



Bounds on the difference between the eccentric distance sum and the degree distance of graphs

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Abstract. The eccentric distance sum and degree distance have been well-studied in the past several years. More recently, many authors have considered the relationships between several distance-based graph invariants. Hua et al. [9] investigated the relationship between the eccentric distance sum $\xi^d(G)$ and the degree distance $D'(G)$ of a graph G . In this paper, we give some further results on $\xi^d(G) - D'(G)$. Firstly, we determine upper and lower bounds on $\xi^d(G) - D'(G)$ among general connected graphs in terms of the number of cut edges, and characterize the corresponding extremal graphs. Meanwhile, we identify the extremal graphs of given girth g having the minimum and maximum $\xi^d(G) - D'(G)$. Secondly, we consider the extremal problems among bipartite graphs on $\xi^d(G) - D'(G)$ in terms of matching number. And then we characterize the extremal bipartite graphs with diameter d having minimum $\xi^d(G) - D'(G)$.

1. Introduction

In this paper, we only consider finite, undirected and simple graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The *eccentricity* of a vertex v in a graph G is defined to be $\epsilon_G(v) = \max\{d_G(u, v) | u \in V(G)\}$. The *diameter* d of G is defined to be $d = \max\{\epsilon_G(v) | v \in V(G)\}$. In a graph G which has at least one cycle, the length of a shortest cycle is called its *girth*.

The well-known *Wiener index* $W(G)$ of a graph G is one of the most studied topological indices which was first introduced by Wiener [26]. It is the summation of distances between all unordered pairs of vertices of G . Many modifications of Wiener index were introduced and studied in literature. Gutman [7] and Nikolić [18] introduced the modified Wiener indices. Vukičević [24] studied the variable Wiener indices.

The Wiener index is also extensively investigated elsewhere, and several recent papers indicate a wide variety of topics studied with respect to the Wiener index. Gupta et al. [5] introduced a graph invariant, namely *eccentricity distance sum*, as an eccentricity weighted version of the Wiener index. In addition,

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Dobrynin and Gutman [4] introduced another graph invariant, namely *degree distance*, as a degree weighted version of the Wiener index.

The eccentricity distance sum of graph G is defined as:

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V(G)} (\epsilon_G(u) + \epsilon_G(v))d_G(u,v) = \sum_{v \in V(G)} \epsilon_G(v)D_G(v),$$

and the degree distance of G is defined as:

$$D'(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) + d_G(v))d_G(u,v) = \sum_{v \in V(G)} d_G(v)D_G(v),$$

where $D_G(v) = \sum_{u \in V(G)} d_G(u,v)$.

The eccentricity distance sum is a novel graph invariant for predicting biological and properties. Recently, Yu et al. [27] characterized the extremal unicyclic graphs with girth g having the minimum and second minimum eccentricity distance sum. Hua, Xu and Shu [11] obtained the sharp lower bound on the eccentricity distance sum among cacti of order n . Geng et al. [8] characterized the extremal trees of order n and domination number γ having the minimal/maximal eccentricity distance sum. Miao, Cao, and Pang [16] considered the similar questions. Miao et al. [17] determined the extremal trees in terms of domination number γ having the maximum eccentricity distance sum, where $4 \leq \gamma \leq \lceil \frac{n}{3} \rceil$.

As mentioned above, the degree distance can be viewed as a degree weighted version of the Wiener index. Ilić et al. [15] obtained the degree distance of partial Hamming graphs. Ilić, Stevanović, Feng, Yu, and Dankelmann [14] determined the extremal graphs with the minimum and maximum degree distance among unicyclic and bicyclic graphs. Hou et al. [12] characterized the extremal unicyclic graphs with maximum degree distance. Du and Zhou [3] determined the maximum degree distance among unicyclic graphs in terms of maximum degree. Tomescu [20–22] and Bucicovschi [1] characterized the extremal graphs having minimum degree distance. Dankelmann et al. [2] gave an asymptotically sharp upper bound of the degree distance of graphs in terms of order and diameter.

As we all known, the eccentricity distance sum and the degree distance can be viewed as two weighted versions of the Wiener index. A natural question arises: How to compare the difference between them?

More recently, Hua, Wang, and Hu [9] investigated the relationship between the eccentric distance sum and the degree distance. They established several sufficient conditions for a connected graph to have a larger/smaller eccentric distance sum than degree distance, respectively. They also investigated extremal problems on the difference between those two graph invariants. Zhang, Meng, and Wu [29] presented upper and lower bounds on $\xi^d(G) - D'(G)$ among all connected graphs with given connectivity (resp. edge number and matching number), and characterized the corresponding extremal graphs.

Motivated by [10, 13, 28], in this paper, we give some further results on $\xi^d(G) - D'(G)$. This paper is organized as follows. In section 2, we introduce some basic definitions and lemmas which will be used in the following sections. In section 3, we determine the upper and lower bounds on $\xi^d(G) - D'(G)$ among general connected graphs in terms of number of cut edges, and characterize the extremal graphs. Meanwhile, we consider the extremal graphs in $\mathcal{G}_n^g$. In section 4, we consider the extremal problems among bipartite graphs on $\xi^d(G) - D'(G)$ in terms of matching number. And then we characterize the extremal bipartite graphs with diameter d having minimum $\xi^d(G) - D'(G)$. In the last section, we conclude our paper.

2. Preliminaries and lemmas

For a positive integer n we will use the notation $[n] = \{1, 2, \dots, n\}$. For two subsets A and B of vertices we write $[A, B]$ for the set of edges $uv \in E(G)$ with $u \in A$ and $v \in B$. An induced subgraph $G[Y]$ is the subgraph of G whose vertex set is Y and whose edge set consists of all edges of G which have both ends in Y . If $V(G_1) \cap V(G_2) = \emptyset$, we denote by $G_1 \cup G_2$ the graph which consists of two components G_1 and G_2 . The join of G_1 and G_2 , denoted by $G_1 \vee G_2$, is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}$. A matching of G is a subset of mutually independent edges

of G . For a graph G , the matching number $\beta(G)$ is the maximum cardinality among the independent sets of edges in G . A cut edge of a connected graph is one whose deletion results in a disconnected graph.

Throughout this paper we use P_n, S_n, C_n, K_n and $\bar{K}_n$ to denote the path graph, star graph, cycle graph, complete graph, and independence set on n vertices, respectively.

In what follows, we give some lemmas which will be used frequently in the proof of main results.

Lemma 2.1. [9] Let G be a connected graph with at least three vertices.

(a) If $G \not\cong K_n$, then $\xi^d(G) - D'(G) > \xi^d(G + e) - D'(G + e)$, where $e \in E(\bar{G})$;

(b) If G has an edge e not being a cut edge, then $\xi^d(G) - D'(G) < \xi^d(G - e) - D'(G - e)$.

Lemma 2.2. [9] Suppose that G_0 is a connected graph and u is any one vertex in G_0 . Let G (resp., G') be a graph obtained by identifying the vertex u of G_0 with a pendent vertex (resp., the maximum degree vertex) of the star S_{s+2} ($s \geq 1$). Then

$$\xi^d(G) - D'(G) > \xi^d(G') - D'(G').$$

Lemma 2.3. [13] Let G be a connected graph on n . For any $v \in V(G)$, it holds

$$\varepsilon_G(v) \leq n - d_G(v).$$

Moreover, all equalities hold together if and only if $G \cong P_4$ or $K_n - iK_2$ ($0 \leq i \leq \lfloor \frac{n}{2} \rfloor$), where for each i , $K_n - iK_2$ is the graph obtained by removing i independent edges from G .

Lemma 2.4. [9] Let T be a tree of order n . Then

$$(n-1)^2 \leq \xi^d(T) - D'(T) \leq \begin{cases} \frac{25n^4}{96} - \frac{5n^3}{6} + \frac{17n^2}{24} - \frac{n}{6} & \text{if } n \text{ is even} \\ \frac{25n^4}{96} - \frac{5n^3}{6} + \frac{31n^2}{48} - \frac{n}{6} + \frac{3}{32} & \text{if } n \text{ is odd} \end{cases}$$

where the left-hand side equality holds if and only if $G \cong S_n$, while the right-hand side equality holds if and only if $G \cong P_n$.

