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Research Article

Ashwini Index of a Graph

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Abstract

Motivated by the terminal Wiener index, we define the Ashwini index $\mathcal{A}$ of trees as

$$\begin{aligned}\mathcal{A}(T) &= \sum_{1\le i<j\le n} d_T(v_i,v_j)[deg_T(N(u_i)) \\ &+ deg_T(N(v_j))],\end{aligned}$$

where $d_T(v_i,v_j)$ is the distance between the vertices $v_i, v_j \in V(T)$, is equal to the length of the shortest path starting at v_i and ending at v_j and $deg_T(N(v))$ is the cardinality of $deg_T(u)$, where $uv \in E(T)$. In this paper, trees with minimum and maximum $\mathcal{A}$ are characterized and the expressions for the Ashwini index are obtained for detour saturated trees $T_3(n)$, $T_4(n)$ as well as a class of Dendrimers D_h.

Keywords : Wiener index; terminal Wiener index, Ashwini index..

1 Introduction

LEt $G = (V, E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m, thus $|V(G)|= n$ and $|E(G)|= m$. By the open neighborhood of a vertex v of G we mean the set $N_G(v) = \{u \in V(G) : uv \in E(G)\}$. The degree of a vertex v, denoted by $deg(v)$, is the cardinality of its open neighborhood. The neighborhood degree of a pendant vertex v, $deg_G(N(v))$ is the cardinality of $deg_G(u)$, where $uv \in E(G)$. The distance between the vertices $v_i, v_j \in V(G)$, is equal to the length of the shortest path starting at v_i and ending at v_j, and will be denoted by $d_G(v_i, v_j)$. For undefined terminologies we refer the reader to [15].

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The oldest molecular index is the one put forward in 1947 by H. Wiener [33], nowadays referred to as the Wiener index and denoted by W. It is defined as the sum of distance between all pairs of vertices of a graph.

$$\begin{aligned}W(G) &= \sum_{\{u,v\subseteq V(G)\}} d_G(u,v) \\ &= \sum_{1\le i<j\le n} d_G(u,v).\end{aligned}$$

For details on its chemical applications and mathematical properties one may refer to [5, 6, 7, 9, 10, 12, 13, 14, 23, 18, 19, 20, 21, 22] and the references cited therein.

If G has k-pendent vertices labeled by $v_1, v_2 \cdots v_k$, then its terminal distance matrix is the square matrix of order k whose (i, j)-th entry is $d_G(v_i, v_j)$. Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic codes [17, 28, 29].

The terminal Wiener index $TW(G)$ of a connected graph G is defined as the sum of the distances between all pairs of its pendent vertices. Thus if $V_T = \{v_1, v_2, \cdots, v_k\}$ is the set of all pendent vertices of G, then

$$\begin{aligned} TW(G) &= \sum_{\{u,v \subseteq V_T(G)\}} d_G(u,v) \\ &= \sum_{1 \le i < j \le k} d_G(u,v) \end{aligned}$$

This distance-based molecular structure descriptor was recently put forward by Gutman et al.[11].

Motivated by the previous researches on terminal Wiener index and its chemical applications [16, 27, 34], we now define the Ashwini index $\mathcal{A}(\mathcal{T})$ of a tree T as follows.

$$\begin{aligned} \mathcal{A}(T) &= \sum_{1 \le i < j \le n} d_T(v_i, v_j)[deg_T(N(u_i)) \\ &+ deg_T(N(v_j))]. \end{aligned} \tag{1.1}$$

In fact, one can rewrite the Ashwini index as

$$\begin{aligned} \mathcal{A}(T) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_T(v_i, v_j)[deg_T(N(v_i)) \\ &+ deg_T(N(v_j))] \end{aligned}$$

As before, in Eq. 1.1 it is assumed that the tree has n vertices of which k vertices, labeled by $v_1, v_2, \cdots, v_k$, are pendent. In order to illustrate (1.1), we show that the Ashwini index is computed for a molecular graph of 3-methylpentane depicted in Fig. 1.

