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Note

Unicyclic and bicyclic graphs having minimum degree distance

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Abstract

In this paper characterizations of connected unicyclic and bicyclic graphs in terms of the degree sequence, as well as the graphs in these classes minimal with respect to the degree distance are given.
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Keywords: Degree distance; Degree sequence; Unicyclic graph; Bicyclic graph

1. Introduction

Let $\mathscr{G}_n$ be the class of connected graphs of order n. We shall consider two subclasses of $\mathscr{G}_n$: $\mathscr{G}_n^1$ and $\mathscr{G}_n^2$ which denote the classes of connected unicyclic and bicyclic graphs, respectively. Note that any graph in $\mathscr{G}_n^1$ contains a unique cycle and it has n edges and every graph in $\mathscr{G}_n^2$ contains two linearly independent cycles, having $n+1$ edges.

For a graph $G \in \mathscr{G}_n$, the distance $d(x, y)$ between vertices x and y is defined as the length of the shortest path between them. The eccentricity of a vertex x is $ecc(x) = \max_{y \in V(G)} d(x, y)$ and the diameter of G is $diam(G) = \max_{x \in V(G)} ecc(x) = \max_{x,y \in V(G)} d(x, y)$. We shall use the notations $D(x) = \sum_{y \in V(G)} d(x, y)$ and $D(G) = \sum_{x \in V(G)} \mathrm{D}(x)$.

Topological indices and graph invariants based on the distances between the vertices of a graph are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds [1–3,10,12].

The Wiener index is a well-known topological index which equals the sum of distances between all pairs of vertices of a molecular graph [6]. It is used to describe molecular branching and cyclicity and establish correlations with various parameters of chemical compounds. Dobrynin and Kotchetova [4] and Gutman [5] introduced a new graph invariant that is more sensitive than the Wiener index. It is defined in the following way: given $G \in \mathscr{G}_n$, the degree distance of a vertex $x \in V(G)$ is defined by $D'(x) = d(x)D(x)$, where $d(x)$ in the degree of x. The degree distance of 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 [11] it was proved that $\min_{G \in \mathscr{G}_n} D'(G) = 3n^2 - 7n + 4$ and the equality holds if and only if G is $K_{1,n-1}$. In the next sections it will be shown that $\min_{G \in \mathscr{G}_n^1} D'(G) = 3n^2 - 3n - 6$, where $n \geqslant 3$, respectively $\min_{G \in \mathscr{G}_n^2} D'(G) = 3n^2 + n - 18$, where $n \geqslant 4$, and the corresponding extremal graphs are unique up to an isomorphism.

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2. Preliminary results

It is well known [7,9], that natural numbers $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n \geqslant 1$ are the degrees of the vertices of a tree if and only if $\sum_{i=1}^{n} d_i = 2n-2$. In the same spirit, the next two lemmas characterize connected unicyclic and bicyclic graphs by their degree sequence.

Lemma 2.1. *Let $n \geqslant 3$. The integers $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n \geqslant 1$ are the degrees of the vertices of a graph $G \in \mathscr{G}_n^1$ if and only if*

(i) $\sum_{i=1}^{n} d_i = 2n$;
(ii) *at least three of them are greater than or equal to* 2.

Proof. Suppose that $G \in \mathscr{G}_n^1$. If G has m edges, its cyclomatic number is $m-n+1=1$, hence $m=n$ and (i) is verified. Additionally, (ii) is also verified since the vertices of the unique cycle have the degrees greater than or equal to 2.

