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Properties of connected graphs having minimum degree distance

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ABSTRACT

The degree distance of a connected graph, introduced by Dobrynin, Kochetova and Gutman, has been studied in mathematical chemistry. In this paper some properties of graphs having minimum degree distance in the class of connected graphs of order n and size $m \geq n-1$ are deduced. It is shown that any such graph G has no induced subgraph isomorphic to P_4, contains a vertex z of degree $n-1$ such that $G-z$ has at most one connected component C such that $|C| \geq 2$ and C has properties similar to those of G.

For any fixed k such that $k = 0$, 1 or $k \geq 3$, if $m = n+k$ and $n \geq k+3$ then the extremal graph is unique and it is isomorphic to $K_1 + (K_{1,k+1} \cup (n-k-3)K_1)$.

1. Introduction

Let $\mathcal{G}(n, m)$ be the set of connected simple graphs of order n and size m $\left(n-1 \leq m \leq \binom{n}{2}\right)$. For a graph $G \in \mathcal{G}(n, m)$ the distance $d(x, y)$ between two vertices $x, y \in V(G)$ is the length of a shortest path between them and the diameter of G, denoted by $\text{diam}(G)$, is $\max_{x,y \in V(G)} d(x, y)$. The eccentricity $\text{ecc}(x)$ of a vertex x is $\text{ecc}(x) = \max_{y \in V(G)} d(x, y)$. If graphs G and H are isomorphic we denote this by $G \cong H$. The join $G + H$ of disjoint graphs G and H is the graph obtained from $G \cup H$ by joining each vertex of G to each vertex of H. We shall use the notation $D(x) = \sum_{y \in V(G)} d(x, y)$ and $D(G) = \sum_{x \in V(G)} D(x)$. Note that the Wiener index $W(G)$, a well-known topological index extensively studied in mathematical chemistry, equals $D(G)/2$.

In some recent papers Dobrynin and Kochetova [5] and Gutman [6] introduced a new graph invariant defined as follows: the degree distance of a vertex x, 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 $\min_{m \geq n-1} \min_{G \in \mathcal{G}(n,m)} D'(G)$ is reached for a connected graph G of order n if and only if $G \cong K_{1,n-1}$, thus solving a conjecture proposed by Dobrynin and Kochetova [5]. The unicyclic graphs with minimal and maximal degree distance were determined in [1,7], respectively.

Note that topological indices and graph invariants based on the distances between vertices of a graph are widely used in mathematical chemistry (see [2–4,8,10]) for the design of so-called quantitative structure–property relations (QSPR) and quantitative structure–activity relations (QSAR), where by "property" are meant the physico-chemical properties and by "activity", the pharmacological and biological activities of the respective chemical compounds. In this paper we study some properties of the graphs in $\mathcal{G}(n, m)$ having minimum degree distance.

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2. Main results

In what follows we shall exclude the trivial case when $m = \binom{n}{2}$ and $G \cong K_n$ and we can suppose that $\operatorname{diam}(G) \geq 2$ and $n \geq 3$. Let x_i denote the number of vertices of degree i of $G \in \mathcal{G}(n, m)$ for every $1 \leq i \leq n-1$. It follows that $\sum_{i=1}^{n-1} x_i = n$ and $\sum_{i=1}^{n-1} ix_i = 2m$. If $d(v) = k$ then $D(v) \geq k + 2(n-k-1) = 2n-k-2$ and equality holds if and only if $\operatorname{ecc}(v) \leq 2$. By defining, as in [9], $F(G) = F(x_1, \ldots, x_{n-1}) = \sum_{k=1}^{n-1} kx_k(2n-k-2)$, we deduce that

$$D'(G) = \sum_{v \in V(G)} d(v)D(v) \geq F(x_1, \ldots, x_{n-1}) \tag{1}$$

and equality holds if and only if $\operatorname{diam}(G) = 2$. We shall prove that all graphs $G \in \mathcal{G}(n, m)$ having minimum degree distance contain a vertex v such that $\operatorname{ecc}(v) = 1$, or equivalently $d(v) = n-1$, which implies that $\operatorname{diam}(G) = 2$.