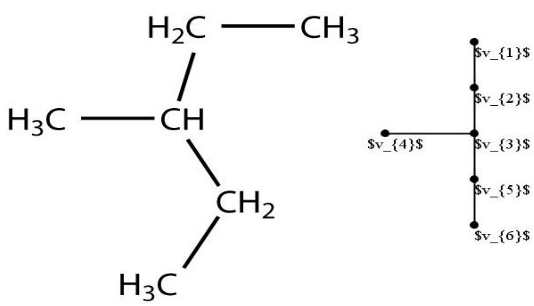

Figure 1: 3-methylpentane and its molecular graph.

The tree T, representing the molecular graph of 3-methylpentane has three pendant vertices v_1, v_4 and v_6. Further, their respective neighborhood

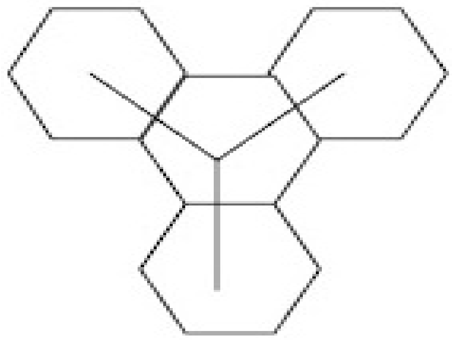

Figure 2: Cata-condensed and its dualist graph.

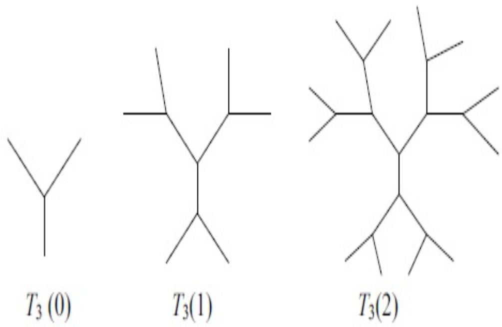

Figure 3: Detour saturated tree for $T_3(0)$, $T_3(1)$ and $T_3(2)$

degrees are $deg_T(N(v_1)) = 2$, $deg_T(N(v_4)) = 3$ and $deg_T(N(v_6)) = 2$. Therefore the summation on the right-hand side of (1.1) contains $\frac{3(3-1)}{2} = 3$ terms and we have:

$$\begin{aligned} \mathcal{A}(T) &= d(v_1, v_4 \setminus T)[deg_T(N(v_1)) + deg_T(N(v_4))] \\ &+ d(v_1, v_6 \setminus T)[deg_T(N(v_1)) + deg_T(N(v_6))] \\ &+ d(v_4, v_6 \setminus T)[deg_T(N(v_4)) + deg_T(N(v_6))] \\ &= 3(2+3) + 4(2+2) + 3(3+2) \\ &= 46. \end{aligned}$$

2 Trees with minimal and maximal Ashwini index

When a new topological index is introduced, one of the first question that need to be answered is for which (molecule) graphs this index assumes minimal and maximal values. Therefore, we characterize trees with minimum and maximum Ashwini index values. For any n-vertex tree T, $4(n-1) \le \mathcal{A}(T) \le 2(n-1)^2(n-2)$. Equality of lower bound holds if and only if $T \cong P_n$ and

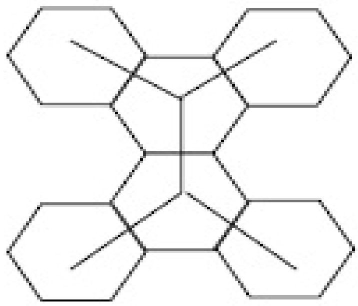

Figure 4: Detour saturated tree of double claw

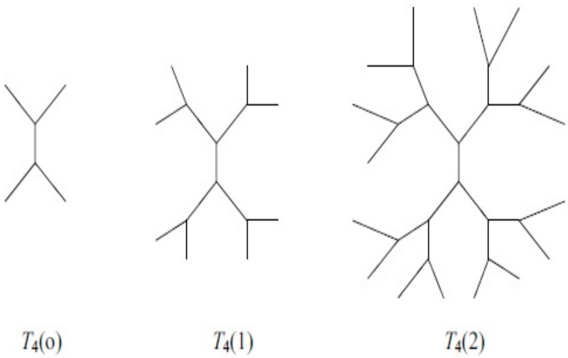

Figure 5: Detour saturated tree for $T_4(0)$, $T_4(1)$ and $T_4(2)$.

the equality of upper bound holds if and only if $T \cong S_n$.

