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Research article

Maximal bond incident degree index for trees and unicyclic graphs with fixed diameter

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Abstract: The bond incident degree index of G is defined as

$$BID(G) = \sum_{u_1u_2 \in E(G)} f(d(u_1), d(u_2)),$$

where $f(y,x) = f(x,y)$ is a real-valued function. In this paper, using graph transformation methods, we respectively established the maximum bond incident degree indices of trees and unicyclic graphs with a fixed diameter. As an application of the sufficient conditions, we verified that six bond incident degree indices satisfy such conditions, among which are the newly introduced Euler Sombor index and the computationally complex general Sombor index.

Keywords: bond incident degree index; trees; unicyclic graphs; diameter
Mathematics Subject Classification: 05C05, 05C09, 05C92

1. Introduction

All graphs $G = (V(G), E(G))$ discussed in this work are connected, simple, and undirected, where $V(G)$ refers to the vertex set of G and $E(G)$ to its edge set. We define a tree (denoted by T) as a graph G with no cycles, a unicyclic graph, by contrast, is a graph G that contains exactly one cycle. Given a vertex $u \in V(G)$, $d_G(u)$ refers to the degree of u, with $N_G(u)$ denoting the neighborhood of u. A vertex u is termed a pendant vertex when $d_G(u) = 1$, and $PV(G)$ is defined as the collection of all pendant vertices in G. The path, cycle, and star graph on n vertices are denoted, respectively, by P_n, C_n, and S_n. Within graph G, a longest path is called a diameter path, denoted by P^d, i.e., $P^d = P_{d+1}$, where d is the diameter of G. Let $G - u_1u_2$ and $G + u_1u_2$ stand for the two graphs constructed by removing edge $u_1u_2 \in E(G)$ from G and adding the edge $u_1u_2 \notin E(G)$ to G, respectively. For other undefined definitions and terminologies, refer to [1].

Mathematical chemistry encompasses several key branches, among which chemical graph theory holds a prominent position. It simulates molecular structures and represents chemical information in a mathematical manner. Specifically, atoms are represented by vertices and chemical bonds by edges between vertices, yielding a molecular graph. The topological index is an important graph-theoretic invariant, which has wide applications in predicting and interpreting physicochemical properties and biological activities, with further utility in drug screening [2–4].

The bond incident degree index of G [5] is defined as

$$BID(G) = \sum_{u_1u_2 \in E(G)} f(d(u_1), d(u_2)).$$

Notably, $f(y, x) = f(x, y)$ is a real-valued function. In particular, let $m_{x,y}$ stand for the count of edges in G satisfying $(d(u), d(v)) = (x, y)$. $BID(G)$ may also be equivalently written as

$$BID(G) = \sum_{1 \le x \le y \le \Delta} m_{x,y} f(x, y).$$

In 2021, Gutman [6] introduced the Sombor index, which originates from geometric distance. The index is expressed as

$$SO(G) = \sum_{u_1u_2 \in E(G)} \sqrt{d(u_1)^2 + d(u_2)^2}.$$

That is, by setting $f(x, y) = \sqrt{x^2 + y^2}$ in the expression of $BID(G)$, then $BID(G) = SO(G)$.

Subsequently, various forms of the bond incident degree indices have been proposed successively, such as the Euler Sombor index [7, 8], atom-bond sum-connectivity (ABS) index [9], and Lanzhou index [10]. Specifically, the ABS index [9] and general Sombor index [11] are formulated as

$$ABS(G) = \sum_{u_1u_2 \in E(G)} \sqrt{\frac{d(u_1) + d(u_2) - 2}{d(u_1) + d(u_2)}}$$

and

$$SO_\alpha(G) = \sum_{u_1u_2 \in E(G)} (d(u_1)^2 + d(u_2)^2)^\alpha,$$

where α is a real number.

Since trees and unicyclic graphs are important components of molecular structures of compounds, in-depth studies have been conducted on bond incident degree indices for trees and unicyclic graphs. In 2021, Gutman [6] derived upper and lower bounds on the Sombor index for arbitrary trees and connected graphs. In 2022, the extremal values of the Sombor index corresponding to trees with predefined parameters such as the pendant vertex number, matching number, and branching number were determined by Chen et al. [12]. Meanwhile, Liu [13] established the largest Sombor index of unicyclic graphs with predefined order and a fixed diameter. In 2023, Nithya et al. [14] identified the first, second, third, and fourth minimum ABS indices of unicyclic graphs with predefined girth g. In 2025, Ahmad and Das [15] completely resolved the open problem concerning the maximum general

Sombor index for chemical trees possessing predefined pendant vertices. In addition, the extremal values of the elliptic Sombor index corresponding to trees with given parameters, namely, the branching number, maximum degree, and so on, were derived by Ahmad et al. [16]. As for additional studies concerning the chemical utility of relevant bond incident degree indices, interested readers may refer to the listed references [17–22].

Beyond directly investigating the extremal problems of a specific index, researchers have also attempted to explore this category of bond incident degree index problems via a universal approach. In 2024, Du et al. [23] established the extreme values of various bond incident degree indices for chemical trees given a fixed number of leaves by analyzing the structural characteristics of chemical trees. In 2025, Gao [24] established the minimum c-cyclic graphs for indices including the reciprocal Randić index, forgotten index, and first Gourava index, by proposing sufficient conditions for trees and c-cyclic graphs to attain the minimum values of bond incident degree indices. Recently, Zhang et al. [25] determined the maximum and minimum ABS indices for graphs with a fixed diameter through various graph transformations and characterized the corresponding extremal graphs.

Inspired by [24] and [25], we attempt to address extremal problems of bond incident degree indices for trees as well as unicyclic graphs with a fixed diameter by adopting a universal method. Let $\mathbb{T}_{n,d}$ and $\mathbb{U}_{n,d}$ denote the collections of trees and unicyclic graphs with n vertices and a diameter d, correspondingly. In Section 2, by characterizing the structural features of trees, we obtain a sufficient condition for a tree $T \in \mathbb{T}_{n,d}$ to achieve the maximum $BID(T)$. In Section 3, via graph transformations, we present a sufficient condition for a unicyclic graph $G \in \mathbb{U}_{n,d}$ to attain the maximum $BID(G)$. As an application of these sufficient conditions, in Section 4, we verify that six bond incident degree indices satisfy the sufficient conditions presented in the preceding two sections, including the recently introduced Euler Sombor index and the computationally complex general Sombor index.

2. Maximal $BID(T)$ of trees with a fixed diameter

In this part, we mainly present a sufficient condition pertaining to trees with a given diameter to achieve the maximum value in BID. Since the structure of tree T is unique when $n = d + 1$ or $n = d + 2$, all trees $T \in \mathbb{T}_{n,d}$ considered in this section satisfy both $d \geq 3$ and $n \geq d + 3$.

Before presenting the following lemma, we first define several special types of tree graphs.

Let $T^i_{n,d}$ denote the graph constructed by connecting one end vertex of each of $(n - d - 1)$ edges P_2 to the vertex u_i of the diameter path $P^d = u_1u_2 \cdots u_du_{d+1}$, where $2 \leq i \leq d$. Specifically, when $i = 2$ or $i = d$, we denote it as $T^i_{n,d} = T^*_{n,d}$.

T_1 denotes the graph formed by attaching one end vertex of each of $(n-d-2)$ edges P_2 to the vertex u_2 of the path $P^d = u_1u_2 \cdots u_du_{d+1}$, and one terminal vertex of one edge P_2 to u_3.

T^i_2 denotes the graph constructed by linking one end vertex of each of $(n - d - 2)$ paths P_2 to the vertex u_2 of the path $P^d = u_1u_2 \cdots u_du_{d+1}$, and one end vertex of one path P_2 to u_i, where $4 \leq i \leq d - 1$.

T_3 denotes the graph constructed by attaching one end vertex of each of $(n - d - 2)$ paths P_2 to the vertex u_2 of the path $P^d = u_1u_2 \cdots u_du_{d+1}$, and one end vertex of one path P_2 to u_d.

Clearly, $T^i_{n,d}, T_1, T^i_2, T_3 \in \mathbb{T}_{n,d}$. For convenience, let $\mathbb{T}^{max}_{n,d} = \{T \in \mathbb{T}_{n,d} \mid BID(T) \text{ is maximizing}\}$.

Lemma 2.1. *(Su [26]) Denote by $P_l = v_1v_2 \cdots , v_l$ an induced subpath of graph G such that $d_G(v_1) \geq 2$ and $d_G(v_l) \geq 2$. Let $G' = G - \sum_{u\in N_G(v_l)\backslash v_{l-1}} v_lu + \sum_{u\in N_G(v_l)\backslash v_{l-1}} v_1u$, see Figure 1. The operation of* *constructing G' based on G is called the path lifting transformation. If $f(x, y)$ fulfills the subsequent conditions:*

(i) $f(x, y)$ is strictly increasing in x;

(ii) $f(x + y - 1, 1) > f(x, y)$ holds for $x, y \geq 2$;

(iii) $f(2, x)$ is strictly convex downward in x,

then $BID(G) < BID(G')$.

