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Minimum of Product of Wiener and Harary Indices

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Abstract

For a connected graph G, the Wiener index W and the Harary index H are defined as $W = \sum_{u,v} d(u,v)$ and $H = \sum_{u,v} 1/d(u,v)$, respectively. Recently, in *MATCH* **91** (2024) 287, the extremal value of the product $W \cdot H$ was studied and shown that $W \cdot H \geq \binom{n}{2}$, with equality for the complete graph. We now extend this result to all graphs of order n and size m, and characterize the respective species with minimum $W \cdot H$-value.

1 Introduction

Let G be a simple graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. The order and size of G are $n = |\mathbf{V}(G)|$ and $m = |\mathbf{E}(G)|$, respectively, and we say that G is an (n,m)-graph. Throughout this paper it is assumed that the graphs considered are connected.

For $u, v \in \mathbf{V}(G)$ we denote by $d(u,v)$ the distance (= length of a shortest path) between u and v. The diameter $d = d(G)$ of a graph G is the largest distance between its vertices.

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The Wiener index and the Harary index of a graph G are defined as

$$W = W(G) = \sum_{\{u,v\}\subset \mathbf{V}(G)} d(u,v) \quad \text{and} \quad H = H(G) = \sum_{\{u,v\}\subset \mathbf{V}(G)} \frac{1}{d(u,v)}$$

respectively. These graph invariants are the best studied distance-based topological indices. For chemical applications and mathematical properties of the Wiener index see [1, 2, 5, 6, 12, 13] and the references cited therein. For analogous data on Harary index see [2, 8, 10, 11, 14].

In the following considerations, we will encounter graphs whose diameter is at most two ($d \leq 2$). For such graphs, the following result holds.

Lemma 1. *If $d \leq 2$, then for any connected (n,m)-graph, the Wiener and Harary indices are fully determined by the parameters n and m, as*

$$W = n(n-1) + m \qquad \textit{and} \qquad H = \frac{1}{4}\left[n(n-1) + 2m\right].$$

Proof. Denote by p_1 and p_2 the number of pairs of vertices whose distance is 1 and 2, respectively. Since $d(G) \leq 2$, $p_1 + p_2$ is equal to the total number of vertex pairs of the graph G, i.e., $p_1 + p_2 = \binom{n}{2}$. Evidently, $p_1 = m$. Therefore, $p_2 = \binom{n}{2} - m$, and Lemma 1 follows by taking into account that $W = p_1 + 2\,p_2$ and $H = p_1 + p_2/2$. ■

Recently, a number of papers appeared, concerned with the product of a topological index and its reciprocal [3, 4, 7, 9]. In [3], the following result was established.

Theorem 1. *For any (connected) graph G of order n,*

$$W(G) \cdot H(G) \geq \binom{n}{2}^2.$$

Equality holds if and only if $G \cong K_n$.

According to Theorem 1, the unique graph of order n, whose $W \cdot H$-value is minimum is the complete graph. The problem that remains is to characterize the non-complete graphs with minimum $W \cdot H$. In [7], the authors solved the following special case of this problem, which earlier was conjectured in [3].

Theorem 2. [7] *For any tree T of order n,*

$$W(T)\cdot H(T) \geq \frac{1}{4}\,(n+2)(n-1)^3.$$

Equality holds if and only if $T \cong S_n$, where S_n is the n-vertex star.

According to Theorem 2, the unique $(n, n-1)$-graph, whose $W\cdot H$-value is minimum is the star. In what follows, we offer an analogous result, pertaining to any (n,m)-graph, for $n \geq 1$, $1 \leq m \leq n-1$.

2 Main results

We define a function of $n-1$ variables as follows:

$$f(x_1, x_2, \ldots, x_{n-1}) = \left(\sum_{i=1}^{n-1} i\, x_i\right)\left(\sum_{i=1}^{n-1} \frac{x_i}{i}\right)$$

where x_1, x_2, …, x_{n-1} are non negative integers.

Lemma 2. *Let n and d be given integers such that $2 \leq d \leq n-1$. Then*

$$f(\underbrace{x_1, \ldots, x_{d-1}, x_d}_{d}, 0, \ldots, 0) > f(\underbrace{x_1, \ldots, x_{d-1} + x_d}_{d-1}, 0, \ldots, 0)\,.$$

