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Bounds for the Adjacent Eccentric Distance Sum

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Abstract

The adjacent eccentric distance sum index of a graph G is defined as $\xi^{sv}(G) = \sum_{v \in V(G)} \frac{\varepsilon(v)D(v)}{deg(v)}$, where $\varepsilon(v)$, $deg(v)$ denote the eccentricity, the degree of the vertex v, respectively, and $D(v) = \sum_{u \in V(G)} d(u, v)$ is the sum of all distances from the vertex v. In this paper we derive some upper or lower bounds for the adjacent eccentric distance sum in terms of some graph invariants or topological indices such as Wiener index, total eccentricity and minimum degree.

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1 Introduction

Throughout this paper, all graphs considered are simple and connected. Let $G = (V(G), E(G))$ be a simple connected graph with n vertices and m edges. For a vertex $v \in V(G)$, $deg(v)$ denotes the degree of v. $\delta(G)$, $\Delta(G)$ represent the minimum and maximum degree of G, respectively. For vertices $u, v \in V(G)$, the *distance* $d(u, v)$ is defined as the length of the shortest path between u and v in G and $D_G(v)$ (or $D(v)$ for short) denotes the sum of all distances

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from v. The *eccentricity* $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. The *radius* $r(G)$ of a graph is the minimum eccentricity of any vertex, while the *diameter* $D(G)$ of a graph is the maximum eccentricity of any vertex in the graph. Let K_n and P_n be a complete graph and a path on n vertices, respectively.

In organic chemistry, topological indices have been found to be useful in chemical documentation, isomer discrimination, structure-property relationships, structure-activity (SAR) relationships and pharmaceutical drug design. These indices include Wiener index [16, 17], Balahan's index [2], Randić index [13] and so on. In recent years, some indices have been derived related to eccentricity such as eccentric connectivity index [7, 12], eccentric distance sum [8], augmented and super augmented eccentric connectivity indices [1, 6], adjacent eccentric distance sum index [14, 15].

The Wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds (for a recent survey on Wiener index see [4]). The *Wiener index* of a graph G, denoted by $W(G)$, is defined as the sum of the distances between all pairs of vertices in graph G, that is, $W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) = \frac{1}{2}\sum_{v\in V(G)} D(v)$. The parameter $DD(G)$ is called the *degree distance* of G and it was introduced by Dobrynin and Kochetova [5] and Gutman [9] as a graph-theoretical descriptor for characterizing alkanes; it can be considered as a weighted version of the Wiener index

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} (deg(u) + deg(v))d(u,v) = \sum_{v\in V(G)} deg(v)\cdot D(v),$$

When G is a tree on n vertices, it has been demonstrated that Wiener index and degree distance are closely related by (see [10]) $DD(G) = 4W(G) - n(n-1)$.

The *total eccentricity* of the graph G (see [3]), denoted by $\zeta(G)$, is defined as the sum of eccentricities of all vertices of graph G, i.e., $\zeta(G) = \sum_{v\in V(G)} \varepsilon(v)$.

The eccentric distance sum of G (EDS) is defined as [8] $\xi^d(G) = \sum_{v\in V(G)} \varepsilon(v)D(v)$.

More recently, the mathematical properties of eccentric distance sum have been investigated. In [11, 18], the authors studied the eccentric distance sum of trees, unicyclic graph with given girth and established some lower and upper bounds for the eccentric distance sum in terms of some graph invariants.

In [14], Sardana and Madan introduced a novel topological descriptor–adjacent eccentric distance sum index (AEDS), which is defined to be

$$\xi^{sv}(G) = \sum_{v\in V(G)} \frac{\varepsilon(v)D(v)}{deg(v)}.$$

Moreover, Sardana and Madan [15] investigated the relationship of Wiener index and adjacent eccentric distance sum index with nitroxide free radicals and their precursors. They shown that high degree of predictions ranges from 0.85 for Wiener index to 0.87 for adjacent eccentric distance sum index. These results promote us to study the mathematical properties of this novel topological descriptor.

In this paper we derive some upper or lower bounds for the adjacent eccentric distance sum in terms of some graph invariants or topological indices such as Wiener index, total eccentricity and minimum degree.

2 Bounds for AEDS in terms of some topological indices

Let $K_n - ke$ be the graph obtained from K_n by deleting k independent edges for $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

Theorem 2.1 *Let G be a connected graph on n vertices. Let n_0 be the number of vertices with eccentricity 1 in graph G. Then*

$$\xi^{sv}(G) \geq n_0 + \frac{2n(n-n_0)}{n-2},$$

with equality holding if and only if $G \cong K_n - \frac{n-n_0}{2}e$, $n - n_0$ is even.

