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Comparing Multiplicative Wiener Index with Other Graph Invariants

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Abstract

The Wiener index (W) of a connected graph is the sum of distances over all vertex pairs in this graph. As a variant of Wiener index, the multiplicative Wiener index (MW) of a connected graph is the product of distances over all vertex pairs in this graph. The first multiplicative Zagreb index (MZ) of a graph is the product of squares of degree over all vertices in this graph. Das and Gutman (2016) proved that for any bipartite connected graph of order $n \ge 5$, MW >W. In this paper, we first generalize Das and Gutman's result by proving that if G is a connected graph of order $n \ge 5$ and size m such that $m \le \lfloor \frac{n}{2} \rfloor \lfloor \frac{n}{2} \rfloor - 1$, then MW >W. Second, we compare MW with MZ for trees, and prove that MW \ge MZ for any tree with at least five vertices. Finally, we compare MW with the independence number, with only two exceptions.

1 Introduction

All graphs considered in this paper will be simple and connected. Let G = (V, E) be a graph whose vertex set and edge set are V = V(G) and E = E(G), respectively. For a vertex v in G, its *degree*, denoted by $d_G(v)$, is defined to be the number of edges incident with v. Let $d_G(u, v)$ be the distance between vertices u and v in G, i.e., the length of one shortest path connecting u and v. The *diameter* of a connected graph G is the maximum distance between all pairs of vertices in G. A path in a connected graph is said to be a *diametral path*, if this path is of length equal to the diameter. A connected graph is said to be a *tree* if it contains no cycles, and said to be a *bipartite graph*, if it contains no

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cycles of odd length. A quasi-tree is a connected graph, in which there exists a vertex whose removal results in a tree. Let P_n , S_n , C_n and K_n be the path, star, cycle and complete graph of order n, respectively. For $a \ge 1$, $b \ge 1$, let S_{a+1} and S_{b+1} be stars on a + 1 and b + 1 vertices, respectively. Then the *double star* $S_{a,b}$ is just the tree obtained by connecting an edge between two centers of S_{a+1} and S_{b+1} . For other notation and terminology not defined here, the readers are referred to [3].

A well-studied graph invariant based on distance of a connected graph G is the Wiener index, denoted by W(G), is defined [30] to be the sum of distances over all unordered vertex pairs in G, namely,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} D_G(u)$$

where $D_G(u) = \sum_{v \in V(G)} d_G(u, v).$

The average distance of G, denoted by $\overline{l}(G)$, is defined to be

$$\bar{l}(G) = \frac{\sum\limits_{\{u,v\} \subseteq V(G)} d_G(u,v)}{\binom{n}{2}} = \frac{2}{n(n-1)} W(G)$$

Results on Wiener index can be found in [7, 13, 25, 26], and so on. For results on average distance, the readers are referred to [4, 5, 6, 12] and the references cited therein.

As a variant of Wiener index, the *multiplicative Wiener index* of a connected graph G, denoted by MW(G), is defined by Gutman et al.[15, 16] to be

$$MW(G) = \prod_{k=1}^{d} k^{\gamma(G;k)}, \qquad (1)$$

where $\gamma(G; k)$ is the number of vertex pairs in G that are at distance k and d is the diameter of G. For recent results on MW(G), see [11, 18] and the references cited therein.

For a (molecular) graph G, two well-studied degree-based topological indices of G are the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$, respectively. They are defined as follows:

$$M_1(G) = \sum_{v \in V(G)} \left(d_G(v) \right)^2, M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v) .$$

In 2010, Todeschini et al. [28, 29] proposed the multiplicative variants of ordinary Zagreb indices, which are defined as follows:

$$\pi_1(G) = \prod_{v \in V(G)} \left(d_G(v) \right)^2, \pi_2(G) = \prod_{uv \in E(G)} d_G(u) d_G(v) \ .$$

Later, I. Gutman [17] called $\pi_1(G)$ and $\pi_2(G)$ the first multiplicative Zagreb index and the second multiplicative Zagreb index of G, respectively. For recent results on $\pi_1(G)$ and $\pi_2(G)$, see [27, 31] and the references cited therein.

During the past few decades, some graph theory scholars have investigated the relationships between various graph invariants, see e.g., [7, 8, 9, 10, 11, 19, 21, 22, 23, 24, 25]. Some of these researches were motivated by Grafitti conjectures [4, 12, 14] or AutoGraphiX conjectures [1, 2, 20, 21]. In particular, Das and Gutman [11] investigated the relationship between the multiplicative Wiener index and Wiener index. They proved that the former index is always greater than the later one for bipartite graphs with at least five vertices.

