length of the longest path between vertices i and j. The detour index of G is the sum of all pairwise longest distances of vertices of G. The aim of this article is to compute the Wiener and detour indices of an infinite class of dendrimer nanostars.

1. Introduction

A graph is a pair G = (V(G) , E(G)) of two non-empty sets V = V(G) and E = E(G) such that $E \subseteq V \times V$. The elements of V and E are called vertices and edges of G, respectively. It is possible to associate a graph to each molecule, named molecular or chemical graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory. In this graph atoms constitute the set of vertices and bonds between atoms are edges of the graph. A topological index is a numeric quantity derived from the structural graph of a molecule. It must be a graph invariant. Obviously, the number of vertices and the number of edges of a graph G are topological indices of G. The first non-trivial topological index was proposed in 1947 by the chemist Harold Wiener [1]. This topological index is defined as the sum of all distances between vertices of the graph.

Let G be a graph with V(G) = {x_1, x_2, …, x_n}. For vertices $u,v \in V(G)$, d(u,v) denotes the length of a minimal path connecting u and v. The distance matrix of G is defined as D(G) = [d_{ij}], where $d_{ij} = d(x_i,x_j)$. The detour matrix DD = [dd_{ij}] can be defined for G with entries $dd_{ii} = 0$ and dd_{ij}, $i \neq j$, as the maximum distance between vertices v_i and v_j. If a graph G is given, the matrix D can be reproduced. The detour matrix was introduced in graph theory some time ago by F. Harary for describing the connectivity in directed graphs [2]. The detour matrix, in contrast to the distance matrix records the length of the longest distance between each pair of vertices. The detour index, defined as the sum of entries in matrix, has recently received some attention in the chemical literature, [3]. We encourage the reader to consult papers [4–10] for background material as well as basic computational techniques.

In some research papers [11–17], Diudea and his co–authors proposed the problem of computing topological indices of nanostructure materials. They computed the Wiener index of some nanotubes and tori. Then Ashrafi and his co-authors [18–24] continued this program to compute the Wiener, PI and Szeged indices of some classes of nanotubes and tori. In this article, the distance and detour matrices of an infinite class of nanostar dendrimers are computed. Our notation is standard and is taken mainly from [25, 26].

2. Main Results

Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention. The topological study of these macromolecules is a new subject of research [27,28]. The aim of this section is to calculate the distance and detour matrices of the nanostar dendrimer NS[n], Figure 1. We also calculate the Wiener and detour indices of these macromolecules.

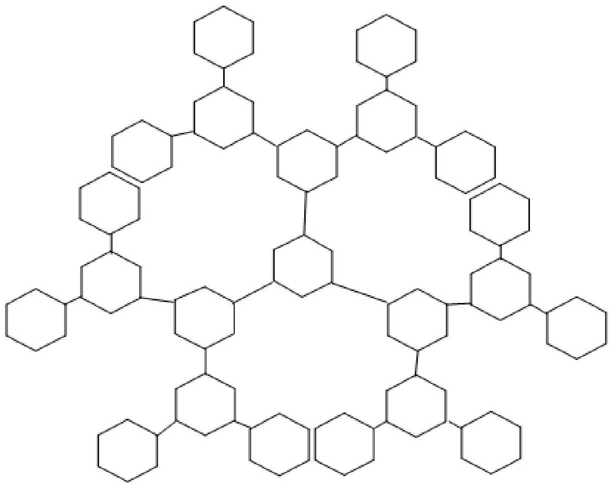

Figure 1. The Nanostar Dendrimer NS[n=2].

We first define the following three matrices which are important for calculating the Wiener matrix of NS[n].

$$B_{Win}=\begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix} \qquad A_{Win}=\begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 3 & 4 & 5 & 4 & 3 \\ 3 & 4 & 5 & 6 & 5 & 4 \\ 2 & 3 & 4 & 5 & 4 & 3 \\ 1 & 2 & 3 & 4 & 3 & 2 \end{bmatrix} \qquad J_i=\begin{bmatrix} i & i & i & i & i & i \\ i & i & i & i & i & i \\ i & i & i & i & i & i \\ i & i & i & i & i & i \\ i & i & i & i & i & i \\ i & i & i & i & i & i \end{bmatrix}.$$

Here the matrices A_{Win} and B_{Win} are distance matrices of a hexagon and two hexagons with a common vertex, respectively. Suppose X and Y are two hexagons. Then d(X,Y) denotes the length of a minimal path connecting a vertex of X to a vertex of Y and [X,Y] denotes a block of distance matrix containing distances between vertices of X and Y. Then $[X,Y] = A_{Win} + J_i$, where $d(X,Y) = i$. For example the distance matrix of the nanostar dendrimer NS[1], is as follows:

