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Wiener index of two special trees

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Abstract

Given a simple connected undirected graph $G = (V, E)$, the Wiener index of G is defined to be $\frac{1}{2}\sum_{u,v\in V} d(u,\, v)$, where $d(u, v)$ is the distance between the vertives u and v in G. In this note, we obtain closed form expressions for the Wiener indices of (a) the complete binary tree of a given depth, and (b) the class of trees (i.e., molecular graphs) derived by maximum substitutions of normal alkyl groups on a normal alkane of a fixed diameter.

1 Introduction

Let $G{=}(V(G), E(G))$ be a simple finite connected undirected graph. The *Wiener index* (or Wiener number) $W(G)$ of G is defined as

$$W\left(G\right) = \frac{1}{2} \sum_{u,v \in V(G)} d\left(u, v\right),$$

where the summation is over all possible pairs u,v and $d\left(u, v\right)$ is the distance between the vertices u and v in G (we define $d(u, u) = 0$ for all $u \in V(G)$). The quantity $W\left(G\right)$ is named after the chemist Harold Wiener who seems to have first studied the correlation between $W\left(G\right)$ and physico-chemical properties of paraffins (hydrocarbons) where G is taken to be the molecular graph of the corresponding chemical compound[1]. In recent times, $W(G)$ has been shown to be a successful topological index of molecular graphs (see for example, [2]) and it has found useful applications in Chemistry in the design of

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molecules with desired properties. The graphical invariant $W(G)$ is also known by other names like *transmission,total status* and *sum of all distances* (see [3], for example). In graph-based models of different types of networks in Computer Science, the related quantity $W(G)/\binom{|V(G)|}{2}$ is of interest, since it is a measure of the average distance traversed by the messages in the network. For a survey of various known results of Wiener index for different classes of trees, reference [4] can be consulted.

In this paper, we derive expressions for $W(G)$ when G is a complete binary tree and when G is a special class of tree (molecular graph) derived by maximum substitutions of (normal) alkyl groups on a normal alkane of a given diameter. The present work is of similar type to the work reported in [5] wherein an expression for the Wiener number of *dendrimers* is obtained.

2 Wiener index of a complete binary tree

In this section we find an explicit expression for the Wiener index of a nontrivial complete binary tree. A binary tree is defined on a finite set of vertices that either, (a) contains no vertices, or (b) is composed of three disjoint sets of vertices: a *root* vertex, a binary tree called its *left subtree* and a binary tree called its *right subtree* (see [6] for more details). We define the root r to be at depth 0. The vertices connected directly to the root are at depth 1. In general, a vertex is at depth $k+1$ if it is a child of a vertex at depth k. A complete binary tree of height k, denoted by T_k, is one that has vertices upto depth k and has the maximum possible number of vertices at each depth. The total number n_{T_k} of vertices in T_k can be seen to be given by

$$n_{T_k} = 2^{k+1} - 1. \tag{1}$$

For a vertex u of a graph G, we define $d^+(u, G)$ as

$$d^+(u, G) = \sum_{v \in G} d(u, v).$$

We thus have,

$$\begin{aligned} d^+(r, T_k) &= \sum_{i=0}^{k} i\, 2^i \\ &= 2 + (k-1)2^{k+1}. \end{aligned} \tag{2}$$

We begin with the following well-known result (see [4]) which we state without proof.

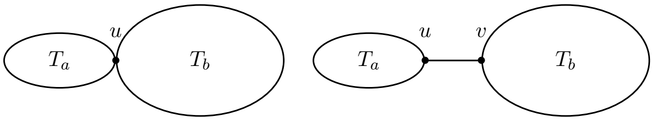
Lemma 1: Let T be a tree obtained from arbitrary trees T_a and T_b of orders n_1 and n_2 respectively and let $u \in V(T_a)$ and $v \in V(T_b)$. Then

(a) If u and v are fused together i.e., identified to be single vertex u (see Fig. 1(a)), then

$$W(T) = W(T_a) + W(T_b) + (n_1 - 1)d^+(u, T_b) + (n_2 - 1)d^+(u, T_a). \tag{3}$$

