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On two eccentricity-based topological indices of graphs

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ABSTRACT

For a connected graph G, the eccentric connectivity index (ECI) and connective eccentricity index (CEI) of G are, respectively, defined as $\xi^c(G) = \sum_{v_i \in V(G)} \deg_G(v_i)\varepsilon_G(v_i)$, $\xi^{ce}(G) = \sum_{v_i \in V(G)} \frac{\deg_G(v_i)}{\varepsilon_G(v_i)}$ where $\deg_G(v_i)$ is the degree of v_i in G and $\varepsilon_G(v_i)$ denotes the eccentricity of vertex v_i in G. In this paper we study on the difference of ECI and CEI of graphs G, denoted by $\xi^D(G) = \xi^c(G) - \xi^{ce}(G)$. We determine the upper and lower bounds on $\xi^D(T)$ and the corresponding extremal trees among all trees of order n. Moreover, the extremal trees with respect to ξ^D are completely characterized among all trees with given diameter d. And we also characterize some extremal general graphs with respect to ξ^D. Finally we propose that some comparative relations between CEI and ECI are proposed on general graphs with given number of pendant vertices.

1. Introduction

We only consider finite, undirected and simple graphs throughout this paper. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots\ldots, v_n\}$ and edge set $E(G)$. The *degree* of $v_i \in V(G)$, denoted by $\deg_G(v_i)$, is the number of vertices in G adjacent to v. For any two vertices v_i, v_j in a graph G, the distance between them, denoted by $d_G(v_i, v_j)$, is the length of a shortest path connecting them in G. Other undefined notations and terminology on the graph theory can be found in [5].

For any vertex of graph G, the eccentricity $\varepsilon_G(v_i)$ is the maximum distance from v_i to other vertices of G, i.e., $\varepsilon_G(v_i) = \max_{v_j \neq v_i} d_G(v_i, v_j)$. If $\varepsilon_G(v_i) = d_G(v_i, v_j)$, then v_j is an *eccentric vertex* of vertex v_i. Moreover, $rad(G) = \min_{v_i \in V(G)}\{\varepsilon_G(v_i)\}$ and $diam(G) = \max_{v_i \in V(G)}\{\varepsilon_G(v_i)\}$ are called the *radius* and the *diameter* of graph G, respectively. The *center* $C(G)$ and the *periphery* $P(G)$ of G are the sets of vertices of minimum, respectively maximum, eccentricity in it, their elements being called *central* resp. *peripheral vertices*. The *eccentricity sequence* of a graph G is just a set of eccentricities of its vertices, that is, $\mathcal{E}(G) = \{\varepsilon_G(v_i) : v_i \in V(G)\}$. If the eccentricity $\varepsilon_G(v_i)$ appears $l_i \geq 1$ times in $\mathcal{E}(G)$, we will write $e_G(v_i)^{(l_i)}$ in it for short. For any graph G, we denote by $\overline{G}$ the complement of G. As usual, let P_n, C_n, and K_n be the path graph, cycle graph, and complete graph, respectively, on n vertices.

As a special distance of graphs, eccentricity of a vertex has some important application in other scientific branches. In pure graph theory, there are several special eccentricity-based graphs. Any graph G with $C(G) = V(G)$ is called a self-centered graph [6]. Recently, based on the application of vertex eccentricity to location theory, two novel classes of graphs with specific central structure have been defined. A graph with $|C(G)| = |V(G)| - 2$ or $|P(G)| = |V(G)| - 1$ is called an *almost self-centered (ASC) graph* [4,22] or *almost-peripheral (AP) graph* [23], respectively. An ASC (AP, resp.) graph with radius r is called an r-ASC (r-AP, resp.) graph. A graph G with $|C(G)| = |V(G)| - 2$ is called a weak almost-peripheral (WAP) graph [35].