Proof. Let $S = \{v_1, v_2, \cdots, v_{n_0}\}$ be the set of vertices with eccentricity 1. It follows that $\varepsilon(v) = 1$ for any $v \in S$ and $\varepsilon(u) \geq 2$, $deg(u) \leq n-2$ for any $u \in V(G) \setminus S$. By the definition of AEDS, we have

$$\begin{aligned}
\xi^{sv}(G) &= \sum_{i=1}^{n_0} \frac{\varepsilon(v_i)D(v_i)}{deg(v_i)} + \sum_{v \in V(G)\setminus S} \frac{\varepsilon(v)D(v)}{deg(v)} \\
&\geq n_0 + \frac{2}{n-2} \sum_{v \in V(G)\setminus S} D(v) \\
&\geq n_0 + \frac{2}{n-2} \sum_{v \in V(G)\setminus S} \big((n-2)+2\big) \\
&= n_0 + \frac{2n(n-n_0)}{n-2}.
\end{aligned}$$

The above equalities hold simultaneously if and only if $\varepsilon(v) = 2$ and $deg(v) = n-2$ for any vertices $v \in V(G) \setminus S$, i.e., $G \cong K_n - \frac{n-n_0}{2}e$, $n - n_0$ is even. ■

Theorem 2.2 *Let G be a connected graph on $n \geq 3$ vertices. Then*

$$\xi^{sv}(G) \geq \zeta(G),$$

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

Proof. Note that $D(v) \geq deg(v)$, with equality if and only if $\varepsilon(v) = 1$. Therefore we have

$$\xi^{sv}(G) \geq \sum_{v \in V(G)} \frac{\varepsilon(v) deg(v)}{deg(v)} = \sum_{v \in V(G)} \varepsilon(v) = \zeta(G),$$

with equality if and only if $\varepsilon(v) = 1$ and $deg(v) = n-1$ for any $v \in V(G)$, i.e., $G \cong K_n$. This implies the result. ■

Theorem 2.3 *Let G be a connected graph on $n \geq 3$ vertices with minimum degree δ. Then*

$$\xi^{sv}(G) \leq \frac{2(n-\delta)}{\delta} W(G),$$

with equality holding if and only if $G \cong K_n$, or $G \cong K_n - \frac{n}{2}e$ for even n.

Proof. It is evident that $\varepsilon(v) \leq n - deg(v)$. So we have

$$\begin{aligned} \xi^{sv}(G) &= \sum_{v \in V(G)} \frac{\varepsilon(v) D(v)}{deg(v)} \\ &\leq \sum_{v \in V(G)} \frac{(n - deg(v)) D(v)}{deg(v)} \qquad (1) \\ &\leq \sum_{v \in V(G)} \frac{(n-\delta) D(v)}{\delta} \qquad (2) \\ &= \frac{2(n-\delta)}{\delta} W(G). \end{aligned}$$

If the equality holds in this theorem, then both (1) and (2) must be equalities. Let $n_i(v)$ be the number of vertices at distance i from the vertex v. It is evident that the equality in (1) holds if and only if $\varepsilon(v) = 1$ and $deg(v) = n-1$, or $\varepsilon(v) \geq 2$ and $n_2(v) = n_3(v) = \cdots = n_{\varepsilon(v)}(v) = 1$. The equality in (2) holds if and only if $deg(v) = \delta$ for any vertex v, that is, G is regular with degree δ.

If $\varepsilon(v) = 1$ and $deg(v) = n-1$ for any $v \in V(G)$, then $G \cong K_n$

If $\varepsilon(v) = 2$ and $deg(v) = n-2$ for any vertex $v \in V(G)$, then $G \cong K_n - \frac{n}{2}e$ for even n.

If $\varepsilon(v) = 2$ and $deg(v) \leq n-3$ for some vertex $v \in V(G)$, then there is no such regular graphs.

If there exists some vertex $u \in V(G)$ such that $\varepsilon(u) \geq 3$. Then the diameter of G is 3. In fact, assume to the contrary that there exists an induced path P with length $D(G) > 3$ in G. Then there exists some vertex $u_i \in V(P)$ such that $\varepsilon(u_i) \geq 2$ and $n_2(u_i) \geq 2$. This contradicts that $n_2(u_i) = 1$. Since $n_2(u) = n_3(u) = \cdots = n_{\varepsilon(u)}(u) = 1$, then $G \cong P_4$. This contradicts that G is regular.

The converse is easy to check. ■

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