Proof. For the convenience, denote $A = \sum\limits_{i=1}^{d-1} \dfrac{x_i}{i}$ and $B = \sum\limits_{i=1}^{d-1} i\, x_i$. Then we have

$$\begin{aligned}
\Delta &= f(\underbrace{x_1, \ldots, x_{d-1}, x_d}_{d}, 0, \ldots, 0) - f(\underbrace{x_1, \ldots, x_{d-1} + x_d}_{d-1}, 0, \ldots, 0)\\
&= (B + d\,x_d)\left(A + \frac{x_d}{d}\right) - \big[B + (d-1)x_d\big]\left(A + \frac{x_d}{d-1}\right)\\
&= \frac{x_d}{d(d-1)}\big[d(d-1)A - B\big]
\end{aligned}$$

and it follows that

$$\begin{aligned}\Delta &= \frac{x_d}{d(d-1)}\sum_{i=1}^{d-1}\left[\frac{d(d-1)-i^2}{i}x_i\right] \\ &> \frac{x_d}{d(d-1)}\sum_{i=1}^{d-1}\left[\frac{d(d-1)-(d-1)^2}{i}x_i\right] = \frac{x_d}{d}\sum_{i=1}^{d-1}\frac{x_i}{i} > 0,\end{aligned}$$

which is our required result. ∎

Note that for any positive integers n and m, such that $n-1 \leq m < n(n-1)/2$, there exist connected graphs of order n and size m with diameter two. For example, the graph obtained from the star S_n by adding $m-n+1$ edges has diameter two. If $m = n(n-1)/2$, then the respective graph is the complete graph K_n, whose diameter is unity.

Theorem 3. *Let G be a connected graph of order n and size m. Then*

$$W \cdot H \geq \frac{1}{4}\left[(n-1)n-m\right]\left[(n-1)n+2m\right]. \tag{1}$$

Equality holds if and only if the diameter of G is at most two.

Proof. Let d be the diameter of G. Suppose first that $d \leq 2$. Then by Lemma 1, it is easy to see that the equality holds in (1).

Suppose now that $d > 2$. Denote by p_i the number of distinct pairs of vertices whose distance in G is exactly i. Then by the definition of the Wiener index and the Harary index, we have

$$W(G) = \sum_{i=1}^{d} i\,p_i \qquad \text{and} \qquad H(G) = \sum_{i=1}^{d}\frac{p_i}{i}.$$

In addition, we have

$$W \cdot H = f(\underbrace{p_1,\ldots,p_{d-1},p_d}_{d},0,\ldots,0),$$

where $p_k > 0$, $1 \leq k \leq d$. This implies

$$\begin{aligned} H(G)\cdot W(G) &> f(\underbrace{p_1, \ldots, p_{d-1} + p_d}_{d-1}, 0, \ldots, 0) \\ &> \cdots > f(p_1, \sum_{i=2}^{d} p_i, 0, \ldots, 0) \qquad (2) \end{aligned}$$

by Lemma 2.

Hence, from the definition of the function f, we get

$$\begin{aligned} f\left(p_1, \sum_{i=2}^{d} p_i, 0, \ldots, 0\right) &= \left(p_1 + 2\sum_{i=2}^{d} p_i\right)\left(p_1 + \frac{1}{2}\sum_{i=2}^{d} p_i\right) \\ &= \Big((n-1)n - m\Big)\left(\frac{(n-1)n}{4} + \frac{m}{2}\right) \qquad (3) \end{aligned}$$

using $p_1 = m$ and $\sum_{i=1}^{d} p_i = \binom{n}{2}$. Therefore, from (2) and (3), we conclude that the inequality in (1) is strict.

This completes the proof. ■

Corollary. *Theorem 1 is the special case of Theorem 3 for* $m = n(n-1)/2$.

Corollary. *Theorem 2 is the special case of Theorem 3 for* $m = n - 1$.

The number of independent cycles in a connected (n, m)-graph is equal to $c = m - n + 1$. Bearing this in mind, using Theorem 3, we can characterize the c-cyclic graphs with minimum $W \cdot H$-values.

According to Theorem 3, and in view of Lemma 1, any connected (n, m)-graph whose diameter is not greater than 2, has a minimum $W \cdot H$-value. Among trees ($c = 0$), this is the star S_n. Among unicyclic graphs ($c = 1$), these are the graphs obtained by adding a new edge to S_n (if $n \geq 3$), and two exceptional graphs – the cycles C_4 and C_5 (if $n = 4$ and $n = 5$, respectively). Among bicyclic graphs ($c = 2$), these are the graphs obtained by adding two edges to S_n (if $n \geq 4$), and the three exceptional graphs depicted in Fig. 1 (if $n = 5$ and $n = 6$, respectively).

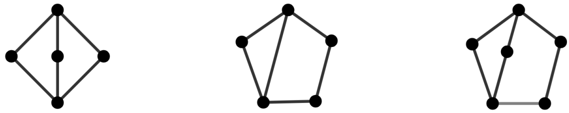

Fig. 1. Exceptional bicyclic graphs with minimum $W \cdot H$.

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