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CONNECTED GRAPHS OF DIAMETER TWO HAVING SMALL DEGREE DISTANCES

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Abstract. Topological indices, like degree distance, introduced by Dobrynin and Kochetova and Gutman were studied in mathematical chemistry. In this paper it is proved that in the class of connected graphs G of order $n \geq 4$ and diameter equal to 2 such that $G \ncong K_{1,n-1}$, the minimum degree distance is reached by $K_{1,n-1} + e$ and it is conjectured that the bistar consisting of vertex disjoint stars $K_{1,n-3}$ and $K_{1,1}$ with central vertices joined by an edge has minimum degree distance in the class of connected graphs G of order n such that $G \ncong K_{1,n-1}$.

1. Introduction

Denote by $\mathcal{G}(n)$ the set of connected graphs of order n. If $G \in \mathcal{G}(n)$ the distance $d(x, y)$ between two vertices $x, y \in V(G)$ is the length of a shortest path between them. The eccentricity $ecc(x)$ of a vertex x is $ecc(x) = \max_{y \in V(G)} d(x, y)$ and the diameter of G, denoted by $\text{diam}(G)$, is $\max_{x \in V(G)} ecc(x) = \max_{x,y \in V(G)} d(x, y)$. If $ecc(x)$ is minimum then x is called a central vertex. Let $V_i(x) = \{y : d(x, y) = i\}$ for every $0 \leq i \leq ecc(x)$.
For $k \geq 2$ let $\mathcal{G}(n; \text{diam}{=}k)$ and $\mathcal{G}(n; \text{diam}{\geq}\ k)$ denote the class of connected graphs of order n and diameter equal to k and greater than or equal to k, respectively.

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If graphs G and H are isomorphic we denote this by $G \cong H$. $K_{1,n-1}, K_{1,n-1}+e$ and $BS(p,q)$, where $p,q \geq 1$ and $p+q=n-2$ will denote the star with n vertices, $K_{1,n-1}$ plus one edge joining two vertices of degree 1 and the bistar of order n consisting of two vertex disjoint stars $K_{1,p}$ and $K_{1,q}$ plus one edge joining the central vertices of $K_{1,p}$ and $K_{1,q}$, respectively. Note that diam$(BS(p,q))$=3. We shall use the notation $D(x)=\sum_{y\in V(G)} d(x,y)$ and $D(G)=\sum_{x\in V(G)} D(x)$. The Wiener index $W(G)$, which is a well-known topological index in mathematical chemistry, equals $D(G)/2$.

Some years ago Dobrynin and Kochetova [5] and Gutman [6] introduced a new graph invariant defined as follows: for a vertex x its degree distance, denoted by $D'(x)$ is defined as $D'(x)=d(x)D(x)$, where $d(x)$ is the degree of x and the degree distance of G, denoted by $D'(G)$ is

$$D'(G)=\sum_{x\in V(G)} D'(x)=\sum_{x\in V(G)} d(x)D(x)=\frac{1}{2}\sum_{x,y\in V(G)} d(x,y)(d(x)+d(y)).$$

In [9] the author showed that for $n \geq 2$ in the class of connected graphs of order n minimum of $D'(G)$ equals $3n^2-7n+4$ and the unique extremal graph is $K_{1,n-1}$, thus solving a conjecture proposed by Dobrynin and Kochetova [5]. In [1] and [10] several properties of connected graphs of fixed order and size were deduced; in [8] it was shown that in the class of connected unicyclic graphs of order n the unique graph having minimum degree distance is $K_{1,n-1}+e$. An ordering of unicyclic graphs by their degree distances was deduced in [2].

Topological indices and graph invariants based on the distances between vertices of a graph are used in mathematical chemistry ([3], [4], [7], [11]) for the design of so-called quantitative structure-property relations (QSPR) and quantitative structure-activity relations (QSAR) of chemical compounds. In this paper we will prove that in the class of connected graphs G of order n and diameter diam(G)=2 such that $G \ncong K_{1,n-1}$, the minimum degree distance is reached only for $K_{1,n-1}+e$.