3. General connected graphs with given parameters

In this section we will give the bounds on $\xi^d(G) - D'(G)$ in terms of girth g , and characterize the extremal graphs. Meanwhile, we consider the extremal graphs with girth g .

Let $\mathcal{B}_n^g$ be the set of all connected graphs of order n with girth g . In this subsection, we characterize the extremal graphs having upper and lower bounds on $\xi^d(G) - D'(G)$ in $\mathcal{B}_n^g$.

3.1 Extremal graphs with regard to $\xi^d(G) - D'(G)$ in $\mathcal{B}_n^g$

Denote by $C(n, g)$ the graph obtained by connecting a vertex of a cycle C_g with a pendent vertex of a path P_{n-g} . We give a lemma which will be used frequently in the proofs of following theorems.

Lemma 3.1. Let $G \in \mathcal{B}_n^g$. Then

$$\xi^d(G) - D'(G) \leq \xi^d(C(n, g)) - D'(C(n, g)),$$

the equality holds if and only if $G \cong C(n, g)$.

Proof. Let $G \in \mathcal{B}_n^g$ be a connected graph having maximum $\xi^d(G) - D'(G)$. By Lemma 2.1, we conclude that G is a unicyclic graph with girth g . In fact, by definition, we know that the value of $\xi^d(G) - D'(G)$ increases when one deletes edges in the graph G . Thus, G must be a unicyclic graph. Let C_g be the induced cycle of G . The hypothesis of G with maximum $\xi^d(G) - D'(G)$ implies that the value $\xi^d(G) - D'(G)$ reaches its maximum when the graph G contains as few edges as possible. Considering that the graph G contains as

few edges as possible, we conclude that $G - E(C_g)$ contains as few edges as possible. That is, $G - E(C_g)$ must be a union of some trees. It implies that $G - E(C_g)$ is a forest.

Let $V(C_g) = \{v_1, v_2, \dots, v_g\}$. Denote by T_{v_i} the component in $G - E(C_g)$ containing v_i for $i \in [g]$. Without loss of generality, suppose $|T_{v_i}| \geq 2$ for $i \in [t]$, where $t \leq g$.

Replace the cycle C_g in G by a copy of K_1 and denote it by v_0 . Then G becomes a tree T with $|T| = n - k + 1$. By Lemma 2.4, we can obtain a new tree $T_0 \cong P_{n-k+1}$ with the special vertex v_0 , such that $\xi^d(T_0) - D'(T_0) > \xi^d(T) - D'(T)$. Then, we replace the vertex $v_0 \in T_0$ by the cycle C_g . Denote this new graph by G_1 . We have $\xi^d(G_1) - D'(G_1) > \xi^d(G) - D'(G)$.

The graph G_1 is a connected graph constructed from C_g by attaching some paths to each $v_i \in C_g$ for $i \in [2]$, where $2 \leq g$. Let $G_1 = G(m_1, m_2)$, where m_i is the number of pendent paths attaching to i th vertex of the cycle C_g for $i \in [2]$.

The remaining proof of this lemma is similar to Theorem 3.16 [29], and we omit it. $\square$

If $g = 3$, then we get the following result easily.

Theorem 3.2. Let $G \in \mathcal{B}_n^3$. Then

$$\xi^d(K_n) - D'(K_n) \leq \xi^d(G) - D'(G) \leq \xi^d(C(n, 3)) - D'(C(n, 3)),$$

where the left-hand side equality holds if and only if $G \cong K_n$, while the right-hand side equality holds if and only if $G \cong C(n, 3)$. Moreover, $\xi^d(K_n) - D'(K_n) = -n^3 + 3n^2 - 2n$.

Proof. By Lemma 3.1, it is easy to see that the upper bound is achieved. By Lemma 2.1, we know that the graphs with minimum $\xi^d(G) - D'(G)$ by adding some edges to a graph such that the resulting graph is in $\mathcal{B}_n^3$. Thus, the extremal graph with minimum $\xi^d(G) - D'(G)$ must be K_n .

Lemma 3.3. [23] Let G be a connected graph with $|E(G)| > \frac{1}{4}|V(G)|^2$. Then G contains at least one triangle.

Lemma 3.4. Let G be a connected triangle-free graph of order $n \geq 4$. Then

$$\xi^d(G) - D'(G) \geq \xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) - D'(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}),$$

the equality holds if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Moreover, $\xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) - D'(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) = 2n(4 - n)(n - 1) - 2(4 - n)\left\lfloor \frac{n^2}{4} \right\rfloor$.

Proof. Let G be a connected triangle-free graph with minimum $\xi^d(G) - D'(G)$. If there exists a vertex $v \in V(G)$ of degree $n - 1$, then $\epsilon_G(v) = 1$. Since G is triangle-free, it is easy to see that $G \cong K_{1, n-1}$. In the following, we suppose that, for all vertices $v \in V(G)$, $d_G(v) \leq n - 2$. It implies that $\epsilon_G(v) \geq 2$, for each vertex $v \in V(G)$. By the definition of $\xi^d(G) - D'(G)$, we have

$$\begin{aligned} \xi^d(G) - D'(G) &= \sum_{v \in V(G)} (\epsilon_G(v) - d_G(v))D_G(v) \\ &\geq \sum_{v \in V(G)} (\epsilon_G(v) - n + 2)D_G(v) \quad (\text{as } d_G(v) \leq n - 2) \\ &\geq \sum_{v \in V(G)} (2 - n + 2)[d_G(v) + 2(n - 1 - d_G(v))] \quad (\text{as } \epsilon_G(v) \geq 2) \\ &= 2n(4 - n)(n - 1) - (4 - n) \sum_{v \in V(G)} d_G(v) \\ &= 2n(4 - n)(n - 1) - 2(4 - n)|E(G)| \\ &\geq 2n(4 - n)(n - 1) - 2(4 - n)\left\lfloor \frac{n^2}{4} \right\rfloor. \quad (\text{by Lemma 3.3}) \end{aligned}$$

We check the equality condition. The three inequalities are equalities if and only if $\epsilon_G(v) = 2$ for all $v \in V(G)$, and $|E(G)| = \lfloor \frac{n^2}{4} \rfloor$ hold together. Combining the hypothesis G is triangle-free and the condition $\epsilon_G(v) = 2$ for all $v \in V(G)$, we know that G is a complete bipartite graph. Suppose that $G \cong K_{a,b}$, where $1 \leq a \leq \lfloor \frac{n}{2} \rfloor$, and $a+b = n$. Considering the well-known *Turán* Theorem, we obtain that $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique triangle-free graph with exactly $\lfloor \frac{n^2}{4} \rfloor$ edges. In what follows, we show that $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique complete bipartite graph with minimum value of $\xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) - D'(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$. It is sufficient to prove the following Claim.

Claim. $\xi^d(K_{a,n-a}) - D'(K_{a,n-a})$ decreases strictly in a for $a \in [1, \lfloor \frac{n}{2} \rfloor]$.

Proof of Claim. For $a \in [2, \lfloor \frac{n}{2} \rfloor]$, we have

$$\begin{aligned} \xi^d(K_{a,n-a}) - D'(K_{a,n-a}) &= a[2 - (n-a)][n-a+2(a-1)] + (n-a)(2-a)[a+2(n-a-1)] \\ &= 3na^2 - 3n^2a + 4n^2 - 4n. \end{aligned}$$

Define a real function $f(x) = 3nx^2 - 3n^2x + 4n^2 - 4n$ in x with $x \in [2, \lfloor \frac{n}{2} \rfloor]$. Since $f'(x) = 6nx - 3n^2 \leq 0$ in the interval $[2, \lfloor \frac{n}{2} \rfloor]$, $f(x)$ is a strictly decreasing function in x for $x \in [2, \lfloor \frac{n}{2} \rfloor]$. That is, $\xi^d(K_{2,n-2}) - D'(K_{2,n-2}) > \xi^d(K_{3,n-3}) - D'(K_{3,n-3}) > \dots > \xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) - D'(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$.

Next, we compare $\xi^d(K_{2,n-2}) - D'(K_{2,n-2})$ and $\xi^d(K_{1,n-1}) - D'(K_{1,n-1})$.

$$[\xi^d(K_{2,n-2}) - D'(K_{2,n-2})] - [\xi^d(K_{1,n-1}) - D'(K_{1,n-1})] = -3n^2 + 10n - 1 < 0. \quad (\text{as } n \geq 4)$$

This completes the proof of Claim 1. $\square$

By Lemma 3.1 and 3.4, it is immediate to get the following theorem.