Suppose that $G \in \mathcal{G}(n, m)$, $u, v, w \in V(G)$, $uv \in E(G)$ but $uw \notin E(G)$. Let $d(v) = p$ and $d(w) = q$. If $G_1 = G - uv + uw$ is connected then $G_1 \in \mathcal{G}(n, m)$ and we get

$$F(G) - F(G_1) = 2(q - p + 1). \tag{2}$$

We shall say that G_1 is obtained from G by a transformation of type 1. If $G \in \mathcal{G}(n, m)$ and there exist four distinct vertices u, v, x, y such that $uv \in E(G)$, $xy \notin E(G)$ and $G_2 = G - uv + xy$ is connected, then $G_2 \in \mathcal{G}(n, m)$ and we shall say that G_2 is deduced from G by a transformation of type 2. Let $d(u) = p$, $d(v) = q$, $d(x) = r$ and $d(y) = s$. We deduce that

$$F(G) - F(G_2) = 2(r + s - p - q + 2). \tag{3}$$

Theorem 2.1. *Let $G \in \mathcal{G}(n, m)$ be an extremal graph with minimum degree distance. Then G has no induced subgraph isomorphic to P_4 and possesses the following property, denoted by (P): G contains a vertex z of degree $|V(G)| - 1$, $G - z$ has at most one connected component C such that $|C| \geq 2$ and the subgraph induced by C also possesses property (P).*

Proof. Let $G \in \mathcal{G}(n, m)$ be a graph with minimum degree distance and z be a vertex of maximum degree of G. Suppose that $d(z) < n-1$. Let $u_1, \ldots, u_r$ $(r \geq 1)$ be the vertices nonadjacent to z. Since G is connected, there exist an index i_1, $1 \leq i_1 \leq r$, and $y_1 \in N(z)$ such that $u_{i_1}y_1 \in E(G)$. The graph $G_1 = G - u_{i_1}y_1 + zu_{i_1}$ obtained from G by a transformation of type 1 is connected and by (2) $F(G) - F(G_1) = 2(d_G(z) - d_G(y_1) + 1) > 0$. Vertex z also has maximum degree in G_1 and there exist another index i_2, $1 \leq i_2 \leq r$, and $y_2 \in N_{G_1}(z)$ such that $u_{i_2}y_2 \in E(G_1)$. By denoting $G_2 = G_1 - u_{i_2}y_2 + zu_{i_2}$ we get $F(G_1) > F(G_2)$. In this way we obtain a sequence of graphs $G_1, \ldots, G_r \in \mathcal{G}(n, m)$ such that $F(G) > F(G_1) > \cdots > F(G_r)$ and $d_{G_r}(z) = n-1$. This implies that $\operatorname{diam}(G_r) = 2$; hence $F(G_r) = D'(G_r)$. It follows that $D'(G) \geq F(G) > F(G_r) = D'(G_r)$, which contradicts the hypothesis that $D'(G)$ is minimum for all graphs in $\mathcal{G}(n, m)$. Hence $d_G(z) = n-1$. Let us observe that $d_{G-z}(v) = d_G(v) - 1$ for every vertex $v \in V(G) \setminus \{z\}$ and in order to apply transformations of type 1 or 2 to $G - z$ we can consider that in (2) and (3) p, q, r, s are the degrees of v, w and u, v, x, y, respectively, in the subgraph $G - z$. Also, since z is adjacent to all vertices of $G - z$ then the resulting graphs G_1 and G_2 are always connected if $u, v, w, x, y \neq z$.

Suppose that $G - z$ has at least two components C_1 and C_2 such that $\min(|C_1|, |C_2|) \geq 2$. It follows that there exist four distinct vertices $x_1, y_1 \in C_1$ and $u_1, v_1 \in C_2$ such that $x_1y_1, u_1v_1 \in E(G)$ and $x_1v_1, y_1u_1 \notin E(G)$. Let $G_1 = G - x_1y_1 + x_1v_1$. Because both G and G_1 have diameter equal to 2 it follows that $D'(G) = F(G)$ and $D'(G_1) = F(G_1)$. The minimality of $D'(G)$ implies by (2) that $d_G(y_1) \geq d_G(v_1) + 1$. By considering the graph $G - u_1v_1 + y_1u_1$ one obtains $d_G(v_1) \geq d_G(y_1) + 1$, a contradiction.