	0	**1**	**2**	**3**	**1_1**	**1_2**	**2_1**	**2_2**	**3_1**	**3_2**
0	B	$A+J_1$	$A+J_1$	$A+J_1$	$A+J_4$	$A+J_4$	$A+J_4$	$A+J_4$	$A+J_4$	$A+J_4$
1	$A+J_1$	B	$A+J_4$	$A+J_4$	$A+J_1$	$A+J_1$	$A+J_7$	$A+J_7$	$A+J_7$	$A+J_7$
2	$A+J_1$	$A+J_4$	B	$A+J_4$	$A+J_7$	$A+J_7$	$A+J_1$	$A+J_1$	$A+J_7$	$A+J_7$
3	$A+J_1$	$A+J_4$	$A+J_4$	B	$A+J_7$	$A+J_7$	$A+J_7$	$A+J_7$	$A+J_1$	$A+J_1$
1_1	$A+J_4$	$A+J_1$	$A+J_7$	$A+J_7$	B	$A+J_4$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$
1_2	$A+J_4$	$A+J_1$	$A+J_7$	$A+J_7$	$A+J_4$	B	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$
2_1	$A+J_4$	$A+J_7$	$A+J_1$	$A+J_7$	$A+J_{10}$	$A+J_{10}$	B	$A+J_4$	$A+J_{10}$	$A+J_{10}$
2_2	$A+J_4$	$A+J_7$	$A+J_1$	$A+J_7$	$A+J_{10}$	$A+J_{10}$	$A+J_4$	B	$A+J_{10}$	$A+J_{10}$
3_1	$A+J_4$	$A+J_7$	$A+J_1$	$A+J_1$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$	B	$A+J_4$
3_2	$A+J_4$	$A+J_7$	$A+J_7$	$A+J_1$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$	$A+J_{10}$	$A+J_4$	B

Theorem 1. The Wiener index of NS[n] is computed as follows:

$$Win(NS[n]) = 486(2n-1)2^{2n+2} + 1755\cdot 2^{n+1} - 270.$$

Proof: It is clear that $|V(NS[n])| = 18.2^{n+1} - 12$ and $|E(NS[n])| = 21.2^{n+1} - 15$. Consider 6×6 matrices A, B, J_1, J_4, …, J_{6n+1}, J_{6n+4}. In the following table the number of appearance of these matrices in the distance matrix of NS[n] are computed as follows:

B	$(3.2^{n+1}-2)$
A	$(9.2^{2n+1}-15.2^{n}+3)$
J_1	$3+3(2^{n+1}-2)$
J_4	$3+9(2^{n}-1)$
J_7	$12+24(2^{n-1}-1)$
J_{10}	$12+36(2^{n-1}-1)$
J_{13}	$[48+96(2^{n-2}-1)$
⋮	⋮
J_{6n+1}	12.2^{2n-2}
J_{6n+4}	12.2^{2n-2}

Therefore,

$$Win(G) = [\sum b_{ij}].[3.2^{n}-1] + [\sum a_{ij}].[9.2^{2n+1} - 15.2^{n}+3]$$

$$+ 4.36[3+9(.2^{n}-1)] + 36\sum_{i=1}^{n}[12.2^{2i-2}+12.2^{2i-1}(2^{n-i}-1)](6i+1)$$

$$+ 36\sum_{i=1}^{n}[12.2^{2i-2}+12.2^{2i-2}.3(\frac{1}{2^{i+1}}.2^{n+1}-1)](6i+4) + 36[3+3(2^{n+1}-2)]$$

$$= 486(2n-1)2^{2n+2} + 17552^{n+1} - 270.$$ ■

The Wiener/Hosoya polynomial of a graph G is defined as $W(G,x) = \sum_{\{x,y\}} x^{d(x,y)}$. From the proof of Theorem 1, it is possible to calculate the Wiener polynomial of these dendrimers. We have:

Theorem 2. Suppose $A_i = 12.2^{2i-2}(2^{n-i+1} - 1)$, $B_i = [12.2^{2i-2}(3.2^{n-i}-2)]$, $C_i = [12.2^{2i}(2^{n-i}-1)]$ and $D_i = 12.2^{2i}(3.2^{n-i-1}-2)$. Then $W(NS_1[n],x) = [21.2^{n+1}-15]x^1 + [30.2^{n+1}-24]x^2 + [33.2^{n+1}-30]x^3 + [69.2^{n}-36]x^4 + [42.2^{n+1}-48]x^5 + [48.2^{n+1}-60]x^6 + [54.2^{n+1} - 75]x^7 + [60.2^{n+1} - 96]x^8 + [66.2^{n+1} - 120]x^9 + [147.2n - 150]x^{10}$

$$+\sum_{i=1}^{n}[8A_i + 4B_i + (4A_i+8B_i)x + (A_i+10B_i+C_i)x^2 + (8B_i+4C_i)x^3 + (4B_i+8C_i)x^4 + (3B_i+7C_i+D_i)x^5]x^{6i+5}.$$