Theorem 3.5. Let $G \in \mathcal{B}_n^4$ be a connected graph of order $n(\geq 4)$. Then

$$\xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) - D'(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) \leq \xi^d(G) - D'(G) \leq \xi^d(C(n, 4)) - D'(C(n, 4)),$$

where the left-hand side equality holds if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$, while the right-hand side equality holds if and only if $G \cong C(n, 4)$. Moreover, $\xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) - D'(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) = 2n(4-n)(n-1) - 2(4-n)\lfloor \frac{n^2}{4} \rfloor$.

Lemma 3.6. [8] If $G \in \mathcal{B}_n^5$, then $|E(G)| \leq \frac{1}{2}n\sqrt{n-1}$.

Theorem 3.7. Let $G \in \mathcal{B}_n^5$ be a connected graph of order n . Then $\xi^d(G) - D'(G) \geq 2n(4-n)(n-1) - n(4-n)\sqrt{n-1}$.

Proof. Let $G \in \mathcal{B}_n^5$ be a connected graph with minimum $\xi^d(G) - D'(G)$. If there exists a vertex $v \in V(G)$ of degree $n-1$, then $\epsilon_G(v) = 1$. Thus, $G \cong K_{1,n-1}$. It is easy to see that $\xi^d(K_{1,n-1}) - D'(K_{1,n-1}) = n^2 - 2n + 1$. In what follows, we suppose that, for all vertices $v \in V(G)$, $d_G(v) \leq n-2$. It implies that $\epsilon_G(v) \geq 2$, for each vertex $v \in V(G)$. By the definition of $\xi^d(G) - D'(G)$, we have

$$\begin{aligned} \xi^d(G) - D'(G) &= \sum_{v \in V(G)} (\epsilon_G(v) - d_G(v))D_G(v) \\ &\geq \sum_{v \in V(G)} (\epsilon_G(v) - n + 2)D_G(v) \quad (\text{as } d_G(v) \leq n-2) \\ &\geq \sum_{v \in V(G)} (2 - n + 2)[d_G(v) + 2(n-1-d_G(v))] \\ &= 2n(4-n)(n-1) - (4-n) \sum_{v \in V(G)} d_G(v) \\ &= 2n(4-n)(n-1) - 2(4-n)|E(G)| \\ &\geq 2n(4-n)(n-1) - n(4-n)\sqrt{n-1}. \quad (\text{by Lemma 3.6}) \end{aligned}$$

Since $n \geq 5$, it is easy to check that $n^2 - 2n + 1 > 2n(4-n)(n-1) - n(4-n)\sqrt{n-1}$. $\square$

Theorem 3.8. Let $G \in \mathcal{B}_n^5$ be a connected graph of order n . Then

$$\xi^d(G) - D'(G) \leq \xi^d(C(n, 4)) - D'(C(n, 4)).$$

3.2 Extremal graphs with regard to $\xi^d(G) - D'(G)$ in terms of cut edges

Let $\mathcal{A}_n^k$ be the set of connected graphs of order n and with $k(> 0)$ cut edges. By Lemma 1.1, adding (resp. deleting) edges will decrease (resp. increase) the value of $\xi^d(G) - D'(G)$. For any graph G without any cut edge, it is easy to see that C_n and K_n have the maximal and minimal value of $\xi^d(G) - D'(G)$. It is natural to ask what are the maximal and minimal values of $\xi^d(G) - D'(G)$, where $G \in \mathcal{A}_n^k$.

Let $K(n, k)$ be a graph obtained by identifying one vertex of K_{n-k} with the center of S_{k+1} . In what follows, we give two theorems to determine the extremal graphs in $\mathcal{A}_n^k$, $1 \leq k \leq n-6$, and calculate the corresponding value of $\xi^d(G) - D'(G)$, respectively.

Theorem 3.9. Let G be a graph $(\in \mathcal{A}_n^k)$ with $1 \leq k \leq n-6$. Then

$$\xi^d(G) - D'(G) \geq \xi^d(K(n, k)) - D'(K(n, k)),$$

with equality holding if and only if $G \cong K(n, k)$.

Moreover, $\xi^d(K(n, k)) - D'(K(n, k)) = -n^3 + 4n^2 + kn^2 + k^2n - 4n - k^3 - 3k^2 - 2k + 1$.

Proof. Let $G \in \mathcal{A}_n^k$ be a graph minimizing the $\xi^d(G) - D'(G)$ with k cut edges. Let E_0 be exactly the set of cut edges of G with $|E_0| = k$.

Claim 1. $G - E_0 = \bigcup_{i=1}^{k+1} K_{n_i}$, where $\sum_{i=1}^{k+1} n_i = n$ with $n_i \geq 1$ and $n_i \neq 2$ for $i \in [k+1]$.

Indeed, if there exists a component in $G - E_0$ that is not a complete subgraph. Then, we can obtain a new graph G_1 from G by adding some edges in this component. Obviously, $G_1 \in \mathcal{A}_n^k$. By Lemma 2.1, we have $\xi^d(G_1) - D'(G_1) < \xi^d(G) - D'(G)$. This is a contradiction to the choice of G . we complete the proof of this claim.

Replace every complete subgraph K_{n_i} for $i \in [k+1]$ by a copy of K_1 . Then G can be viewed as a tree T with $|T| = k+1$. By Lemma 2.4, we can obtain a new tree $T_0 \cong S_{k+1}$ with central vertex v , such that $\xi^d(T_0) - D'(T_0) \leq \xi^d(T) - D'(T)$. This means that the *star-like* structure G has minimum value $\xi^d(G) - D'(G)$. Suppose that the vertex v in T_0 corresponds to a complete graph K_{n_j} in G , where $j \in [k+1]$. Let $V(K_{n_j}) = \{w_1, w_2, \dots, w_{n_j}\}$. Now, we replace every vertex $u \in T_0 \setminus \{v\}$ by the corresponding complete graph K_{n_i} for $i \in [k+1] \setminus \{j\}$. That is, this graph is a *star-like* connected graph by replacing every vertex of a star with a complete subgraph K_{n_i} for $i \in [k+1]$. Denote this resulting graph by G_2 . According to the above argument, we have $\xi^d(G_2) - D'(G_2) \leq \xi^d(G) - D'(G)$.

In what follows, we choose G_2 with $\xi^d(G_2) - D'(G_2)$ as small as possible.

Let K_{n_l} be a pendent complete graph, and let xy_l be an edge connecting K_{n_l} and K_{n_j} with $x \in K_{n_j}$, $y_l \in K_{n_l}$, where $l \in [k+1] \setminus \{j\}$. Construct a graph G_3 from G_2 by deleting all edges $\{y_l z | z \in K_{n_l} \setminus \{y_l\}\}$, and adding all edges $\{wz | z \in K_{n_l} \setminus \{y_l\}, w \in K_{n_j}\}$. For every $i \in [k-1] \setminus \{j\}$, we use the similar above-method to obtain a graph G_4 , which is a connected graph by attaching $n-k$ pendent vertices to a complete graph K_{n-k} . Next, we prove that G_3 have smaller value $\xi^d(\cdot) - D'(\cdot)$ than G_2 .