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In chemical graph theory, various graphical invariants are used for establishing correlations of chemical structures with various physical properties, chemical reactivity, or biological activity. These graphical invariants are called topological indices of (molecular) graphs in this field. There are some eccentricity-based topological indices in chemical graph theory. In 2000, Gupta et al. [13] introduced a novel, adjacency-cum-path length based, topological descriptor named as connective eccentricity index (CEI) when investigating the antihypertensive activity of derivatives of N-benzylimidazole. They showed that the results obtained using the connective eccentricity index were better than the corresponding values obtained using Balabans mean square distance index [2,3] and the accuracy of prediction was found to be about 80 percents in the active range [13]. Moreover, Sharma et al. [30] introduced the eccentric connectivity index, for a graph, which has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature [12,29,30]. Some nice results on other attractive distance-based topological indices of graphs can be found in a survey paper [37] and the reference therein.

In 1997, Sharma, Goswami and Madan [30] introduced a distance-based molecular structure descriptor, which is named as "eccentric connectivity index" and defined as

$$\xi^c(G) = \sum_{v_i \in V(G)} \deg_G(v_i)\varepsilon_G(v_i).$$

The eccentric connectivity index (ECI) has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature [11,28,29]. The ECI also can be written as follows:

$$\xi^c(G) = \sum_{v_i v_j \in E(G)} \big(\varepsilon_G(v_i) + \varepsilon_G(v_j)\big).$$

Some properties of ECI have been reported in [7,19,26,42].

In 2000, the connective eccentricity index (CEI) $\xi^{ce}(G)$ of a graph G was introduced in [13], which is defined as

$$\xi^{ce}(G) = \sum_{v_i \in V(G)} \frac{deg_G(v_i)}{\varepsilon_G(v_i)}.$$

Clearly, the CEI can also be rewritten in the following way:

$$\xi^{ce}(G) = \sum_{v_i v_j \in E(G)} \Big(\frac{1}{\varepsilon_G(v_i)} + \frac{1}{\varepsilon_G(v_j)}\Big).$$

Some recent results on the CEI of graphs can be found in [1,34,38,40]. For some recent results on other eccentricity-based graph invariants, please see [10,14,24,25,31,32,36,39].

From the definitions, we have $\xi^c(G) \geq \xi^{ce}(G)$ for any connected graph G of order $n > 1$ with equality holding if and only if $G \cong K_n$. We denote by $\xi^D(G)$ the difference between ECI and CEI of connected graphs G, that is, $\xi^D(G) = \xi^c(G) - \xi^{ce}(G)$. For some results on the difference between other distance-based graph invariants, please see [21]. The nth harmonic number is $H_n = \sum_{k=1}^{n} \frac{1}{k}$. For any two integers n and d with $1 \leq d \leq n-1$, let $\mathcal{T}_n(d)$ be the set of trees of order n and with diameter d.

The paper is organized as follows. In Section 2, we first determined the extremal (minimum and maximum) trees of order n with respect to ξ^D. Also the extremal trees are characterized with minimum and maximum values of ξ^D, respectively, among all trees from $\mathcal{T}_n(d)$. Using this result, we determine the trees with second minimum and second maximum value of ξ^D among all trees of order n. In Section 3, we deal with some extremal general graphs with respect to ξ^D, including connected graphs of order n, the graphs with given minimum degree, the graphs with diameter 2, and the graphs with exactly two distinct eccentricities. In Section 4, we establish some comparative relations between CEI and ECI of general graphs with given number of pendant vertices.

2. The ξ^D of trees

In this section we characterize the extremal (minimal and maximal) trees of order n with respect to ξ^D. Also the trees from $\mathcal{T}_n(d)$ with minimum and maximum ξ^D are determined, respectively. By using this result, we determine, respectively, the trees of order $n \geq 6$ with second minimum and second maximum ξ^D.

Theorem 2.1. *Let T be a tree order $n \geq 4$. Then*

$$\frac{3}{2}(n-1) \leq \xi^D(T) \leq \begin{cases} \frac{3}{2}(n-1)^2 + \frac{n+3}{2(n-1)} - 4\big(H_{n-1} - H_{\frac{n}{2}-1}\big), & n \geq 4 \text{ is even}; \\ \frac{3}{2}(n-1)^2 - \frac{2}{n-1} - 4\big(H_{n-1} - H_{\frac{n-1}{2}}\big), & n \geq 5 \text{ is odd} \end{cases}$$

with left equality holding if and only if $T \cong S_n$, right equality holding if and only if $T \cong P_n$.