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The relationship between the eccentric connectivity index and Zagreb indices

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ABSTRACT

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as follows:

$$M_1(G) = \sum_{v\in V(G)} (d_G(v))^2,$$

and

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v),$$

where $d_G(v)$ is the degree of vertex v in G. The eccentric connectivity index of a graph G, denoted by $\xi^c(G)$, is defined as

$$\xi^c(G) = \sum_{v\in V(G)} d_G(v)ec_G(v),$$

where $ec_G(v)$ is the eccentricity of v in G. Recently, Das and Trinajstić (2011) [11] compared the eccentric connectivity index and Zagreb indices for chemical trees and molecular graphs. 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 this paper, we compare the eccentric connectivity index and Zagreb indices for some graph families. We first give some sufficient conditions for a graph G satisfying $\xi^c(G) \le M_i(G), i = 1,\ 2$. Then we introduce two classes of composite graphs, each of which has larger eccentric connectivity index than the first Zagreb index, if the original graph has larger eccentric connectivity index than the first Zagreb index. As a consequence, we can construct infinite classes of graphs having larger eccentric connectivity index than the first Zagreb index.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. As usual, we use n to denote the order of a graph G, namely, the number of vertices in $V(G)$. For a graph G, we let $d_G(v)$ be the *degree* of a vertex v in G. The *maximum vertex degree* in G is denoted by $\Delta(G)$. For each $v \in V(G)$, the set of neighbors of the vertex v is denoted by $N_G(v)$. The distance between two vertices u and v in G, namely, the length of the shortest path between u and v is denoted by $d_G(u,\ v)$.

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The *eccentricity* of a vertex v in a graph G is defined to be $ec_G(v) = \max\{d_G(u, v)|u \in V(G)\}$. The *diameter* of a graph G, denoted by $d(G)$, is the maximum distance between any two vertices of G. The *average degree* of a graph G is denoted by $\overline{d}(G)$ and is defined by

$$\overline{d}(G) = \frac{\sum_{v \in V(G)} d_G(v)}{n}. \tag{1}$$

Therefore, the average degree of each graph containing n vertices and m edges is equal to $2m/n$.

Among the oldest and most studied topological indices, there are two classical vertex-degree based topological indices—the *first Zagreb index* and *second Zagreb index*. These two indices first appeared in [16], and were elaborated in [17]. Later they were used in the structure–property model (see [30]). The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined, respectively, as

$$M_1(G) = \sum_{v \in V(G)} (d_G(v))^2,$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v).$$

During the past decades, numerous results concerning Zagreb indices have been put forward, see [6,18,7–10,12,19,20,24,27,31,35,36] and the references cited therein.

The *eccentric connectivity index* (see [15,28,29]) of G, denoted by $\xi^c(G)$, is defined as

$$\xi^c(G) = \sum_{v \in V(G)} d_G(v)\, ec_G(v),$$

where $ec_G(v)$ is the eccentricity of v. The eccentric connectivity index provides good correlations with regard to both physical and biological properties (see [1,14,21,25]). 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 [2,22,26,37] and the references cited therein.

More recently, Das and Trinajstić [11] investigated the relation between the eccentric connectivity index and Zagreb indices for chemical trees and molecular graphs. They proved that for almost all chemical trees G, it holds that $\xi^c(G) \geq M_i(G)$, $i = 1, 2$. Moreover, they verified that for each molecular graph G of diameter at least 7, $\xi^c(G) > M_1(G)$. However, the comparison between eccentric connectivity index and Zagreb indices, in the case of general trees and general graphs, remains an open problem.

In this paper, we compare the eccentric connectivity index with Zagreb indices for some graph families. This paper is organized as follows. In Section 2, we give some sufficient conditions for a connected graph G satisfying $\xi^c(G) \leq M_i(G)$, $i = 1, 2$. In Section 3, we introduce two classes of composite graphs, each of which has larger eccentric connectivity index than first Zagreb index, if the original graph has larger eccentric connectivity index than first Zagreb index. As a consequence, we construct infinite classes of graphs having larger eccentric connectivity index than first Zagreb index.

Before proceeding, we introduce some further notation and terminology. A connected graph with maximum vertex degree not exceeding 4 is said to be a *molecular graph*. A tree in which the maximum vertex degree does not exceed 4 is said to be a *chemical tree*. As usual, we denote by P_n, $K_{1,\,n-1}$, C_n and K_n the path, star, cycle and complete graph of order n, respectively. Denote by $DS_{p+1,q+1}$ $(p \geq q)$, a double star which is constructed by joining the central vertices of two stars $K_{1,\,p}$ and $K_{1,\,q}$. Other notation and terminology not defined here will conform to those in [3].

2. Graphs satisfying $\xi^c(G) \leq M_i(G)$ for $i = 1, 2$

In this section, we give some sufficient conditions for a connected graph G satisfying $\xi^c(G) \leq M_i(G)$ for $i = 1, 2$.

From the definition of the eccentric connectivity index and first Zagreb index, we can rewrite them as

$$\xi^c(G) = \sum_{uv \in E(G)} (ec_G(u) + ec_G(v)) \tag{2}$$

and

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)), \tag{3}$$

respectively.

In fact, by (2), we know that each edge uv contributes $ec_G(u)$ and $ec_G(v)$ to eccentricity connectivity index, respectively. So, all edges incident to u contribute $d_G(u)ec_G(u)$ to the eccentricity connectivity index and all edges incident to v contribute $d_G(v)ec_G(v)$ to eccentricity connectivity index, respectively. Therefore, for each vertex x in G, it contributes $d_G(x)ec_G(x)$ to eccentricity connectivity index. Summing the contributions of all vertices, we get the required formula given in Section 1 for eccentricity connectivity index. Similarly, we can get formula (3) for first Zagreb index.