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On the extremal total reciprocal edge-eccentricity of trees ☆

Shuchao Li, Lifang Zhao *

Faculty of Mathematics and Statistics, Central China Normal University, Wuhan 430079, PR China

A R T I C L E I N F O

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A B S T R A C T

The total reciprocal edge-eccentricity is a novel graph invariant with vast potential in structure activity/property relationships. This graph invariant displays high discriminating power with respect to both biological activity and physical properties. If $G = (V_G, E_G)$ is a simple connected graph, then the total reciprocal edge-eccentricity (REE) of G is defined as $\xi^{ee}(G) = \sum_{uv \in E_G}(1/\varepsilon_G(u) + 1/\varepsilon_G(v))$, where $\varepsilon_G(v)$ is the eccentricity of the vertex v. In this paper we first introduced four edge-grafting transformations to study the mathematical properties of the reciprocal edge-eccentricity of G. Using these elegant mathematical properties, we characterize the extremal graphs among n-vertex trees with given graphic parameters, such as pendants, matching number, domination number, diameter, vertex bipartition, et al. Some sharp bounds on the reciprocal edge-eccentricity of trees are determined.

1. Introduction

Throughout this paper, we only consider simple connected graph $G = (V_G, E_G)$ on n vertices and m edges (so $n = |V_G|$ is its order, and $m = |E_G|$ is its size). The *distance* between two vertices u, v of G, written $d_G(u, v)$, is the length of a shortest u–v path in G. The *eccentricity* $\varepsilon_G(v)$ of a vertex v is the distance between v and a furthest vertex from v in G. For any edge $e = uv \in E_G$, we may define *edge-eccentricity* of e as $\mathrm{ec}(e) = \varepsilon_G(u) + \varepsilon_G(v)$; whereas its *reciprocal edge-eccentricity* is defined as $\mathrm{ree}(e) = \frac{1}{\varepsilon_G(u)} + \frac{1}{\varepsilon_G(v)}$. When the graph is clear from the context, we will omit the subscript G from the notation. We follow the notation and terminology in [3] except if otherwise stated.

Molecular descriptors play an important role in mathematical chemistry, especially in the QSPR and QSAR modeling [1]. Among them, a special place is reserved for the so-called topological indices, or graph invariant. The well-studied distance-based graph invariant probably is the *Wiener index* [35], one of the most well used chemical indices that correlate a chemical compound's structure with the compound's physical–

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* Corresponding author.
E-mail addresses: lscmath@mail.ccnu.edu.cn (S. Li), zhaolfmath@163.com (L. Zhao).

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chemical properties. The Wiener index, introduced in 1947, is defined as the sum of distances between all pairs of vertices, namely that

$$W(G) = \sum_{\{u,v\} \subseteq V_G} d_G(u, v).$$

For more results on Wiener index one may be referred to those in [10,23,24,32] and the references cited therein.

Another distance-based graph invariant, defined [18,31] in a fully analogous manner to Wiener index, is the *Harary index*, which is equal to the sum of reciprocal distances over all unordered vertex pairs in G, that is,

$$H(G) = \sum_{\{u,v\} \subseteq V_G} \frac{1}{d_G(u, v)}.$$

For more results on Harary index, one may be referred to [5,17,21,27,31,36].

More recently, the distance-based graph invariants involving eccentricity have attracted much attention. These graph invariants mainly include the average eccentricity [4], the superaugmented eccentric connectivity index [7], the reformed eccentric connectivity index [20], the eccentric distance sum [11], augmented eccentric connectivity index [33], etc. In particular, the *average eccentricity* [4,6,14,15], and the *eccentric distance sum* [10] of the graph G, written by $\xi(G)$ and $\xi^d(G)$ are defined, respectively, as

$$\xi(G) = \frac{1}{n} \sum_{u \in V_G} \varepsilon_G(u), \qquad \xi^d(G) = \sum_{\{u,v\} \subseteq V_G} (\varepsilon_G(u) + \varepsilon_G(v)) d_G(u, v).$$

Recently, mathematical properties of the eccentric distance sum of graphs have been studied. Mukungunugwa and Mukwembi [30] obtained the asymptotically sharp upper bounds on $\xi^d(G)$ with respect to the order and minimal degree of G. Geng, Zhang and one of the present authors [8] studied the relationship between ξ^d and some other parameters, such as domination number, pendants and so on of trees. For more results on $\xi^d(G)$, one may be referred to [16,25,26,28] and the references therein.

The *total edge-eccentricity* of a graph G is defined as

$$\xi^c(G) = \sum_{e=uv \in E_G} (\varepsilon_G(u) + \varepsilon_G(v)).$$

The total edge-eccentricity of the graph G can be defined alternatively as

$$\xi^c(G) = \sum_{u \in V_G} \varepsilon_G(u) d_G(u).$$

This graph invariant is just the *eccentric connectivity index*, which is a distance-based molecular structure descriptor, proposed by Sharma, Goswami and Madan [34] in 1997. The index $\xi^c(G)$ was successfully used for mathematical models of biological activities of diverse nature [7,9]. For the study of its mathematical properties one may be referred to [12,15,29] and the references therein.

Bearing in mind that the relation between Wiener index and Harary index, we study here a novel graph invariant named the *total reciprocal edge-eccentricity* (REE), i.e.,

$$\xi^{ee}(G) = \sum_{e=uv \in E_G} \left(\frac{1}{\varepsilon_G(u)} + \frac{1}{\varepsilon_G(v)} \right),$$

which can be defined alternatively as

$$\xi^{ee}(G) = \sum_{u \in V_G} \frac{d_G(u)}{\varepsilon_G(u)}.$$