If G were to contain an induced P_4: u, v, w, t, then $uw, vt \notin E(G)$ and in the same way we deduce that $d_G(v) \geq d_G(w) + 1$ (relatively to u) and $d_G(w) \geq d_G(v) + 1$ (relatively to t), a contradiction. By the same reasoning as above we deduce that the subgraph induced by C possesses property (P). □

This theorem enables us to find easily some extremal sparse graphs in $\mathcal{G}(n, m)$.

Corollary 2.2. *If $G \in \mathcal{G}(n, m)$ has minimum degree distance then:*

(a) *for $m = n-1$ and $n \geq 2$, $G \cong K_{1,n-1}$;*
(b) *for $m = n$ and $n \geq 3$, $G \cong K_1 + (K_2 \cup (n-3)K_1)$;*
(c) *for $m = n+1$ and $n \geq 4$, $G \cong K_1 + (K_{1,2} \cup (n-4)K_1)$;*
(d) *for $m = n+2$: $G \cong K_4$ for $n = 4$ and $G \cong K_1 + (K_3 \cup (n-4)K_1)$ or $G \cong K_1 + (K_{1,3} \cup (n-5)K_1)$ for $n \geq 5$;*
(e) *for $m = n+3$: $G \cong K_1 + (K_1 + (K_1 \cup K_2))$ for $n = 5$ and $G \cong K_1 + (K_{1,4} \cup (n-6)K_1)$ for $n \geq 6$;*
(f) *for $m = n+4$: $G \cong K_1 + (K_1 + K_{1,2})$ for $n = 5$; $G \cong K_1 + (K_1 \cup (K_1 + K_{1,2}))$ or $G \cong K_1 + (K_1 + (K_2 \cup 2K_1))$ for $n = 6$; $G \cong K_1 + (K_{1,5} \cup (n-7)K_1)$ for $n \geq 7$.*

Proof. If $G \in \mathcal{G}(n, m)$ has minimum degree distance then by Theorem 2.1 there exists a vertex z having $d(z) = n-1$ and $G - z$ has at most one component C with $|C| = r \geq 2$. It follows that $r - 1 \leq m - n + 1 \leq \binom{r}{2}$ and $n \geq r + 1$. Also, in C there exists a vertex x such that $d_C(x) = r - 1$ and $C - x$ has at most one component containing at least two vertices. In view of this, cases (a)–(c) are immediate.

(d) We have $r = 3$ or $r = 4$. If $r = 3$ then $n \geq 4$. If $n = 4$ then $G \cong K_4$. Otherwise $n \geq 5$ and x is adjacent to u and v in C and $uv \in E(G)$. The resulting graph, denoted by G_1, is isomorphic to $K_1 + (K_3 \cup (n-4)K_1)$. If $r = 4$ then $n \geq 5$ and C induces a subgraph isomorphic to $K_{1,3}$; the resulting graph, denoted by G_2, is isomorphic to $K_1 + (K_{1,3} \cup (n-5)K_1)$. For G_1, let y stand for a vertex of degree 1. We have $d(u) + d(v) = d(x) + d(y) + 2 = 6$; hence by a transformation of type 2, G_1 goes into G_2 such that $D'(G_1) = D'(G_2)$ by (3). In this case there exist two extremal graphs.