Claim 2. $\xi^d(G_2) - D'(G_2) > \xi^d(G_4) - D'(G_4)$

Proof of Claim 2. Consider the difference between $\xi^d(G_2) - D'(G_2)$ and $\xi^d(G_4) - D'(G_4)$.

$$\begin{aligned} & [\xi^d(G_2) - D'(G_2)] - [\xi^d(G_4) - D'(G_4)] \\ &= \left(\sum_{i=1, i \neq j}^{k+1} \sum_{u \in V(K_{n_i}) \setminus \{y_i\}} + \sum_{i=1, i \neq j}^{k+1} \sum_{u=y_i} + \sum_{u \in V(K_{n_j})} \right) (\varepsilon_{G_2}(u) - d_{G_2}(u)) D_{G_2}(u) \\ & \quad - \left(\sum_{v \in V(K_{n-k})} (\varepsilon_{G_4}(u) - d_{G_4}(u)) D_{G_4}(u) + 2k(2n+k-4) \right) \\ &= \sum_{i=1, i \neq j}^{k+1} (n_i - 1)(6 - n_i)(5n - 4n_i - 2n_j - k - 1) + \sum_{i=1, i \neq j}^{k+1} (4 - n_i)(4n - 3n_i - 2n_j - k - 1) \\ & \quad + n_j(4 - n_j)(3n - n_i - 2n_j - k - 7) - (n - k)(3 - n + k)(n + k - 1) - 2k(2n + k - 4) \\ & > k(n_1 - 1)(6 - n_k)(5n - 6n_k - k - 1) + k(4 - n_k)(4n - 5n_k - k - 1) \end{aligned}$$

$$\begin{aligned}
& + n_1(4 - n_k)(3n - 3n_k - k - 7) - (n - k)(3 - n - k - 1) - 2k(2n + k - 4) \\
& > n^2 + (k^2 - 5)n_1n_k + k(16n_k - 10n_1) + (3k + 6kn_1 - k)n_k^2 + 12k \\
& > 0
\end{aligned}$$

Let $G_4 = G(m_1, m_2, \dots, m_t)$, where m_i is the number of pendent vertices adjacent to i th vertex of the graph K_{n_i} for $i \in [t]$ with $\sum_{i=1}^t m_i = k$. Suppose that $m_1 \geq m_2 \geq \dots \geq m_t$.

Claim 3. $G \cong K(n, k)$

Proof of Claim 3. According to the definition of graph $G(m_1, m_2, \dots, m_t)$, we know that $G(\sum_{i=1}^t m_i, 0, \dots, 0) \cong K(n, k)$. Let $G_4 = G(m_1, m_2, \dots, m_t)$, and $G_5 = G(m_1 + 1, m_2, \dots, m_t - 1)$. Next, we consider the difference of $\xi^d(G_4) - D'(G_4)$ and $\xi^d(G_5) - D'(G_5)$.

$$\begin{aligned}
& [(\xi^d(G_4) - D'(G_4)) - (\xi^d(G_5) - D'(G_5))] \\
& = \sum_{v \in V(G_4)} (\varepsilon_{G_4}(v) - d_{G_4}(v))D_{G_4}(v) - \sum_{v \in V(G_5)} (\varepsilon_{G_5}(v) - d_{G_5}(v))D_{G_5}(v) \\
& = 2m_t(2n - m_t + k - 1) + 2m_1(2n - m_1 + k - 1) + (3 - n + k - m_t)(n - m_t + k - 1) \\
& \quad + (3 - n + k - m_1)(n - m_1 + k - 1) - 2(m_t - 1)(2n - (m_t - 1) + k - 1) \\
& \quad - 2(m_1 + 1)(2n - (m_1 + 1) + k - 1) - (3 - n + k - (m_t - 1))(n - (m_t - 1) + k - 1) \\
& \quad - (3 - n + k - (m_1 + 1))(n - (m_1 + 1) + k - 1) \\
& = 2m_1 - 2m_t + 2 \quad (\text{as } m_1 \geq m_t) \\
& > 0.
\end{aligned}$$

Repeating the above several times, we obtain that $\xi^d(\cdot) - D'(\cdot)$ decreases by the following graph operations, namely, $G(m_1, m_2, \dots, m_t) \rightarrow G(m_1 + 1, m_2, \dots, m_t - 1) \rightarrow \dots \rightarrow G(m_1 + m_t, m_2, \dots, 0) \rightarrow \dots \rightarrow G(\sum_{i=1}^t m_i, 0, \dots, 0) \cong K(n, k)$.

We complete the proof of this Theorem. $\square$

4. Bipartite graphs with given parameters

4.1 Extremal bipartite graphs with regard to $\xi^d(G) - D'(G)$ in terms of matching number

Let $\mathcal{D}_n^\beta$ be the class of all bipartite graphs of order n with matching number β . In this section, we give the lower bound on the $\xi^d(G) - D'(G)$ of all connect graphs $G \in \mathcal{D}_n^\beta$. The corresponding extremal graph is determined.

Theorem 4.1. Let G be a connected graph in $\mathcal{D}_n^\beta$, then

$$\xi^d(G) - D'(G) \geq \xi^d(K_{\beta, n-\beta}) - D'(K_{\beta, n-\beta}),$$

with equality if and only if $G \cong K_{\beta, n-\beta}$. Moreover, $\xi^d(K_{\beta, n-\beta}) - D'(K_{\beta, n-\beta}) = 4n^2 - 3\beta n^2 + 3\beta^2 n - 4n$.

Proof. By a simple calculation, it is easy to see that

$$\begin{aligned}
& \xi^d(K_{\beta, n-\beta}) - D'(K_{\beta, n-\beta}) \\
& = \beta(2 - n + \beta)(n - \beta + 2(\beta - 1)) + (n - \beta)(2 - \beta)(\beta + 2(n - \beta - 1)) \\
& = 4n^2 - 3\beta n^2 + 3\beta^2 n - 4n.
\end{aligned}$$

Choose G in $\mathcal{D}_n^\beta$ such that the value of $\xi^d(G) - D'(G)$ is as small as possible. Let X, Y be the bipartition of the vertex set of $\mathcal{D}_n^\beta$, and let M be a maximal matching of G . Suppose $|X| \geq |Y| \geq \beta$, $X_0 = X \cap V(G[M])$, and $Y_0 = Y \cap V(G[M])$. Note that $|X_0| = |Y_0| = \beta$. As we all known that $\beta \leq \lfloor \frac{n}{2} \rfloor$, we consider two cases according to the value of β .

Case 1. $\beta = \lfloor \frac{n}{2} \rfloor$. In this case, it is easy to see that $|X| = \lceil \frac{n}{2} \rceil$, $|Y| = \lfloor \frac{n}{2} \rfloor$. By Lemma 2.1, we find that the value of

$\xi^d(G) - D'(G)$ of a graph G decreases by adding edges between the sets X and Y . Thus, the extremal graph is just $K_{\beta, n-\beta}$.

Case 2. $\beta < \lfloor \frac{n}{2} \rfloor$. According to Lemma 2.1, if $|Y| = \beta$, the extremal graph is $K_{\beta, n-\beta}$. In what follows, we assume that $|Y| > \beta$. Note that $[X \setminus X_0, Y \setminus Y_0] = \emptyset$. Otherwise, if $[X \setminus X_0, Y \setminus Y_0] \neq \emptyset$, we can find a new matching $M \cup \{e\}$ of G , where $e \in [X \setminus X_0, Y \setminus Y_0]$. This contradicts the maximality of M .

We obtain a new graph G_1 from G by adding all possible edges between the sets X_0 and Y_0 , X_0 and $Y \setminus Y_0$, Y_0 and $X \setminus X_0$, respectively. We have $\xi^d(G_1) - D'(G_1) < \xi^d(G) - D'(G)$. Let $n_1 = |Y \setminus Y_0|$, $n_2 = |X \setminus X_0|$. Suppose $n_1 \leq n_2$. Let M_0 be a subset of matching of $K_{\beta, \beta}$ induced by $G_1[X_0 \cup Y_0]$, and let $|M_0| < \beta$. The matching numbers of $G_1[X_0 \cup Y \setminus Y_0]$ and $G_1[Y_0 \cup X \setminus X_0]$ are both at least $\beta - |M_0|$. Then, the matching number of G_1 is $|M_0| + 2(\beta - |M_0|) = \beta + (\beta - |M_0|) \geq \beta + 1$. Hence, $G_1 \notin \mathcal{D}_n^\beta$ and $G_1 \neq G$. We construct a new graph G_2 from G_1 by deleting and adding edges, (see Fig.2), which satisfies $[X_0, Y \setminus Y_0] = \emptyset$, and $G_2[Y_0 \cup (Y \setminus Y_0)] = K_{n_1, \beta}$.