(b) If u and v are linked by an edge (see Fig. 1(b)), then

$$W(T) = W(T_a) + W(T_b) + n_1 d^+(v, T_b) + n_2 d^+(u, T_a) + n_1 n_2. \tag{4}$$



(a) (b)

Figure 1: A tree T : u is a cut-vertex in (a) and uv is a cut-edge in (b)

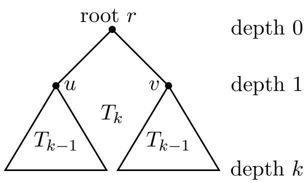


Figure 2: A complete binary tree T_k with two subtrees T_{k-1}

Remark : It may be noted that lemma 1 holds good even when T_a and T_b are connected graphs.

Theorem 1: The Wiener index of a complete binary tree of height k is given by

$$W(T_k) = (k+4)2^{k+1} + (k-2)2^{2(k+1)}.$$

Proof: The proof is based on an application of lemma 1. Let T_k be the complete binary tree of height k whose root is r. Let u,v be the children of r – that is, u and v are the roots of T_{k-1}. Then T_k can be formed using two subtrees T_{k-1} as shown in Fig. 2. We first identify T_k as a tree of the type as shown in Fig. 1(a). We take T_a to be $T_{k-1} \cup (edge(ur))$ and T_b to be $T_{k-1} \cup (edge(vr))$ so that r is a cut-vertex of T_k with $T_a \cap T_b = \{r\}$. Then invoking (3) we have

$$W(T_k) = 2\,W(T_a) + \left(2^{k+1} - 2\right) d^+(u, T_a). \tag{5}$$

(Note: we have applied (1) and we have taken T_b to be T_a as they are isomorphic). By invoking (4), it follows that

$$W(T_a) = W(T_{k-1}) + (k-1)2^k + 1. \tag{6}$$

Also by using (2) it follows that

$$d^+(u, T_a) = (k-1)2^k + 1. \tag{7}$$

Substituting (6) and (7) in (5) we finally get

$$W\,(T_k) = 2\,W\,(T_{k-1}) + 2^{2k+1}\,(k-1) + 2^{k+1}.$$

Solution to the above recurrence relation yields $W(T_k)$ as desired. □

We use the expression for $W(T_k)$ given in Theorem 1 to compute the actual values of $W(T_k)$ for $k = 1, \ldots, 8$ – this is given in Table 1.

k	1	2	3	4	5	6	7	8
$W(T_k)$	4	48	368	2304	12864	66816	330496	1579008

Table 1: Wiener index of T_k for $k = 1, \ldots, 8$.

3 Wiener index of the trees A_{2k+1} and A_{2k}

We define a class of trees A_{2k+1} with a parameter k (where k is a positive integer) that corresponds to the molecular graphs of alkanes with diameter $2k$ where every H-atom is substituted by normal alkyl groups (having the longest possible path). In Fig. 3 the graphs A_3, A_5 and A_7 are depicted. We can define the tree A_{2k+1} with diameter $2k$ as follows:

(a) A_3 is the tree given in Fig. 3 (a)

(b) A_{2k+1} is obtained from A_{2k-1} in the following manner:
Add three pendant vertices (two 'vertical' and one 'horizontal') to the left most and the right most pendant vertices of A_{2k-1} ; next, add a pendant vertex ('vertically') to every other pendant vertex of A_{2k-1} .

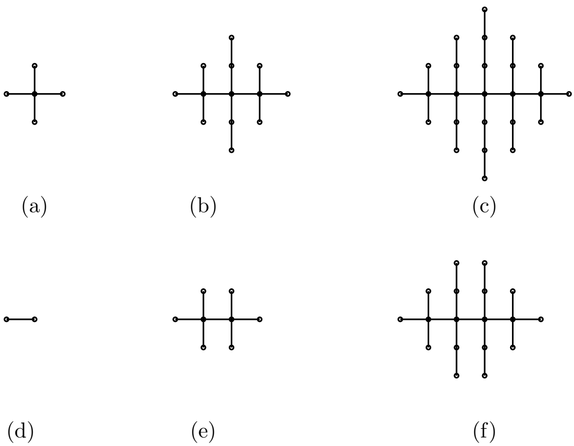


Figure 3: The trees A_3, A_5, A_7, A_2, A_4 and A_6.

