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Research article

Bond incident degree indices of stepwise irregular graphs

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Abstract: The bond incident degree (BID) index of a graph G is defined as $BID_f(G) = \sum_{uv\in E(G)} f(d(u), d(v))$, where $d(u)$ is the degree of a vertex u and f is a non-negative real valued symmetric function of two variables. A graph is stepwise irregular if the degrees of any two of its adjacent vertices differ by exactly one. In this paper, we give a sharp upper bound on the maximum degree of stepwise irregular graphs of order n when $n \equiv 2 (\mathrm{mod}\ 4)$, and we give upper bounds on BID_f index in terms of the order n and the maximum degree Δ. Moreover, we completely characterize the extremal stepwise irregular graphs of order n with respect to BID_f.

Keywords: maximum degree; stepwise irregular graph; BID index; bipartite graph
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1. Introduction

In molecular graphs, the vertices correspond to atoms, while the edges represent covalent bonds between atoms. A molecular structure can be characterized using many numerical descriptors which are usually defined by formulas involving atoms and bonds. Such numerical descriptor is called molecular structure descriptor or topological index. During the last decade, topological indices are being be widely used in theoretical chemistry and pharmaceutical researchers. Among them, a large number of topological indices depend only vertex degrees of the molecular graph. Such index is called vertex-degree-based topological index.

Let $G = (V, E)$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $d(v)$, the degree of a vertex v of G. The maximum degree Δ and minimum degree δ of a graph G is the maximum and minimum value of the degrees of vertices in G, respectively.

The general form of vertex-degree-based topological index is defined as

$$BID_f(G) = \sum_{uv \in E(G)} f(d(u), d(v))$$

and called the bond incident degree index, where $f(x, y)$ is a non-negative real valued symmetric function. The general form BID index $\sum_{uv\in E(G)} f(d_u, d_v)$ was first proposed in [13], and an early one with constraint on f was considered in [27].

The most studied vertex-degree-based topological indices are the first and second Zagreb indices and defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)) \text{ and } M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

These topological indices have been intensively studied for the last fifty years, see [4, 5, 8, 11]. Moreover, the relation between these indices and the reduced form of the second Zagreb index RM_2 which is called the reduced second Zagreb index, were studied in [7, 9, 10, 12, 18].

Recently, Gutman introduced new degree based topological indices which are called the Sombor index and the reduced Sombor index. They are defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

and

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2}.$$

It invented in the Summer of 2020, and made publicly available in early 2021. In less than one year, more than fifty research papers on this topological index were produced, see [16, 17, 19, 20, 23, 26] and cited therein.

Two multiplicative versions of Zagreb indices are defined as

$$\Pi_2(G) = \prod_{uv \in E(G)} d_G(u) d_G(v) \text{ and } \Pi_1^*(G) = \prod_{uv \in E(G)} (d_G(u) + d_G(v)),$$

and called the multiplicative second Zagreb index and the multiplicative sum Zagreb index, respectively. Recent results related to them can be found in [14, 21, 24, 28].

The Zagreb indices, the Sombor index, the reduced Sombor index and the reduced form of the second Zagreb index are direct special cases of the bond incident index, in particular

$$M_1(G) = BID_{f_1}(G), \ \ M_2(G) = BID_{f_2}(G) \text{ and } RM_2(G) = BID_{f_3}(G),$$

and

$$SO(G) = BID_{f_4}(G) \text{ and } SO_{red}(G) = BID_{f_5}(G),$$

where $f_1(x, y) = x + y$, $f_2(x, y) = xy$, $f_3(x, y) = (x - 1)(y - 1)$, $f_4(x, y) = \sqrt{x^2 + y^2}$ and $f_5(x, y) = \sqrt{(x - 1)^2 + (y - 1)^2}$.

The above multiplicative versions of Zagreb indices are indirect special cases, but are related as

$$\ln \Pi_2(G) = BID_{f_6}(G) \text{ and } \ln \Pi_1^*(G) = BID_{f_7}(G),$$

where $f_6(x, y) = \ln xy$ and $f_7(x, y) = \ln(x + y)$.