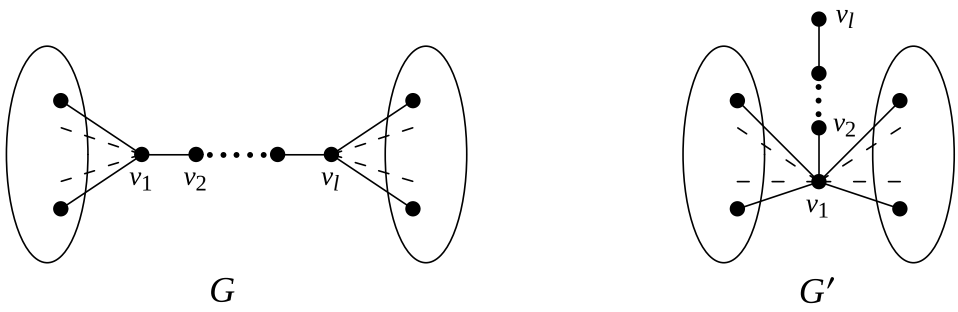

Figure 1. Graphs of G and G' in Lemma 2.1.

Lemma 2.2. *Denote by T_1, T_2^i (T_2 for short), T_3, and $T_{n,d}^i$ the trees defined above, where $3 \leq i \leq d - 1$. If $f(x, y)$ meets the subsequent conditions:*

(i) $f(x, y)$ is strictly increasing in x;

(ii) $f(x + 1, y - 1) > f(x, y)$ holds for $x \geq y$;

(iii) $f(1, x)$ is strictly convex downward in x,

then $BID(T_{n,d}^i) > BID(T_j)$ holds for $1 \leq j \leq 3$.

Proof. First, by condition (i), we have $f(n - d + 1, 1) > f(n - d, 1)$ and $f(n - d + 1, 2) > f(3, 2)$. Condition (ii) yields $f(n - d + 1, 2) > f(n - d, 3)$, and condition (iii) gives $f(1, 3) - f(1, 2) < f(1, n - d + 1) - f(1, n - d)$. Therefore, based on the structures of $T_{n,d}^i$ and T_1, we obtain

$$\begin{aligned}BID(T_{n,d}^i) - BID(T_1) &= (n - d - 1)f(n - d + 1, 1) + 2f(n - d + 1, 2) + (d - 4)f(2, 2)\\ &\quad + 2f(1, 2) - (n - d - 1)f(1, n - d) - f(3, n - d)\\ &\quad - (d - 4)f(2, 2) - f(1, 3) - f(2, 3) - f(1, 2)\\ &> f(1, n - d + 1) - f(1, n - d) + f(1, 2) - f(1, 3) > 0.\end{aligned}$$

That is, $BID(T_{n,d}^i) > BID(T_1)$.

Next, condition (i) implies $f(n-d+1, x) > f(n-d, x)$ and $f(n-d+1, 2) > f(3, 2)$. It follows from condition (iii) that

$$\begin{aligned}BID(T_{n,d}^i) - BID(T_2^i) &= (n - d - 1)(f(1, n - d + 1) - f(1, n - d)) + f(2, n - d + 1)\\ &\quad - f(2, n - d) + f(2, n - d + 1) - f(2, 3) + f(1, 2) - f(1, 3)\\ &> f(1, n - d + 1) + f(1, 2) - f(1, n - d) - f(1, 3) > 0.\end{aligned}$$

$$\begin{aligned}BID(T_{n,d}^i) - BID(T_3) &= (n - d - 1)(f(1, n - d + 1) - f(1, n - d)) + f(2, n - d + 1)\\ &\quad - f(2, n - d) + f(2, n - d + 1) - f(2, 3) + 2(f(1, 2) - f(1, 3))\\ &> 2(f(1, n - d + 1) + f(1, 2)) - 2(f(1, n - d) + f(1, 3)) > 0.\end{aligned}$$

Consequently, $BID(T^i_{n,d}) > BID(T^i_2)$ and $BID(T^i_{n,d}) > BID(T_3)$. □

Theorem 2.1. *Let $T \in \mathbb{T}_{n,d} \backslash T^*_{n,d}$. If $f(x,y)$ fulfills the following requirements:*
(i) $f(x,y)$ is strictly increasing in x;
(ii) $f(x+1,y-1) > f(x,y)$ holds for $x \geq y$;
(iii) $f(1,x)$ and $f(2,x)$ are strictly convex downward in x;
(iv) $\varphi(x,y) = f(x,y) - f(x-1,y)$ is strictly increasing with x while strictly decreasing with y, then

$$BID(T) \leq BID(T^i_{n,d}) = (n-d-1)f(1,n-d+1) + (d-4)f(2,2) + 2f(2,n-d+1) + 2f(1,2)$$

holds precisely when $T \cong T^i_{n,d}$, where $i = 3,4,\cdots,d-1$.

Proof. Let $T \in \mathbb{T}^{max}_{n,d} \backslash T^*_{n,d}$, and let $P^d = u_1u_2\cdots u_du_{d+1}$ be a diameter path of T.
Claim 1. There exists no non-pendant edge uv in T satisfying $uv \notin E(P^d)$.
Proof of Claim 1. Assume for contradiction that there exists a non-pendant edge u_iv with $u_iv \notin E(P^d)$. By Lemma 2.1 and the path lifting transformation, we obtain $T' \in \mathbb{T}_{n,d} \backslash T^*_{n,d}$ satisfying $BID(T') > BID(T)$, which contradicts $T \in \mathbb{T}^{max}_{n,d} \backslash T^*_{n,d}$. □

Therefore, T is a tree formed by attaching $d_T(u_i) - 2$ pendant vertices to each vertex u_i (where $3 \leq i \leq d-1$) of the diameter path P^d. Next, we prove $T \cong T^i_{n,d}$. Assume for contradiction that $T \ncong T^i_{n,d}$. Consequently, there are vertices u_i and u_j satisfying $d_T(u_i) \geq 3$ and $d_T(u_j) \geq 3$. We let $i < j$ and $d_T(u_i) \geq d_T(u_j)$. In the proof, we need to consider three special cases of graphs T_1, T^i_2, and T_3. For convenience, denote $d_T(u_{i-1}) = a$, $d_T(u_{j+1}) = b$, $d_T(u_i) = x$, and $d_T(u_j) = y$, where $x \geq y$.
Case 1. $j = i+1$.

We define $N_T(u_i) = \{v_1, v_2, \cdots, v_{d_T(u_i)-2}, u_{i-1}, u_j\}$ and $N_T(u_j) = \{w_1, w_2, \cdots, w_{d_T(u_j)-2}, u_i, u_{j+1}\}$. By Lemma 2.2, $T \ncong T_1$. As established earlier, $u_iu_j \in E(P^d)$ and $x \geq y \geq 3$, so T is depicted in Figure 2.

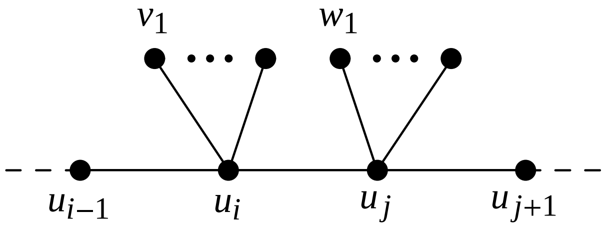

Figure 2. Tree T in Transformation 1.

Transformation 1: $T' = T - u_jw_1 + w_1u_i$.

We have that $T' \in \mathbb{T}_{n,d} \backslash T^*_{n,d}$. By condition (i), $f(x+1,1) \geq f(y+1,1)$ and $\varphi(x,y) = f(x,y) - f(x-1,y) > 0$. Repeatedly applying condition (iv), we obtain

$$\begin{aligned} BID(T') - BID(T) &= f(x+1,y-1) - f(x,y) + f(a,x+1) + (x-1)f(1,x+1) + (y-3)f(1,y-1) \\ &\quad + f(b,y-1) - f(a,x) - (x-2)f(1,x) - (y-2)f(1,y) - f(b,y) \\ &\geq \varphi(x+1,a) - \varphi(y,b) + (x-2)\varphi(x+1,1) - (y-3)\varphi(y,1) + f(1,x+1) - f(1,y) \\ &\geq \varphi(x+1,a) - \varphi(y,b) + (x-2)\varphi(x+1,1) - (y-3)\varphi(y,1) + f(1,y+1) - f(1,y) \\ &> \varphi(x+1,a) - \varphi(y,b) + (y-3)(\varphi(x+1,1) - \varphi(y,1)) + \varphi(y+1,1) \\ &> \varphi(y+1,1) - \varphi(y,b) \geq \varphi(y+1,1) - \varphi(y,1) > 0. \end{aligned}$$

This contradicts $T \in \mathbb{T}_{n,d}^{max} \backslash T_{n,d}^*$.

Case 2. $j \geq i + 2$.