It is easy to see that A_{2k+1} has (a) $2k(k+1)+1$ vertices (b) $4k$ pendant vertices, and (c) $2k-1$ vertices of degree 4.
In a manner analogous to the above, we define the class of trees $A_{2k} (k \geq 1)$ with

diameter $2k-1$ starting with A_2 shown in Fig. 3 (d). We note that A_{2k} has (a) $2k^2$ vertices (b) $2(2k-1)$ pendant vertices and (c) $2k-2$ vertices of degree 4.
In this section, we obtain the Wiener index of the trees A_{2k+1} and A_{2k} . We begin with following lemmas.

Lemma 2: Let P_n denote a path on n (≥ 2)vertices. Then $W\left(P_n\right)=\binom{n+1}{3}$.

Proof: Follows from a simple counting (see also [4]).

Lemma 3: Let B_n be the n^{th} Bernoulli number (see [7]) and let r and k be positive integers. Then the sum of the r^{th} powers of the first k natural numbers is given by

$$\sum_{m-1}^{k} m^r = \sum_{j-1}^{r+1} \binom{r+1}{j} \frac{B_{r+1-j}}{(r+1)} (k+1)^j .$$

Proof : For a proof see [8].

Remark. An application of lemma 3 calls for the values of Bernuolli numbers. For example the sum $S_4(k)$ of the fourth powers of the first k natural numbers can be seen to be given by

$$S_4(k) = B_4(k+1) + 2B_3(k+1)^2 + 2B_2(k+1)^3 + B_1(k+1)^4 + (k+1)^5.$$

Noting that $B_0 = \frac{1}{5}$, $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_3 = 0$, $B_4 = -\frac{1}{30}$, it follows that

$$S_4\left(k\right) = \frac{1}{30} k\left(k+1\right)\left(2k+1\right)\left(3k^2\ +3k\ +1\right).$$

Lemma 4: Let v_k denote the middle vertex of P_{2k+1} and let w denote a pendant vertex of P_{k+1} . Then

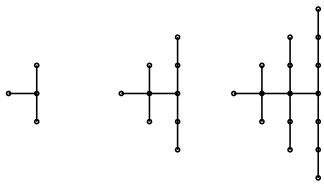
$$d^+\left(v_k, P_{2k+1}\right) = k\left(k+1\right) \quad \text{, and}$$

$$d^+\left(w, P_{k+1}\right) = \frac{k\left(k+1\right)}{2}.$$

Proof: Again, follows from a simple counting.

Lemma 5: Let G_3 be the tree shown in Fig. 4 (a). We construct the tree G_{2k+1} (with parameter k) in the following manner. In G_{2k-1} , let u_{k-1} denote the vertex of degree 3 on the longest path. Add an edge $u_{k-1}v_k$, connecting G_{2k-1} and a path P_{2k+1} , where v_k is the middle vertex of P_{2k+1} . In Fig. 4 (b) and in Fig. 4 (c), we depict G_5 and G_7 respectively (note that the vertex v_k becomes the vertex u_k of G_{2k+1}). Then

$$D_k = d^+\left(u_k, G_{2k+1}\right) = \frac{k\left(k\ +1\right)\left(4k\ +5\right)}{6}.$$



(a) (b) (c)

Figure 4: The trees G_3, G_5 and G_7.

Proof: Using simple counting, we get the following equations:

$$\begin{aligned}
D_1 &= 3 \\
D_2 &= D_1 + 2^2 + 2\sum_{i=1}^{2} i \\
D_3 &= D_2, +3^2 + 2\sum_{i=1}^{3} i \\
&\vdots \\
D_k &= D_{k-1} + k^2 + 2\sum_{i=1}^{k} i
\end{aligned}$$

By direct summation of the above equations we get $d^+(u_k, G_{2k+1})$ as desired.