(e) In this case $r = 4$ or $r = 5$. If $r = 4$ we have $n \geq 5$; in C x is adjacent to u, v, w and $uv \in E(G)$; the resulting graph $G_3 \cong K_1 + ((K_1 + (K_1 \cup K_2)) \cup (n-5)K_1)$. If $r = 5$, $n \geq 6$ and the resulting graph $G_4 \cong K_1 + (K_{1,4} \cup (n-6)K_1)$. If y stands for a vertex of degree 1 in G_3 for $n \geq 6$, we get $6 = d(u) + d(v) < d(x) + d(y) + 2 = 7$; hence by (3) we have $D'(G_4) < D'(G_3)$ and the extremal graph coincides with G_4 for every $n \geq 6$. The case (f) can be treated in a similar way. □

The number of extremal graphs may be even greater than 2. For example, for $n = 7$ and $m = 13$ there exist three extremal graphs: $K_1 + (K_1 + (K_{1,2} \cup 2K_1))$, $K_1 + (K_1 \cup (K_1 + K_{1,3}))$ and $K_1 + (K_1 \cup (K_1 + (K_3 \cup K_1)))$. A case when the extremal graph is unique is given by the next theorem.

Theorem 2.3. *Let $k \geq 3$ be a fixed natural number, $m = n + k$ and $n \geq k + 3$. If $G \in \mathcal{G}(n, m)$ has minimum degree distance then $G \cong K_1 + (K_{1,k+1} \cup (n-k-3)K_1)$.*

Proof. Let $G \in \mathcal{G}(n, n+k)$ where $n \geq k + 3$ having minimum degree distance and $z \in V(G)$ such that $d(z) = n - 1$. Then $G - z$ has $k + 1$ edges, $n - 1 \geq k + 2$ vertices, one component C such that $|C| = r \geq 2$ and $n - 1 - r$ isolated vertices. Since $r - 1 \leq k + 1 \leq \binom{r}{2}$ it follows that $r \leq k + 2$ and $k \geq 3$ implies $r \geq 4$.

If $r = k + 2$ then C induces a subgraph isomorphic to $K_{1,k+1}$ and in this case $G \cong K_1 + (K_{1,k+1} \cup (n-k-3)K_1)$. We will show that this is the unique case when G has minimum degree distance. If $r = k + 1$ then C induces the subgraph $K_1 + (K_2 \cup (k-2)K_1)$, consisting of a vertex x adjacent to the remaining k vertices of C. Also, there exist two adjacent vertices u, v in C adjacent to x and let y be a vertex adjacent only to z in G. Let G_1 stand for the graph in $\mathcal{G}(n, n+k)$ deduced in this way. We have $6 = d(u) + d(v) < d(x) + d(y) + 2 = k + 4$; hence by a transformation of type 2, G_1 goes to $K_1 + (K_{1,k+1} \cup (n-k-3)K_1)$ and its degree distance decreases strictly by (3).

Now let $r \leq k$. Define $r - 1 = q \leq k - 1$ and $p = k + 1 - q \geq 2$. Since $r \geq 4$ it follows that $q \geq 3$. We deduce that $G - z$ has a component C with $q + 1$ vertices and $n - 1 - r = n - k + p - 3$ isolated vertices. Furthermore, there exists a vertex x in C adjacent to other q vertices of C. We shall prove that all graphs deduced in this way have a degree distance strictly greater than that of the graph obtained when $r = k + 2$. The graph $K_1 + (K_{1,k+1} \cup (n-k-3)K_1)$ has parameters $x_1 = n - k - 3$, $x_2 = p + q$, $x_{p+q+1} = 1$ and $x_{n-1} = 1$. We denote the corresponding parameters for G by x'_i for $1 \leq i \leq n - 1$ and $i \neq q + 1$. For $i = q + 1$, x'_{q+1} stands for the number of vertices of G of degree $q + 1$ different from x. We have $x'_1 = n - k - 3 + p$, $x'_{q+2} = \cdots = x'_{n-2} = 0$, $x'_{n-1} = 1$ and x has degree $q + 1$. We get $F(K_1 + (K_{1,k+1} \cup (n-k-3)K_1)) - F(G) = 2(p+q)(2n-4) + (p+q+1)(2n-p-q-3) - p(2n-3) - (q+1)(2n-q-3) - \sum_{k=2}^{q+1} kx'_k(2n-k-2) = -5p - 4q - p^2 - 2pq + \sum_{k=2}^{q+1} k^2 x'_k$ since $\sum_{k=2}^{q+1} kx'_k = 2(p+q)$. We shall prove that

$$\sum_{k=2}^{q+1} k^2 x'_k < p^2 + 2pq + 5p + 4q, \tag{4}$$

where

$$\sum_{k=2}^{q+1} x'_k = q \quad \text{and} \quad \sum_{k=2}^{q+1} kx'_k = 2p + 2q. \tag{5}$$