Denote $N_T(u_i) = \{v_1, v_2, \cdots, v_{d_T(v_i)-2}, u_{i-1}, u_{i+1}\}$ and $N_T(u_j) = \{w_1, w_2, \cdots, w_{d_T(v_j)-2}, u_{j-1}, u_{j+1}\}$. By Lemma 2.2, $T \ncong T_2^i$ and $T \ncong T_3$. Moreover, $u_iu_j \notin E(P^d)$, and $x \geq y \geq 3$. Similar to Case 1, we perform Transformation 1 to obtain the new graph T'. Repeatedly applying condition (iv), we deduce

$$\begin{aligned}
BID(T') - BID(T) &= f(a, x+1) + (x-1)f(1, x+1) + (y-3)f(1, y-1) + f(b, y-1) + f(2, x+1) \\
&\quad + f(2, y-1) - f(a, x) - (x-2)f(1, x) - (y-2)f(1, y) - f(b, y) - f(2, x) - f(2, y) \\
&> \varphi(x+1, a) - \varphi(y, b) + (x-2)\varphi(x+1, 1) - (y-3)\varphi(y, 1) \\
&\quad + \varphi(x+1, 2) - \varphi(y, 2) + \varphi(y+1, 1) \\
&> \varphi(x+1, a) - \varphi(y, b) + (y-3)(\varphi(x+1, 1) - \varphi(y, 1)) + \varphi(y+1, 1) \\
&> \varphi(y+1, 1) - \varphi(y, b) > 0.
\end{aligned}$$

This contradicts $T \in \mathbb{T}_{n,d}^{max} \backslash T_{n,d}^*$, and the theorem is proven. □

Theorem 2.2. *Let $T \in \mathbb{T}_{n,d}$ for integers $d \geq 3$ and $n \geq d+3$. If $f(x,y)$ fulfills the subsequent requirements:*

(i) $f(x,y)$ is strictly increasing in x;

(ii) $f(x+1, y-1) > f(x,y)$ holds for $x \geq y \geq 2$;

(iii) $f(1,x)$ and $f(2,x)$ are strictly convex downward in x;

(iv) $\varphi(x,y) = f(x,y) - f(x-1,y)$ is strictly increasing with x and strictly decreasing with y,

then

$$BID(T) \leq BID(T_{n,d}^*) = (n-d)f(1, n-d+1) + (d-3)f(2,2) + f(2, n-d+1) + f(1,2)$$

holds precisely when $T \cong T_{n,d}^*$.

Proof. First, by Theorem 2.1, we have $BID(T) \leq BID(T_{n,d}^i)$ for $T \in \mathbb{T}_{n,d} \backslash T_{n,d}^*$ and $3 \leq i \leq d-1$. Furthermore, since $n - d \geq 3$ and by condition (iv), we obtain

$$\begin{aligned}
BID(T_{n,d}^*) - BID(T_{n,d}^i) &= (n-d)f(1, n-d+1) + (d-3)f(2,2) + f(2, n-d+1) + f(1,2) \\
&\quad - (n-d-1)f(1, n-d+1) - (d-4)f(2,2) - 2f(2, n-d+1) - 2f(1,2) \\
&= \varphi(2,2) - \varphi(2, n-d+1) > 0.
\end{aligned}$$

Thus, the theorem is proven. □

3. Maximal $BID(G)$ of unicyclic graphs with a fixed diameter

In this section, we mainly present the sufficient conditions for unicyclic graphs with a fixed diameter to achieve the maximal BID. Before stating the relevant results, we first define several classes of special graphs.

Let S_n^+ denote the graph constructed by introducing one additional edge to the n-vertex star graph S_n.

A_n denotes the graph formed by attaching one end of each of $(n-5)$ copies of the path P_2 to a common vertex of the cycle C_5.

$B_n(a,b)$ denotes the graph formed by attaching one end vertex of each of a paths P_2 and b paths P_2 to two adjacent vertices of the cycle C_4, with the constraints $a+b+4=n$ and $a \geq b$. Specifically, we denote $B_n^* = B_n(n-4,0)$.

$C_n(a,b,c)$ represents the graph formed by attaching one end vertex of each of a paths P_2, b paths P_2, and c paths P_2 to the three vertices of the cycle C_3, respectively, where $a+b+c+3=n$ and $a \geq b \geq c$. Specifically, we denote $C_n^* = C_n(n-4,1,0)$.

Let D denote the graph constructed by linking one end vertex of the path P_3 to one vertex of the 3-cycle C_3. $D_n(a,b)$ represents the graph formed by linking a paths P_2 and b paths P_2 to the 3-degree vertex and the non-cycle 2-degree vertex of graph D, respectively, where $a+b=n-5$. Specifically, we denote $D_n^* = D_n(n-5,0)$. $B_n(a,b)$, $C_n(a,b,c)$, and $D_n(a,b)$ are depicted in Figure 3.

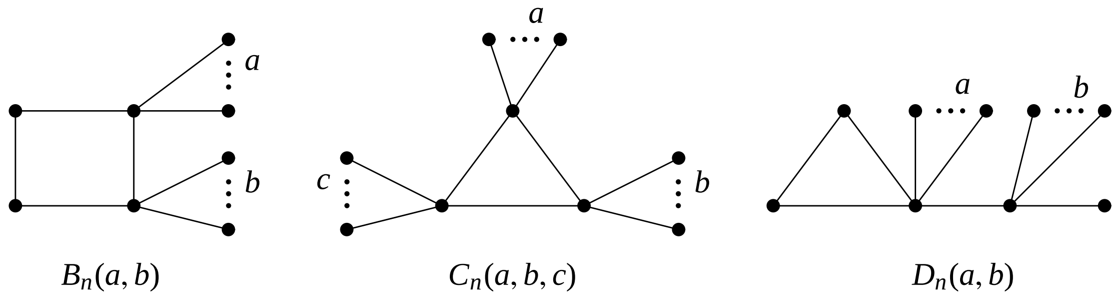

Figure 3. Trees of $B_n(a,b)$, $C_n(a,b,c)$, and $D_n(a,b)$.

Clearly, $S_n^+ \in \mathbb{U}_{n,2}$, A_n, $B_n(a,b)$, $C_n(a,b,c)$, $D_n(a,b) \in \mathbb{U}_{n,3}$. Immediately, we derive

$$BID(S_n^+) = (n-3)f(1,n-1) + 2f(2,n-1) + f(2,2),$$

$$BID(A_n) = (n-5)f(1,n-3) + 2f(2,n-3) + 3f(2,2),$$

$$BID(B_n^*) = (n-4)f(1,n-2) + 2f(2,n-2) + 2f(2,2),$$

$$BID(C_n^*) = (n-4)f(1,n-2) + f(2,n-2) + f(3,n-2) + f(2,3) + f(1,3),$$

$$BID(D_n^*) = (n-5)f(1,n-2) + 3f(2,n-2) + f(2,2) + f(1,2).$$

Theorem 3.1. *Let $G \in \mathbb{U}_{n,2}$ with $n \geq 4$. If $f(x,y)$ fulfills the subsequent requirements:*

(i) $f(x,y)$ is strictly increasing in x;

(ii) $f(x+y-1,1) > f(x,y)$ holds for $x,y \geq 2$,

then

$$BID(G) \leq BID(S_n^+) = (n-3)f(1,n-1) + 2f(2,n-1) + f(2,2)$$

holds precisely when $G \cong S_n^+$.

Proof. Since the diameter $d=2$, there are three possible structures for unicyclic graphs satisfying $G \in \mathbb{U}_{n,2}$, namely, $G \cong C_4$, $G \cong C_5$, and $G \cong S_n^+$. If $G \cong C_4$, then $BID(C_4) = 4f(2,2)$. By conditions (i) and (ii), we obtain $f(2,2) < f(2,3)$ and $f(2,2) < f(1,3)$, respectively. Therefore,

$$\begin{aligned} BID(S_n^+) - BID(C_4) &= (n-3)f(1,n-1) + 2f(2,n-1) + f(2,2) - 4f(2,2) \\ &\geq f(1,3) + 2f(2,3) - 3f(2,2) > 0. \end{aligned}$$

Similarly, if $G \cong C_5$, we can deduce $BID(S_n^+) > BID(C_5) = 5f(2,2)$. Thus, the theorem is proven. □

Theorem 3.2. *Let $G \in \mathbb{U}_{n,3}$ with $n \geq 5$. If $f(x, y)$ fulfills the following requirements:*
(i) $f(x, y)$ is strictly increasing in x;
(ii) $f(x + 1, y - 1) > f(x, y)$ holds for $x \geq y$;
(iii) $f(1, x)$ and $f(2, x)$ are strictly convex downward in x,
then

$$BID(G) \leq BID(C_n^*) = (n - 4)f(1, n - 2) + f(2, n - 2) + f(3, n - 2) + f(2, 3) + f(1, 3)$$

holds precisely when $G \cong C_n^*$.

Proof. Since $d = 3$, there are exactly five structures for unicyclic graphs satisfying $G \in \mathbb{U}_{n,3}$, namely, $G \cong C_6$ or C_7, $G \cong A_n$, $G \cong B_n(a, b)$, $G \cong C_n(a, b, c)$, and $G \cong D_n(a, b)$. Four cases are discussed in what follows.
Case 1. $G \cong C_6$, C_7, or $G \cong A_n$. Similar to Theorem 3.1, by conditions (i) and (ii), direct calculations yield that

$$BID(C_n^*) > BID(C_6),\ BID(C_n^*) > BID(C_7),\ BID(C_n^*) > BID(A_n).$$

Case 2. $G \cong B_n(a, b)$. Let $d_G(u) = a$, $d_G(v) = b$, and let $N_G(v) = \{w, u, v_1, v_2, \cdots v_b\}$.
Transformation 2: $G' = G - vv_1 + uv_1$.