In the recent years, several articles associated with the BID indices of molecular graphs were published. In [25], authors studied the behavior of BID indices over catacondensed pentagonal systems and derived a general expression for calculating them. In [22], authors determined the bond incident degree indices of complex structures in drugs called nanostar dendrimers and compute the closed formula for these indices. They also obtained some results which will be applicable to the physiochemical properties, chemical reactivity or biological activities. Ali and his colleagues computed BID indices of several nanostructures and pentagonal chains [2, 3]. They also characterized graphs with maximum values of BID indices among tree, unicyclic, bicyclic, tricyclic and tetracyclic graphs [1].

In 2018, Gutman [15] introduced the class of stepwise irregular graphs and studied their properties. A graph is stepwise irregular (SI) if the degrees of any two of its adjacent vertices differ by exactly one. In [6], authors give some sharp upper bounds on the maximum degree of SI graphs of order n when $n \not\equiv 2 (\text{mod } 4)$, and give upper bounds on the size of SI graphs in terms of the order n and the maximum degree Δ. In this paper, we consider BID_f indices over the class of SI graphs. For the class of SI graphs, we can assume $f(x, y)$ as a function of a single variable, i.e., $f(x, y) = f(x, x-1)$.

This paper is organized as follows. In Section 2, we introduce some notations and some previously known results. In Section 3, we give an upper sharp bound on the maximum degree of SI graphs of order n when $n \equiv 2 (\text{mod } 4)$. In Section 4, we give sharp upper bounds on the BID index of SI graphs in term of the order for $f(x, x-1)$ which is increasing on $[1, \infty)$.

2. Preliminaries

For notations and terminologies, we follow [6]. Let G be a SI graph of order n with the maximum degree Δ and minimum degree δ. Denote by A_k the set of vertices of degree $\Delta - k$ in G for $k = 0, 1, \ldots, \Delta - \delta$. Denote $|A_k| = a_k$.

Let u and v be vertices of degree Δ and δ. Then all vertices in $N(u)$ and $N(v)$ have degree $\Delta - 1$ and $\delta + 1$, respectively. Hence, $N(u) \subseteq A_1$ and $N(v) \subseteq A_{\Delta-\delta-1}$. It follows that

$$a_1 \geq \Delta \tag{2.1}$$

and

$$a_{\Delta-\delta-1} \geq \delta. \tag{2.2}$$

Similarly, for $1 \leq k \leq \Delta - \delta - 1$, let w be a vertex of degree $\Delta - k$. Then $N(w)$ is a subset of $A_{k-1} \cup A_{k+1}$ since the degree of any vertex adjacent to w is $d(w) + 1$ or $d(w) - 1$. Hence one can see easily that

$$\Delta - k \leq a_{k-1} + a_{k+1} \quad \text{for} \quad 1 \leq k \leq \Delta - \delta - 1. \tag{2.3}$$

For $0 \leq i \leq \Delta - \delta$, denote by $E(A_i)$ the sets of edges incident with a vertex in A_i. Then $|E(A_i)| = a_i(\Delta - i)$ and $E(A_i) \subseteq E(A_{i-1} \cup A_{i+1})$ for $1 \leq i \leq \Delta - \delta - 1$. Therefore

$$a_i(\Delta - i) \leq a_{i-1}(\Delta - i + 1) + a_{i+1}(\Delta - i - 1). \tag{2.4}$$

On the other hand, since $E(A_0) \subseteq E(A_1)$ and $E(A_{\Delta-\delta}) \subseteq E(A_{\Delta-\delta-1})$, we have

$$\Delta a_0 \leq (\Delta - 1)a_1 \tag{2.5}$$

and

$$\delta a_{\Delta-\delta} \leq (\delta + 1)a_{\Delta-\delta-1}, \tag{2.6}$$

respectively. The equalities in (2.5) and (2.6) hold if and only if $\delta = \Delta - 1$.

Let $a_0 + a_2 = \Delta - 1$. Then from (2.1) and (2.4), we get

$$\Delta(\Delta - 1) \leq a_1(\Delta - 1) \leq a_0\Delta + a_2(\Delta - 2) = \Delta(a_0 + a_2) - 2a_2 = \Delta(\Delta - 1) - 2a_2$$

and it follows that $a_2 = 0$. Therefore, we have

$$a_0 + a_2 \geq \Delta, \text{ if } a_2 > 0 \text{ (or } \delta < \Delta - 1) \tag{2.7}$$

by (2.3).