The sufficiency will be proved by induction on n. For $n=3$ we deduce that $d_1=d_2=d_3=2$ and the cycle $C_3 \in \mathscr{G}_3^1$ is the only graph having this degree sequence. Suppose that $n \geqslant 4$ and that the statement is true for all $n' \leqslant n-1$. If $d_n \geqslant 2$ it follows that $d_1=d_2=\cdots=d_n=2$ and the cycle $C_n \in \mathscr{G}_n^1$ has these degrees. Otherwise, one has $d_n=1$. If $d_i \leqslant 2$ for all $1 \leqslant i \leqslant n-1$ then $\sum_{i=1}^{n} d_i \leqslant 2n-1$, which contradicts the hypothesis. Hence there exists a maximal index j, $1 \leqslant j \leqslant n-1$ such that $d_j \geqslant 3$, $d_{j+1} \leqslant 2$ and $d_1 \geqslant \cdots \geqslant d_{j-1} \geqslant d_j > d_{j+1} \geqslant \cdots \geqslant d_n = 1$. We have $\sum_{k=1,k\neq j}^{n-1} d_k + (d_j-1) = 2(n-1)$ and at least three numbers of the sequence $d_1, d_2, \ldots, d_{j-1}, d_j-1, d_{j+1}, \ldots, d_{n-1}$ are greater than or equal to 2. By the induction hypothesis there exists a graph $G_1 \in \mathscr{G}_{n-1}^1$ having this degree sequence. By adding a new vertex, joined by an edge with the vertex of degree d_j-1 of G_1, we get a connected unicyclic graph of order n having the degree sequence $d_1, \ldots, d_n$, where $d_n=1$. $\square$

Lemma 2.2. *Let $n \geqslant 4$. The integers $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n \geqslant 1$ are the degrees of the vertices of a graph $G \in \mathscr{G}_n^2$ if and only if*

(i) $\sum_{i=1}^{n} d_i = 2n+2$;
(ii) *at least four of them are greater than or equal to* 2;
(iii) $d_1 \leqslant n-1$.

Proof. Let $G \in \mathscr{G}_n^2$. Because G has the cyclomatic number $m-n+1=2$, it follows that $m=n+1$, hence $\sum_{i=1}^{n} d_i = 2n+2$. Two cycles contain together at least four vertices of degrees greater than or equal to 2 and (ii) is verified. Also, $d_1 \leqslant |V(G)|-1 = n-1$.

The sufficiency will be shown also by induction on n. For $n=4$ we deduce that $d_1=d_2=3$ and $d_3=d_4=2$. In this case, $C_4+e \in \mathscr{G}_4^2$ is the only graph having this degree sequence. Let $n \geqslant 5$ and suppose that the statement is true for all $n' \leqslant n-1$. If $d_n \geqslant 2$ then the only possibilities are: (a) $d_1=4$, $d_2=d_3=\cdots=d_n=2$ and (b) $d_1=d_2=3$, $d_3=d_4=\cdots=d_n=2$. In the first case, any graph consisting of two cycles C_p and C_{n+1-p} having a common vertex $(3 \leqslant p \leqslant n-2)$ is in $\mathscr{G}_n^2$ and has the above mentioned degree sequence. In the second case, any cycle with a chord C_n+e has this degree sequence.

The remaining case is $d_n=1$. If $d_1=n-1$ then the only possibilities are $d_1=n-1$, $d_2=d_3=d_4=d_5=2$, $d_6=\cdots=d_n=1$ and $d_1=n-1$, $d_2=3$, $d_3=d_4=2$, $d_5=\cdots=d_n=1$. These degree sequences have unique realizations in $\mathscr{G}_n^2$, namely $K_{1,n-1}$ plus two vertex disjoint edges and two edges having a common extremity, respectively. Suppose that $d_1 \leqslant n-2$. If $d_i \leqslant 2$ for each $1 \leqslant i \leqslant n-1$ then $\sum_{i=1}^{n} d_i \leqslant 2n-1$, a contradiction. By the same reasoning as above, we can find a maximal index j, $1 \leqslant j \leqslant n-1$ such that $d_j \geqslant 3$, $d_{j+1} \leqslant 2$ and $d_1 \geqslant \cdots \geqslant d_{j-1} \geqslant d_j > d_{j+1} \geqslant \cdots \geqslant d_n = 1$. At least four numbers of the sequence $d_1, \ldots, d_{j-1}, d_j-1, d_{j+1}, \ldots, d_{n-1}$ are greater than or equal to 2, $d_1 \leqslant n-2$ and $\sum_{k=1,k\neq j}^{n-1} d_k + (d_j-1) = 2(n-1)+2$. Applying the induction hypothesis, there exists a graph $G_2 \in \mathscr{G}_{n-1}^2$ having this degree sequence. By adding a new vertex, joined by an edge with the vertex of degree d_j-1 of G_2 we obtain a connected bicyclic graph of order n having the degree sequence $d_1, \ldots, d_n$, where $d_n=1$. $\square$

We note that a slightly different characterization was obtained for unicyclic and bicyclic graphs by Schocker in [8]. However, it is not convenient for our approach.

