Discrete Applied Mathematics 171 (2014) 35–41

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

Comparison between the Wiener index and the Zagreb indices and the eccentric connectivity index for trees

Kinkar Ch. Das [a,*], Han-ul Jeon [a], Nenad Trinajstić [b]

[a] *Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea*

[b] *The Rugjer Bošković Institute, HR-10002 Zagreb, Croatia*

ARTICLE INFO

Article history:
Received 16 September 2013
Received in revised form 21 February 2014
Accepted 26 February 2014
Available online 18 March 2014

Keywords:
Graph
First Zagreb index
Second Zagreb index
Eccentric connectivity index
Wiener index
Diameter

ABSTRACT

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 Todeschini and Consonni (2000, 2009). Recently, we carried out comparison between several topological indices for various classes of graphs and trees (Das et al., 2012; Das and Trinajsti, 2010, 2011, 2012; Horoldagva and Das, 2012; Hua and Das, 2013). In this report, we compare the Wiener index and the Zagreb indices and the eccentric connectivity index for trees.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, we let $d_G(v_i)$ be the *degree* of a vertex v_i in G. The *maximum vertex degree* in G is denoted by $\Delta(G)$. For each $v_i \in V(G)$, the set of neighbors of the vertex v_i is denoted by $N_G(v_i)$. The distance between two vertices v_i and v_j in G, namely, the length of the shortest path between v_i and v_j is denoted by $d_G(v_i, v_j)$. The *eccentricity* of a vertex v_i in a graph G is defined to be $ec_G(v_i) = \max\{d_G(v_i, v_j) | v_j \in V(G)\}$. The *diameter* of a graph G, denoted by d, is the maximum distance between any two vertices of G.

Among the oldest and most studied topological indices, there are two classical vertex-degree based topological indices—the *first Zagreb index* and the *second Zagreb index*. These two indices first appeared in [14], and were elaborated in [13]. Later they were used in the structure–property modeling (see [27,28]). The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined, respectively, as

$$M_1(G) = \sum_{v_i \in V(G)} d_G(v_i)^2 = \sum_{v_i v_j \in E(G)} \Big(d_G(v_i) + d_G(v_j)\Big) \tag{1}$$

and

$$M_2(G) = \sum_{v_i v_j \in E(G)} d_G(v_i)\, d_G(v_j). \tag{2}$$

* Corresponding author. Tel.: +82 31 299 4528; fax: +82 31 290 7033.
E-mail addresses: kinkardas2003@googlemail.com, kinkar@lycos.com (K.Ch. Das), polychoron@naver.com (H.-u. Jeon), trina@irb.hr (N. Trinajstić).

http://dx.doi.org/10.1016/j.dam.2014.02.022

During the past decades, numerous results concerning Zagreb indices have been put forward, see [2,3,6,7,15,19,21,23,24,29,32] and the references cited therein.

One of the oldest and most thoroughly studied distance based molecular structure descriptors is the Wiener index [25,31]. Hosoya [16] produced the formula in which the sum of the distances between all pairs of vertices of a given graph G:

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

For details on the Wiener index see the review [11], the recent papers [5,30] and the references cited therein. Let e be an edge of the graph G (which may contain cycles or be acyclic), connecting the vertices v_i and v_j. Define two sets $N_i(e|G)$ and $N_j(e|G)$ as

$$N_i(e|G) = \{v_k \in V(G) | d(v_k, v_i|G) < d(v_k, v_j|G)\}$$
$$N_j(e|G) = \{v_k \in V(G) | d(v_k, v_j|G) < d(v_k, v_i|G)\}.$$