Proof. We prove this theorem by considering the following cases.

Case 1. First consider the lower bound for Ashwini index. Let us consider the minimum possibility of any n-vertex tree T such that Ashwini index exists. Let $u, v \in V(T)$ such that $d(u, v)_T \leq n-1$ and $deg_T(N(u)) = 2 = deg_T(N(v))$. Now employing (1.1), we get $4(n-1) \leq \mathcal{A}(T)$.

Now for the equality of lower bound, consider the case path P_n, there two pendant vertices v_1 and v_2 respectively, such that $deg_{P_n}(N(v_1)) = 2$ and $deg_{P_n}(N(v_n)) = 2$. Now employing (1.1), to the path P_n, we get $\mathcal{A}(P_n) = 4(n-1)$.

Conversely, if $\mathcal{A}(G) = 4(n-1)$ and $G \neq P_n$, then G contains a pair of vertices $v_i, v_j \in V(G)$ such that $d_G(v_i, v_j) < n-1$. Hence employing (1.1) to G we get $\mathcal{A}(G) < 4(n-1)$, a contradiction.

Case 2. Now for the upper bound, let us consider a n-vertex tree T together with maximum number of pendant vertices and corresponding max-

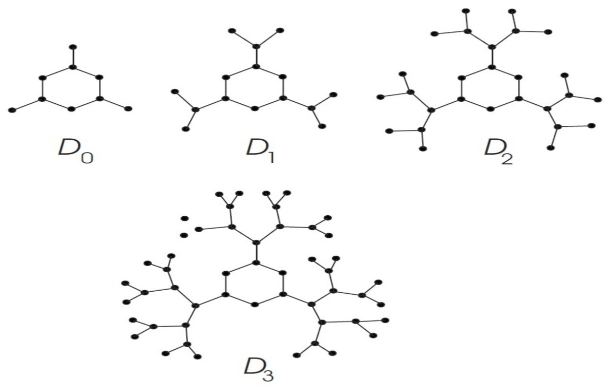

Figure 6

imum neighborhood degrees. We know that for any n-vertex tree T, there exists at most $n-1$ pendant vertices and maximum neighborhood degree $n-1$. Also by (1.1), we can see that every pendant vertex counts at most $(n-2)$ times together with corresponding neighborhood degree. Hence by enumeration techniques, we could see that $\mathcal{A}(T) \leq 2(n-1)^2(n-2)$.

Now for the equality of upper bound, in the case of the star S_n, there are $n-1$ pendant vertices, and the neighborhood degree of each pendant vertex is $(n-1)$. Therefore $\mathcal{A}(S_n) = 2(n-1)^2(n-2)$.

Conversely, if $\mathcal{A}(G) = 2(n-1)^2(n-2)$ and $G \neq S_n$ then G contains a pair of vertices $v_i, v_j \in V(G)$ such that $d_G(v_i, v_j) \geq 3$. Hence employing (1.1) to G we get $\mathcal{A}(G) < 2(n-1)^2(n-2)$, a contradiction. Thus, the path is the tree with minimal Ashwini index and the star is the tree with maximal Ashwini index.