In this paper, we investigate the relationship between the multiplicative Wiener index and Wiener index, the relationship between the multiplicative Wiener index and first multiplicative Zagreb index, and the relationship between the multiplicative Wiener index and independence number. We first generalize Das and Gutman's result by proving that if G is a connected graph of order $n \geq 5$ and size m such that $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$, then the multiplicative Wiener index is greater than Wiener index. Second, we compare he multiplicative Wiener index with first multiplicative Zagreb index for trees, and prove that the multiplicative Wiener index is greater than or equal to the first multiplicative Zagreb index for any tree with at least five vertices. Finally, we compare the multiplicative Wiener index with independence number for connected graph, and we prove that the multiplicative Wiener index is greater than independence number, with only two exceptions.

2 Main results

In this section, we investigate the relationship between the multiplicative Wiener index and Wiener index, the relationship between the multiplicative Wiener index and first multiplicative Zagreb index, and the relationship between the multiplicative Wiener index and independence number. We will proceed by dividing our discussions into three subsections.

2.1 The multiplicative Wiener index and Wiener index

In this subsection, we investigate the relationship between the multiplicative Wiener index and Wiener index. In fact, Das and Gutman [11] have investigated the relationship between the multiplicative Wiener index and Wiener index. They proved the following result.

Theorem 2.1. Let G be a connected bipartite graph of order n > 4. Then

$$MW(G) - W(G) \ge 2^{\left(\frac{n(n-1)}{2} - \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil\right)} - n(n-1) + \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$$

with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

As a result, they obtained the following corollary.

Corollary 2.2. Let G be a connected bipartite graph of order n > 4. Then MW(G) > W(G).



Figure 1. Graphs occurred in the proof of Theorem 2.3.

Now, we use the same techniques as those used in [11] to generalize Das and Gutman's result to general connected graphs with a restricted condition on the number of edges. We improve Theorem 2.1 as follows.

Theorem 2.3. Let G be a connected graph of order $n \ge 4$ and size m. If $m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$, then

$$MW(G) - W(G) > 2^{\left(\frac{n(n-1)}{2} - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil\right)} - n(n-1) + \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil$$

Proof. Let d be the diameter of G. Since $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$, we have $G \ncong K_n$. Then $d \geq 2$. We consider the following two cases.

Case 1. d = 2.

Since d = 2, we have $m + \gamma(G; 2) = \frac{n(n-1)}{2}$. So, $MW(G) = 2^{\gamma(G; 2)} = 2^{\frac{n(n-1)}{2}-m}$ and $W(G) = m + 2\gamma(G; 2) = n(n-1) - m$. Then

$$MW(G) - W(G) = 2^{\frac{n(n-1)}{2} - m} - n(n-1) + m.$$

Now, we consider the function $f(x) = 2^{\frac{n(n-1)}{2}-x} - n(n-1) + x$ $(x < \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil)$. Then $f'(x) = -\ln 2 \cdot 2^{\frac{n(n-1)}{2}-x} + 1$. Since $x < \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$, we have

$$\frac{n(n-1)}{2} - x > \frac{n(n-1)}{2} - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil$$
$$= \begin{cases} \frac{n^2 - 2n}{4} & \text{if } n \text{ is even,} \\ \frac{n^2 - 2n + 1}{4} & \text{if } n \text{ is odd.} \end{cases}$$

Thus,

$$2^{\frac{n(n-1)}{2}-x} > \begin{cases} 2^{\frac{n^2-2n}{4}} & \text{if } n \text{ is even,} \\ \\ 2^{\frac{n^2-2n+1}{4}} & \text{if } n \text{ is odd.} \end{cases}$$

and then

$$2^{\frac{n(n-1)}{2}-x} \cdot \ln 2 > \begin{cases} 2^{\frac{n^2-2n-4}{4}} \cdot \ln 4 & \text{if } n \text{ is even,} \\ 2^{\frac{n^2-2n-3}{4}} \cdot \ln 4 & \text{if } n \text{ is odd.} \end{cases}$$
$$> \begin{cases} \ln 4 & \text{if } n \ge 4, \\ \ln 4 & \text{if } n \ge 3. \end{cases}$$

Therefore, when $n \ge 4$, we have f'(x) < 0, that is, f(x) is strictly decreasing on the interval $(-\infty, \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil]$ when $n \ge 4$.

