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Eccentric distance sum index for some classes of connected graphs

ABSTRACT. In this paper we show some properties of the eccentric distance sum index which is defined as follows $\xi^d(G) = \sum_{v \in V(G)} D(v)\varepsilon(v)$. This index is widely used by chemists and biologists in their researches. We present a lower bound of this index for a new class of graphs.

1. Introduction. In this paper we will be considering simple and connected graphs. We will start with a few definitions. Let $G = (V(G), E(G))$ be a simple connected graph of order $n = |V(G)|$ and size $m = |E(G)|$.

For a vertex $v \in V(G)$, we denote a set of neighbours of v by $N(v)$. Degree is denoted by $\deg(v)$ and defined as $\deg(v) = |N(v)|$. Vertex of degree equal to 1 is called a pendant vertex. For vertices $u, v \in V(G)$, we define a distance $d(u, v)$ as the length of the shortest path between u and v. What is more, $D(v)$ denotes the sum of all distances from the vertex v. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum of distances between v and all other vertices. The minimum eccentricity over all vertices is denoted by $\mathrm{rad}(G)$ and called the radius of the graph G, while the maximum eccentricity is denoted by $\mathrm{diam}(G)$ and called the diameter of the graph G.

Let K_n be a complete graph and P_n be a path on n vertices. For graphs G and H we denote the join operation by $G + H$ and by $G \cup H$ we mean a disjoint sum of those graphs.

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A vertex in a graph is called a cutpoint when the number of components in a graph increases after removal of this vertex. Graph which is connected, nontrivial and has no cutpoints is called nonseparable graph. A block of a graph G is a maximal nonseparable subgraph of G. A cactus is a connected graph, each of whose block is isomorphic to a cycle or a path of order 2. A spanning tree of a connected graph G is a subtree of G which includes all of the vertices of G. Not defined notations one can find in [1].

The eccentric distance sum index is defined as follows:

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

The eccentric distance sum index was introduced in 2002 by Gupta, Singh and Madana [2]. The authors showed that this graph invariant can be used for predicting some biological and physical properties. It has a vast potential in quantitative structure-activity relationship. Some structure-activity studies using the eccentric distance sum index were proved [2] to be better than the corresponding values obtained using the Wiener index of a graph defined in 1947 [6] as:

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

The eccentric distance sum index properties were studied recently. Yu, Feng and Ilić [7] described the extremal tree with respect to the eccentric distance sum index among all n-vertex trees. They proved it also for unicyclic graphs. Hua, Xu, Wen [4] gave then a short and unified proof of their results.

Ilić, Yu and Feng [5] showed also some lower and upper bounds for the eccentric distance sum index in terms of the Wiener index, degree distance and some other graph invariants.

2. Eccentric distance sum index for cacti and some other classes of connected graphs. In this section there is a research done for lower bound of the eccentric distance sum index for some generalization of cacti. In Theorem 2.1 we present an interesting result of Hua, Xu and Wen [4] for cacti.

Theorem 2.1 (Hua, Xu and Wen [4]). *Let G be a cactus with $n \geq 4$ vertices and $k_2 \geq 0$ cycles. Then $\xi^d(G) \geq 4n^2 - 9n - 4k_2 + 5$, with the equality if and only if $G \cong Cat_{n,k_2}$, where Cat_{n,k_2} is the cactus obtained by introducing k_2 independent edges among pendant vertices of n-vertex star $K_{1,n-1}$.*

Lemma 2.2. *Let G be a graph of order n and size m. If* $\operatorname{rad}(G) \geq 2$, *then*

$$\xi^d(G) \geq 4n(n-1) - 4m$$

with equality holding if and only if $\operatorname{rad}(G) = 2$.

