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Further results on the eccentric distance sum

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ABSTRACT

The eccentric distance sum (EDS) is a novel graph invariant which can be used to predict biological and physical properties, and has a vast potential in structure activity/property relationships. For a connected graph *G*, its EDS is defined as $\xi^d(G) = \sum_{v \in V(G)} ecc_G(v)D_G(v)$, where $ecc_G(v)$ is the eccentricity of a vertex v in *G* and $D_G(v)$ is the sum of distances of all vertices in *G* from v. In this paper, we obtain some further results on EDS. We first give some new lower and upper bounds for EDS in terms of other graph invariants. Then we present two Nordhaus–Gaddum-type results for EDS. Moreover, for a given nontrivial connected graph, we give explicit formulae for EDS of its double graph and extended double cover, respectively. Finally, for all possible k values, we characterize the graphs with the minimum EDS within all connected graphs on n vertices with k cut edges and all graphs on n vertices with edge-connectivity k, respectively.

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1. Introduction

Let *G* be a simple connected graph with the vertex set *V*(*G*). For a graph *G*, let deg_{*G*}(*v*) be the degree of a vertex *v* in *G*, $\delta(G) = \min\{\deg_G(v)|v \in V(G)\}$ and $\Delta(G) = \max\{\deg_G(v)|v \in V(G)\}$. For $S \subseteq V(G)$, we use *G*[*S*] to denote the subgraph of *G* induced by *S*. The distance between two vertices *u* and *v*, namely, the length of the shortest path between *u* and *v*, in a graph *G* is denoted by $d_G(u, v)$. The *eccentricity* of a vertex *v* in a connected graph *G* is defined as $ecc_G(v) = \max\{d_G(v, u)|u \in V(G)\}$. Let $D_G(v)$ be the sum of distances of all vertices in *G* from *v*, that is, $D_G(v) = \sum_{u \in V(G)} d_G(v, u)$. Denote by P_n, S_n, C_n and K_n the path, star, cycle and complete graph on *n* vertices, respectively. For other notation and terminology not defined here, the reader is referred to [3].

Recently, two eccentricity-based topological indices, the eccentric connectivity index (ECI), defined as [17]:

$$\xi^{c}(G) = \sum_{v \in V(G)} \operatorname{ecc}_{G}(v) \operatorname{deg}_{G}(v)$$

and the eccentric distance sum (EDS), defined as [9]:

$$\xi^{d}(G) = \sum_{v \in V(G)} \operatorname{ecc}_{G}(v) D_{G}(v)$$

were proposed and studied.

The ECI was successfully used for mathematical models of biological activities of diverse nature [8,15–17]. For the mathematical properties of ECI, see [2,13,20] and a recent survey [12].

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The EDS was a novel distance-based molecular structure descriptor which can be used to predict biological and physical properties. It has a vast potential in structure activity/property relationships. The authors [9] have shown that some structure activity and quantitative structure-property studies using eccentric distance sum were better than the corresponding values obtained by using the Wiener index [6,7,10], defined as

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \frac{1}{2} \sum_{v\in V(G)} D_G(v).$$

More recently, the mathematical properties of EDS have been investigated [11,14,18]. Yu et al. [18] characterized the extremal tree and unicyclic graph with respect to EDS among all *n*-vertex trees and unicyclic graphs, respectively. Ilić et al. [14] gave explicit formulae for EDS of the Cartesian graph product and some lower and upper bounds for EDS in terms of other graph invariants, such as the Wiener index, the degree distance, eccentric connectivity index, independence number, connectivity, and so on. Hua et al. [11] gave a short and unified proof of Yu et al.'s results on the EDS of trees and unicyclic graphs.

This paper is organized as follows. In Section 2, we give some new lower and upper bounds for EDS in terms of other graph invariants. In Section 3, we present two Nordhaus-Gaddum-type results for EDS. In Section 4, for a given nontrivial connected graph, we give explicit formulae for EDS of its double graph and extended double cover, respectively. In Section 5, for all possible k values, we characterize the graphs with the minimum EDS within all connected graphs on n vertices with k cut edges and all graphs on n vertices with edge-connectivity k, respectively.

2. Lower and upper bounds

In this section, we give some lower and upper bounds for EDS of connected graphs in terms of some graph invariants. such as, the degree sequence, the number of pendent vertices and the Wiener index, and so on.

Theorem 1. Let *G* be a connected graph on n > 2 vertices. Then

$$\xi^{d}(G) \ge \frac{4}{n(n-1)} (W(G))^{2},$$

with equality if and only if $G \cong K_n$.

Proof. By the definition of eccentricity, for any vertex $u \in V(G) \setminus \{v\}$, we have $ec_G(v) > d_G(u, v)$. Thus,

$$\xi^{d}(G) = \frac{1}{n-1} \sum_{v \in V(G)} [(n-1) \operatorname{ecc}_{G}(v)] D_{G}(v)$$

$$\geq \frac{1}{n-1} \sum_{v \in V(G)} (D_{G}(v))^{2}$$

$$\geq \frac{1}{n(n-1)} \left(\sum_{v \in V(G)} D_{G}(v) \right)^{2}$$

$$= \frac{4}{n(n-1)} (W(G))^{2}.$$

On one hand, the equality holds in the above first inequality only if $ecc_G(v) = d_G(u, v)$ for each vertex v and any $u \in V(G) \setminus \{v\}$, that is, $\operatorname{ecc}_G(v) = d_G(u, v) = 1$. The equality holds in the above second inequality only if $D_G(v)$ is a constant. So, we have $\xi^d(G) \ge \frac{4}{n(n-1)}(W(G))^2$, with equality only if G is K_n . On the other hand, if G is K_n , then $\xi^d(G) = n(n-1) = \frac{4}{n(n-1)}(W(G))^2$, as $W(G) = \frac{n(n-1)}{2}$. This completes the proof. \Box

Recall that the *Harary index* [5,7,19] is defined as $H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u,v)}$. From this definition, we immediately have $W(G) \ge H(G)$, with the equality if and only if $G \cong K_n$. Then by Theorem 1, we have

Corollary 1. Let G be a connected graph on $n \ge 2$ vertices. Then

$$\xi^{d}(G) \ge \frac{4}{n(n-1)}(H(G))^{2},$$

with equality if and only if $G \cong K_n$.

Theorem 2. Let *G* be a connected graph on $n \ge 2$ vertices with degree sequence (d_1, d_2, \ldots, d_n) . Then

$$\xi^{d}(G) \leq (n-1) \sum_{i=1}^{n} (n-d_{i})^{2},$$

with equality if and only if $d_1 = d_2 = \cdots = d_n = n - 1$, that is, $G \cong K_n$.

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