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Note on the Product of Wiener and Harary Indices

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Abstract

For a simple graph G, we use $d(u,v)$ to denote the distance between two vertices u,v in G. The Wiener index is defined as the sum of distances between all unordered pairs of vertices in a graph. In other word, given a connected graph G, the Wiener index $W(G)$ of G is $W(G) = \sum_{\{u,v\}\subseteq G} d(u,v)$. Another index of graphs closely related to Wiener index is the Harary index, defined as $H(G) = \sum_{\{u,v\}\subseteq G, u\neq v} 1/d(u,v)$. Recently, Gutman posed the following conjecture: For a positive integer $n \geq 5$, let T_n be any n-vertex tree different from the star S_n and the path P_n. Then $W(S_n)\cdot H(S_n) < W(T_n)\cdot H(T_n) < W(P_n)\cdot H(P_n)$. In this paper, we confirm the lower bound of the conjecture and disproof the upper bound of it.

1 Introduction

In this paper, we consider only finite, undirected and simple graphs. Let G be a graph. We use n and m to denote the number of vertices and the number of edges of G, respectively. For terminology and notation not defined here, we refer the reader to [1]. In 1947, Harold Wiener introduced

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the Wiener index of a (molecular) graph for the purpose of determining the approximation formula of the boiling point of paraffin [9]. For a connected graph G, the Wiener index $W(G)$ of G is defined by

$$W(G) = \sum_{\{u,v\}\subseteq G} d(u,v),$$

where $d(u,v)$ denotes the distance of u and v in G.

Another index of a graph related to the Wiener index is the Harary index, which was introduced by Plavšić et al. [8] and Ivanciuc et al. [5]. For a connected graph G, the Harary index $H(G)$ of G is defined by

$$H(G) = \sum_{\{u,v\}\subseteq G, u\neq v} 1/d(u,v).$$

The fundamental properties of the Wiener index and Harary index in the case of extrema have been proved in many articles. For example, let $n \geq 5$ and T_n be a n-vertex tree, different from the star S_n and the path P_n. Entringer [2] and Gutman [3, 4] proved

$$W(S_n) < W(T_n) < W(P_n),$$

independently. In fact, Gutman in [3] also proved

$$H(P_n) < H(T_n) < H(S_n).$$

For more results about the Wiener index and Harary index, please refer to [6] and [7, 10].

Recently, by computer search, Gutman discovered a remarkable regularity and posed the following conjecture:

Conjecture 1. *Let $n \geq 5$ and T_n be any n-vertex tree, different from the star S_n and the path P_n. Then*

$$W(S_n) \cdot H(S_n) < W(T_n) \cdot H(T_n) < W(P_n) \cdot H(P_n).$$

In this paper, we will confirm the lower bound of Conjecture 1 and disproof the upper bound of it. The following results are obtained.

Theorem 1. *Let $n \geq 5$ and T_n be an n-vertex tree different from the star S_n. Then $W(S_n)H(S_n) < W(T_n)H(T_n)$.*

Theorem 2. *For sufficiently large integer n, there is an n-vertex tree T_n different from the path P_n such that $W(T_n)H(T_n) > W(P_n)H(P_n)$. Therefore, the path P_n cannot be the (unique) n-vertex tree that achieves the maximal value of the product of the two indices.*

We feel that the upper bound of the product is achieved by a class of trees, not by a single tree.

2 Proofs of our results

Before we start our proofs, we introduce the following results, which are easily seen, or can be found in some published papers, see [6, 10].

Lemma 1. *Let S_n be a star with n vertices and P_n be a path with n vertices. Then $W(S_n) = (n-1)^2$ and $W(P_n) = \binom{n+1}{3}$*

Lemma 2. *Let S_n be a star with n vertices and P_n be a path with n vertices. Then $H(S_n) = \frac{n^2+n-2}{4}$ and $H(P_n) = 1 + n\sum_{i=2}^{n-1}\frac{1}{i}$*

Lemma 3. *When $x_1 > x_2 > 1$, the following inequality holds:*

$$x_1 + \frac{1}{x_1} > x_2 + \frac{1}{x_2} > 2.$$

Now we give the proofs of our results.