Claim 1. $G_2 \cong K_{\beta, n-\beta}$. It is routine to check that $\xi^d(G_1) - D'(G_1) > \xi^d(G_2) - D'(G_2)$. It is easy to see that $V(G_1) = V(G_2) = X_0 \cup (X \setminus X_0) \cup Y_0 \cup (Y \setminus Y_0)$. For all vertices $x \in X \setminus X_0$ (resp. $y' \in Y_0, x' \in X_0, y \in Y \setminus Y_0$), we have

$$\begin{aligned} (\varepsilon_{G_1}(x) - d_{G_1}(x))D_{G_1}(x) &= (3 - \beta)(3\beta + 3n_1 + 2n_2 - 2), & (\varepsilon_{G_2}(x) - d_{G_2}(x))D_{G_2}(x) &= (2 - \beta)(3\beta + 2n_1 + 2n_2 - 2), \\ (\varepsilon_{G_1}(y') - d_{G_1}(y'))D_{G_1}(y') &= (2 - n_2 - \beta)(3\beta + 2n_1 + n_2 - 2), & (\varepsilon_{G_2}(y') - d_{G_2}(y'))D_{G_2}(y') &= (2 - n_1 - n_2 - \beta)(3\beta + n_1 + n_2 - 2), \\ (\varepsilon_{G_1}(x') - d_{G_1}(x'))D_{G_1}(x') &= (2 - n_1 - \beta)(3\beta + 2n_2 + n_1 - 2), & (\varepsilon_{G_2}(x') - d_{G_2}(x'))D_{G_2}(x') &= (2 - \beta)(3\beta + 2n_1 + 2n_2 - 2), \\ (\varepsilon_{G_1}(y) - d_{G_1}(y))D_{G_1}(y) &= (3 - \beta)(3\beta + 3n_2 + 2n_1 - 2), & (\varepsilon_{G_2}(y) - d_{G_2}(y))D_{G_2}(y) &= (2 - \beta)(3\beta + 2n_2 + 2n_1 - 2). \end{aligned}$$

Now, consider the difference of $\xi^d(G_1) - D'(G_1)$ and $\xi^d(G_2) - D'(G_2)$.

$$\begin{aligned} & [\xi^d(G_1) - D'(G_1)] - [\xi^d(G_2) - D'(G_2)] \\ &= \sum_{v \in V(G)} [(\varepsilon_{G_1}(v) - d_{G_1}(v))D_{G_1}(v) - (\varepsilon_{G_2}(v) - d_{G_2}(v))D_{G_2}(v)] \\ &= \left(\sum_{v \in X \setminus X_0} + \sum_{v \in Y_0} + \sum_{v \in X_0} + \sum_{v \in Y \setminus Y_0} \right) [(\varepsilon_{G_1}(v) - d_{G_1}(v))D_{G_1}(v) - (\varepsilon_{G_2}(v) - d_{G_2}(v))D_{G_2}(v)] \\ &= n_2[(3 - \beta)(3\beta + 3n_1 + 2n_2 - 2) - (2 - \beta)(3\beta + 2n_1 + 2n_2 - 2)] \\ &\quad + \beta[2 - n_2 - \beta)(3\beta + 2n_1 + n_2 - 2) - (2 - n_1 - n_2 - \beta)(3\beta + n_1 + n_2 - 2)] \\ &\quad + \beta[(2 - n_1 - \beta)(3\beta + 2n_2 + n_1 - 2) - (2 - \beta)(3\beta + 2n_1 + 2n_2 - 2)] \\ &\quad + n_1[(3 - \beta)(3\beta + 3n_2 + 2n_1 - 2) - (2 - \beta)(3\beta + 2n_2 + 2n_1 - 2)] \\ &= 10n_1n_2 - 2n_2 - 2n_1 + 3n_1\beta + 3n_2\beta + 2n_1^2 + 2n_2^2 \\ &= 2n_1^2 + 2n_2^2 + 10n_1n_2 + (3\beta - 2)(n_2 + n_1) \\ &> 0. \end{aligned}$$

This implies that $G_2 \cong K_{\beta, n-\beta}$.

Combining the Case 1 and Case 2, we complete the proof of this theorem.

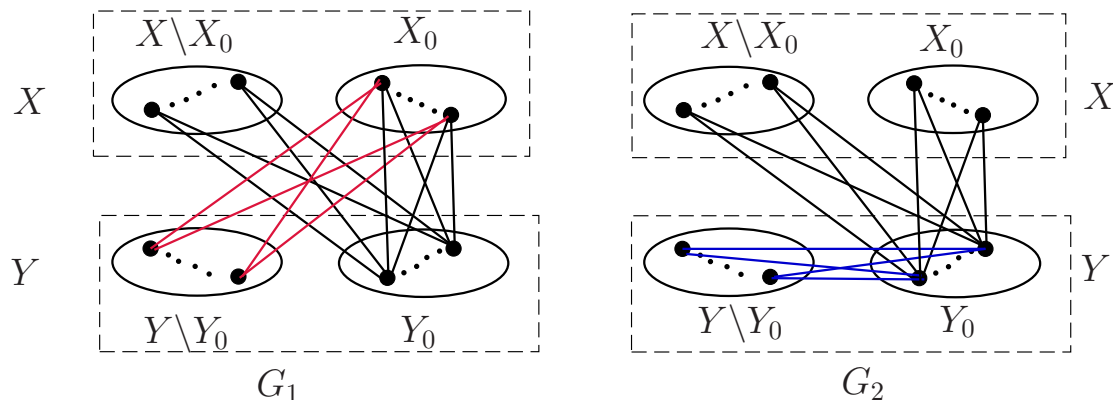


Fig.2. G_2 obtained from G_1 by deleting red edges and adding blue edges4.2 Extremal bipartite graphs with regard to $\xi^d(G) - D'(G)$ in terms of diameter

Let $\mathcal{F}_n^d$ be the class of all bipartite graphs of order n with diameter d .

Let $G \in \mathcal{F}_n^d$, and let d be the diameter of G . Then, there exist two vertices u and v in G , such that $d_G(u, v) = d$. The shortest path connecting u and v , denoted by $P_{u,v} (= P_{u=u_0, u_1, \dots, u_d=v})$, is called diametral path. Let $V_i = \{w \in V(G) | d_G(u, w) = i\}$, and let $n_i = |V_i|$ for $i \in [d] \cup \{0\}$. Clearly, $n_0 = 1$. Then, we get a partition $V(G) = \bigcup_{i=0}^d V_i$ such that $u_i \in V_i$ for $i \in [d] \cup \{0\}$.

Lemma 4.2. [4] For any graph $E \in \mathcal{F}_n^d$ with the above partition of V_G , $G[V_i]$ induces an empty graph (i.e. containing no edge) for each $i \in \{0, 1, \dots, d\}$.

Define a graph G^* (resp. G^{**}) that corresponds to d being odd (resp. even) as extremal graph in the following theorem. Those two graphs can be constructed by the following way.

Recall that $P_{u,v} (= P_{u=u_0, u_1, \dots, u_d=v})$ of length d is a diametral path. The graph G_1 can be constructed from $P_{u,v}$ by replacing $u_{\frac{d-1}{2}}$ and $u_{\frac{d+1}{2}}$ with $\bar{K}_{\lfloor \frac{n-d+1}{2} \rfloor}$ and $\bar{K}_{\lceil \frac{n-d+1}{2} \rceil}$, respectively. That is, $V_{\frac{d-1}{2}} = V(\bar{K}_{\lfloor \frac{n-d+1}{2} \rfloor})$ and $V_{\frac{d+1}{2}} = V(\bar{K}_{\lceil \frac{n-d+1}{2} \rceil})$. We obtain the graph G^* from G_1 by adding edges such that induced subgraphs $G^*[u_{\frac{d-3}{2}}, V_{\frac{d-1}{2}}]$, $G^*[V_{\frac{d-1}{2}}, V_{\frac{d+1}{2}}]$ and $G^*[V_{\frac{d+1}{2}}, u_{\frac{d+3}{2}}]$ are all complete bipartite subgraphs.

The graph G_2 can be constructed from $P_{u,v}$ by replacing $u_{\frac{d-2}{2}}$ and $u_{\frac{d+2}{2}}$ with $\bar{K}_{\lfloor \frac{n-d+2}{4} \rfloor}$ and $\bar{K}_{\lceil \frac{n-d+2}{4} \rceil}$, respectively. That is, $V_{\frac{d-2}{2}} = V(\bar{K}_{\lfloor \frac{n-d+2}{4} \rfloor})$, $V_{\frac{d}{2}} = V(\bar{K}_{\lceil \frac{n-d+2}{4} \rceil})$ and $V_{\frac{d+2}{2}} = V(\bar{K}_{\lfloor \frac{n-d+2}{4} \rfloor})$. We obtain the graph G^{**} from G_2 by adding edges such that induced subgraphs $G^{**}[u_{\frac{d-4}{2}}, V_{\frac{d-2}{2}}]$, $G^{**}[V_{\frac{d-2}{2}}, V_{\frac{d}{2}}]$, $G^{**}[V_{\frac{d}{2}}, V_{\frac{d+2}{2}}]$ and $G^{**}[V_{\frac{d+2}{2}}, u_{\frac{d+4}{2}}]$ are all complete bipartite subgraphs.