2. Main result

By direct computation we get

Lemma 2.1. $D'(BS(n-3,1))=3n^2-3n-8$.

Lemma 2.2. *Let G be a connected graph of order n and $x \in V(G)$ such that $ecc(x) = p$. Then $D'(x) = (n-1)^2$ for $p = 1$, $D'(x) = d(x)(2n-2-d(x))$ for $p = 2$ and $D'(x) \geq d(x)(2n - d(x) + (p^2 - 3p)/2 - 1)$ for $p \geq 3$.*

Proof: If $p = 2$ then $|V_1(x)| = d(x)$ and $|V_2(x)| = n - 1 - d(x)$. For $p \geq 3$ the minimum value of $D'(x)$ is reached for $|V_i(x)| = 1$ for every $3 \leq i \leq p$, which implies that $D'(x) \geq d(x)(d(x) + 2(n - d(x) - p + 1) + 3 + 4 + \ldots + p) = d(x)(2n - d(x) + (p^2 - 3p)/2 - 1)$. □

Theorem 2.3. *For every $n \geq 4$ we have*

$$\min_{G \in \mathcal{G}(n;\ diam=2) \setminus \{K_{1,n-1}\}} D'(G) = 3n^2 - 3n - 6$$

and the unique extremal graph is $K_{1,n-1} + e$.

Proof: We deduce that $D'(K_{1,n-1} + e) = 3n^2 - 3n - 6$. Let $n \geq 4$ and $G \in \mathcal{G}(n;\text{diam=2})$. It follows that every $x \in V(G)$ has $1 \leq ecc(x) \leq 2$, which implies, by Lemma 2.2 that

$$D'(G) = r(n-1)^2 + \sum_{x \in V(G);\ ecc(x)=2} d(x)(2n - 2 - d(x)),$$

where r denotes the number of vertices x having $ecc(x) = 1$ and the sum has $n - r$ terms. Suppose that $r = 0$. If $x \in V(G)$ has $d(x) = 1$ then the unique vertex y which is adjacent to x has $ecc(y) = 1$, which contradicts the hypothesis. It follows that $2 \leq d(x) \leq n - 2$ for every $x \in V(G)$. The expression $d(x)(2n - 2 - d(x))$ has its minimum equal to $2(2n - 4)$, which implies $D'(G) \geq 2n(2n - 4) > 3n^2 - 3n - 6$ for $n \geq 4$. We deduce that the graph $G \in \mathcal{G}(n;\text{ diam=2}) \setminus \{K_{1,n-1}\}$ having minimum degree distance has $r \geq 1$. The function $d(x)(2n-2-d(x))$ is strictly increasing for $d(x) = 1, \ldots, n-1$ having a maximum equal to $(n-1)^2$. It follows that if $G \in \mathcal{G}(n;\text{ diam=2}) \setminus \{K_{1,n-1}\}$ then $D'(G)$ is minimum only if $r = 1$, i.e., there exists exactly one vertex x with $ecc(x) = 1$, two vertices of degree equal to 2 and other vertices of degree 1, hence $G \cong K_{1,n-1} + e$, since the degree sequence $n-1, k, 1, \ldots, 1$ with $2 \leq k \leq n-1$ has no graphical realization.

□

Note that the arguments used above yield a new proof of the conjecture proposed by Dobrynin and Kochetova.

Finally, we propose the following conjectures:

Conjecture 1 The connected graphs of order $n \geq 4$ having smallest degree distances are $K_{1,n-1}, BS(n-3,1)$ and $K_{1,n-1}+e$; moreover $D'(K_{1,n-1}) = 3n^2 - 7n + 4, D'(BS(n-3,1)) = 3n^2 - 3n - 8$ and $D'(K_{1,n-1}+e) = 3n^2 - 3n - 6$.

Conjecture 2 For every $n \geq 4$ we have

$$\min_{G \in \mathcal{G}(n;\ diam=3)} D'(G) = \min_{G \in \mathcal{G}(n;\ diam \geq 3)} D'(G) = 3n^2 - 3n - 8$$

and the unique extremal graph is $BS(n-3,1)$.

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