Proof. By the definition of the eccentric distance sum index:

$$\begin{aligned}\xi^d(G) \geq 2\sum_{v\in V(G)} D(v) &= 2\Big(\sum_{v\in V(G)}\deg(v) + \sum_{v\in V(G)}\sum_{u\in V(G)\setminus N(v)} d(v,u)\Big)\\ &\geq 2\Big(\sum_{v\in V(G)}\deg(v) + \sum_{v\in V(G)}\sum_{u\in V(G)\setminus N(v)} 2\Big)\\ &= 2\Big[\sum_{v\in V(G)}\deg(v) + \sum_{v\in V(G)} 2(n-\deg(v)-1)\Big]\\ &= 2\Big[2n(n-1) - \sum_{v\in V(G)}\deg(v)\Big]\\ &= 4n(n-1) - 4m. \qquad \square\end{aligned}$$

Let us now consider another graph structure than cactus. Let n, k_2, k_3 be integers with $k_2, k_3 \geq 0$ and $n \geq 2k_2 + 3k_3 + 1$. Let $\mathcal{G}_{n,k_2,k_3}$ be a class of connected graphs of order n consisting of blocks: k_2 cycles with no chords, k_3 cycles with one chord and paths P_2. Some examples are presented in Figure 1 (note that we have $\xi^d(G_5) = \xi^d(G_6) = 191$).

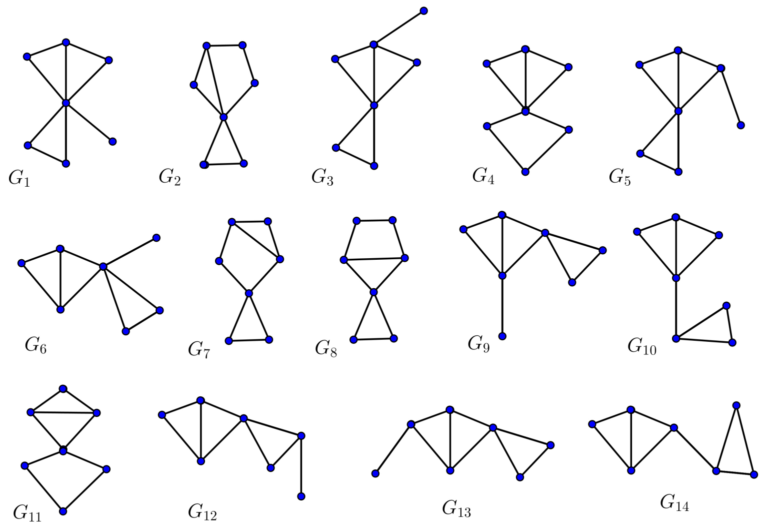

FIGURE 1. Graphs from the class $\mathcal{G}_{n,k_2,k_3}$ with $n = 7$, $k_2 = 1$ and $k_3 = 1$. Values of the eccentric distance sum index: $\xi^d(G_1) = 126$, $\xi^d(G_2) = 174$, $\xi^d(G_3) = 175$, $\xi^d(G_4) = 189$, $\xi^d(G_5) = 191$, $\xi^d(G_6) = 191$, $\xi^d(G_7) = 195$, $\xi^d(G_8) = 196$, $\xi^d(G_9) = 197$, $\xi^d(G_{10}) = 217$, $\xi^d(G_{11}) = 254$, $\xi^d(G_{12}) = 255$, $\xi^d(G_{13}) = 264$, $\xi^d(G_{14}) = 286$.

For this class of graphs we present the lower bound of the eccentric distance sum index and it is an extended result of Theorem 2.1. The idea of the proof is based on the proof of Theorem 2.1.

Theorem 2.3. *Let n, k_2, k_3 be integers with $k_2, k_3 \geq 0$ and $n \geq 2k_2+3k_3+1$. Let $G \in \mathcal{G}_{n,k_2,k_3}$ be a graph of order $n \geq 5$. Then*

$$\xi^d(G) \geq 4n^2 - 9n - 8k_3 - 4k_2 + 5$$

with the equality if and only if $G \cong \widehat{G}_{n,k_2,k_3}$, where

$$\widehat{G}_{n,k_2,k_3} = K_1 + (k_3P_3 \cup k_2P_2 \cup (n-1-2k_2-3k_3)K_1).$$

Proof. We are considering a graph G from a class $\mathcal{G}_{n,k_2,k_3}$.

Let S_i be the set of vertices with eccentricity equal to i and $n_i = |S_i|$. Let us consider first $n_1 > 0$. Let v be a vertex with $\varepsilon(v) = 1$. Then each vertex $u \in V(G)\backslash\{v\}$ is adjacent to v. As $n \geq 5$ and $G \in \mathcal{G}_{n,k_2,k_3}$, then G can only be a graph obtained by introducing k_3 independent paths P_3 and k_2 independent paths P_2 among pendant vertices of a star $K_{1,n-1}$. That is $G \cong \widehat{G}_{n,k_2,k_3}$. An example of this graph you can see in Figure 2.