Lemma 4.3. Let d, d', n , and i are all positive integers, and $d > d'$. Let n_i (resp. n'_i) be positive integers for $i \in [d]$ (resp. $[d']$). Let $n_i \geq n'_i$ for any $i \in [d']$, and $\sum_{i=1}^d n_i = \sum_{i=1}^{d'} n'_i = n - 1$. Then

$$\sum_{i=1}^d i \cdot n_i > \sum_{i=1}^{d'} i \cdot n'_i.$$

Proof. Define a function $f(n_1, n_2, \dots, n_d) = \sum_{i=1}^d i \cdot n_i$. For some $j \in [d-1]$, we consider the difference between $f(n_1, n_2, \dots, n_j, \dots, n_d)$ and $f(n_1, n_2, \dots, n_j + 1, \dots, n_d - 1)$.

$$\begin{aligned} & f(n_1, n_2, \dots, n_j, \dots, n_d) - f(n_1, n_2, \dots, n_j + 1, \dots, n_d - 1) \\ &= \left(\sum_{i, i \neq j, d} i \cdot n_i + d \cdot n_d + j \cdot n_j \right) - \left(\sum_{i, i \neq j, d} i \cdot n_i + d \cdot (n_d - 1) + j \cdot (n_j + 1) \right) \\ &= d - j > 0. \end{aligned}$$

From the above, we find that the function $f(n_1, n_2, \dots, n_j, \dots, n_d)$ decreases when the pair (n_j, n_d) changes by the following chain $(n_j, n_d) \rightarrow (n_j + 1, n_d - 1) \rightarrow \dots \rightarrow (n_j + n_d, 0)$.

Now, let $n'_i = n_i$ for $i \in [d] \setminus \{j, d\}$, $n'_j = n_j + n_d$, and $d' = d - 1$. We complete the proof of this lemma.

Theorem 4.4. Let G is in $\mathcal{F}_n^d$ with minimum value of $\xi^d(G) - D'(G)$.

(I) If $d = 2$, then $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

(II) If $d \geq 3$, then $G \cong G^*$ for odd d and $G \cong G^{**}$ for even d .

Proof. Let $G \in \mathcal{F}_n^d$ be a connected bipartite graph with bipartition (U, V) such that the value of $\xi^d(G) - D'(G)$ is as small as possible.

(I) If $d = 2$. By Lemma 2.1, we know that adding edges will decrease the value of $\xi^d(G) - D'(G)$, then G must be a complete graph. Let $G \cong K_{n-t,t}$, where $\min\{t, n-t\} \geq 2$. Let $|U| = n-t, |V| = t$. Then we can easily calculate the value of $\xi^d(G) - D'(G)$ as following.

For each vertex u (resp. v) in U (resp. V), we have $(\varepsilon_G(u) - d_G(u))D_G(u) = (2-t)(2n-t-2)$, and $(\varepsilon_G(v) - d_G(v))D_G(v) = (2-n+t)(n+t-2)$.

Thus

$$\begin{aligned} & \xi^d(K_{n-t,t}) - D'(K_{n-t,t}) \\ &= \left(\sum_{w \in U} + \sum_{w \in V} \right) (\varepsilon_{K_{n-t,t}}(w) - d_{K_{n-t,t}}(w)) D_{K_{n-t,t}}(w) \\ &= (n-t)(2-t)(2n-t-2) + t(2-n+t)(n+t-2) \\ &= 3nt^2 - 3n^2t + 4n^2 - 4n. \end{aligned}$$

Define a function $f(x) = 3nx^2 - 3n^2x + 4n^2 - 4n$, which is a real function in x . $f(x)$ reaches its minimum value when $x = \frac{n}{2}$.

If n is odd, that is, $t = \frac{n-1}{2}$ or $\frac{n+1}{2}$, then $\xi^d(K_{n-t,t}) - D'(K_{n-t,t}) \geq -\frac{3}{4}n^3 + 4n^2 - \frac{13}{4}n$.

If n is even, that is, $t = \frac{n}{2}$, then $\xi^d(K_{n-t,t}) - D'(K_{n-t,t}) \geq -\frac{3}{4}n^3 + 4n^2 - 4n$.

Combining above two cases, we have $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

(II) Recall that $|V_i| = n_i$ for $i \in [d] \cup \{0\}$. We first give two claims.

Claim 1. $G[V_i \cup V_{i+1}] \cong K_{n_i, n_{i+1}}$ for $i \in [d-1] \cup \{0\}$, and $|n_d| = 1$ for $d \geq 3$.

Proof of Claim 1. By Lemma 4.2, $E(G[V_i]) = \emptyset$ for $i \in [d] \cup \{0\}$. Suppose that there exists some $k \in [d-1] \cup \{0\}$ such that $G[V_k \cup V_{k+1}] \not\cong K_{n_k, n_{k+1}}$. So, we can obtain a new graph G' by adding some edges between two sets V_k and V_{k+1} . By Lemma 2.1, we get that $\xi^d(G') - D'(G') < \xi^d(G) - D'(G)$. This contradicts the minimality of $\xi^d(G) - D'(G)$.

In what follows, we prove the second part of Claim 1. If $|n_d| \geq 2$, we choose a vertex $w \in V_d \setminus \{u_d\}$, and add edge wx , where $x \in V_{d-3}$. Then, we get a new graph $G'' = G + wx$ with $G'' \in \mathcal{B}_n^d$. By Lemma 2.1, we have $\xi^d(G'') - D'(G'') < \xi^d(G) - D'(G)$. This contradicts to the choice of G . We complete the proof of Claim 1.

Claim 2. Let $V(G) = \bigcup_{i=0}^d V_i$.

(a) If d is odd, then $n_i = 1$ for $i \in [d] \cup \{0\} \setminus \{\frac{d-1}{2}, \frac{d+1}{2}\}$, and $|n_{\frac{d-1}{2}} - n_{\frac{d+1}{2}}| \leq 1$.

(b) If d is even, then $n_i = 1$ for $i \in [d] \cup \{0\} \setminus \{\frac{d-2}{2}, \frac{d}{2}, \frac{d+2}{2}\}$, and $n_{\frac{d}{2}} - (n_{\frac{d-2}{2}} + n_{\frac{d+2}{2}}) \leq 1$.

Proof of Claim 2.(a) We only prove (a), and omit the proof of (b). Note that $n_0 = n_d = 1$. Since we can use similar method to prove $n_i = 1$ for $i \in [d] \cup \{0\} \setminus \{\frac{d-1}{2}, \frac{d+1}{2}\}$, it suffices to show that $n_1 = 1$.

Indeed, if $d = 3$, the result is trivial. So, suppose $d \geq 5$. If $n_1 \geq 2$, then choose $u'_1 \in V_1 \setminus \{u_1\}$ and let $G' = G - u_0u'_1 + \{u'_1x | x \in V_4\}$. Obviously, $\sum_{i=4}^d n_i \geq d-3 \geq d - \lceil \frac{d}{2} \rceil = \lfloor \frac{d}{2} \rfloor > n_0 = 1$. In what follows, we consider the difference between $\xi^d(G) - D'(G)$ and $\xi^d(G') - D'(G')$. For any vertex $x \in V(G) \cap V(G')$, we let $\Delta(x) = (\varepsilon_G(x) - d_G(x))D_G(x) - (\varepsilon_{G'}(x) - d_{G'}(x))D_{G'}(x)$, $n_G^i(v) = |\{w \in V(G) | d_G(v, w) = i\}|$, and $n_{G'}^i(v) = |\{w \in V(G') | d_{G'}(v, w) = i\}|$.