We introduce some results and main properties of SI graphs [6, 15].

Lemma 2.1. [6, 15] *Let G be a SI graph. Then the following properties hold:*

(i) *G is bipartite.*
(ii) *The number of edges of G is even.*
(iii) *Let X and Y be the parts of G. Then either $|X|$ or $|Y|$ is even.*

In [6], authors presented that for a positive integer n such that $n \equiv 0(\text{mod } 4)$, there is the unique SI graph G of order n with the maximum degree $n/2$ such that $V(G) = A_0 \cup A_1 \cup A_2$, $|A_0| = n/4$, $|A_1| = n/2$ and $|A_2| = n/4$. Further, this unique SI graph will be denoted by G_n.

Lemma 2.2. [6] *Let G be a SI graph of order n with the maximum degree Δ, the minimum degree δ. Let X and Y be the parts of G. Then the following inequalities hold:*

(i) $\Delta \leq \left\lfloor \frac{n+1}{2} \right\rfloor$ with equality if and only if $G \cong K_{\Delta,\Delta-1}$ when n is odd or $G \cong G_n$ when $n \equiv 0(4)$.
(ii) If $||X| - |Y|| \geq 2$ or $\delta \leq \Delta - 4$ then $\Delta \leq (n + 9)/4$.
(iii) If $||X| - |Y|| \geq 2$ and $\delta > \Delta - 4$ then $\Delta < (n + 6)/4$.

Lemma 2.3. [6] *Let G be a SI graph of order n with maximum degree Δ. Then*

$$|E(G)| \leq \frac{\Delta(\Delta - 1)n}{2\Delta - 1}$$

with equality if and only if $\delta = \Delta - 1$.

Lemma 2.4. [6] *Let G be a SI graph of order n with maximum degree Δ. Then*

$$|E(G)| \leq \frac{(n - 1)\Delta}{2}$$

with equality if and only if $G \cong K_{\Delta,\Delta-1}$.

Lemma 2.5. [6] *Let G be a stepwise irregular graph of order n with maximum degree Δ which is different from $K_{\Delta,\Delta-1}$. Then*

$$|E(G)| \leq (\Delta - 1)(n - \Delta)$$

with equality if and only if $\delta = \Delta - 2$.

When $n \equiv 2(\text{mod } 4)$, denote by $\mathcal{G}_n$ the set of all SI graphs of order n with the maximum degree $(n+2)/4$ such that $V(G) = A_0 \cup A_1$, $|A_0| = (n-2)/2$, $|A_1| = (n+2)/2$.

Lemma 2.6. [6] *Let G be a SI graph of order n.*

(i) If n is odd then $|E(G)| \leq (n^2 - 1)/4$ with equality if and only if $G \cong K_{(n+1)/2,(n-1)/2}$.

(ii) If $n \equiv 0(\text{mod } 4)$ then $|E(G)| \leq (n^2 - 2n)/4$ with equality if and only if $G \cong G_n$.

(iii) If $n \equiv 2(\text{mod } 4)$ then $|E(G)| \leq (n^2 - 4)/8$ with equality if and only if $G \in \mathcal{G}_n$.

3. Upper bounds on the maximum degree of SI graphs

In this section, our purpose is to give a sharp upper bound on the maximum degree of SI graphs of order n when $n \equiv 2(\text{mod } 4)$.

Let G be a SI graph of order $n \equiv 2(\text{mod } 4)$ with the maximum degree Δ and X, Y be the parts of G in which X contains the maximum degree vertex. Then by Lemma 2.1(iii), $||X| - |Y|| \geq 2$. Since Lemma 2.2(ii) and $n \equiv 2(\text{mod } 4)$, it follows that

$$\Delta \leq \frac{(n+6)}{4}.$$

In the Lemmas 3.1–3.5, we will show that the latter inequality holds strictly.