3 Ashwini index of detour saturated trees

A graph is said to be detour–saturated if the addition of any edge results in an increased greatest path length [24]. A benzenoid graph is called catacondensed if its characteristic graph is a tree. The characteristic graph of a hexagonal chain is isomorphic to the path [8]. In the new definition [1], Cata-condensed species have dualist graphs, which are detour saturated trees, while those Peri-condensed species contain at least one circuit. The dualist graph of Cata-condensed species is a claw. The claw is the detour-saturated tree T_3, which is depicted in Fig. 2. The general detour-saturated tree $T_3(n)$ [2] for odd $n \geq 5$ is obtained from $T_3(n-1)$ by attaching two new leave to each of the old leaves. The Ashwini index of detour saturated tree $T_3(n)$ is

$$\mathcal{A}(T_3(n)) = 18 \cdot 2^{n-1}\Bigg[\sum_{i=1}^{n+1} i2^i + (n+1)2^{n+1}\Bigg] \tag{3.2}$$

Proof. Let n be the number of steps in the formation of detour trees. Then claerly, $T_3(n)$ contains $3{\cdot}2^n$ leaves. Further note that the neighborhood degree of each leaf is 3. Therefore by the definition of Ashwini index

$$\mathcal{A}(G) = \frac{1}{2}\sum_{i=1}^{3\cdot 2^n}\sum_{j=1}^{3\cdot 2^n} d(v_i,v_j)[deg_G(N(v_i)) + deg_G(N(v_j))].$$

$\mathcal{A}(T_3(0)) = \frac{1}{2}3[2(6)+2(6)] = \frac{1}{2}18[4]$

$\mathcal{A}(T_3(1)) = \frac{1}{2}3{\cdot}2^1[2(6)+4(6)+4(6)+4(6)+4(6)] = \frac{1}{2}18\cdot 2^1[2+(4+4)+(4+4)]$

$\mathcal{A}(T_3(2)) = \frac{1}{2}18\cdot 2^2[2+(4+4)+(6+6+6+6)+(6+6+6+6)]$

$\mathcal{A}(T_3(3)) = \frac{1}{2}18\cdot 2^3\Big[2+(4+4)+(6+6+6+6)+\underbrace{8+8+\cdots+8}_{8times}+\underbrace{8+8+\cdots+8}_{8times}\Big]$ and so on.

With this background now, we are able to prove (3.2) by mathematical induction.

$\mathcal{A}(T_3(0)) = \frac{3\cdot 2^0}{2}[2(2(6))] = 36$, is true for $n=0$.

$\mathcal{A}(T_3(1)) = \frac{3\cdot 2}{2}[2(6)+2(2^2)(6)] + \frac{3\cdot 2}{2}[2(2^2)(6)] = 324$ is true for $n=1$.

Assume the result is true for $n = k-1$. Then

$\mathcal{A}(T_3(k-1)) = \frac{18\cdot 2^{k-1}}{2}[2+2(2^2)+3(2^3)+\cdots+k2^k] + \frac{18\cdot 2^{k-1}}{2}[k2^k]$

$\mathcal{A}(T_3(k-1)) = \frac{18\cdot 2^{k-1}}{2}\Big[\sum_{i=1}^{k} i2^i\Big] + \frac{18\cdot 2^{k-1}}{2}(k)2^k$

To prove $\mathcal{A}(T_3(k))$ is true for $n=k$

$$\begin{aligned}\mathcal{A}(T_3(k)) &= \frac{18\cdot 2^{k-1}}{2}\Bigg[\sum_{i=1}^{k} i2^i\Bigg] \\ &+ \frac{18\cdot 2^{k-1}}{2}\Big[(k+1)2^{k+1}\Big] \\ &+ \frac{18\cdot 2^{k}}{2}(k+1)2^{k+1} \\ &= \frac{18\cdot 2^{k}}{2}\Bigg[\sum_{i=1}^{k+1} i2^i\Bigg] \\ &+ \frac{18\cdot 2^{k}}{2}(k+1)2^{k+1} \\ &= 18\cdot 2^{k-1}\Bigg[\sum_{i=1}^{k+1} i2^i \\ &+ (k+1)2^{k+1}\Bigg] \\ &= 18\cdot 2^{n-1}\Bigg[\sum_{i=1}^{n+1} i2^i \\ &+ (n+1)2^{n+1}\Bigg].\end{aligned}$$