We have that $G' \in \mathbb{U}_{n,3}$. It follows from condition (i) that $f(b, 1) < f(a + 1, 1)$. Condition (iii) gives $f(2, b) + f(2, a) < f(2, a + 1) + f(2, b - 1)$ and $f(1, b) + f(1, a) < f(1, a + 1) + f(1, b - 1)$. By virtue of condition (ii), $f(a + 1, b - 1) > f(a, b)$. Therefore, we have

$$\begin{aligned} BID(G') - BID(G) &= f(1, a + 1) - f(1, b) + f(2, b - 1) - f(2, b) \\ &\quad + f(2, a + 1) - f(2, a) + f(a + 1, b - 1) - f(a, b) \\ &\quad + \sum_{i=1}^{a-2} (f(1, a + 1) - f(1, a)) + \sum_{i=2}^{b-2} (f(1, b - 1) - f(1, b)) > 0. \end{aligned}$$

Repeatedly applying Transformation 2 to $B_n(a, b)$ yields B_n^*, with $BID(B_n^*) > BID(G)$.
On the other hand, by condition (iii) and condition (i), we obtain

$$\begin{aligned} BID(C_n^*) - BID(B_n^*) &= (n - 4)f(1, n - 2) + f(2, n - 2) + f(3, n - 2) + f(2, 3) + f(1, 3) \\ &\quad - (n - 4)f(1, n - 2) - 2f(2, n - 2) - 2f(2, 2) \\ &> f(3, n - 2) - f(2, n - 2) + f(3, 2) - f(2, 2) > 0. \end{aligned}$$

Case 3. $G \cong C_n(a, b, c)$. Let $d_G(u) = a$, $d_G(v) = b$, and let $N_G(v) = \{w, u, v_1, v_2, \cdots v_a\}$. Exactly similar to Case 2, we perform Transformation 2. Through calculation, we deduce $BID(G') > BID(G)$. Repeatedly applying Transformation 2 to $C_n(a, b, c)$ yields $C_n(a + b, c, 0)$ with $BID(G) < BID(C_n(a + b, c, 0))$. We further apply Transformation 2 repeatedly to $C_n(a + b, c, 0)$ until it becomes C_n^*. By calculation, we have $BID(C_n^*) > BID(C_n(a + b, c, 0))$. Thus, Case 3 is proven.
Case 4. $G \cong D_n(a, b)$. Let $d_G(u) = a$, $d_G(v) = b$, and denote $N_G(v) = \{w, u, v_1, v_2, \cdots v_a\}$. We perform Transformation 2, and obtain $G' \in \mathbb{U}_{n,3}$.
Case 4.1. If $a - 2 \geq b$. Condition (i) yields $f(a + 1, 1) - f(b, 1) > 0$ and $f(a + 1, 2) - f(a, 2) > 0$. As a result of condition (ii), $f(a+1, b-1) - f(a, b) > 0$. It follows from condition (iii) that $f(1, b) + f(1, a) <$

$f(1, a+1) + f(1, b-1)$. Consequently,

$$\begin{aligned} BID(G') - BID(G) &= f(a+1,1) - f(b,1) + 2(f(a+1,2) - f(a,2)) + f(a+1,b-1) \\ &\quad - f(a,b) + \sum_{i=1}^{a-3}(f(a+1,1) - f(a,1)) + \sum_{i=2}^{b}(f(1,b-1) - f(1,b)) \\ &> \sum_{i=1}^{a-3}(f(1,a+1) - f(a,1)) + \sum_{i=2}^{b}(f(b-1,1) - f(1,b)) \\ &> (a-2-b)(f(1,a+1) - f(a,1) + f(b-1,1) - f(1,b)) > 0. \end{aligned}$$

Repeatedly applying Transformation 2 to $D_n(a, b)$ yields D_n^* with $BID(D_n^*) > BID(G)$.

On the other hand, by condition (i), $f(1, 2) + f(2, 2) < f(1, 3) + f(2, 3)$. From condition (iii), it follows that $f(3, n-2) + f(1, n-2) > 2f(2, n-2)$. Thus, we get

$$\begin{aligned} BID(C_n^*) - BID(D_n^*) &= (n-4)f(1,n-2) + f(2,n-2) + f(3,n-2) + f(3,2) + f(1,3) \\ &\quad - (n-5)f(1,n-2) - 3f(2,n-2) - f(2,2) - f(1,2) \\ &= f(1,n-2) + f(3,n-2) - 2f(2,n-2) > 0. \end{aligned}$$

Case 4.2. If $a - 2 + 1 \leq b$. Combining $a \geq 3$ and $a + b = n$, we deduce $\frac{n-1}{2} \leq b \leq n-3$. Therefore,

$$BID(D_n(a,b)) = (b-1)f(1,b) + f(b,n-b) + 2f(2,n-b) + (n-3-b)f(1,n-b) + f(2,2).$$

By condition (i) with $\frac{n-1}{2} \leq b \leq n-3$, we derive that $(n-4)f(1, n-2) - (b-1)f(1, b) > (n-3-b)f(1, n-2)$. Condition (ii) also gives $f(1, 3) > f(2, 2)$ and $f(b, n-b) < f(2, n-2)$. Again using condition (i) and $\frac{n-1}{2} \leq b \leq n-3$, it follows that $f(2, n-2) < f(3, n-2)$ and $f(2, n-b) < f(2, n-\frac{n-1}{2}) = f(2, \frac{n+1}{2})$. Furthermore, by condition (iii), $f(2, n-2) + f(2, 3) - 2f\left(2, \frac{n+1}{2}\right) > 0$. Consequently, we have

$$\begin{aligned} BID(C_n^*) - BID(D_n(a,b)) &= (n-4)f(1,n-2) + f(2,n-2) + f(3,n-2) + f(2,3) + f(1,3) \\ &\quad - (b-1)f(1,b) - f(b,n-b) - 2f(2,n-b) - (n-3-b)f(1,n-b) - f(2,2) \\ &> (n-3-b)(f(1,n-2) - f(1,n-b)) + f(3,n-2) + f(2,3) - 2f(2,n-b) \\ &> f(2,n-2) + f(2,3) - 2f(2,\frac{n+1}{2}) > 0. \end{aligned}$$

Thus, based on all the above cases, if $G \not\cong C_n^*$, we have $BID(C_n^*) > BID(G)$. □

For convenience, let $\mathbb{U}_{n,d}^{max} = \{G \in \mathbb{U}_{n,d} \mid BID(G) \text{ is maximizing}\}$. Specifically, $\mathcal{U}_{n,d}$ is constructed by attaching the two end vertices of a path P_3 to the vertices v_2 and v_4 of a diametral path $P^d = v_1v_2\cdots v_dv_{d+1}$, and attaching one end vertex of each of $(n-d-2)$ paths P_2 to the vertex v_2. Clearly, $\mathcal{U}_{n,d} \in \mathbb{U}_{n,d}$, and we have

$$BID(\mathcal{U}_{n,d}) = (n-d-1)f(n-d+1,1) + 2f(n-d+1,2) + \begin{cases} (n-5)f(2,2) + 3f(2,3) + f(1,2), & d \geq 5; \\ 2f(2,3) + f(1,3), & d = 4. \end{cases}$$

Theorem 3.3. *Let $G \in \mathbb{U}_{n,d}$ with $d \geq 4$ and $n = d + 2$. If $f(x, y)$ satisfies the subsequent requirements:*

(i) $f(x, y)$ is strictly increasing in x;

(ii) $f(x + y - 1, 1) > f(x, y)$ holds when $x, y = 2$;

(iii) $\varphi(3, x) = f(3, x) - f(2, x)$ is strictly decreasing in x,

then $BID(G) \leq BID(\mathcal{U}_{d+2,d})$ holds precisely when $G \cong \mathcal{U}_{d+2,d}$.

Proof. Suppose $G \in \mathbb{U}_{n,d}^{max}$, where C_k is the only cycle and $P^d = v_1v_2\cdots v_dv_{d+1}$ is the diameter path. There is a vertex $u \notin V(P^d)$, for which $C_k = v_iv_{i+1}uv_i$ or $C_k = v_iv_{i+1}v_{i+2}uv_i$, i.e., $k = 3$ or 4. Otherwise, $k \geq 5$, which contradicts $n = d + 2$.

Claim 1. $v_1 \notin V(C_k)$ and $v_{d+1} \notin V(C_k)$.

Proof of Claim 1. Suppose for contradiction that $v_1 \in V(C_k)$ (the case $v_{d+1} \in V(C_k)$ can be proven analogously). Then G is depicted in Figure 4.

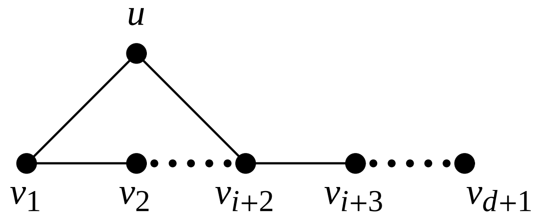

Figure 4. Graph G in Transformation 3.

Transformation 3: $G' = G - v_1u + uv_j$, where $j = 3$ if $k = 3$, and $j = 2$ if $k = 4$.

If $k = 3$ or $k = 4$. Condition (i) yields $f(2,2) < f(3,3)$, and it follows from condition (ii) that $f(2,2) < f(3,1)$. Thus, we deduce

$$BID(G') - BID(G) = f(3,3) + f(3,1) - 2f(2,2) > 0.$$

A contradiction with $G \in \mathbb{U}_{n,d}^{max}$ is derived. □

Claim 2. $C_k = C_4$.

Proof of Claim 2. As analyzed earlier, we only need to prove $C_k \neq C_3$. Assume for contradiction that $C_3 = v_iv_{i+1}uv_i$ exists. It then follows from Claim 1 that $v_{i-1}, v_{i+1} \notin PV(G)$ and $2 \leq i \leq d-1$. We only consider $v_{i-1} \notin PV(G)$ (the case $v_{i+2} \notin PV(G)$ is similar), so $d_G(v_{i-2}) \leq 2$.

Transformation 4: $G' = G - v_iu + uv_{i-1}$.