Lemma 3.1. *Let G be a SI graph of order $n \equiv 2(\text{mod } 4)$ with the maximum degree Δ and the minimum degree δ. If $\delta \leq \Delta - 8$ then*

$$\Delta < \frac{n+6}{4}.$$

Proof. Conversely, suppose $\Delta = (n+6)/4$. Then $n = 4\Delta - 6$. Since $\delta \leq \Delta - 8$, clearly $a_8 \geq 1$ and $\Delta \geq 9$. Since (2.1), (2.3), (2.7), $a_7 \geq 1$ and $a_8 \geq 1$, we have

$$|Y| \geq a_1 + a_3 + a_5 + a_7 + a_9 \geq \Delta + (\Delta - 4) + 1 + 0 = 2\Delta - 3$$

and

$$|X| \geq a_0 + a_2 + a_4 + a_6 + a_8 \geq \Delta + (\Delta - 5) + 1 = 2\Delta - 4.$$

Hence, we get $|Y| = 2\Delta - 2$ and $|X| = 2\Delta - 4$ because $|X| + |Y| = 4\Delta - 6$. Moreover, we get $a_0 + a_2 = \Delta, a_4 + a_6 = \Delta - 5, a_8 = 1, a_{10} = 0$. Therefore, we have

$$\begin{aligned}|E(G)| &= a_0\Delta + a_2(\Delta - 2) + a_4(\Delta - 4) + a_6(\Delta - 6) + a_8(\Delta - 8)\\ &= (a_0 + a_2)\Delta + (a_4 + a_6)(\Delta - 4) + (\Delta - 8) - 2a_2 - 2a_6\\ &= 2\Delta^2 - 8\Delta + 12 - 2(a_2 + a_6). \qquad (3.1)\end{aligned}$$

On the other hand, we have

$$|E(G)| = a_1(\Delta - 1) + a_3(\Delta - 3) + a_5(\Delta - 5) + a_7(\Delta - 7) + a_9(\Delta - 9)$$

$$= (a_1 + a_3 + a_5 + a_7 + a_9)(\Delta - 9) + 8a_1 + 4(a_3 + a_5) + 2a_3 + 2a_7$$
$$= (2\Delta - 2)(\Delta - 9) + 8a_1 + 4(a_3 + a_5) + 2a_3 + 2a_7$$
$$= 2\Delta^2 - 8\Delta + 2 + 8(a_1 - \Delta) + 4(a_3 + a_5 - \Delta + 4) + 2a_3 + 2a_7. \quad (3.2)$$

If $a_1 \geq \Delta + 1$ or $a_3 + a_5 \geq \Delta - 3$ then

$$\begin{aligned}|E(G)| &= 2\Delta^2 - 8\Delta + 2 + 8(a_1 - \Delta) + 4(a_3 + a_5 - \Delta + 4) + 2a_3 + 2a_7 \\ &\geq 2\Delta^2 - 8\Delta + 10 > 2\Delta^2 - 8\Delta + 12 - 2(a_2 + a_6) = |E(G)|\end{aligned}$$

since a_2, a_3, a_6 and a_7 are positive integers. Hence, we have $a_1 = \Delta$ and $a_3 + a_5 = \Delta - 4$. Since $|Y| = 2\Delta - 2$, we get $a_7 + a_9 = 2$. Also from (3.1) and (3.2), one can see that $a_2 + a_3 + a_6 + a_7 = 5$.

If $a_2 = 1$ then $a_0 = \Delta - 1$ and $a_1 = \Delta$ which contradicts to $a_0\Delta < a_1(\Delta - 1)$. Therefore, $a_2 = 2$ and $a_3 = a_6 = a_7 = 1$. Then $a_9 = 1$ and since $a_6 + a_8 \geq \Delta - 7$, it follows $\Delta \leq 9$. This is a contradiction to $a_9 = 1$. □

Lemma 3.2. *Let G be a SI graph of order* $n \equiv 2 \pmod 4$ *with the maximum degree* Δ *and the minimum degree* δ*. If* $\delta = \Delta - 7$ *then*

$$\Delta < \frac{n+6}{4}.$$

Proof. Suppose $\Delta = (n + 6)/4$. Then $n = 4\Delta - 6$. Since $\delta = \Delta - 7$, it is clear that $a_7 \geq 1, a_8 = 0$ and $\Delta \geq 8$. From (2.1), (2.3) and $a_7 \geq 1$, we get

$$|Y| = a_1 + a_3 + a_5 + a_7 \geq \Delta + \Delta - 4 + 1 = 2\Delta - 3. \quad (3.3)$$