Thus, when $n \ge 4$, we have

$$\begin{aligned} MW(G) - W(G) &= f(m) > f\left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rfloor\right) \\ &= 2^{\left(\frac{n(n-1)}{2} - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil\right)} - n(n-1) + \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil \end{aligned}$$

Case 2. $d \ge 3$.

If n = 4, by our assumption that $3 \le m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1 = 3$ and $d \ge 3$, G must be isomorphic to P_4 . It is easy to check that the theorem holds. Now, we assume that $n \ge 5$. When n = 5, as $d \ge 3$ and $m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1 = 5$, G must be isomorphic to P_5 or one of graphs as shown in Fig. 1. It is not difficult to check that the theorem holds. So, we may assume that $n \ge 6$.

The proof of the remaining part is completely identical to that in [11] for the case $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$ (because their proof of this part is also applicable to non-bipartite graphs).

This completes the proof.

By Theorem 2.3, we immediately have

Corollary 2.4. Let G be a connected graph of order $n \ge 5$. If $m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$, then MW(G) > W(G).

Remark 2.5. Among all bipartite graphs of order n, the graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique graph having $\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ edges. All other bipartite graphs of order n have less than $\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ edges. Thus, our Theorem 2.3 generalizes Theorem 2.1, and Corollary 2.4 generalizes Corollary 2.2.

Since $\overline{d} = \frac{2m}{n} \leq \Delta$, by Corollary 2.4, we immediately have

Corollary 2.6. Let G be a connected graph of order $n \ge 5$ with maximum degree \triangle . If

$$\Delta \le \frac{2\left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - 1\right)}{n}$$

then MW(G) > W(G).

Corollary 2.7. Let G be a quasi-tree of order $n \ge 8$. Then MW(G) > W(G).

Proof. Suppose that G has m edges. By the definition of the quasi-tree, we have $m \le (n-1) + (n-2) = 2n-3$. It is easy to check that if $n \ge 8$, then $m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$. According to Corollary 2.4, we have MW(G) > W(G).

Corollary 2.8. Let G be a simple maximal planar graph of order $n \ge 11$. Then MW(G) > W(G).

Proof. Suppose that G has m edges. Since G is a maximal plannar graph, we have $m \leq 3n-6$. It is easy to check that if $n \geq 11$, then $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$. In view of Corollary 2.4, we have MW(G) > W(G).

2.2 The multiplicative Wiener index and the first multiplicative Zagreb index

In this subsection, we investigate the relationship between the multiplicative Wiener index and the first multiplicative Zagreb index. To find the relationship between these two kinds of indices, we first consider the following two examples.

Example 2.1. For the complete graph K_n , we have

 $MW(K_n) = 1 < (n-1)^{2n} = \pi_1(K_n)$

for $n \geq 3$.

Example 2.2. For the path P_n $(n \ge 5)$, we have

$$\pi_1(P_n) = \left(2^2\right)^{n-2} = 4^{n-2}.$$

Now, we consider the multiplicative Wiener index of the path P_n . We label all vertices of the path P_n successively as v_1, v_2, \dots, v_n . Then

$$MW(P_n) > \prod_{x \in V(G) \setminus \{v_1\}} d_G(x, v_1) \cdot \prod_{y \in V(G) \setminus \{v_1, v_n\}} d_G(y, v_n) \ge (n-1) \left[(n-2)! \right]^2 .$$

Thus, for $n \geq 5$, we have

$$\ln MW(P_n) \geq \ln(n-1) + 2[\ln(n-2) + \dots + \ln 2] > \ln(n-1) + 2(n-3)\ln 2$$

$$\geq 2\ln 2 + 2(n-3)\ln 2 = (n-2)\ln 4 = \ln \pi_1(P_n) .$$

So, for $n \ge 5$, we have $MW(G) > \pi_1(P_n)$.

From two examples given above, one can conclude that the multiplicative Wiener index and the first multiplicative Zagreb index are incomparable in case of general connected graphs. So, it is natural for us to restrict our attention only to trees.

First, we establish the relationship between the multiplicative Wiener index and the first multiplicative Zagreb index for double-stars. We need the following result.