Let x_i denote the number of vertices of degree i of $G \in \mathcal{G}_n$, for $1 \leqslant i \leqslant n-1$. If $d(v)=k$ then $D(v) \geqslant k+2(n-k-1)=2n-k-2$ and the equality holds if and only if $ecc(x) \leqslant 2$. Consequently,

$$D'(G) = \sum_{v \in V(G)} d(v)D(v) \geqslant \sum_{k=1}^{n-1} kx_k(2n-k-2),$$

where the equality holds if and only if $diam(G) \leqslant 2$.

By denoting as in [11]

$$F(x_1, \dots, x_{n-1}) = \sum_{k=1}^{n-1} kx_k(2n-k-2),$$

we will find the minimum of $F(x_1, \dots, x_{n-1})$ over all natural numbers $x_1, \dots, x_{n-1} \geqslant 0$ satisfying the conditions in Lemmas 2.1 and 2.2.

Rewriting Lemmas 2.1 and 2.2 in terms of the above notations, yields:

Corollary 2.3. *Let $n \geqslant 3$. The integers $x_1, \dots, x_{n-1} \geqslant 0$ are the multiplicities of the degrees of a graph $G \in \mathcal{G}_n^1$ if and only if*:

(i) $\sum_{i=1}^{n-1} x_i = n$;

(ii) $\sum_{i=1}^{n-1} ix_i = 2n$;

(iii) $x_1 \leqslant n-3$.

Corollary 2.4. *Let $n \geqslant 4$. The integers $x_1, \dots, x_{n-1} \geqslant 0$ are the multiplicities of the degrees of a graph $G \in \mathcal{G}_n^2$ if and only if*:

(i) $\sum_{i=1}^{n-1} x_i = n$;

(ii) $\sum_{i=1}^{n-1} ix_i = 2n+2$;

(iii) $x_1 \leqslant n-4$.

Denote by Δ_1 and Δ_2 the sets of vectors $(x_1, \dots, x_{n-1})$ where $x_1, \dots, x_{n-1}$ are non-negative integers satisfying the conditions (i)–(iii) in Corollaries 2.3 and 2.4, respectively.

Let $G \in \mathcal{G}_n$ with the associated multiplicities of the degrees $(x_1, \dots, x_{n-1})$ and let $m \geqslant 2,\ p > 0,\ m+p \leqslant n-2,\ x_m \geqslant 1,\ x_{m+p} \geqslant 1$. Now consider the transformation t_1 defined as follows:

$$\begin{aligned} t_1(x_1, \dots, x_{n-1}) &= (x_1', \dots, x_{n-1}') \\ &= (x_1, \dots, x_{m-1}+1, x_m-1, \dots, x_{m+p}-1, x_{m+p+1}+1, \dots, x_{n-1}). \end{aligned}$$

We have $x_i' = x_i$ for $i \notin \{m-1, m, m+p, m+p+1\}$ and $x_{m-1}' = x_{m-1}+1,\ x_m' = x_m-1,\ x_{m+p}' = x_{m+p}-1,\ x_{m+p+1}' = x_{m+p+1}+1$.