In order to find the maximum of $H(x'_2, \ldots, x'_{q+1}) = \sum_{i=2}^{q+1} i^2 x'_i$ where $(x'_2, \ldots, x'_{q+1})$ satisfies (5), suppose that $3 \leq s < t \leq q$, $x'_s \geq 1$, $x'_t \geq 1$ and define $y_{s-1} = x'_{s-1} + 1$, $y_s = x'_s - 1$, $y_t = x'_t - 1$, $y_{t+1} = x'_{t+1} + 1$ and $y_i = x'_i$ for every $2 \leq i \leq q + 1$, $i \neq s - 1, s, t, t + 1$. The system of values $(y_2, \ldots, y_{q+1})$ satisfies conditions (5) and

$$H(x'_2, \ldots, x'_{q+1}) - H(y_2, \ldots, y_{q+1}) = 2(s - t - 1) < 0.$$

If there exists s, $3 \leq s \leq q$, such that $x'_s \geq 2$ we shall define $y_{s-1} = x'_{s-1} + 1$, $y_s = x'_s - 2$, $y_{s+1} = x'_{s+1} + 1$ and $y_i = x'_i$ for every $2 \leq i \leq q + 1$, $i \neq s - 1, s, s + 1$. $(y_2, \ldots, y_{q+1})$ satisfies (5) and

$$H(x'_2, \ldots, x'_{q+1}) - H(y_2, \ldots, y_{q+1}) = -2.$$

It follows that the maximum of $H(x'_2, \ldots, x'_{q+1})$ is reached when: A. $x'_3 = \cdots = x'_q = 0$; or B. There exists an index α, $3 \leq \alpha \leq q$, such that $x'_\alpha = 1$ and $x'_i = 0$ for every $3 \leq i \leq q$ and $i \neq \alpha$.

For the case A, from (5) we deduce $x'_2 = q - 2p/(q-1)$ and $x'_{q+1} = 2p/(q-1)$. It follows that

$$H(x'_2, \ldots, x'_{q+1}) \leq 4(q - \frac{2p}{q-1}) + (q+1)^2 \frac{2p}{q-1} = 4q + 2p(q+3);$$

$$H(x'_2, \ldots, x'_{p+1}) - p^2 - 2pq - 5p - 4q \leq p - p^2 < 0.$$

For the case B, $x'_2 = q - 1 - (2p + \alpha + 2)/(q - 1)$, $x'_\alpha = 1$ and $x'_{q+1} = (2p - \alpha + 2)/(q - 1)$. It follows that

$$\begin{aligned} H(x'_2, \ldots, x'_{q+1}) &\le 4\left(q - 1 - \frac{2p - \alpha + 2}{q - 1}\right) + (q + 1)^2 \frac{2p - \alpha + 2}{q - 1} + \alpha^2 \\ &= 6q + 6p + 2pq - \alpha q + \alpha^2 - 3\alpha + 2; \\ H(x'_2, \ldots, x'_{q+1}) - p^2 - 2pq - 5p - 4q &\le (\alpha - 2)(\alpha - 1 - q) + p - p^2 < 0. \end{aligned}$$

Since (4) holds it follows that the graph $G \in \mathcal{G}(n, n + k)$ having $D'(G)$ minimum is unique and it is isomorphic to $K_1 + (K_{1,k+1} \cup (n - k - 3)K_1)$. □

Note that by Corollary 2.2 under the conditions of Theorem 2.3 the extremal graph is unique even for $k = 0$ or $k = 1$, but for $k = 2$ there exist two extremal graphs.

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