By condition (iii) and $d_G(v_{i-2}) \leq 2$, we deduce $f(3, d_G(v_{i-2})) - f(2, d_G(v_{i-2})) \geq f(3,2) - f(2,2) > f(3,3) - f(2,3)$. Consequently,

$$BID(G') - BID(G) = f(3, d_G(v_{i-2})) - f(2, d_G(v_{i-2})) + f(2,3) - f(3,3) > 0.$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and Claim 2 is proven. □

We now return to the proof of the theorem. From Claims 1 and 2, it follows that $2 \leq i \leq d-1$ and $C_k = C_4$. If $i \neq 2$ or $i \neq d-2$, condition (iii) gives $f(3,2) - f(2,2) < f(3,1) - f(2,1)$, so we have

$$BID(\mathcal{U}_{d+2,d}) - BID(G) = f(3,1) + f(2,2) - f(3,2) - f(2,1) > 0.$$

This again contradicts $G \in \mathbb{U}_{n,d}^{max}$. Therefore, $G \cong \mathcal{U}_{d+2,d}$, and the theorem is proven. □

Lemma 3.1. *Let $G \in \mathbb{U}_{n,d}^{max}$ with $4 \leq d \leq n-3$. Suppose C_k is the unique cycle and $P^d = v_1v_2\cdots v_dv_{d+1}$ is a diameter path. Let $v \in PV(G)$ with $vv_2 \in E(G)$ or $vv_d \in E(G)$. If $f(x,y)$ fulfills the subsequent requirements:*

(i) $f(x,y)$ is strictly increasing with x;

(ii) $f(x+y-1,1) > f(x,y)$ holds for $x, y \geq 2$;

(iii) $\varphi(2,x) = f(2,x) - f(1,x)$ is strictly decreasing in x,

then $|V(C_k) \cap V(P^d)| \geq 2$.

Proof. Assume for contradiction that $|V(C_k) \cap V(P^d)| \leq 1$, and we consider two cases as follows.
Case 1. $|V(C_k) \cap V(P^d)| = 0$.

There exists a path $v_i u_1 u_2 \cdots u_l$ connecting C_k and P^d, where $v_i \in V(P^d)$ and $u_l \in V(C_k)$. Since $3 \leq i \leq d-1$, we deduce that $v_{i-1} \notin PV(G)$ and $v_{i+1} \notin PV(G)$, i.e., $d_G(v_{i-1}) \geq 2$ and $d_G(v_{i+1}) \geq 2$.
Case 1.1. $l = 1$.

We apply the lifting transformation in Lemma 2.1 to $v_i u_1$ in G, yielding $G' \in \mathbb{U}_{n,d}$. From condition (i), it follows that $f(5,x) > f(3,x)$. Additionally, condition (ii) yields $f(3,3) < f(5,1)$. Consequently,

$$\begin{aligned} BID(G') - BID(G) &= f(5, d_G(v_{i-1})) + f(5, d_G(v_{i+1})) - f(3, d_G(v_{i-1})) - f(3, d_G(v_{i+1})) \\ &\quad + 2f(5,2) - 2f(3,2) + f(5,1) - f(3,3) \\ &> f(5,1) - f(3,3) > 0. \end{aligned}$$

Case 1.2. $l \geq 2$.
Transformation 5: $G' = G - u_1u_2 + u_2v_i$.

If $l = 2$, condition (i) gives $f(4,x) > f(3,x)$ and $f(4,3) > f(2,3)$. Furthermore, condition (ii) implies $f(2,3) < f(4,1)$, and we deduce

$$\begin{aligned} BID(G') - BID(G) &= f(4, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) + f(4, d_G(v_{i+1})) - f(3, d_G(v_{i+1})) \\ &\quad + f(4,3) + f(4,1) - 2f(2,3) \\ &> f(4,1) - f(2,3) > 0. \end{aligned}$$

If $l \geq 3$, by condition (i), we obtain

$$\begin{aligned} BID(G') - BID(G) &= f(4, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) + f(4, d_G(v_{i+1})) - f(3, d_G(v_{i+1})) + f(2,4) - f(2,3) \\ &> 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$.
Case 2. $|V(C_k) \cap V(P^d)| = 1$.

Let $C_k = u_1 u_2 \cdots u_k u_1$, where $u_1 = v_i$ is the common vertex of C_k and P^d. Since $d \geq 4$, for $2 \leq i \leq d$, either $d_G(v_{i-1}) \geq 2$ or $d_G(v_{i+1}) \geq 2$. For simplicity, assume $d_G(v_{i+1}) \geq 2$, so we deduce $d_G(v_i) \geq 4$ and $d_G(v_{i+2}) \geq 1$. Thus, the graph G is depicted in Figure 5.

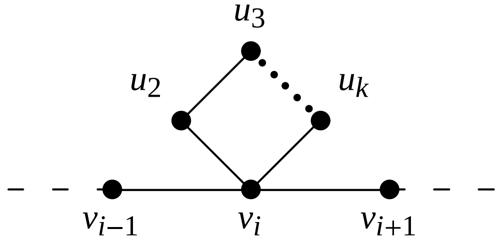

Figure 5. Graph G in Transformation 6.

Transformation 6: $G' = G - u_2u_3 + u_jv_{i+3-j}$, where $j = 2$ if $k = 3$, and $j = 3$ if $k \geq 4$.

We have that $G' \in \mathbb{U}_{n,d}$. If $k = 3$, condition (i) gives $f(d_G(v_{i+1}) + 1, x) > f(d_G(v_{i+1}), x)$ and $f(d_G(v_{i+1}) + 1, 2) \geq f(3, 2)$. Condition (ii) yields $f(2, 2) < f(1, 3)$. Furthermore, by condition (iii) and $d_G(v_i) \geq 4$, we deduce $f(1, d_G(v_i)) - f(2, d_G(v_i)) > f(1, 3) - f(2, 3)$. Thus,

$$\begin{aligned} BID(G') - BID(G) = {} & f(d_G(v_i), d_G(v_{i+1}) + 1) - f(d_G(v_i), d_G(v_{i+1})) \\ & + f(d_G(v_{i+1}) + 1, d_G(v_{i+2})) - f(d_G(v_{i+1}), d_G(v_{i+2})) \\ & + f(1, d_G(v_i)) - f(2, d_G(v_i)) + f(2, d_G(v_{i+1}) + 1) - f(2, 2) \\ & > f(1, d_G(v_i)) - f(2, d_G(v_i)) + f(2, 3) - f(1, 3) > 0. \end{aligned}$$

If $k \geq 4$, condition (i) gives $f(5, x) > f(4, x)$. Additionally, condition (ii) yields $f(2, 2) < f(1, 3)$. Thus, we deduce

$$\begin{aligned} BID(G') - BID(G) = {} & f(5, d_G(v_{i-1})) - f(4, d_G(v_{i-1})) + f(5, d_G(v_{i+1})) - f(4, d_G(v_{i+1})) \\ & + f(1, 5) - f(2, 2) + 2(f(5, 2) - f(4, 2)) \\ & > f(1, 5) - f(2, 2) > 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and the lemma is thus proven. □

Lemma 3.2. *Suppose $G \in \mathbb{U}_{n,d}^{max}$ with $4 \leq d \leq n - 3$. If $f(x, y)$ satisfies the following conditions:*
(i) $f(x, y)$ is strictly increasing with x;
(ii) $f(2, x)$ is strictly convex downward in x;
(iii) $\varphi(3, x) = f(3, x) - f(2, x)$ is strictly decreasing in x,
then there is a vertex $v_0 \in PV(G)$ for which $G - v_0 \in \mathbb{U}_{n-1,d}$.

Proof. First, we claim that $G \ncong C_n$. Otherwise, let $G' = C_{n-1} + e \in \mathbb{U}_{n,d}$. By (i) and (ii), we have

$$BID(G) = nf(2, 2) < (n - 3)f(2, 2) + 2f(3, 2) + f(3, 1) = BID(G').$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and hence $PV(G) \neq \emptyset$. In the following, assume for contradiction that for all $v \in PV(G)$, $G - v \in \mathbb{U}_{n-1,d-1}$. Since $3 \leq d \leq n - 3$, G contains a diameter path $P^d = v_1 v_2 \cdots v_d v_{d+1}$ with $v_1 \in PV(G)$. Immediately, we deduce $v = v_1$ or $v = v_{d+1}$. By Lemma 3.1, $|V(C_k) \cap V(P^d)| \geq 2$. We thus let $C_k = v_i v_{i+1} \cdots v_{i+j} u_l u_{l-i} \cdots u_3 u_2 u_1$, where $j \geq 1$, $l \geq 3$, and $j \leq l$. So, we deduce $d_G(v_{i-1}) \geq 1$, $d_G(v_i) = 3$, $d_G(u_2) = d_G(u_3) = 2$, and G is depicted in Figure 6.

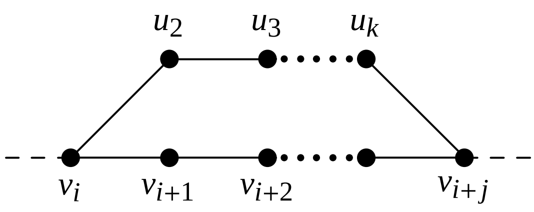

Figure 6. Graph G in Transformation 7.

Case 1. $3 \leq l = j$.
Transformation 7: $G' = G - v_i u_2 - u_2 u_3 + u_2 v_{i+1} + u_3 v_{i+1}$.