Lemma 2.5. *Let $(x_1, \dots, x_{n-1}) \in \Delta_1$. Then $t_1(x_1, \dots, x_{n-1}) \in \Delta_1$ unless $m=2$ and $x_1 = n-3$. Also, if $(x_1, \dots, x_{n-1}) \in \Delta_2$ then $t_1(x_1, \dots, x_{n-1}) \in \Delta_2$ unless $m=2$ and $x_1 = n-4$. Moreover*

$$F(t_1(x_1, \dots, x_{n-1})) < F(x_1, \dots, x_{n-1}).$$

Proof. We obtain $\sum_{i=1}^{n-1} x_i' = \sum_{i=1}^{n} x_i$, $\sum_{i=1}^{n-1} ix_i' = \sum_{i=1}^{n-1} ix_i$. If $(x_1, \dots, x_{n-1}) \in \Delta_1$ then $x_1' > n-3$ if and only if $m=2$ and $x_1 = n-3$; a similar conclusion holds if $(x_1, \dots, x_{n-1}) \in \Delta_2$. By a simple calculation we get $F(x_1, \dots, x_{n-1}) - F(t_1(x_1, \dots, x_{n-1})) = 2p+2 > 0$. $\square$

We shall consider a second transformation t_2 which acts on the vectors from $\Delta_1 \cup \Delta_2$ as follows. Let m such that $2 \leqslant m \leqslant n-2$ and $x_m \geqslant 2$. We define

$$t_1(x_1, \ldots, x_{n-1}) = (x'_1, \ldots, x'_{n-1})$$
$$= (x_1, \ldots, x_{m-1}+1, x_m-2, x_{m+1}+1, \ldots, x_{n-1}).$$

i.e. $x'_i = x_i$ for $i \notin \{m-1, m, m+1\}$ and $x'_{m-1} = x_{m-1}+1,\ x'_m = x_m - 2,\ x'_{m+1} = x_{m+1}+1$.

Lemma 2.6. *Let* $(x_1, \ldots, x_{n-1}) \in \Delta_1$. *We have* $t_2(x_1, \ldots, x_{n-1}) \in \Delta_1$ *unless* $m=2$ *and* $x_1 = n-3$; *if* $(x_1, \ldots, x_{n-1}) \in \Delta_2$ *then* $t_2(x_1, \ldots, x_{n-1}) \in \Delta_2$ *unless* $m=2$ *and* $x_1 = n-4$. *Also*

$$F(t_2(x_1, \ldots, x_{n-1})) < F(x_1, \ldots, x_{n-1}).$$

Proof. The proof is similar to the proof of the previous lemma, taking $p=0$. □

3. Main results

Theorem 3.1. *For every* $n \geqslant 3$ *we have*

$$\min_{G \in \mathcal{G}_n^1} D'(G) = 3n^2 - 3n - 6$$

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

Proof. In order to find the minimum of $D'(G)$ over all $G \in \mathcal{G}_n^1$, we will find $\min_{(x_1,\ldots,x_{n-1}) \in \Delta_1} F(x_1, \ldots, x_{n-1})$. Firstly, let us consider the case $n=3$. The only graph $G \in \mathcal{G}_3^1$ is C_3 and $D'(C_3) = 12 = \varphi(3)$, where $\varphi(n) = 3n^2 - 3n - 6$; moreover $C_3 = K_{1,2}+e$ and the theorem is proved in this case.

Let $n \geqslant 4$. If $x_{n-1} \geqslant 2$ consider two different vertices $x, y \in V(G)$ such that $d(x) = d(y) = n-1$. Since $n \geqslant 4$ we can choose two different vertices $z, t \in V(G) \backslash \{x, y\}$. We have $xy,\ xz,\ xt,\ yz,\ yt \in E(G)$, hence G has at least two cycles x, y, z, x and x, y, t, x, which contradicts the hypothesis. Therefore $x_{n-1} \leqslant 1$.

Let us analyse the possible values for $x_3, \ldots, x_{n-2}$ in the case of minimum. If there exist $3 \leqslant i < j \leqslant n-2$ such that $x_i \geqslant 1$ and $x_j \geqslant 1$, then, by applying t_1 for the positions i and j, we obtain a new vector $(x'_1, \ldots, x'_{n-1}) \in \Delta_1$ for which $F(x'_1, \ldots, x'_{n-1}) < F(x_1, \ldots, x_{n-1})$. Similarly, if there exists $3 \leqslant i \leqslant n-2$ such that $x_i \geqslant 2$, then by t_2 we obtain a new degree sequence in Δ_1 for which $F(x'_1, \ldots, x'_{n-1}) < F(x_1, \ldots, x_{n-1})$.

