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A Note on Comparison Between the Wiener Index and the Zagreb Indices

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Abstract: In this note, we correct a wrong result in a paper of Das *et al.* with regard to the comparison between the Wiener index and the Zagreb indices for trees (Das K C, Jeon H, Trinajstić N. The comparison between the Wiener index and the Zagreb indices and the eccentric connectivity index for trees. Discrete Appl. Math., 2014, 171: 35–41), and give a simple way to compare the Wiener index and the Zagreb indices for trees. Moreover, the comparison between the Wiener index and the Zagreb indices for unicyclic graphs is carried out.

Key words: Wiener index, Zagreb indice, tree, unicyclic graph

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1 Introduction

Throughout this paper, let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The order and size of G are defined as $n = |V(G)|$ and $m = |E(G)|$, respectively. For a simple connected graph G, if $m = n - 1$, then G is called a tree; if $m = n$, then G is called a unicyclic graph. The degree of a vertex $v_i \in V(G)$ in G is denoted by $d_G(v_i)$. The distance between two vertices v_i, $v_j \in V(G)$ is the length of the shortest path between v_i and v_j, denoted by $d_G(v_i, v_j)$.

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Molecular descriptors play an important role in mathematical chemistry, especially in the QSPR and QSAR modeling. Among them, a special place is reserved for the so called topological indices. Nowadays, there exists a legion of topological indices that found applications in various areas of chemistry (see [1]). Among the oldest and most studied topological indices, there are two classical vertex-degree based topological indices: the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$, which are defined, respectively, as

$$M_1(G) = \sum_{v_i \in V(G)} d_G(v_i)^2, \qquad M_2(G) = \sum_{v_i v_j \in E(G)} d_G(v_i) d_G(v_j).$$

Many works on the Zagreb indices have been proposed (see [1] and [2] and the references cited therein). Moreover, one of the oldest and most thoroughly studied distance based on molecular structure descriptors is the Wiener index (see [3] and [4]):

$$W(G) = \sum_{1 \le i < j \le n} d_G(v_i, v_j).$$

For details on the Wiener index see the review [5] and the references cited therein.

Recently, Das *et al.*[6] compared the Wiener index and the Zagreb indices for trees. However, we found that one of the main results in [6] was incorrect.

In this note, we correct the wrong result in [6] and give a simple way to compare the Wiener index and the Zagreb indices for trees. Besides, the comparison between the Wiener index and the Zagreb indices for unicyclic graphs is carried out.

2 Comparison Between the Wiener Index and the Zagreb Indices for Trees

Error 2.1 ([6], Corollary 2.3) *Let T be a tree of order n $(n > 3)$. Then $W(T) \ge M_1(T)$.*

As usual, we denote by $K_{1,n-1}$ (or S_n) the star of order n $(n \ge 2)$, P_n the path of order n $(n \ge 2)$, and C_n the cycle of order n $(n \ge 3)$, respectively. Denote by $DS_{p,q}$ $(p \ge q \ge 1$, $n = p + q + 2)$, a double star of order n $(n \ge 4)$ which is constructed by joining the central vertices of two stars $K_{1,p}$ and $K_{1,q}$. Other notations and terminology are not defined here which will conform to those in [7].

Example 2.1 *For the star S_n of order n $(n \ge 2)$,*

$$W(S_n) = (n-1)^2 < n(n-1) = M_1(S_n).$$

It can be seen that the star S_n $(n \ge 2)$ is a counter example for Corollary 2.3 in [6].

Lemma 2.1[8],[9] *Let $n \ge 4$, and T be a tree of order n. If $T \ncong S_n$, $DS_{n-3,1}$ (see Fig. 2.1), then $M_1(T) \le M_1(DS_{n-3,1}) < M_1(S_n)$, $M_2(T) < M_2(S_n)$.*

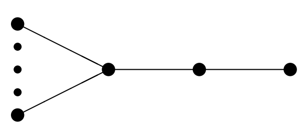

Fig. 2.1 $DS_{n-3,1}$