Double claw can be connected to the species in the form of Polyhexes. Double claw is denoted by $T_4(n)$ and can be constructed inductively by adding two new leaves at each of the old leaves of $T_4(n-1)$, $n \geq 6$. The Ashwini index of detour saturated tree $T_4(n)$ is

$$\mathcal{A}(T_4(n)) = 6\cdot 2^{n+1}\Bigg[\sum_{i=1}^{n+1} i2^i + (2n+3)2^{n+1}\Bigg]. \tag{3.3}$$

Proof. Let n be the number of steps in the formation of detour trees. Clearly the detour saturated tree $T_4(n)$ has 2^{n+2} leaves and note that the neighborhood degree of each leaf is 3. Hence, by the definition of Ashwini index,

$$\mathcal{A}(G) = \frac{1}{2}\sum_{i=1}^{2^{n+2}}\sum_{j=1}^{2^{n+2}} d(v_i,v_j)[deg_G(N(v_i)) + deg_G(N(v_j))].$$

$$\begin{aligned}
\mathcal{A}(T_4(0)) &= \frac{1}{2}\Big\{4\cdot 2^0[2(6)+(3(6)\\
&+ 3(6))]\Big\}\\
\mathcal{A}(T_4(1)) &= \frac{1}{2}\Big\{(4\cdot 2)[2(6)+(4+4)(6)\\
&+ (5+5+5+5)(6)]\Big\}\\
\mathcal{A}(T_4(2)) &= \frac{1}{2}\Big\{(4\cdot 2^2)[2(6)+(4+4)(6)\\
&+ (6+6+6+6)(6)\\
&+ \underbrace{(7+7+\cdots+7)}_{8times}(6)]\Big\}\\
\mathcal{A}(T_4(3)) &= \frac{1}{2}\Big\{(4\cdot 2^3)\Big[2(6)+(4+4)(6)\\
&+ (6+6+6+6)(6)\\
&+ \underbrace{(8+8+\cdots+8)(6)}_{8times}\\
&+ \underbrace{(9+9+\cdots+9)}_{16times}(6)\Big]\Big\}
\end{aligned}$$

and so on. With this background now we are in a position to prove (3.3).

$\mathcal{A}(T_4)(0) = \frac{4\cdot 2^0}{2}\Big[2(2^0)+(2+2)+(1+1)\Big](6) = 96$ is true for $n=0$.

$\mathcal{A}(T_4)(1) = \frac{4\cdot 2^1}{2}\Big[2 + 2(2^2) + 2(2^2) + 2(2^2) + 2(2)\Big](6) = 720$, is true for $n=1$.

Now assume the result is true for $n = k-1$.

$\mathcal{A}(T_4)(k-1) = \frac{4\cdot 2^{k-1}}{2}\Big\{[2+2(2^2)+3(2^3)+\cdots+ k(2^k)] + k(2^k) + k(2^k) + 2^k\Big\}$

$\mathcal{A}(T_4)(k-1) = \frac{4\cdot 2^{k-1}}{2}\Big\{\sum_{i=1}^{k} i2^i + k(2^k) + k(2^k) + 2^k\Big\}.$

To prove the result is true for $n=k$

$$\begin{aligned}
\mathcal{A}(T_4)(k) &= \frac{4\cdot 2^k}{2}\Big\{[2+2(2^2)+3(2^3)\cdots+k(2^k)\\
&+ (k+1)2^{k+1}](6)\\
&+ [((k+1)(2^{k+1}))+((k+1)(2^{k+1}))\\
&+ 2^{k+1}](6)\Big\}\\
&= \frac{4\cdot 2^k}{2}\Big\{\sum_{i=1}^{k+1} i2^i + ((k+1)(2^{k+1}))\\
&+ ((k+1)(2^{k+1}))+2^{k+1}\Big\}(6)\\
&= 6\cdot 2^{k+1}\Big[\sum_{i=1}^{k+1} i2^i + (2k+3)2^{k+1}\Big]\\
&= 6\cdot 2^{n+1}\Big[\sum_{i=1}^{n+1} i2^i + (2n+3)2^{n+1}\Big].
\end{aligned}$$