Lemma 6 : Let G_{2k+1} be as defined in lemma 5. Then the Wiener index $W(G_{2k+1})$ is given by the following formula :

$$\begin{aligned}
W(G_{2k+1}) &= \frac{1}{6}(W_1 + W_2 + W_3 + W_4) \qquad (8)\\
W_1 &= \frac{7}{15}k(k+1)(2k+1)(3k^2+3k-1) \\
W_2 &= 6\,k^2(k+1)^2 \\
W_3 &= \frac{13}{6}k(k+1)(2k+1) \\
W_4 &= \frac{3}{2}k(k+1).
\end{aligned}$$

Proof : Let the edge $u_{k-1}v_k$ in definition of $W(G_{2k+1})$ (see lemma 5) be identified as the cut-edge in lemma 1 (case (b)). By an application of (4), we can write $W(G_{2k+1})$ as

$$W(G_{2k+1}) = W(G_{2k-1}) + W(P_{2k+1}) + (2k+1)\left[d^+(u_{k-1}, G_{2k-1})\right] + k^2\left[d^+(v_k, P_{2k+1})\right] + k^2(2k+1).$$

Invoking the results of lemmas 2, 4 and 5 and simplifying, the above equation reduces to

$$W(G_{2k+1}) = W(G_{2k-1}) + \frac{1}{6}\left[14\,k^4 + 24\,k^3 + 13\,k^2 + 3\,k\right]. \tag{9}$$

In (9) above, we first successively replace k by $k-1$, $k-2$, …, 2, 1 and add all the resulting equations to (9). We then use the fact that $W(G_1) = 0$ and we use the result of lemma 3. Upon subsequent simplification we get $W(G_{2k+1})$ as desired.

Theorem 2: The Wiener index $W(A_{2k+1})$ of the tree A_{2k+1} is given as under:

$$W(A_{2k+1}) = c_1\,k^5 + c_2\,k^4 + c_3\,k^3 + c_4\,k^2 + c_5\,k,$$
$$\text{where}\quad c_1 = \frac{34}{15},\quad c_2 = \frac{16}{3},\quad c_3 = \frac{16}{3},\quad c_4 = \frac{8}{3}\quad \textit{and}\quad c_5 = \frac{2}{5}.$$

Proof : We first we identify the graph A_{2k+1} as a graph consisting of two connected subgraphs $T_a = G_{2k+1}$, $T_b = G_{2k-1}$ with cut-edge uv where u and v are the vertices of degree 3 on the longest path in G_{2k+1} and G_{2k-1} respectively (we thus identify A_{2k+1} to be a graph of the type as shown in Fig.1(b)). Applying lemma 1 (case (b)) and using the fact that $n_1 = (k+1)^2$ and $n_2 = k^2$ we get

$$W(A_{2k+1}) = W(G_{2k+1}) + W(G_{2k-1}) + (k+1)^2\,d^+(v, G_{2k-1}) + k^2\,d^+(u, G_{2k+1}) + k^2\,(k+1)^2\,.$$

Using the result of lemma 5, we get

$$W(A_{2k+1}) = W(G_{2k+1}) + W(G_{2k-1}) + (k+1)^2\,\frac{[(k-1)(k)(4k+1)]}{6} + k^2\frac{[k(k+1)(4k+5)]}{6} + k^2\,(k+1)^2\,.$$

We next invoke lemma 6 (for getting the expressions for $W(G_{2k+1})$ and $W(G_{2k-1})$) and simplify the resultant expression to get $W(A_{2k+1})$ as stated in the theorem. □

In a manner similar to the above proof, i.e., by fitting A_{2k} to be a type of the graph as in Fig. 1(b) (wherein we take both T_a and T_b to be G_{2k-1}) we can derive the expression for $W(A_{2k})$ as follows:

$$W(A_{2k}) = c_1'\,k^5 + c_2'\,k^4 + c_3'\,k^3 + c_4'\,k^2 + c_5'\,k,$$

$$\text{where}\quad c_1' = \frac{34}{15},\quad c_2' = -\frac{1}{3},\quad c_3' = -\frac{4}{3},\quad c_4' = \frac{1}{3}\quad \textit{and}\quad c_5' = \frac{1}{15}.$$

By using the above expressions for $W(A_{2k+1})$ and $W(A_{2k})$, we find that the Wiener indices of A_2, A_3, A_4, A_5, A_6 to be respectively 1, 16, 58, 212, and 491.

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