Condition (iii) gives $f(2, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) \geq f(2, 1) - f(3, 1)$. From condition (ii), we have $2f(2, 2) < f(2, 1) + f(2, 3)$. Combined with condition (i), we get

$$\begin{aligned}
BID(G') - BID(G) &= f(2, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) + 3f(2, 4) + f(1, 4) - 2f(2, 2) - 2f(2, 3) \\
&> f(2, 1) - f(3, 1) + 3f(2, 4) + f(1, 4) - 2f(2, 2) - 2f(2, 3) \\
&> f(2, 1) + f(2, 4) - 2f(2, 2) > 0.
\end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$.
Case 2. $l > j$.
Transformation 8: $G' = G - u_2u_3 + u_3v_i$.

By condition (i), $f(4, x) > f(3, x)$. Condition (ii) also gives $f(2, 2) - f(2, 1) < f(2, 4) - f(2, 3)$. Thus, we obtain

$$\begin{aligned}
BID(G') - BID(G) &= f(4, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) + f(4, d_G(v_{i+1})) - f(3, d_G(v_{i+1})) \\
&\quad + f(2, 4) + f(1, 4) - f(2, 2) - f(2, 3) \\
&> f(2, 4) + f(1, 4) - f(2, 2) - f(2, 3) > 0.
\end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and the lemma is proven. □

Lemma 3.3. *Let $G \in \mathbb{U}_{n,d}^{max}$ with $4 \leq d \leq n - 3$. Define $A = \{v \in PV(G) \mid G - v \in \mathbb{U}_{n-1,d}\}$, $B = \{u \in N_G(v) \mid v \in A\}$, and $C_G(u) = \{w \in N_G(u) \mid u \in B, d_G(w) \geq 2\}$ with $|C_G(u)| \geq 1$. Given that $f(x, y)$ fulfills the following requirements:*

(i) $f(x, y)$ is strictly increasing in x;

(ii) $f(x + 1, y - 1) > f(x, y)$ holds for $x \geq y \geq 2$;

(iii) $f(1, x)$ and $f(2, x)$ are strictly convex downward in x;

(iv) $\varphi(x, y) = f(x, y) - f(x - 1, y)$ is strictly increasing with x and strictly decreasing with y,
then there is a vertex $v_0 \in PV(G)$ for which $v_0 \in A$ and $|C_G(N_G(v_0))| \geq 2$.

Proof. First, Lemma 3.2 implies that $A \neq \emptyset$, and hence $|C_G(u)| \geq 1$. Assume for contradiction that $|C_G(u)| = 1$ for all $u \in B$. Denote the diameter path as $P^d = v_1v_2 \cdots v_dv_{d+1}$ and the only cycle as $C_k = u_1u_2 \cdots u_ku_1$.
Claim 1. $A \subseteq N_G(v_2) \cup N_G(v_d)$.
Proof of Claim 1. Assume for contradiction that there is a vertex $v \in A$ satisfying $v \notin N_G(v_2) \cup N_G(v_d)$. Let $N_G(v) = u$, and then $u \notin \{v_1, v_2, v_d, v_{d+1}\}$. Otherwise, the diameter d would increase. On the other hand, $|C_G(u)| = 1$ for all $u \in B$ implies $u \notin V(P^d) \cup V(C_k)$. Let $w \in N_G(u)$ and $N_G(w) = \{u, z_1z_2 \cdots z_t\}$), where $d_G(w) = t + 1$ and $t \geq 1$. Thus, the graph G is depicted in Figure 7.

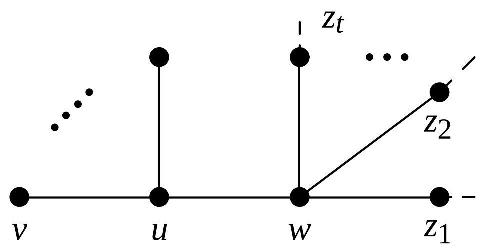

Figure 7. Graph G in Transformation 9.

Transformation 9: $G' = G - \{\bigcup_{1\le i\le t} wz_i\} + \{\bigcup_{1\le i\le t} vz_i\}$.

Condition (i) implies $f(t + d_G(u), x) > f(t + 1, x)$ and $f(t + d_G(u), 1) > f(d_G(u), 1)$. It follows from condition (ii) that $f(d_G(u) + t, 1) > f(d_G(u), t + 1)$. Consequently, we obtain

$$\begin{aligned} BID(G') - BID(G) = &\sum_{i=1}^{t} (f(t + d_G(u), d_G(z_i)) - f(t + 1, d_G(z_i))) + f(d_G(u) + t, 1) \\ &- f(d_G(u), t + 1) + (d_G(u) - 1)(f(t + d_G(u), 1) - f(d_G(u), 1)) \\ &> f(d_G(u) + t, 1) - f(d_G(u), t + 1) > 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and Claim 1 holds. □

Thus, there exists $v \in A$, such that $v \in N_G(v_2)$ and $|C_G(u)| = 1$. In G, it follows that $v_1, v_2 \notin C_k$, $d_G(v_2) \ge 3$, and $d_G(v_{i-1}) \ge 1$. These satisfy the conditions of Lemma 3.1, so $|V(C_k) \cap V(P^d)| \ge 2$. Similar to Lemma 3.2, we can write $C_k = v_i v_{i+1} \cdots v_{i+j} u_l u_{l-1} \cdots u_3 u_2 u_1$, where $u_1 = v_i$, $j \ge 1$, and $j \le l$.

Claim 2. $|V(C_k)\backslash V(P^d)| = 1$.

Proof of Claim 2. Suppose for contradiction that $|V(C_k)\backslash V(P^d)| \ge 2$, so $l \ge 2$. If $l = j$, we perform the following transformation.

Transformation 10: $G' = G - v_i u_2 - u_2 u_3 + u_2 v_{i+1} + u_3 v_{i+1}$.

By condition (i), $f(4, d_G(v_{i+2})) > f(2, d_G(v_{i+2}))$. Condition (iv) gives $f(2, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) > f(2, 1) - f(3, 1)$, and condition (iii) yields $f(2, 2) - f(2, 1) < f(2, 4) - f(2, 3)$. Thus, combined with condition (i), we deduce

$$\begin{aligned} BID(G') - BID(G) = &f(4, d_G(v_{i+2})) - f(2, d_G(v_{i+2})) + f(2, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) \\ &+ 2(f(2, 4) - f(2, 3)) + f(1, 4) - f(2, 2) \\ &> f(2, 1) - f(3, 1) + 2f(2, 4) - 2f(2, 3) + f(1, 4) - f(2, 2) \\ &> f(2, 1) + f(2, 4) + f(2, 2) - f(2, 3) > 0. \end{aligned}$$

If $l > j$, we perform the following transformation.

Transformation 11: $G' = G - u_2 u_3 + u_3 v_i$.

By condition (i), $f(4, x) > f(3, x)$ and $f(4, 2) > f(2, 2)$. Furthermore, condition (ii) gives $f(4, 1) > f(2, 3)$. Thus, we obtain

$$\begin{aligned} BID(G') - BID(G) = &f(4, d_G(v_{i-1})) - f(3, d_G(v_{i-1})) + f(4, d_G(v_{i+1})) - f(3, d_G(v_{i+1})) \\ &+ f(4, 2) + f(4, 1) - f(2, 2) - f(2, 3) > 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and Claim 2 is proven. □

Consequently, from Claim 2, $|V(C_k)\backslash V(P^d)| = 1$ yields $k = |V(C_k)| = 3$ or 4. Therefore, for the rest of the lemma's proof, it suffices to consider $k = 3$ and 4.

Claim 3. $d_G(v_1) = d_G(v_{d+1}) = 1$.

Proof of Claim 3. We only present the proof for $d_G(v_1) = 1$, and the case for $d_G(v_{d+1}) = 1$ can be proven analogously. Suppose for contradiction that $d_G(v_1) \ge 2$. Then $d_G(v_1) = 2$. Otherwise, $d_G(v_1) \ge 3$ yields that the diameter d would increase. Moreover, $|C_G(u)| = 1$ for all $u \in B$ implies v_d is not adjacent to any pendant vertices. Therefore, we derive $d_G(v_4) \ge 2$ from the condition of $d \ge 4$.

Transformation 12: $G' = G - v_1 w + w v_r$, where $r = 3$ if $k = 3$, and $r = 2$ if $k = 4$.

When $k = 3$, the unique cycle is $C_3 = v_1v_2wv_1$. By conditions (i) and (ii), we have

$$\begin{aligned} BID(G') - BID(G) &= f(3, d_G(v_{d-2})) - f(2, d_G(v_{d-2})) + f(3,3) + f(3,1) + f(2,3) - 2f(2,3) - f(2,2) \\ &> f(3,1) - f(2,2) > 0. \end{aligned}$$

When $k = 4$, the unique cycle is $C_4 = v_1v_2v_3wv_1$. Similar to the case where $k = 3$, we obtain

$$BID(G') - BID(G) = f(3,3) + f(1,3) - 2f(2,2) > 0.$$

This contradicts $G \in \mathbb{U}^{max}_{n,d}$, and Claim 3 is proven. □

Claim 4. $k = |V(C_k)| = 4$.

Proof of Claim 4. Suppose for contradiction that $k = 3$, i.e., $C_3 = v_iv_{i+1}wv_i$ with $3 \le i \le d-1$. Otherwise, this contradicts Claim 3 and the assumption that $|C_G(u)| = 1$. Hence, the graph G is depicted in Figure 8. Since $A \neq \emptyset$ and $d_G(v_2) \ge 3$, two subcases are considered herein.

If $i = 3$. We perform the following transformation.