Lemma 2.9. For any positive real number x > 4, it holds that

$$2^x > x^2.$$

Proof. Let $f(x) = 2^x - x^2$. We shall prove that f(x) > 0 for x > 4. It is easy to obtain that $f'(x) = 2^x \ln 2 - 2x$ and $f''(x) = 2^x (\ln 2)^2 - 2$. When $x \ge 3$, we have $f''(x) = 2^{x-2}(2\ln 2)^2 - 2 > 2^{x-2} - 2 \ge 0$. So, f'(x) is strictly increasing on the interval $[3, +\infty)$. Thus, $f'(x) > f'(4) = 2^4 \ln 2 - 2 \times 4 > 0$. Hence, f(x) is strictly increasing on the interval $[4, +\infty)$. Thus, $f(x) > f(4) = 2^4 - 4^2 = 0$.

This completes the proof.

Proposition 2.10. For the double star $S_{a,b}$ (a + b = n - 2, $a \ge 1$ and $b \ge 1$), if $(a, b) \ne (1, 1)$, then

$$MW(S_{a,b}) > \pi_1(S_{a,b}).$$

Proof. By the definitions of the multiplicative Wiener index and the first multiplicative Zagreb index, we have

$$MW(S_{a,b}) = 3^{ab} \cdot 2^{a+b} > 2^{ab+1} \cdot 2^{a+b} (as (a, b) \neq (1, 1)) = 2^{ab+a+b+1}$$
(2)

and

$$\pi_1(S_{a,b}) = (a+1)^2 \cdot (b+1)^2 = (ab+a+b+1)^2.$$
(3)

Since $(a, b) \neq (1, 1)$, we have $ab + a + b + 1 \ge 6$. By Lemma 2.9, (2) and (3), we have $MW(S_{a,b}) > \pi_1(S_{a,b})$.

Now, we are in a position to state and prove our second result, which deals with the relationship between the multiplicative Wiener index and the first multiplicative Zagreb index of trees.

Theorem 2.11. Let T be a tree of order n. Then

(a).
$$\pi_1(T) = MW(T)$$
 for $n = 2$,

(b). $\pi_1(T) > MW(T)$ for n = 3, 4;

(c). $MW(T) \ge \pi_1(T)$ for $n \ge 5$, and the equality holds if and only if $T \cong S_5$.

Proof. If n = 2, 3, then $T \cong P_2$ and P_3 , respectively. Clearly, we have $MW(P_2) = 1 = \pi_1(P_2)$ and $MW(P_3) = 2 < 4 = \pi_1(P_3)$. If n = 4, then $T \cong P_4$ or S_4 . Clearly, we have $MW(P_4) = 3 \cdot 2^2 = 12 < 16 = 2^2 \cdot 2^2 = \pi_1(P_4)$; and $MW(S_4) = 2^3 = 8 < 9 = 3^2 = \pi_1(S_4)$. Now, we consider the case when $n \ge 5$.

We prove that (c) holds by induction on n for $n \ge 5$. First, we consider the case of n = 5. Let d be the diameter of T. If d = 2, then $T \cong S_5$, and $MW(S_5) = 2^4 = 4^2 = \pi_1(S_5)$. Now, we assume that $d \ge 3$. Since n = 5 and $d \ge 3$, we must have $T \cong P_5$ or $S_{1,2}$. Note that $MW(P_5) = 4 \cdot 3^2 \cdot 2^3 > 2^6 = \pi_1(P_5)$. Also, by Proposition 2.10, we have $MW(S_{1,2}) > \pi_1(S_{1,2})$. So, the statement of (c) holds for n = 5.

Now, we let $n \ge 6$ and assume that (c) holds for smaller values of n. Let $P_{d+1} = v_0v_1 \cdots v_d$ be a diametral path in T. If $T \cong P_n$, then the theorem is true by Example 2.2. Suppose now that $T \ncong P_n$. So, $d \le n-2$. There exists at least one pendent vertex, say v, lying outside the diametral path. Let u be the unique neighbor of v. Set $T' = T - \{v\}$. It is obvious that T' is connected. If d = 2, then $T \cong S_n$ $(n \ge 6)$, and $MW(S_n) = 2^{n-1} > (n-1)^2 = \pi_1(S_n)$ by Lemma 2.9. So, we assume that $d \ge 3$.