The two remaining cases are (a) $x_3 = x_4 = \cdots = x_{n-2} = 0$ and (b) there is only one index i, $3 \leqslant i \leqslant n-2$ such that $x_i = 1$ and $x_k = 0$ for all $3 \leqslant k \leqslant n-2,\ k \neq i$. Let us prove that in the latter one $F(x_1, \ldots, x_{n-1})$ cannot be minimum. We will show that we can apply t_1 for the positions 2 and i. But for this to be possible we need to have $x_2 \geqslant 1$ and $x_1 \leqslant n-4$.

Indeed, suppose that $x_2 = 0$. It follows that $x_1 + x_{n-1} = n-1$. Prior, we have seen that $x_{n-1} \leqslant 1$. If $x_{n-1} = 0$ then $x_1 = n-1$, and $x_{n-1} = 1$ implies $x_1 = n-2$. Both of these subcases contradict condition (iii) of Corollary 2.3. Thus we have $x_2 \geqslant 1$.

Consider now that $x_1 > n-4$, which again, by condition (iii) entails $x_1 = n-3$. Condition (i) can be written $n-3+x_2+1+x_{n-1} = n$, hence $x_2 = 2 - x_{n-1}$. Condition (ii) implies that $n-3+2x_2+i+(n-1)x_{n-1} = 2n$ or $n+4+(i-3)+(n-3)x_{n-1} = 2n$, which, by the fact that $i \geqslant 3$ leads to $(n-3)x_{n-1} \leqslant n-4$. If $x_{n-1} = 0$ then $x_2 = 2$ and, by (ii), we deduce $i = n-1$, a contradiction. If $x_{n-1} = 1$ then $x_2 = 1$ and, by (ii), we have $i = 2$, also a contradiction. Finally, $x_1 \leqslant n-4$ and now it is possible to apply t_1 for positions 2 and i, obtaining a new vector $(x'_1, \ldots, x'_{n-1}) \in \Delta_1$ for which $F(x'_1, \ldots, x'_{n-1}) < F(x_1, \ldots, x_{n-1})$.

Therefore case (a) holds, thus implying $x_3 = \cdots = x_{n-2} = 0$. The degree sequence at this point is $(x_1, x_2, 0, \ldots, 0, x_{n-1})$ with $x_{n-1} \in \{0, 1\}$. Let us consider the case $x_{n-1} = 0$. We have $x_1 + x_2 = n$ and $x_1 + 2x_2 = 2n$, implying that $x_2 = n$ and $x_1 = 0$ (the corresponding graph in $\mathcal{G}_n^1$ being C_n). In this case, $(0, n, 0, \ldots, 0)$ cannot be a point of minimum in Δ_1 since transformation t_2 can be applied to this vector. The remaining case is $x_{n-1} = 1$. Conditions (i) and (ii) of Corollary 2.3 imply that $x_2 = 2$ and $x_1 = n-3$.

It follows that $F(x_1,\dots,x_{n-1})$ is minimum if and only if $x_1=n-3$, $x_2=2$, $x_3=\cdots=x_{n-2}=0$, $x_{n-1}=1$ and the corresponding graph is $K_{1,n-1}+e$. Hence,

$$\min_{G\in\mathcal{G}_n^1} D'(G)\geqslant \min_{(x_1,\dots,x_{n-1})\in\Delta_1} F(x_1,\dots,x_{n-1})$$

$$=F(n-3,2,0,\dots,0,1)=3n^2-3n-6=D'(K_{1,n-1}+e),$$

which concludes the proof. □

Note that $\min_{G\in\mathcal{G}_n^1} D'(G)=\min_{(x_1,\dots,x_{n-1})\in\Delta_1} F(x_1,\dots,x_{n-1})$ since $K_{1,n-1}+e$ has diameter 2 and $D(v)=2n-k-2$ for every v of degree k in $V(K_{1,n-1}+e)$.

Theorem 3.2. *For every $n\geqslant 4$ we have*

$$\min_{G\in\mathcal{G}_n^2} D'(G)=3n^2+n-18.$$

The extremal graph is unique and may be obtained from $K_{1,n-1}$ by adding two edges having a common extremity.