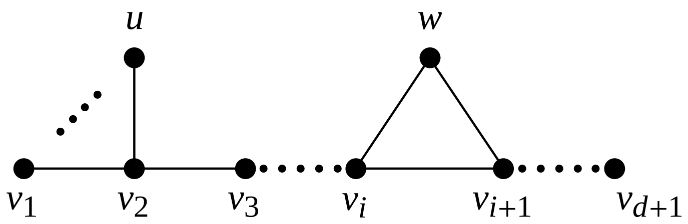

Figure 8. Graph G in Transformations 13 and 14.

Transformation 13: $G' = G - v_3w + wv_2$.

By condition (i), $f(1, d_G(v_2) + 1) > f(1, d_G(v_2))$. When combined with condition (ii), this yields $f(3,3) < f(d_G(v_2), 3) < f(d_G(v_2) + 1, 2)$. Consequently, we deduce

$$\begin{aligned} BID(G') - BID(G) &= f(1, d_G(v_2) + 1) - f(1, d_G(v_2)) + 2f(d_G(v_2) + 1, 2) - f(d_G(v_2), 3) - f(3,3) \\ &> 2f(d_G(v_2) + 1, 2) - 2f(d_G(v_2) + 1, 2) = 0. \end{aligned}$$

If $i \ge 4$. We construct the following transformation.

Transformation 14: $G' = G - v_iw - v_{i+1}w + v_2w + v_4w$.

Note that $d_G(v_2) \ge 3$ and $d_G(v_{i+2}) \ge 1$. From condition (iii), we have $f(1, d_G(v_2)+1) - f(1, d_G(v_2)) \ge f(1,4) - f(1,3)$. Condition (iv) implies $f(2, d_G(v_{i+2})) - f(3, d_G(v_{i+2})) \ge f(2,1) - f(3,1)$. By virtue of condition (ii), $f(3,3) < f(d_G(v_2), 3) < f(d_G(v_2) + 1, 2)$. Moreover, condition (iii) leads to $f(1,3) - f(1,2) < f(1,4) - f(1,3)$. Therefore, we get

$$\begin{aligned} BID(G') - BID(G) &= (d_G(v_2) - 1)(f(1, d_G(v_2) + 1) - f(1, d_G(v_2))) + 2f(d_G(v_2) + 1, 2) \\ &\quad - f(d_G(v_2), 2) - f(3,3) + f(2, d_G(v_{i+2})) - f(3, d_G(v_{i+2})) \\ &> 2f(1,4) - 2f(1,3) + 2f(d_G(v_2) + 1, 2) - f(d_G(v_2), 2) - f(3,3) + f(1,2) - f(1,3) \\ &> 2f(1,4) + f(1,2) - 3f(1,3) > 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}^{max}_{n,d}$, and Claim 4 is proven. □

Claim 5: $d_G(v_2) = n - d$ and $d_G(v_d) = 2$.

Proof of Claim 5. Otherwise, it follows from Claims 1–4 that the graph G is depicted in Figure 9, where $d_G(v_2) = a$, $d_G(v_d) = b$, and we may assume that $a \geq b$. Let $d_G(v_3) = x$ and $d_G(v_{d-1}) = y$, and then $2 \leq x, y \leq 3$.

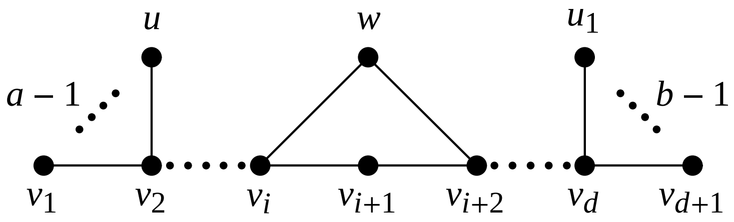

Figure 9. Graph G in Transformation 15.

Transformation 15: $G' = G - v_d u_1 + v_2 u_1$.

By condition (iii), we have $f(1, a+1) - f(1, a) > f(1, b) - f(1, b-1)$. From condition (iv), it holds that $f(a+1, 1) - f(b, 1) \geq f(b+1) - f(b, 1) > f(b, 1) - f(b-1, 1) > f(b, y) - f(b-1, y)$. Consequently,

$$\begin{aligned} BID(G') - BID(G) &= af(a+1,1) - (a-1)f(a,1) + (b-2)f(b-1,1) - (b-1)f(b,1) \\ &\quad + f(a+1,x) - f(a,x) + f(b-1,y) - f(b,y) \\ &> f(a+1,1) - f(b,1) + f(a+1,x) - f(a,x) + f(b-1,y) - f(b,y) \\ &> f(a+1,x) - f(a,x) > 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$. □

We now return to the proof of the lemma. From the five claims, we immediately deduce that the unique 4-cycle $C_4 = v_i v_{i+1} v_{i+2} w v_i$ is connected to the diameter path via vertex v_i, where $3 \leq i \leq d-2$. Moreover, we have $d_G(v_2) \geq 3$, $d_G(v_{i+1}) = 2$, and $d_G(v_{i+3}) \geq 1$. In what follows, we compare the values of $BID(G)$ and $BID(\mathcal{U}_{n,d})$ in two cases to derive a contradiction.

Case 1. $i = 3$. By condition (iii), $f(1, d_G(v_2)+1) - f(1, d_G(v_2)) \geq f(1,4) - f(1,3)$. Condition (iv) gives $f(2, d_G(v_6)) - f(3, d_G(v_6)) \geq f(2,1) - f(3,1)$. From condition (ii), $f(d_G(v_2), 3) < f(d_G(v_2)+1, 2)$. Condition (iii) also yields $2f(1,3) < f(1,4) + f(1,2)$. Thus, we have

$$\begin{aligned} BID(\mathcal{U}_{n,d}) - BID(G) &= (d_G(v_2)-1)(f(1, d_G(v_2)+1) - f(1, d_G(v_2))) + 2f(d_G(v_2)+1, 2) \\ &\quad - f(d_G(v_2), 3) - f(2,3) + f(2, d_G(v_6)) - f(3, d_G(v_6)) \\ &\geq 2f(1,4) - 2f(1,3) + 2f(d_G(v_2)+1, 2) - f(d_G(v_2), 3) - f(2,3) + f(1,2) - f(1,3) \\ &> 2f(1,4) - 3f(1,3) + f(d_G(v_2)+1, 2) - f(2,3) + f(1,2) \\ &> 2f(1,4) + f(1,2) - 3f(1,3) > 0. \end{aligned}$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$.

Case 2. $4 \leq i \leq d-2$. From condition (iii), $f(1, d_G(v_2)+1) - f(1, d_G(v_2)) \geq f(1,4) - f(1,3)$. Condition (iv) gives $f(2, d_G(v_{i+3})) - f(3, d_G(v_{i+3})) \geq f(2,1) - f(3,1)$. Condition (iii) also yields

$f(2, d_G(v_2) + 1) + f(2, 1) > f(2, d_G(v_2)) + f(2, 2)$. Since $d_G(v_2) \geq 3$, we deduce

$$\begin{aligned} BID(\mathcal{U}_{n,d}) - BID(G) &= (d_G(v_2) - 1)(f(1, d_G(v_2) + 1) - f(1, d_G(v_2))) + 2f(d_G(v_2) + 1, 2) \\ &- f(d_G(v_2), 2) - 2f(2, 3) + f(2, 2) + f(2, d_G(v_{i+3})) - f(3, d_G(v_{i+3})) \\ &> 2(f(1, 4) - f(1, 3)) + 2f(d_G(v_2) + 1, 2) - f(d_G(v_2), 2) \\ &- 2f(2, 3) + f(2, 2) + f(2, 1) - f(3, 1) \\ &> 2f(1, 4) + f(d_G(v_2) + 1, 2) + f(d_G(v_2), 2) + 2f(2, 2) \\ &- (3f(1, 3) + 2f(2, 3) + f(d_G(v_2), 2)) \\ &> 2f(1, 4) + f(4, 2) + 2f(2, 2) - (3f(1, 3) + 2f(2, 3)). \end{aligned}$$

Furthermore, condition (iii) gives $f(2, 4) + f(2, 2) > 2f(2, 3)$ and $f(1, 4) + f(1, 2) > 2f(1, 3)$. Thus,

$$BID(\mathcal{U}_{n,d}) - BID(G) > f(1, 4) - f(1, 3) > 0.$$

This contradicts $G \in \mathbb{U}_{n,d}^{max}$, and the proof is done. □

Theorem 3.4. *Let $G \in \mathbb{U}_{n,d}$ with $d \geq 4$ and $n \geq d + 2$. If $f(x, y)$ fulfills the following requirements:*
(i) $f(x, y)$ is strictly increasing in x;
(ii) $f(x + 1, y - 1) > f(x, y)$ holds for $x \geq y \geq 2$;
(iii) $f(1, x)$ and $f(2, x)$ are strictly convex downward in x;
(iv) $\varphi(x, y) = f(x, y) - f(x - 1, y)$ is strictly increasing with x and strictly decreasing with y,
then $BID(G) \leq BID(\mathcal{U}_{n,d})$ holds precisely when $G \cong \mathcal{U}_{n,d}$.