Firstly, we give a partition of G with

$$V(G) = V(G') = \{u\} \cup \{u'_1\} \cup ((V_1 \setminus \{u'_1\}) \cup V_2 \cup V_3) \cup V_4 \cup (\bigcup_{i=5}^d V_i)$$

• For vertex u'_1 , we have $\varepsilon_G(u'_1) - d_G(u'_1) = d - n_2 - 2$, $\varepsilon_{G'}(u'_1) - d_{G'}(u'_1) = d - n_2 - n_4 - 3$. So, $\varepsilon_G(u'_1) > \varepsilon_{G'}(u'_1)$. Since $D_G(u'_1) = \sum_{i=1}^{d-1} i \cdot n_G^i(v)$, and $D_{G'}(u'_1) = \sum_{i=1}^{d-3} i \cdot n_{G'}^i(v)$, by Lemma 4.3, we have $D_G(u'_1) > D_{G'}(u'_1)$. Then, $\Delta(u'_1) > 0$.

Moreover,

$$\Delta(u'_1) > 2(d - n_2 - n_4 - 3)(\sum_{i=4}^d n_i - 1). \quad (7)$$

• For vertex u , we have $(\varepsilon_G(u) - d_G(u))D_G(u) = (d - n_1)D_G(u)$, $(\varepsilon_{G'}(u) - d_{G'}(u))D_{G'}(u) = (d - n_1 + 1)D_{G'}(u)$. We have

$$\Delta(u) = (d - n_1)(D_G(u) - D_{G'}(u)) - D_{G'}(u) > -2(d - n_1) - \frac{n(n-1)}{2}. \quad (8)$$

• For each vertex $v \in (V_1 \setminus \{u'_1\}) \cup V_2 \cup V_3$, we have $\Delta(v) = 0$. Then

$$\sum_{v \in (V_1 \setminus \{u'_1\}) \cup V_2 \cup V_3} \Delta(v) = 0 \quad (9)$$

- For each vertex $v \in V_4$, we have $(\varepsilon_G(v) - d_G(v))D_G(v) = (d - 4 - n_3 - n_5)D_G(v)$, $(\varepsilon_{G'}(v) - d_{G'}(v))D_{G'}(v) = (d - 5 - n_3 - n_5)D_{G'}(v)$. So, $\Delta(v) > (d - 5 - n_3 - n_5)(D_G(v) - D_{G'}(v)) > 2(d - 5 - n_3 - n_5)$. Then,

$$\sum_{v \in V_4} \Delta(v) > 2n_4(d - 5 - n_3 - n_5) \geq 2(d - 5 - n_3 - n_5). \quad (10)$$

- For each vertex $v \in \cup_{i=5}^d V_i$, we have $D_G(v) - D_{G'}(v) = 2$. Since,

$$\Delta(x) > \begin{cases} 2(d - i - n_{i-1} - n_{i+1}) & \text{if } i \in \{5, 6, \dots, \lfloor \frac{d}{2} \rfloor\} \\ 2(i - n_{i-1} - n_{i+1}) & \text{if } i \in \{\lceil \frac{d}{2} \rceil, \lceil \frac{d}{2} \rceil + 1, \dots, d\} \end{cases}$$

We have

$$\begin{aligned} \sum_{v \in \cup_{i=5}^d V_i} \Delta(v) &> \left(\sum_{i=\lceil \frac{d}{2} \rceil}^{d-5} + \sum_{i=\lceil \frac{d}{2} \rceil}^d \right) 2i - 4 \sum_{i=4}^d n_i \\ &= \frac{(3d-9)(d-9)}{2} + \frac{(d+1)(3d+1)}{2} - 4 \sum_{i=4}^d n_i. \end{aligned} \quad (11)$$

Combining (7) – (11), we have

$$\begin{aligned} &[\xi^d(G) - D'(G)] - [\xi^d(G') - D'(G')] \\ &= \left(\sum_{v \in \{u, u'_1\}} + \sum_{v \in (V_1 \setminus \{u'_1\}) \cup V_2 \cup V_3} + \sum_{v \in V_4} + \sum_{v \in \cup_{i=5}^d V_i} \right) \Delta(v) \\ &> 2(d - n_2 - n_4 - 3) \left(\sum_{i=4}^d n_i - 1 \right) - 2(d - n_1) - \frac{n(n-1)}{2} \\ &\quad + 2(d - 5 - n_3 - n_5) + \frac{(3d-9)(d-9)}{2} + \frac{(d+1)(3d+1)}{2} - 4 \sum_{i=4}^d n_i \\ &> 0. \end{aligned}$$

That is, $\xi^d(G) - D'(G) > \xi^d(G') - D'(G')$. This is a contradiction to the choice of G . Hence, $n_1 = 1$.

In what follows, we prove $|n_{\frac{d-1}{2}} - n_{\frac{d+1}{2}}| \leq 1$ for n odd. Suppose that $|n_{\frac{d-1}{2}} - n_{\frac{d+1}{2}}| \geq 2$, and $n_{\frac{d-1}{2}} > n_{\frac{d+1}{2}}$. Choose a vertex $v \in V_{\frac{d-1}{2}}$. We construct a new graph G'' from G by deleting all edges incident with v , and moving v from $V_{\frac{d-1}{2}}$ to $V_{\frac{d+1}{2}}$. Finally, add all edges between $\{v\}$ and $V_{\frac{d-1}{2}} \cup V_{\frac{d+3}{2}}$. Let $\Delta(x) = (\varepsilon_G(x) - d_G(x))D_G(x) - (\varepsilon_{G''}(x) - d_{G''}(x))D_{G''}(x)$. In what follows, we consider the difference between $\xi^d(G) - D'(G)$ and $\xi^d(G'') - D'(G'')$. According to the first part of Claim 2(a), we give a partition of G with

$$V(G) = V(G'') = \left(\cup_{i=0}^{\frac{d-5}{2}} \{u_i\} \right) \cup \left(\cup_{i=\frac{d+5}{2}}^d \{u_i\} \right) \cup \{u_{\frac{d-3}{2}}\} \cup \{u_{\frac{d+3}{2}}\} \cup \left(V_{\frac{n-1}{2}} \setminus \{v\} \right) \cup V_{\frac{n+1}{2}} \cup \{v\}.$$

- If $i \in [\frac{d-5}{2}] \cup \{0\}$, $D_G(u_i) - D_{G'}(u_i) = -1$. If $i \in [\frac{d-5}{2}]$, $\varepsilon_G(u_i) - d_G(u_i) = \varepsilon_{G'}(u_i) - d_{G'}(u_i) = d - i - 2$. If $i = 0$, $\varepsilon_G(u_0) - d_G(u_0) = \varepsilon_{G'}(u_0) - d_{G'}(u_0) = d - 1$. Then,

$$\sum_{x \in \cup_{i=0}^{\frac{d-5}{2}} \{u_i\}} \Delta(x) = -(1 + \sum_{i=\frac{d+1}{2}}^{d-2} i). \quad (12)$$

- If $i \in \{\frac{d+5}{2}, \frac{d+7}{2}, \dots, d\}$, $D_G(u_i) - D_{G'}(u_i) = 1$. If $i \in \{\frac{d+5}{2}, \frac{d+7}{2}, \dots, d-1\}$, $\varepsilon_G(u_i) - d_G(u_i) = \varepsilon_{G'}(u_i) - d_{G'}(u_i) = i - 2$. If $i = d$, $\varepsilon_G(u_d) - d_G(u_d) = \varepsilon_{G'}(u_d) - d_{G'}(u_d) = d - 1$. Then,

$$\sum_{x \in \cup_{i=\frac{d+5}{2}}^d \{u_i\}} \Delta(x) = 1 + \sum_{i=\frac{d+1}{2}}^{d-2} i. \quad (13)$$

- If $i = \frac{d-3}{2}$, we have $\Delta(u_{\frac{d-3}{2}}) = -(\frac{d+3}{2} - n_{\frac{d-1}{2}}) - D_G(u_{\frac{d-3}{2}})$ (14)

- If $i = \frac{d-3}{2}$, we have $\Delta(u_{\frac{d+3}{2}}) = \frac{d+3}{2} - n_{\frac{d+1}{2}} - 2 + D_G(u_{\frac{d+3}{2}})$ (15)

- For each vertex $x \in (V_{\frac{d-1}{2}} \setminus \{v\})$, we have $\Delta(x) = \frac{d+1}{2} - n_{\frac{d+1}{2}} - 2 + D_G(x)$. Then,

$$\sum_{x \in \frac{d-1}{2} \setminus \{v\}} \Delta(x) = (n_{\frac{d-1}{2}} - 1) \left(\frac{d+1}{2} - n_{\frac{d+1}{2}} - 2 + D_G(x) \right). \quad (16)$$