We now calculate the detour index of this dendrimer nanostar. To do this, we apply a similar argument as above. We first calculate the detour matrix of the graph under consideration, see Figure 2. In what follows, the detour matrix of the nanostar dendrimer NS[1] is computed as follows:

	0	1	2	3	1_1	1_2	2_1	2_2	3_1	3_2
0	B	$A+J_1$	$A+J_1$	$A+J_1$	$A+J_6$	$A+J_6$	$A+J_6$	$A+J_6$	$A+J_6$	$A+J_6$
1	$A+J_1$	B	$A+J_6$	$A+J_6$	$A+J_1$	$A+J_1$	$A+J_{11}$	$A+J_{11}$	$A+J_{11}$	$A+J_{11}$
2	$A+J_1$	$A+J_6$	B	$A+J_6$	$A+J_{11}$	$A+J_{11}$	$A+J_1$	$A+J_1$	$A+J_{11}$	$A+J_{11}$
3	$A+J_1$	$A+J_6$	$A+J_6$	B	$A+J_{11}$	$A+J_{11}$	$A+J_{11}$	$A+J_{11}$	$A+J_1$	$A+J_1$
1_1	$A+J_6$	$A+J_1$	$A+J_{11}$	$A+J_{11}$	B	$A+J_6$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$
1_2	$A+J_6$	$A+J_1$	$A+J_{11}$	$A+J_{11}$	$A+J_6$	B	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$
2_1	$A+J_6$	$A+J_{11}$	$A+J_1$	$A+J_{11}$	$A+J_{16}$	$A+J_{16}$	B	$A+J_6$	$A+J_{16}$	$A+J_{16}$
2_2	$A+J_6$	$A+J_{11}$	$A+J_1$	$A+J_{11}$	$A+J_{16}$	$A+J_{16}$	$A+J_6$	B	$A+J_{16}$	$A+J_{16}$
3_1	$A+J_6$	$A+J_{11}$	$A+J_{11}$	$A+J_1$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$	B	$A+J_6$
3_2	$A+J_6$	$A+J_{11}$	$A+J_{11}$	$A+J_1$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$	$A+J_{16}$	$A+J_6$	B

Theorem 3. $dd(NS[n]) = 2619.2^{n+1} + (1620n - 594)2^{2n+2} - 342$.

Proof. We first define the following three matrices which are important for calculating the Wiener matrix of NS[n].

$$B_{Det}=\begin{bmatrix} 0 & 5 & 4 & 3 & 4 & 5 \\ 5 & 0 & 5 & 4 & 3 & 4 \\ 4 & 5 & 0 & 5 & 4 & 3 \\ 3 & 4 & 5 & 0 & 5 & 4 \\ 4 & 3 & 4 & 5 & 0 & 5 \\ 5 & 4 & 3 & 4 & 5 & 0 \end{bmatrix} \quad \text{and} \quad A_{Det}=\begin{bmatrix} 0 & 5 & 4 & 3 & 4 & 5 \\ 5 & 10 & 9 & 8 & 9 & 10 \\ 4 & 9 & 8 & 7 & 8 & 9 \\ 3 & 8 & 7 & 6 & 7 & 8 \\ 4 & 9 & 8 & 7 & 8 & 9 \\ 5 & 10 & 9 & 8 & 9 & 10 \end{bmatrix}$$

We consider 6 × 6 matrices A_{Det}, B_{Det}, J_1, J_6, …, J_{10n+1}, J_{10n+6}. In the following table the number of appearance of these matrices in the detour matrix of NS[n] are computed as follows:

B_{Det}	$(3.2^{n+1}-2)$	J_{21}	$[48+96(2^{n-2}-1)$
A_{Det}	$(9.2^{2n+1}-15.2^n+3)$	$\vdots$	$\vdots$
J_1	$3+3(2^{n+1}-2)$	J_{10n+1}	12.2^{2n-2}
J_6	$3+9(2^n-1)$	J_{10n+6}	12.2^{2n-2}
J_{11}	$12+24(2^{n-1}-1)$		
J_{16}	$12+36(2^{n-1}-1)$		

Therefore using some tedious calculations, we have $dd(NS[n]) = 2619.2^{n+1} + (1620n – 594)2^{2n+2} – 342$. ∎

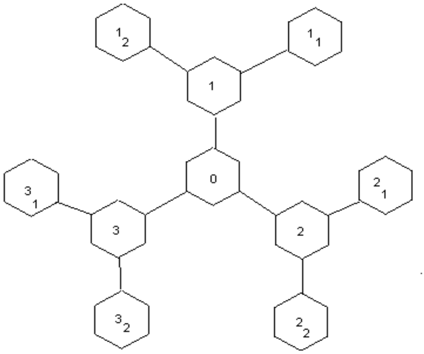

Figure 2. The Hexagon Labeled Nanostar Dendrimer NS[1].

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