Proof. Let $G\in\mathcal{G}_n^2$ be a connected bicyclic graph with the multiplicities of the degrees $(x_1,\dots,x_{n-1})\in\Delta_2$. As for Theorem 3.1, in order to find the minimum of $D'(G)$ over all $G\in\mathcal{G}_n^2$, we will find the minimum of $F(x_1,\dots,x_{n-1})$ over all $(x_1,\dots,x_{n-1})\in\Delta_2$.

Firstly, for $n=4$ the only graph $G\in\mathcal{G}_n^2$ is C_4+e and $D'(C_4+e)=34=\psi(4)$, where $\psi(n)=3n^2+n-18$.

Let $n\geqslant 5$. By a similar reasoning as before, we have $x_{n-1}\leqslant 1$. Similarly, on positions $4,\dots,n-2$ we cannot have two values greater than or equal to 1 or one value greater than or equal to 2. Let us show that all vectors $(x_1,\dots,x_{n-1})\in\Delta_2$ realizing the minimum of F have $x_4=x_5=\cdots=x_{n-2}=0$.

Indeed, suppose that there is an index $4\leqslant i\leqslant n-2$ such that $x_i=1$ and $x_k=0$ for all $4\leqslant k\leqslant n-2$, $k\neq i$. In this case, if $x_3\geqslant 1$ we can apply t_1 for positions 3 and i and obtain a smaller value for F. Suppose that $x_3=0$. As $x_{n-1}\in\{0,1\}$, we will analyse separately the two cases: (a) $x_{n-1}=1$ and (b) $x_{n-1}=0$.

(a) In this case $x_{n-1}=x_i=1$, where $i\geqslant 4$. We can consider different vertices $x,y,u,v,w\in V(G)$ such that $d(x)=n-1\geqslant 4$, $d(y)=i\geqslant 4$, $xy, xu, xv, xw, yu, yv, yw\in E(G)$. We have found three linearly independent cycles x,y,u,x; x,y,v,x; x,y,w,x, which contradicts the hypothesis about G.

(b) If $x_{n-1}=0$ then Δ_2 is characterized by $x_1+x_2=n-1$, $x_1+2x_2+i=2n+2$ and $x_1\leqslant n-4$. We deduce that $x_1=i-4\leqslant n-6$ and $x_2=n+3-i\geqslant 1$. In this case we can apply t_1 for positions 2 and i and deduce a smaller value for F.

To sum up, we have $x_4=x_5=\cdots=x_{n-2}=0$ and $x_{n-1}\in\{0,1\}$. If $x_{n-1}=0$, then $x_1+x_2=n-x_3$ and $x_1+2x_2=2n+2-3x_3$, which imply $x_1=x_3-2$. It follows that $x_3\geqslant 2$; by applying t_2 for position 3 we obtain a smaller value for F. If $x_{n-1}=1$ then $x_1+x_2+x_3=n-1$ and $x_1+2x_2+3x_3=n+3$. If $x_3=0$ we obtain $(n-5,4,0,\dots,0,1)\in\Delta_2$ and if $x_3=1$ we get $(n-4,2,1,0,\dots,0,1)\in\Delta_2$. But $t_2(n-5,4,0,\dots,0,1)=(n-4,2,1,0,\dots,0,1)$. It follows that $F(x_1,x_2,\dots,x_{n-1})$ is minimum in Δ_2 if and only if $x_1=n-4$, $x_2=2$, $x_3=1$, $x_4=\cdots=x_{n-2}=0$ and $x_{n-1}=1$. The corresponding graph is $K_{1,n-1}+2e$, where the additional edges have a common extremity. This graph has also diameter 2. As in Theorem 3.1, we have

$$\min_{G\in\mathcal{G}_n^2} D'(G)\geqslant \min_{(x_1,\dots,x_{n-1})\in\Delta_2} F(x_1,\dots,x_{n-1})$$

$$=F(n-4,2,1,0,\dots,0,1)=3n^2+n-18=D'(K_{1,n-1}+2e).\qquad\square$$

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