We also get $|X| = a_0 + a_2 + a_4 + a_6 \geq \Delta + \Delta - 5 = 2\Delta - 5$ since (2.3) and (2.7). Hence one can easily see that $|X| = 2\Delta - 4$ and $|Y| = 2\Delta - 2$ because $|X| + |Y| = 4\Delta - 6$ and $|X|, |Y|$ are even. Also we have $a_0 + a_2 = \Delta$ or $a_0 + a_2 = \Delta + 1$. Therefore

$$\begin{aligned}|E(G)| &= (a_0 + a_2 + a_4 + a_6)(\Delta - 6) + 6a_0 + 4a_2 + 2a_4 \\ &= (2\Delta - 4)(\Delta - 6) + 6a_0 + 4a_2 + 2a_4 \\ &= \begin{cases} 2\Delta^2 - 12\Delta + 24 + 2a_0 + 2a_4 & \text{if } a_0 + a_2 = \Delta \\ 2\Delta^2 - 12\Delta + 28 + 2a_0 + 2a_4 & \text{if } a_0 + a_2 = \Delta + 1 \end{cases}.\end{aligned} \quad (3.4)$$

From (2.2), we have $2\Delta - 4 = a_0 + a_2 + a_4 + a_6 \geq a_0 + a_2 + a_4 + \Delta - 7$ and it follows that

$$a_4 \leq \begin{cases} 3 & \text{if } a_0 + a_2 = \Delta \\ 2 & \text{if } a_0 + a_2 = \Delta + 1 \end{cases}. \quad (3.5)$$

Similarly, using (2.2) and (2.3), we have $2\Delta - 4 = a_0 + a_2 + a_4 + a_6 \geq a_0 + \Delta - 3 + \Delta - 7$ and it follows that

$$a_0 \leq 6. \quad (3.6)$$

Using (3.4)–(3.6), we get

$$|E(G)| \leq \begin{cases} 2\Delta^2 - 12\Delta + 42 & \text{if } a_0 + a_2 = \Delta \\ 2\Delta^2 - 12\Delta + 44 & \text{if } a_0 + a_2 = \Delta + 1 \end{cases}. \quad (3.7)$$

The equality in (3.7) holds if and only if $a_0 = 6, a_4 = 3, a_0 + a_2 = \Delta$ or $a_0 = 6, a_4 = 2, a_0 + a_2 = \Delta + 1$. On the other hand, we have

$$|E(G)| = (a_1 + a_3 + a_5 + a_7)(\Delta - 7) + 6a_1 + 2(a_3 + a_5) + 2a_3. \tag{3.8}$$

From (3.8), (2.3) and $a_3 \geq 1$, we get

$$\begin{aligned} |E(G)| &\geq (2\Delta - 2)(\Delta - 7) + 6a_1 + 2(\Delta - 4) + 2 \\ &= 2\Delta^2 - 14\Delta + 8 + 6a_1. \end{aligned} \tag{3.9}$$

The equality in (3.9) holds if and only if $a_3 = 1, a_5 = \Delta - 5$. From (3.7) and (3.9), we get

$$\Delta + 18 \geq 3a_1.$$

If $a_1 \geq \Delta + 1$ then we get $\Delta < 8$ which is a contradiction to $\delta = \Delta - 7$. Hence $a_1 = \Delta$ and $8 \leq \Delta \leq 9$.

Let $\Delta = 9$. From (3.7) and (3.9), we get

$$98 = 2\Delta^2 - 12\Delta + 44 \geq |E(G)| \geq 2\Delta^2 - 14\Delta + 8 + 6a_1 = 98$$

By the equalities conditions of (3.7) and (3.9), we have $a_0 = 6$, $a_4 = 2$, $a_2 = 4, a_3 = 1$. But this contradicts to $a_0\Delta + a_2(\Delta - 2) < a_1(\Delta - 1) + a_3(\Delta - 3)$.

Let $\Delta = 8$. Since (3.3), $|Y| = 2\Delta - 2$ and $a_1 = \Delta$, it follows that $a_3 + a_5 = \Delta - 4, a_7 = 2$ or $a_3 + a_5 = \Delta - 3, a_7 = 1$. Now we distinguish the following four cases.