Proof of Theorem 1: Choose an n-vertex tree T_n different from the star S_n, we will prove $W(S_n)H(S_n) < W(T_n)H(T_n)$. For the star S_n, note that $W(S_n)H(S_n)$ equals to the sum of all entries in the following Table 1. Let $\ell = \binom{n}{2}$ and $(d_1, d_2, ..., d_\ell)$ be the sequence of distances such that $d_1 \leq d_2 \leq \cdots \leq d_\ell$ in T_n. Then $W(T_n)H(T_n) = (\sum_{i=1}^{\ell} d_i) \cdot (\sum_{i=1}^{\ell} \frac{1}{d_i})$. Since T_n contains exactly $n-1$ edges, which implies $d_1 = d_2 = \cdots = d_{n-1} = 1$ and $d_i \geq 2$ for each $i \in \{n, n+1, ..., \ell\}$. In Tables 1 and 2, we use $a_{i,j}$ and $b_{i,j}$ to denote the entry lying in row i and column j, respectively.

$\times$	d_1	d_2	$\cdots$	d_{n-1}	d_n	d_{n+1}	$\cdots$	d_ℓ
$\frac{1}{d_1}$	1	1	$\cdots$	1	2	2	$\cdots$	2
$\frac{1}{d_2}$	1	1	$\cdots$	1	2	2	$\cdots$	2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\frac{1}{d_{n-1}}$	1	1	$\cdots$	1	2	2	$\cdots$	2
$\frac{1}{d_n}$	$\frac{1}{2}$	$\frac{1}{2}$	$\cdots$	$\frac{1}{2}$	1	1	$\cdots$	1
$\frac{1}{d_{n+1}}$	$\frac{1}{2}$	$\frac{1}{2}$	$\cdots$	$\frac{1}{2}$	1	1	$\cdots$	1
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\frac{1}{d_\ell}$	$\frac{1}{2}$	$\frac{1}{2}$	$\cdots$	$\frac{1}{2}$	1	1	$\cdots$	1

Table 1. $W(S_n) \times H(S_n)$

$\times$	d_1	d_2	$\cdots$	d_{n-1}	d_n	d_{n+1}	$\cdots$	d_ℓ
$\frac{1}{d_1}$	1	1	$\cdots$	1	d_n	d_{n+1}	$\cdots$	d_ℓ
$\frac{1}{d_2}$	1	1	$\cdots$	1	d_n	d_{n+1}	$\cdots$	d_ℓ
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\frac{1}{d_{n-1}}$	1	1	$\cdots$	1	d_n	d_{n+1}	$\cdots$	d_ℓ
$\frac{1}{d_n}$	$\frac{1}{d_n}$	$\frac{1}{d_n}$	$\cdots$	$\frac{1}{d_n}$	1	$\frac{d_{n+1}}{d_n}$	$\cdots$	$\frac{d_\ell}{d_n}$
$\frac{1}{d_{n+1}}$	$\frac{1}{d_{n+1}}$	$\frac{1}{d_{n+1}}$	$\cdots$	$\frac{1}{d_{n+1}}$	$\frac{d_n}{d_{n+1}}$	1	$\cdots$	$\frac{d_\ell}{d_{n+1}}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\frac{1}{d_\ell}$	$\frac{1}{d_\ell}$	$\frac{1}{d_\ell}$	$\cdots$	$\frac{1}{d_\ell}$	$\frac{d_n}{d_\ell}$	$\frac{d_{n+1}}{d_\ell}$	$\cdots$	1

Table 2. $W(T_n) \times H(T_n)$

For each integer $i \in \{n, n+1, ..., \ell\}$, note that $d_i \geq 2$ in Table 2.

For any two integers $i \in \{1, 2, ..., n-1\}$ and $j \in \{1, 2, ..., n-1\}$, we have $b_{ij} = 1 = a_{ij}$;

For any two integers $i \in \{n, n+1, ..., \ell\}$ and $j \in \{1, 2, ..., n-1\}$, we have $b_{ji} + b_{ij} = d_i + \frac{1}{d_i} \geq 2 + \frac{1}{2} = a_{ji} + a_{ij}$ from Lemma 3. Note that the equality holds if and only if $b_{ji} = d_i = 2$;

For any two integers $i \in \{n, n+1, ..., \ell\}$ and $j \in \{n, n+1, ..., \ell\}$, we have $b_{ji} + b_{ij} = \frac{d_i}{d_j} + \frac{d_j}{d_i} \geq 2 = a_{ji} + a_{ij}$. Note that the equality holds if and only if $d_i = d_j$.