Let D_0, D_1, $D_2, \cdots$ be a series of dendrimer graphs. Let for $h = 1, 2, \cdots$, the dendrimer graph D_h be obtained so that k leaves are attached to each leaf of D_{h-1}. For an illustration see Fig. 6. The Ashwini index of the dendrimer graph D_h is

$$\begin{aligned}
\mathcal{A}(D_h) &= 18\cdot 2^{n-1}\Big[\sum_{i=1}^{n} i2^i\\
&+ (n+2)2^{n+2}\Big] \qquad (3.4)
\end{aligned}$$

Proof. Let n be the number of steps in the formation of dendrimer graph. Clearly the dendrimer graph D_h has $3\cdot 2^n$ leaves and note that the neighborhood degree of each leaf is 3. Hence, by the definition of Ashwini index,

$$A(G) = \frac{1}{2}\sum_{i=1}^{3\cdot 2^n}\sum_{j=1}^{3\cdot 2^n} d(v_i,v_j)[deg_G \quad (3.5)$$
$$(N(v_i)) + deg_G(N(v_j))].$$

$$\begin{aligned}
\mathcal{A}(D_0) &= \frac{1}{2}[3(4(6)+4(6))]\\
&= 72
\end{aligned}$$

$$\begin{aligned}
\mathcal{A}(D_1) &= \frac{3\cdot 2^1}{2}\Big[2(6)+(6+6)(6)\\
&+ (6+6)(6)\Big]\\
&= 468
\end{aligned}$$

$$\begin{aligned}\mathcal{A}(D_2) &= \frac{3\cdot 2^2}{2}\Big[2(6)+(4+4)(6)\\ &+ \underbrace{(8+8+8+8)}_{4times}(6)\\ &+ \underbrace{(8+8+8+8)}_{4times}(6)\Big]\\ &= 2664\end{aligned}$$

$$\begin{aligned}\mathcal{A}(D_3) &= \frac{3\cdot 2^2}{2}\Big[2(6)+(4+4)(6)\\ &+ (6+6+6+6)(6)\\ &+ \underbrace{(10+10+\cdots+10)}_{8times}(6)\end{aligned}$$

$$+\underbrace{(10+10+\cdots+10)}_{8times}(6)\Big]$$
$$= 13968$$

and so on. Now we are in a position to prove (3.4) by mathematical induction
$\mathcal{A}(D_0)=\frac{3\cdot 2^0}{2}[2(4)]=12$ is true for $n=0$
$\mathcal{A}(D_1)=\frac{3\cdot 2^1}{2}\Big[2(6)+3(2^3)(6)\Big]=468$, is true for $n=1$.
Now assume that the result is true for $n=k-1$.

$$\begin{aligned}\mathcal{A}(D_{k-1}) &= \frac{3\cdot 2^{k-1}}{2}\Big[2(6)+\\ 2(2^2)(6)+\cdots &+ (k-1)2^{k-1}(6)\Big]+\end{aligned}$$
$$\frac{3\cdot 2^{k-1}}{2}[(k+1)2^{k+1}](6)$$
$$= \frac{18\cdot 2^{k-1}}{2}\left[\sum_{i=1}^{k-1} i2^i\right]+$$
$$\frac{18\cdot 2^{k-1}}{2}(k+1)2^{k+1}$$

To prove the result is true for $n=k$

$$\mathcal{A}(D_k) = \frac{18\cdot 2^{k-1}}{2}\left[\sum_{i=1}^{k-1} i2^i\right]$$
$$+\frac{18\cdot 2^{k-1}}{2}[k2^k]$$
$$+ \frac{18\cdot 2^k}{2}[(k+2)2^{k+2}]$$
$$= \frac{18\cdot 2^k}{2}\left[\sum_{i=1}^{k} i2^i\right]+$$
$$\frac{18\cdot 2^k}{2}[(k+2)2^{k+2}]$$
$$= 18\cdot 2^{k-1}$$
$$\left[\sum_{i=1}^{k} i2^i+(k+2)2^{k+2}\right]$$
$$= 18\cdot 2^{n-1}$$
$$\left[\sum_{i=1}^{n} i2^i+(n+2)2^{n+2}\right].$$

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