The number of elements of $N_i(e|G)$ and $N_j(e|G)$ are denoted by $n_i(e|G)$ and $n_j(e|G)$, respectively. Thus, $n_i(e|G)$ counts the vertices of G lying closer to the vertex v_i than to vertex v_j. The meaning of $n_j(e|G)$ is analogous. Vertices equidistant from both ends of the edge v_iv_j belong neither to $N_i(e|G)$ nor to $N_j(e|G)$. Note that for any edge e of G, $n_i(e|G) \ge 1$ and $n_j(e|G) \ge 1$, because $v_i \in N_i(e|G)$ and $v_j \in N_j(e|G)$. One long known property of the Wiener index is the formula [31]

$$W(T) = \sum_{v_iv_j \in E(T)} n_i(e|T)\, n_j(e|T). \tag{3}$$

The *eccentric connectivity index* (see [12,26]) of G, denoted by $\xi^c(G)$, is defined as

$$\xi^c(G) = \sum_{v_i \in V(G)} d_G(v_i) ec_G(v_i) = \sum_{v_iv_j \in E(G)} \Big(ec_G(v_i) + ec_G(v_j)\Big), \tag{4}$$

where $ec_G(v_i)$ is the eccentricity of v_i in G. The eccentric connectivity index provides good correlations with regard to both physical and biological properties (see [20]). The simplicity amalgamated with high correlating ability of this index can be easily exploited in QSPR/QSAR studies. Such studies can easily provide valuable leads for the development of potential therapeutic agents. For the mathematical properties of eccentric connectivity index, the reader is referred to [17,18,22] and the references cited therein.

Recently, Das and Trinajstić [9] compared the eccentric connectivity index and Zagreb indices for chemical trees and molecular graphs. In that paper it has been proved that for almost all chemical trees T, $M_i(T) \le \xi^c(T)$, $i = 1,\ 2$. Moreover, they showed that $M_1(G) < \xi^c(G)$ for each molecular graph G of diameter at least 7. However, the comparison between the eccentric connectivity index and Zagreb indices, in the case of general trees and general graphs, is very hard and remains unsolved till now. In [17], we compare the eccentric connectivity index and Zagreb indices for some graph families. Moreover, we carried out comparison between several topological indices for various classes of graphs and trees [6,8,10,15]. In this paper we continue our research in that direction. In this paper we compare the Wiener index with Zagreb indices for trees. Moreover, we compare the Wiener index with eccentric connectivity index for trees. As usual, we denote by $K_{1,\,n-1}$ the star of order n. Let S_n^* be the tree of order n with maximum degree $n-2$. Denote by $DS_{p,\,q}$ ($p \ge q$, $n = p+q+2$), a double star of order n which is constructed by joining the central vertices of two stars $K_{1,\,p}$ and $K_{1,\,q}$. In particular, $DS_{n-3,\,1} \cong S_n^*$. Other notation and terminology not defined here will conform to those in [1].

The paper is organized as follows. In Section 2, we compare between the Wiener index and Zagreb indices for trees. In Section 3, we compare between the Wiener index and eccentric connectivity index for trees.

2. Comparison between the Wiener index and Zagreb indices for trees

In this section we compare between the Wiener index and Zagreb indices for trees. For this we need the following result:

Lemma 2.1 (*[4]*). *Let $f(x) = x(n-x-k)$, k is any real number. Then $f(x)$ is an increasing function on $0 \le x \le (n-k)/2$ and a decreasing function on $x \ge (n-k)/2$.*

Now we are ready to compare between the Wiener index and first Zagreb index for trees.

Theorem 2.2. *Let T ($\ncong K_{1,\,n-1}$) be a tree of order n. Then*

$$W(T) \ge M_1(T) + 2(n-4) \tag{5}$$

with equality holding if and only if $T \cong S_n^*$ ($DS_{n-3,\,1} \cong S_n^*$).

Proof. Let d be the diameter of tree T. Since $T \ncong K_{1,\,n-1}$, then we have $d \ge 3$. We now consider two cases (i) $d = 3$ and (ii) $d \ge 4$.

Case (i): $d = 3$. If $T \cong S_n^*$, then $W(T) = n^2 - n - 2 = M_1(T) + 2(n-4)$ and hence the equality holds in (5). Otherwise, $T \ncong S_n^*$. In this case T must be a double star and hence $T \cong DS_{p,\,q}$, $p \ge q \ge 2$, $n = p+q+2$ (see Fig. 1). For $2 \le p \le 3$, we have $T \cong DS_{2,\,2}$ or $DS_{3,\,2}$ or $DS_{3,\,3}$ as $p \ge q \ge 2$. One can see easily that the inequality in (5) is strict for $DS_{2,\,2}$, $DS_{3,\,2}$ and $DS_{3,\,3}$.