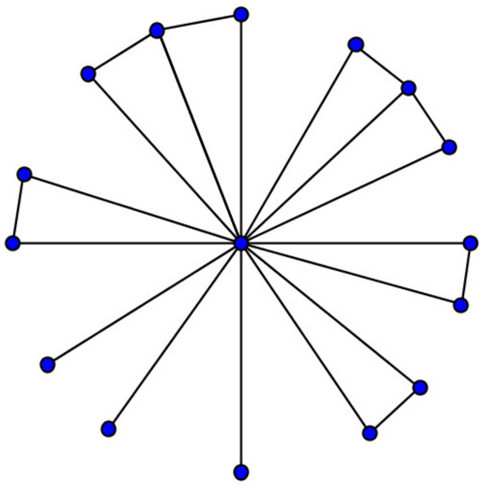

FIGURE 2. An example of a graph $\widehat{G}_{n,k_2,k_3}$ with $n = 16$, $k_2 = 3$ and $k_3 = 2$.

Since $n_1 = 1$, we have the following result:

$$\begin{aligned}\xi^d(\widehat{G}_{n,k_2,k_3}) &= (n-1) && \text{(for a vertex } v \text{ with } \varepsilon(v)=1)\\ &+ 4(k_2+k_3)(2(n-3)+2) && \text{(for vertices } v \text{ with } \deg(v)=2)\\ &+ 2k_3(2(n-4)+3) && \text{(for vertices } v \text{ with } \deg(v)=3)\end{aligned}$$

$$+\,2(n-1-3k_3-2k_2)(2(n-2)+1) \quad \text{(for vertices } v \text{ with } \deg(v)=1)$$
$$=4n^2-9n-8k_3-4k_2+5.$$

Let us now consider the case where $G \in \mathcal{G}_{n,k_2,k_3}$ with $n_1 = 0$. Here we have $\varepsilon(v) \geq 2$ for every vertex v in a graph. By Lemma 2.2 we have $\xi^d(G) \geq 4n(n-1) - 4m$.

By the structure of the graph we have $m = n-1+2k_3+k_2$, where $n-1$ is the number of edges in a spanning tree of our graph and $2k_3+k_2$ is the sum of edges which do not belong to this spanning tree.

The result is as follows:

$$\begin{aligned}\xi^d(G)-\xi^d(\widehat{G}_{n,k_2,k_3}) &\geq [4n(n-1)-4m]-[4n^2-9n-8k_3-4k_2+5]\\ &=[4n(n-1)-4(n-1+2k_3+k_2)]\\ &\quad -[4n^2-9n-8k_3-4k_2+5]\\ &=n-1>0.\end{aligned}$$

This completes the proof. □

Theorem 2.3 cannot be expanded for $n=4$ with $k_3=1$ since in this case $\xi^d(K_1+(P_2\cup K_1))=29$, but $\xi^d(K_2+2K_1)=22$.

Remark 2.4. After applying $k_3=0$ in Theorem 2.3, we immediately get the result of Theorem 2.1 for $n \geq 5$.

In Theorem 2.5 we will give a lower bound for $\xi^d(G)$ for the class of graphs defined below.

Let p, q be positive integers, where $q \geq p \geq 1$ and let $k_p, k_{p+1}, \ldots, k_q$ be a sequence of integers, where $k_i \geq 0$ for $p \leq i \leq q$; $k_p, k_q \geq 1$ and $n = 1 + \sum_{i=p}^{q} k_i i$. Let $\mathcal{G}$ be a class of connected graphs of order n with k_i blocks isomorphic to $K_1 + P_i$, $p \leq i \leq q$. Numbers p, q are the lengths of the shortest and the longest paths P_i, respectively. This class is audited in the next theorem.

Theorem 2.5. *Let $G \in \mathcal{G}$ be a graph of order $n \geq 5$. Then*

$$\xi^d(G) \geq 4n^2-9n+5-4\sum_{i=p}^{q} k_i(i-1)$$

with the equality if and only if $G \cong K_1 + \bigcup_{i=p}^{q} k_i P_i$, where $n = 1+\sum_{i=p}^{q} k_i i$ and p, q are the lengths of the shortest and the longest paths P_i, respectively.