Proof. This theorem is established via induction on n. First, combining conditions (i), (ii), and (iv) with Theorem 3.3, the conclusion is valid when $n = d + 2$. In what follows, we restrict our attention to the scenario that $4 \leq d \leq n - 3$. Assume the theorem holds for $n - 1$, i.e., for any $G' \in \mathbb{U}_{n-1,d}$,

$$BID(G') \leq BID(\mathcal{U}_{n-1,d}) = (n - d - 2)f(1, n - d) + 2f(2, n - d) + (d - 5)f(2, 2) + 3f(2, 3) + f(1, 2).$$

On the other hand, the conditions satisfy Lemma 3.3, so there must exist a vertex $v \in PV(G)$, for which $G - v \in \mathbb{U}_{n-1,d}$. Let $u \in N_G(v)$, and there exist two edges $uu_1, uu_2 \in E(G)$ with $d_G(u_1) \geq 2$ and $d_G(u_2) \geq 2$, where $3 \leq d_G(u) \leq n - d + 1$. In this case, we may assume $N_G(u) = \{v, u_1, u_2, \cdots, u_{d_G(u)-1}\}$.

Let $G' = G - v$, and it follows that $G' \in \mathbb{U}_{n-1,d}$. Next, we consider two cases: $d = 4$ and $d \geq 5$. When $d \geq 5$, by condition (iv), $f(x, y) - f(x - 1, y) \leq f(x, 1) - f(x - 1, 1)$ for all $y \geq 1$. Thus,

$$\begin{aligned} BID(G) &= BID(G') + f(d_G(v), d_G(u)) + \sum_{i=1}^{d_G(u)-1} (f(d_G(u), d_G(u_i)) - f(d_G(u) - 1, d_G(u_i))) \\ &\leq BID(G') + f(1, d_G(u)) + 2(f(d_G(u), 2) - f(d_G(u) - 1, 2)) \\ &+ \sum_{i=3}^{d_G(u)-1} (f(d_G(u), d_G(u_i)) - f(d_G(u) - 1, d_G(u_i))) \\ &\leq BID(G') + f(1, d_G(u)) + 2(f(d_G(u), 2) - f(d_G(u) - 1, 2)) \\ &+ (d_G(u) - 3)(f(d_G(u), 1) - f(d_G(u) - 1, 1)). \end{aligned}$$

Since $d_G(u) \leq n - d + 1$, by condition (iii), $f(2, d_G(u)) - f(2, d_G(u) - 1) \leq f(2, n - d + 1) - f(2, n - d)$, and $f(1, d_G(u)) - f(1, d_G(u) - 1) \leq f(1, n - d + 1) - f(1, n - d)$. Combined with condition (i), we have

$$\begin{aligned} BID(G) &\leq BID(G') + f(1, n - d + 1) + 2(f(2, n - d + 1) - f(2, n - d)) \\ &\quad + (d_G(u) - 3)(1, n - d + 1) - f(1, n - d)) \\ &\leq BID(G') + (n - d - 1)f(1, n - d + 1) + 2f(2, n - d + 1) - 2f(2, n - d) \\ &\quad - (n - d - 2)f(1, n - d). \end{aligned}$$

Substituting the induction hypothesis into the above,

$$\begin{aligned} BID(G) &\leq (n - d - 2)f(1, n - d) + 2f(2, n - d) + (d - 5)f(2, 2) + 3f(2, 3) + f(1, 2) \\ &\quad + (n - d - 1)f(1, n - d + 1) + 2f(2, n - d + 1) - 2f(2, n - d) - (n - d - 2)f(1, n - d) \\ &= (n - d - 1)f(1, n - d + 1) + 2f(2, n - d + 1) + (d - 5)f(2, 2) + 3f(2, 3) + f(1, 2) \\ &= BID(\mathcal{U}_{n,d}). \end{aligned}$$

This holds precisely when $d_G(u) = n - d + 1$, $G' \in \mathbb{U}_{n-1,d}$, $d_G(v) = 1$, $d_G(u_1) = d_G(u_2) = 2$, and $d_G(u_i) = 1$ for $3 \leq i \leq d_G(u) - 1$. That is, $G \cong \mathcal{U}_{n,d}$.

When $d = 4$, the proof is completely analogous to the case where $d \geq 5$, except that $(d - 5)f(2, 2)$ $+3f(2, 3) + f(1, 2)$ is replaced with $2f(2, 3) + f(1, 3)$. Following the same derivation, we obtain $BID(G) \leq BID(\mathcal{U}_{n,4})$, with equality precisely when $G \cong \mathcal{U}_{n,4}$. Thus, the theorem is proven. □

4. Application of the sufficient conditions

As an application of the sufficient conditions, in this section, we verify the topological indices that meet the sufficient conditions for the maximum *BID* of trees and unicyclic graphs with a fixed diameter, where these conditions were derived in the previous two sections. Through direct calculations, we can obtain the following conclusion, and the detailed calculation processes are omitted herein.

Proposition 4.1. *The bond incident degree indices in Table 1 satisfy the requirements:*
(i) $f(x, y)$ is strictly increasing in x;
(ii) $f(x + 1, y - 1) > f(x, y)$ holds for $x \geq y \geq 2$;
(iii) $f(1, x)$ and $f(2, x)$ are strictly convex downward in x;
(iv) $\varphi(x, y) = f(x, y) - f(x - 1, y)$ is strictly increasing with x and strictly decreasing with y.

Table 1. The bond incident degree indices with determined maximal values of *BID*.

No.	$f(x, y)$	Indices	$\mathbb{T}_{n,d}^{Max}$	$\mathbb{U}_{n,2}^{Max}$	$\mathbb{U}_{n,3}^{Max}$	$\mathbb{U}_{n,d}^{Max}$ $(d \geq 4)$
1	$\sqrt{x^2 + y^2}$	Sombor index	$T_{n,d}^*$ [12]	S_n^+	C_n^*	$\mathcal{U}_{n,d}$ [13]
2	$\sqrt{(x-1)^2 + (y-1)^2}$	Reduced Sombor index	$T_{n,d}^*$	S_n^+	C_n^*	$\mathcal{U}_{n,d}$
3	$\sqrt{2}\pi \frac{x^2+y^2}{x+y}$	Third Sombor index	$T_{n,d}^*$	S_n^+	C_n^*	$\mathcal{U}_{n,d}$
4	$\frac{\pi}{2}(\frac{x^2+y^2}{x+y})^2$	Fourth Sombor index	$T_{n,d}^*$	S_n^+	C_n^*	$\mathcal{U}_{n,d}$
5	$\sqrt{x^2 + y^2 + xy}$	Euler Sombor index	$T_{n,d}^*$	S_n^+	C_n^*	$\mathcal{U}_{n,d}$
6	$(x^2 + y^2)^\alpha$ $(\frac{1}{2} \leq \alpha < 1)$	General Sombor index	$T_{n,d}^*$	S_n^+	C_n^*	$\mathcal{U}_{n,d}$

Therefore, from Theorem 2.2 and Proposition 4.1, we directly arrive at the following Theorem 4.1. Furthermore, Theorems 4.2–4.4 are derived, respectively, from Theorems 3.1, 3.2, 3.4 and Proposition 4.1.

Theorem 4.1. *Let $T \in \mathbb{T}_{n,d}$ with $d \geq 3$ and $n \geq d+3$. For the bond incident degree indices listed in Table 1, we have that*

$$BID(T) \leq BID(T^*_{n,d}) = (n-d)f(1, n-d+1) + (d-3)f(2,2) + f(2, n-d+1) + f(1,2)$$

holds precisely when $T \cong T^*_{n,d}$.

Theorem 4.2. *Let $G \in \mathbb{U}_{n,2}$ with $n \geq 4$. For the bond incident degree indices listed in Table 1, we have that*

$$BID(G) \leq BID(S^+_n) = (n-3)f(1, n-1) + f(2,2) + 2f(2, n-1)$$

holds precisely when $G \cong S^+_n$.

Theorem 4.3. *Let $G \in \mathbb{U}_{n,3}$ with $n \geq 5$. Regarding the bond incident degree indices listed in Table 1, we have that*

$$BID(G) \leq BID(C^*_n) = (n-4)f(1, n-2) + f(2, n-2) + f(3, n-2) + f(2,3) + f(1,3)$$

holds precisely when $G \cong C^*_n$.

Theorem 4.4. *Let $G \in \mathbb{U}_{n,d}$ with $d \geq 4$ and $n \geq d+2$. Concerning the bond incident degree indices listed in Table 1, we have that*

$$BID(G) = (n-d-1)f(1, n-d+1) + 2f(2, n-d+1) + \begin{cases} (n-5)f(2,2) + 3f(2,3) + f(1,2), & d \geq 5; \\ 2f(2,3) + f(1,3), & d = 4, \end{cases}$$

holds precisely when $G \cong \mathcal{U}_{n,d}$.

5. Concluding remarks

Our main work is to obtain the sufficient conditions for the maximum *BID* of bond incident degree topological indices for trees and unicyclic graphs with a fixed diameter, respectively, by means of various graph transformations based on the structural characteristics of these graphs, and characterizing the associated extremal graphs. When applying the sufficient conditions, we verify that six types of bond incident degree topological indices satisfy these conditions, which indicates that the proposed sufficient conditions have certain applicability and generalization ability.

Obviously, the method of exploring bond incident degree index problems by seeking sufficient conditions can avoid repetitive calculations for individual indices and thus exhibits good generalization performance. Moreover, bond incident degree topological indices share certain commonalities to some extent, for example, the ABS index and the forgotten index satisfy two and three of the four conditions in Theorem 3.4, respectively. It will be an important direction for further research to investigate the sufficient conditions of topological indices, thereby addressing the extremal problems for more graph classes and more indices. Naturally, we pose an open problem.

Problem 5.1. *What are the sufficient conditions for the extremal topological indices of bicyclic and tricyclic graphs with a fixed diameter?*

Use of Generative-AI tools declaration

The author declares they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The author declares no conflict of interest.

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