- For each vertex $y \in V_{\frac{d+1}{2}}$, we have $\Delta(y) = -(\frac{d+1}{2} - n_{\frac{d-1}{2}}) - D_G(y)$. Then,

$$\sum_{y \in \frac{d+1}{2}} \Delta(y) = n_{\frac{d+1}{2}} \left(-\frac{d+1}{2} + n_{\frac{d-1}{2}} - D_G(y) \right). \quad (17)$$

• For vertex v , we have $\Delta(v) = \left(\frac{d+1}{2} - n_{\frac{d+1}{2}} - 1 \right) D_G(v) - \left(\frac{d+1}{2} - n_{\frac{d-1}{2}} \right) D_{G''}(v)$. By Lemma 4.3, we have $D_G(v) > D_{G''}(v)$. Then, $\Delta(v) = \left(\frac{d+1}{2} - n_{\frac{d+1}{2}} - 1 \right) D_G(v) - \left(\frac{d+1}{2} - n_{\frac{d-1}{2}} \right) D_{G''}(v) > \left(n_{\frac{d-1}{2}} - n_{\frac{d+1}{2}} - 1 \right) D_{G''}(v) > 0$. That is, $\Delta(v) > 0$. (18)

Combining (12) – (18), we have

$$\begin{aligned} & [\xi^d(G) - D'(G)] - [\xi^d(G'') - D'(G'')] \\ &= \left(\sum_{x \in \bigcup_{i=0}^{\frac{d-5}{2}} \{u_i\}} + \sum_{x \in \bigcup_{i=\frac{d+3}{2}}^d \{u_i\}} + \sum_{x \in V_{\frac{d-1}{2}} \setminus \{v\}} + \sum_{x \in V_{\frac{d+1}{2}} \setminus \{v\}} + \sum_{x \in \{v\}} \right) \Delta(x) \\ &= -\left(1 + \sum_{i=\frac{d+1}{2}}^{d-2} i \right) + \left(1 + \sum_{i=\frac{d-3}{2}}^{d-2} i \right) - \left(\frac{d+3}{2} - n_{\frac{d-1}{2}} \right) - D_G(u_{\frac{d-3}{2}}) \\ &\quad + \frac{d+3}{2} - n_{\frac{d+1}{2}} - 2 + D_G(u_{\frac{d+3}{2}}) + (n_{\frac{d-1}{2}} - 1) \left(\frac{d+1}{2} - n_{\frac{d+1}{2}} - 2 + D_G(x) \right) \\ &\quad + n_{\frac{d+1}{2}} \left(-\frac{d+1}{2} + n_{\frac{d-1}{2}} - D_G(y) \right) + \Delta(v) \\ &> D_G(u_{\frac{d+3}{2}}) - D_G(u_{\frac{d-3}{2}}) + n_{\frac{d+1}{2}} (D_G(x) - D_G(y)) \\ &> 0. \end{aligned}$$

In view of Claim 2(a), we know that $n_{\frac{d-1}{2}} + n_{\frac{d+1}{2}} = n - d + 1$, and $|n_{\frac{d-1}{2}} - n_{\frac{d+1}{2}}| \leq 1$. Then, we get that $G \cong G^*$.

This completes the proof.

5. Concluding remarks

In this paper, we give some further results on $\xi^d(G) - D'(G)$. Firstly, we determine the upper and lower bounds on $\xi^d(G) - D'(G)$ among general connected graphs in terms of number of cut edges, and characterize the extremal graphs. Meanwhile, we consider the extremal graphs in $\mathcal{B}_n^g$. Secondly, we consider the extremal problems among bipartite graphs on $\xi^d(G) - D'(G)$ in terms of matching number. And then we characterize the extremal bipartite graphs with diameter d having minimum $\xi^d(G) - D'(G)$.

Author contributions

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References

- [1] O. Bucicovschi, S. M. Cioabă. The minimum degree distance of graphs of given order and size, *Discrete Appl. Math.* **156** (2008) 3518-3521.
- [2] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart. On the degree distance of a graph. *Discrete Appl. Math.* **157** (2009) 2773-2777.
- [3] Z. Du, B. Zhou. Degree distance of unicyclic graphs, *Filomat* **24** (2010) 95-120.
- [4] A. Dobrynin, R. Entringer, I. Gutman. Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211-249.
- [5] S. Gupta, M. Singh, A. K. Madan. Application of graph theory: relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity, *J. Math. Anal. Appl.* **266** (2002) 259-268.
- [6] I. Gutman. Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087-1089.
- [7] I. Gutman, J. Žerovnik. Corroborating a modification of the Wiener index, *Croat. Chem. Acta* **75** (2002) 603-612.
- [8] X. Y. Geng, S. C. Li, M. Zhang. Extremal values on the eccentric distance sum of trees, *Discrete Appl. Math.* **161** (2013) 2427-2439.
- [9] H. Hua, H. Wang, X. Hu. On eccentric distance sum and degree distance of graphs, *Discrete Appl. Math.* **250** (2018) 262-275.

- [10] H. Hua. On the quotients between the eccentric connectivity index and the eccentric distance sum of graphs with diameter 2, *Discrete Appl. Math.* **285** (2020) 297-300.
- [11] H. Hua, K. Xu, W. Shu. A short and unified proof of Yu et al.'s two results on the eccentric distance sum, *J. Math. Anal. Appl.* **382** (2011) 364-366.
- [12] Y. Hou, A. Chang. The unicyclic graphs with maximum degree distance, *J. Math. Study* **39** (2006) 18-24.
- [13] A. Ilić, Yu G, L. Feng. On the eccentric distance sum of graphs, *J. Math. Anal. Appl.* **381** (2011) 590-600.
- [14] A. Ilić, D. Stevanović, L. Feng, G. Yu, P. Dankelmann. Degree distance of unicyclic and bicyclic graphs, *Discrete Appl. Math.* **159** (2011) 779-788.
- [15] A. Ilić, S. Klavžar, D. Stevanović. Calculating the degree distance of partial Hamming graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 411-424.
- [16] L. Y. Miao, Q. Q. Cao, S. Y. Pang. On the extremal values of the eccentric distance sum of trees, *Discrete Appl. Math.* **186** (2015) 199-206.
- [17] L. Y. Miao, S. Y. Pang, F. Liu, E. Y. Wang, X. Q. Guo. On the extremal values of the eccentric distance sum of trees with a given domination number, *Discrete Appl. Math.* **229** (2017) 113-120.
- [18] S. Nikolić, N. Trinajstić, M. Randić. Wiener index revisited, *Chem. Phys. Lett.* **333** (2001) 319-321.
- [19] T. Pisanski, J. Žerovnik. Edge-contributions of some topological indices and arboreality of molecular graphs, *Ars Math. Contemp.* **2** (2009) 49-58.
- [20] I. Tomescu. Some extremal properties of the degree distance of a graph. *Discrete Appl. Math.* **98** (1999) 159-163.
- [21] I. Tomescu. Properties of connected graphs having minimum degree distance. *Discrete Math.* **309** (2008) 2745-2748.
- [22] I. Tomescu. Unicyclic and bicyclic graphs having minimum degree distance, *Discrete Appl. Math.* **156** (2008) 125-130.
- [23] P. Turán. Eine Extremalaufgabe aus der Graphentheorie. *Mat. Fiz. Lapok* **48** (1941) 436-452.
- [24] D. Vukičević, J. Žerovnik J. Variable Wiener indices, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 385-402.
- [25] H. Wang, L. Kang. Further properties on the degree distance of graphs, *J. Comb. Optim.* **31** (2016) 427-446.
- [26] H. Wiener. Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69**(1947)17-20.
- [27] G. H. Yu, L. H. Feng, A. Ilić. On the eccentric distance sum of trees and unicyclic graphs, *J. Math. Anal. Appl.* **375** (1) (2011) 99-107.
- [28] H. Zhang, S. Li, B. Xu. Extremal graphs of given parameters with respect to the eccentricity distance sum and the eccentric connectivity index, *Discrete Appl. Math.* **254** (2019) 204-221.
- [29] W. Zhang, J. Meng, B. Wu. Extremal graphs with respect to two distance-based topological indices, *Discrete Appl. Math.* **317** (2022) 63-74.