Proof. For our graph G the number of vertices with eccentricity equal to one (denoted by n_1) is $n_1 \leq 1$ as $n \geq 5$.

Case 1. If $\varepsilon(v)=1$ for a vertex v in G, then every vertex $u \in V(G)\backslash\{v\}$ is adjacent to v. Now we know that in this situation G can only be a graph isomorphic to $K_1 + \bigcup_{i=p}^{q} k_i P_i$.

Now we will show how to compute $\xi^d(K_1 + \bigcup_{i=p}^{q} k_i P_i)$. There is only one vertex v for which $\varepsilon(v) = 1$ and it is clear that $D(v) = n - 1$. For every other vertex u in G we have $\varepsilon(u) \geq 2$. Each introduced path P_i has two "ends" (every "end" of the path has exactly two vertices at the distance equal to one and it has the distance equal to two to every other vertex) and $(i-2)$ internal vertices of P_i (every internal vertex has exactly three vertices at the distance equal to one).

Note that the number of pendant vertices is $n - 1 - \sum_{i=p}^{q} ik_i$. So, this is what we have:

$$\xi^d\left(K_1 + \bigcup_{i=p}^{q} k_i P_i\right) = n - 1 \qquad \text{(for vertex } v \text{ with } \varepsilon(v) = 1)$$

$$+ 2 \cdot 2 \cdot (2 \cdot (n-3) + 2) \sum_{i=p}^{q} k_i \qquad \text{(for "ends" of paths)}$$

$$+ 2 \cdot (2 \cdot (n-4) + 3) \sum_{i=p}^{q} (i-2) k_i \qquad \text{(for internal vertices in paths)}$$

$$+ 2 \cdot (2 \cdot (n-2) + 1) \left(n - 1 - \sum_{i=p}^{q} ik_i\right) \qquad \text{(for vertices with degree 1)}$$

$$= n - 1 + (8n - 16) \sum_{i=p}^{q} k_i + (4n - 10) \sum_{i=p}^{q} ik_i$$

$$- 2(4n - 10) \sum_{i=p}^{q} k_i + (4n - 6)(n - 1) - (4n - 6) \sum_{i=p}^{q} ik_i$$

$$= (n - 1)(4n - 5) + (8n - 16 - 8n + 20) \sum_{i=p}^{q} k_i$$

$$+ (4n - 10 - 4n + 6) \sum_{i=p}^{q} ik_i$$

$$= 4n^2 - 9n + 5 + 4 \sum_{i=p}^{q} k_i - 4 \sum_{i=p}^{q} ik_i$$

$$= 4n^2 - 9n + 5 - 4 \sum_{i=p}^{q} k_i (i - 1).$$

Case 2. Let us now consider the case when $n_1 = 0$. In this case we have $\varepsilon(v) \geq 2$ for every vertex v in G. By Lemma 2.2 we have

$$\xi^d(G) \geq 4n(n-1) - 4m.$$

We also have $m = n - 1 + \sum_{i=p}^{q} k_i(i-1)$. Hence

$$\begin{aligned}
\xi^d(G) - \xi^d\left(K_1 + \bigcup_{i=p}^{q} k_i P_i\right) &\geq [4n(n-1) - 4m] \\
&\quad - \left[4n^2 - 9n + 5 - 4\sum_{i=p}^{q} k_i(i-1)\right] \\
&= \left[4n(n-1) - 4\left(n - 1 + \sum_{i=p}^{q} k_i(i-1)\right)\right] \\
&\quad - \left[4n^2 - 9n + 5 - 4\sum_{i=p}^{q} k_i(i-1)\right] \\
&= n - 1 > 0.
\end{aligned}$$

This is the end of the proof. □

3. Conclusions. In this paper we presented a lower bound for the eccentric distance sum index for some generalization of cacti. This result extends the result of Hua, Xu and Wen [4] for cacti. There remains an open problem of how to order graphs in a class by the values of the eccentric distance sum index. Note that $\mathcal{G}_{n,k_2,k_3}$ cannot be ordered by $\xi^d(G)$ for $n = 7$, $k_2 = 1$, $k_3 = 1$.

In the future we will study the problem mentioned above for $n > 7$.

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