Since T_n is not a star, it follows that there are two integers $i \in \{n, n+1, ..., \ell\}$ and $j \in \{n, n+1, ..., \ell\}$ such that $d_i \neq d_j$. Then $W(T_n)H(T_n) > W(S_n)H(S_n)$. The proof is now complete. ■

Before starting the proof of Theorem 2, we introduce the graph in Figure 1, which we call the meteor graph M_n:

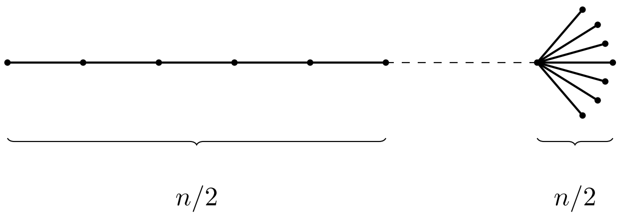

Figure 1. Meteor graph

The meteor graph can be obtained from $P_{\frac{n}{2}}$ and $S_{\frac{n}{2}}$ by joining one end vertex of $P_{\frac{n}{2}}$ and the center vertex of $S_{\frac{n}{2}}$. Now, we can calculate the Wiener index and Harary index of the meteor graph.

$$
\begin{aligned}
W(M_n) = &\binom{\frac{n}{2}+1}{3} + (\frac{n}{2}-1)^2 + 1 + (\frac{n}{2}-1)2 + 2 + (\frac{n}{2}-1)3 + \cdots \\
&+ \frac{n}{2} + (\frac{n}{2}-1)(\frac{n}{2}+1) \\
= &\frac{5}{48}n^3 + \frac{5}{8}n^2 - \frac{5}{3}n + 1,
\end{aligned}
$$

$$\begin{aligned}
H(M_n) &= 1 + \frac{n}{2}\sum_{i=2}^{\frac{n}{2}-1}\frac{1}{i} + \frac{(\frac{n}{2})^2 + \frac{n}{2} - 2}{4} + 1 + (\frac{n}{2}-1)\frac{1}{2} + \frac{1}{2} + (\frac{n}{2}-1)\frac{1}{3} \\
&\quad + \cdots + \frac{1}{\frac{n}{2}} + (\frac{n}{2}-1)\frac{1}{\frac{n}{2}+1} \\
&= 1 + \frac{n}{2}\sum_{i=1}^{\frac{n}{2}}\frac{1}{i} - \frac{n}{2} - 1 + \frac{n^2+2n-8}{16} + \frac{n}{2}\sum_{i=1}^{\frac{n}{2}}\frac{1}{i} \\
&\quad + (\frac{n}{2}-1)(\frac{n}{2}\sum_{i=1}^{\frac{n}{2}}\frac{1}{i} - 1 + \frac{1}{\frac{n}{2}+1}) \\
&= \frac{1}{16}n^2 + \frac{n}{2}\sum_{i=1}^{\frac{n}{2}}\frac{1}{i} - \frac{7}{8}n + \frac{3}{2} - \frac{4}{n+2}.
\end{aligned}$$

Proof of Theorem 2: Note that $\sum_{i=1}^{n}\frac{1}{i} = \ln n + C$. Now we estimate the values of the products of the Wiener index and Harary index for the path and meteor, respectively. That is,

$$W(P_n)H(P_n) = \frac{1}{6}n^4 \ln n + O(n^4),$$

and

$$W(M_n)H(M_n) = \frac{5}{768}n^5 + O(n^4 \ln n).$$

It is clear that $W(M_n)H(M_n) > W(P_n)H(P_n)$ when n is sufficiently large.

■

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References

[1] J. A. Bondy, U. S. R. Murty, Graph Theory, *Graduate Texts in Mathematics, No.244*, Springer, 2008.

[2] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czechoslovak Math.J.* (1976) 283–296.

[3] I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.* **36A** (1997) 128–132.

[4] I. Gutman, W. Linert, I. Lukovits, A. A. Dobrynin, Trees with extremal hyper-Wiener index: Mathematical basis and chemical applications, *J. Chem. Inf. Comput. Sci.* **37** (1997) 349–354.

[5] O. Ivanciuc, T. S. Balaban, A. T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices, *J. Math. Chem.* **12** (1993) 309–318.

[6] M. Knor, R. Škrekovski, A. Tepeh, Selected topics on Wiener index, arXiv:2303.11405.

[7] X. Lin, Y. Fan, The connectivity and the Harary index of a graph, *Discrete Appl. Math.* **181** (2015) 167–173.

[8] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.

[9] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[10] B. Zhou, X. Cai, N. Trinajstić, On Harary index, *J. Math. Chem.* **44** (2008) 611–618.