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On Wiener and multiplicative Wiener indices of graphs

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ABSTRACT

Let G be a connected graph of order n with m edges and diameter d. The Wiener index $W(G)$ and the multiplicative Wiener index $\pi(G)$ of the graph G are equal, respectively, to the sum and product of the distances between all pairs of vertices of G. We obtain a lower bound for the difference $\pi(G) - W(G)$ of bipartite graphs. From it, we prove that $\pi(G) > W(G)$ holds for all connected bipartite graphs, except P_2, P_3, and C_4. We also establish sufficient conditions for the validity of $\pi(G) > W(G)$ in the general case. Finally, a relation between $W(G)$, $\pi(G)$, n, m, and d is obtained.

1. Introduction

In this paper we are concerned with connected simple graphs. Let $G = (V(G), E(G))$ be such a graph, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $E(G)$ are the vertex and edge sets of G; $|V(G)| = n$ and $|E(G)| = m$. The distance $d_G(v_i, v_j)$ between the vertices v_i and v_j of the graph G is equal to the length of (number of edges in) the shortest path that connects v_i and v_j [1]. The Wiener index of G is then defined as

$$W = W(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} d_G(v_i, v_j).$$

If we denote by $d(G, k)$ the number of vertex pairs of G, whose distance is equal to k, then the Wiener index of G can be expressed as

$$W(G) = \sum_{k\geq 1} k\, d(G, k).$$

Recall that $d(G, 1) = m$. The maximum value of k for which $d(G, k)$ is non-zero, is the diameter of the graph G, and will be denoted by d.

The Wiener index is one of the oldest and most thoroughly studied distance based molecular structure descriptors [8,16]. Numerous of its chemical applications were reported (see e.g., [15,17]). Mathematical properties of the Wiener index are reasonably well understood (see the surveys [3,19,11], the recent papers [5,18,2,10,12,13], and the references cited therein).

In [6,7], the multiplicative version of the Wiener index of G was put forward as

$$\pi = \pi(G) = \prod_{\{v_i,v_j\}\subseteq V(G)} d_G(v_i, v_j)$$

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which can be written also as

$$\pi(G) = \prod_{k\geq 1} k^{d(G,k)}.$$

In [6,7], it was shown that in the case of alkanes there exists a very good correlation between π and W, and that there exists an (either linear or slightly curvilinear) correlation between π and W among a variety of classes of isomeric alkanes, monocycloalkanes, bicycloalkanes, benzenoid hydrocarbons, and phenylenes. Recently, Hua et al. [9] studied the mathematical properties of the multiplicative Wiener index.

From the definition of the indices W and π, we see that both depend on the distances between pairs of vertices. Therefore, it may be of some interest to compare them. This we do in the subsequent section.

2. Comparing Wiener and multiplicative Wiener indices

In this section we compare the Wiener and the multiplicative Wiener indices.

As usual, by P_n, C_n, K_n, and $K_{p,q},\ p+q=n$, we denote, respectively, the path, cycle, complete graph and complete bipartite graph of order n.

Directly from the definitions of W and π it follows:

$$W(K_n) = \binom{n}{2}, \qquad \pi(K_n) = 1$$

$$W(K_n-e) = \binom{n}{2} + 1, \qquad \pi(K_n-e) = 2$$

where $e \in E(K_n)$, and

$$W(K_{p,q}) = p^2 + pq + q^2 - (p+q), \qquad \pi(K_{p,q}) = 2^{[p(p-1)+q(q-1)]/2}. \tag{1}$$

For $G \cong C_4$, K_n or K_n-e, we have $\pi(G) < W(G)$. On the other hand, if $n \geq 5$, then $\pi(K_{n-1,1}) > W(K_{n-1,1})$. Therefore, in the general case π and W are incomparable.

It is easy to verify that among connected bipartite graphs of order n, the complete bipartite graph $K_{\lceil n/2\rceil,\lfloor n/2\rfloor}$ has minimal W– and π-values. As a special case of (1), we get

$$W\left(K_{\lceil n/2\rceil,\lfloor n/2\rfloor}\right) = n(n-1) - \left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor$$

and

$$\pi\left(K_{\lceil n/2\rceil,\lfloor n/2\rfloor}\right) = 2^{\left(n(n-1)/2-\lceil n/2\rceil\lfloor n/2\rfloor\right)}.$$

Bearing this in mind, we have the following result.

Theorem 1. *Let G be a bipartite graph of order $n > 4$. Then*

$$\pi(G) - W(G) \geq 2^{\left(n(n-1)/2-\lceil n/2\rceil\lfloor n/2\rfloor\right)} - n(n-1) + \left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor \tag{2}$$

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

Proof. Since G is bipartite, $m \leq \lceil n/2\rceil\lfloor n/2\rfloor$. We have to distinguish between the following two cases:

Case (i): $d = 2$. In this case $G \cong K_{p,q}$ $(p+q = n \geq 5,\ p \geq q)$. Thus we have $p \geq \lceil\frac{n}{2}\rceil$. Now, $m = pq$ and $d(G,2) = \frac{1}{2}[p(p-1)+q(q-1)]$. Thus,

$$m + d(G,2) = pq + \frac{1}{2}[p(p-1)+q(q-1)] = \frac{1}{2}\,n(n-1)$$

and

$$W(G) = n(n-1) - p(n-p); \qquad \pi(G) = 2^{\left(n(n-1)/2-p(n-p)\right)}.$$

Consider now the function

$$f(x) := 2^{\left(n(n-1)/2-x(n-x)\right)} - n(n-1) + x(n-x), \quad x \geq \left\lceil\frac{n}{2}\right\rceil$$

for which

$$f'(x) = (2x-n)\left[2^{\left(n(n-1)/2-x(n-x)\right)}\ \ln 2 - 1\right] \geq 0 \quad \text{as } x \geq \left\lceil\frac{n}{2}\right\rceil,\ n \geq 5.$$