Clearly,

$$MW(T) = MW(T') \cdot \prod_{x \in V(T) \setminus \{v\}} d_T(v, x).$$

$$\tag{4}$$

 $\prod_{x \in V(T) \setminus \{v\}} d_T(v, x) > d_T(v, v_0) d_T(v, v_d) \ge d_T(v, v_0) + d_T(v, v_d) - 1 \ge (d+2) - 1 \ge 4.$ (5)

By (4) and (5), we obtain

$$MW(T) > 4MW(T'). (6)$$

$$\pi_1(T') = \frac{\pi_1(T)}{(d_T(u))^2} \cdot (d_T(u) - 1)^2 \ge \frac{1}{4}\pi_1(T) \quad (\text{as } d_T(u) \ge 2).$$
(7)

Note that $T' \ncong S_5$, by the induction hypothesis, $MW(T') > \pi_1(T')$. This, in joint with (6) and (7) gives $MW(T) \ge \pi_1(T)$ for $n \ge 5$, with equality holding if and only if $T \cong S_5$. This completes the proof.

In the following, we give a sufficient condition for a general connected graph to have a larger multiplicative Wiener index than first multiplicative Zagreb index.

Theorem 2.12. Let G be a connected graph of order n with average degree \overline{d} and diameter $d \ (\geq 3)$. If $\ln d + 2 \sum_{i=2}^{d-1} \ln i \geq 2n \ln \overline{d}$, then

$$MW(G) > \pi_1(G).$$

Proof. By the Geometry-Arithmetic Mean Inequality, we have

$$\pi_1(G) \leq \left(\frac{\sum\limits_{i=1}^n d_i}{n}\right)^{2n} = \overline{d}^{2n}$$

with equality if and only if $d_1 = \cdots = d_n$, that is, G is regular.

Also, as proved in Example 2.2,

$$MW(G) \geq d\left[(d-1)!\right]^2$$

It is not difficult to see that the above equality is attained if and only if $G \cong P_4$.

Since P_4 is not regular, by our assumption that $\ln d + 2 \sum_{i=2}^{d-1} \ln i \ge 2n \ln \overline{d}$, we have $MW(G) > \pi_1(G)$.

2.3 The multiplicative Wiener index and independence number

In the last subsection, we investigate the relationship between the multiplicative Wiener index and independence number. Our result is as follows.

Theorem 2.13. Let G be a connected graph of order n. Then

$$MW(G) \ge \alpha(G)$$

with equality if and only if $G \cong K_n$ $(n \ge 2)$ or $G \cong K_n - e$ $(n \ge 3)$.

Proof. Let *m* be the number of edges in *G*. For $m = \frac{n(n-1)}{2}$, we have $G \cong K_n$, hence $MW(G) = 1 = \alpha(G)$. For $m = \frac{n(n-1)}{2} - 1$, we have $G \cong K_n - e$. Then $MW(G) = 2 = \alpha(G)$, again the equality holds. Otherwise, $m \leq \frac{n(n-1)}{2} - 2$. Now,

$$MW(G) \ge 2^{\binom{\alpha(G)}{2}} = 2^{\frac{\alpha(G)(\alpha(G)-1)}{2}}$$

If $\alpha(G) \geq 3$, then we obtain $MW(G) \geq 2^{\alpha(G)} > \alpha(G)$. So, we consider the case of $\alpha(G) = 2$. Thus we have $MW(G) \geq 4 > 2 = \alpha(G)$.

This completes the proof.

The following result was reported by Chung in [4].

Theorem 2.14. Suppose G is a connected graph of order n. Let $\alpha(G)$ and $\overline{l}(G)$ be the independence number and average distance of G, respectively. Then

$$\alpha(G) \ge \overline{l}(G) \tag{8}$$

with equality if and only if $G \cong K_n$.

By Theorems 2.13 and 2.14, we have

Corollary 2.15. Let G be a connected graph of order n with the average distance $\overline{l}(G)$ and the multiplicative Wiener index MW(G). Then

$$MW(G) \ge \overline{l}(G)$$

with equality if and only if $G \cong K_n$.

3 Concluding remarks

In this paper, we investigated the relationship between the multiplicative Wiener index and Wiener index, the relationship between the multiplicative Wiener index and first multiplicative Zagreb index, and the relationship between the multiplicative Wiener index and independence number. We first generalized Das and Gutman's result by proving that if G is a connected graph of order $n \geq 5$ and size m such that $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$, then the multiplicative Wiener index is greater than Wiener index. Second, we compared he multiplicative Wiener index with first multiplicative Zagreb index for trees, and proved that the multiplicative Wiener index is greater than or equal to the first multiplicative Zagreb index for any tree with at least five vertices. Finally, we compared the multiplicative Wiener index with independence number for connected graph, and we proved that the multiplicative Wiener index is greater than independence number, with only two exceptions. It may be interesting to compare other topological indices and graph invariants.

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