Case 1. $a_0 + a_2 = \Delta, a_3 + a_5 = \Delta - 4$. Then $a_7 = 2$ and from $|X| = 2\Delta - 4$, one can see that $a_4 + a_6 = \Delta - 4 = 4$. By using (3.4), (3.8), we get $7 + a_3 = a_0 + a_4$. Since $a_7 = 2$, it follows $a_6 \geq 2$ and $a_4 \leq 2$. Thus, $7 + a_3 = a_0 + a_4 \leq 6 + 2$ and $a_3 \leq 1$. Hence, $a_3 = 1, a_0 = 6, a_4 = 2$. Then $a_2 = 2$. But this contradicts to $a_2 + a_4 \geq \Delta - 3$.

Case 2. $a_0 + a_2 = \Delta, a_3 + a_5 = \Delta - 3$. Then $a_7 = 1$ and by using (3.4), (3.8), we get $8 + a_3 = a_0 + a_4$. From $|X| = 2\Delta - 4$, one can see that $a_4 + a_6 = \Delta - 4 = 4$. From (3.5), (3.6), we see that $8 + a_3 = a_0 + a_4 \leq 6 + 3$. Thus $a_3 = 1, a_0 = 6, a_4 = 3$. Then $a_2 = 2$. Since $a_3 = 1$ and $a_2 + a_4 = 5$, the unique vertex in A_3 is adjacent to all vertices in $A_2 \cup A_4$. Therefore, the number of edges between A_1 and A_2 must be $a_2(\Delta - 3)$. On the other hand, it is equal to $a_1(\Delta - 1) - a_0\Delta$. But $a_2(\Delta - 3) > a_1(\Delta - 1) - a_0\Delta$ and a contradiction.

Case 3. $a_0 + a_2 = \Delta + 1, a_3 + a_5 = \Delta - 4$. Then $a_7 = 2$ and by using (3.4), (3.8), we get $5 + a_3 = a_0 + a_4$. From $|X| = 2\Delta - 4$, one can see that $a_4 + a_6 = \Delta - 5 = 3$. Since $a_7 = 2$, we have $a_6 \geq 2$ and $a_4 \leq 1$. Thus, $a_4 = 1$ and $a_6 = 2$. Therefore, $5 + a_3 = a_0 + a_4 \leq 6 + 1$. It follows that $a_3 \leq 2$ and $a_5 \geq 2$. But

$$8 = a_4(\Delta - 4) + a_6(\Delta - 6) > a_5(\Delta - 5) + a_7(\Delta - 7) = 3a_5 + 2 \geq 3 \cdot 2 + 2 = 8,$$

which is a contradiction.

Case 4. $a_0 + a_2 = \Delta + 1, a_3 + a_5 = \Delta - 3$. Then $a_7 = 1$ and by using (3.4), (3.8), we get $6 + a_3 = a_0 + a_4$. From $|X| = 2\Delta - 4$, one can see that $a_4 + a_6 = \Delta - 5 = 3$. It follows $a_4 \leq 2$ and $6 + a_3 = a_0 + a_4 \leq 8$. Therefore, we get $a_3 \leq 2$ and $a_5 \geq 3$ since $a_3 + a_5 = 5$. But

$$\begin{aligned} 10 = 2 \cdot 3 + 2 \cdot 2 \geq 2(a_4 + a_6) + 2a_4 &= a_4(\Delta - 4) + a_6(\Delta - 6) \\ &> a_5(\Delta - 5) + a_7(\Delta - 7) = 3a_5 + 1 \geq 3 \cdot 3 + 1 = 10, \end{aligned}$$

which is a contradiction.

From the above all, the proof is completed. □

Lemma 3.3. *Let G be a SI graph of order $n \equiv 2 (\mathrm{mod}\ 4)$ with the maximum degree Δ and the minimum degree δ. If $\delta = \Delta - 6$ then*

$$\Delta < \frac{n+6}{4}.$$

Proof. Conversely, Suppose $\Delta = (n+6)/4$. From $\delta = \Delta - 6$, $a_6 \geq 1, a_7 = 0$ and $\Delta \geq 7$. We have $|Y| = a_1 + a_3 + a_5 \geq 2\Delta - 4$ and $|X| \leq 2\Delta - 2$ from $|X| + |Y| = 4\Delta - 6$. Now we distinguish the following two cases.

Case 1. Let $|X| \geq |Y| + 2$. Then $|X| = 2\Delta - 2$ and $|Y| = 2\Delta - 4$. Thus, $a_1 = \Delta, a_3 + a_5 = \Delta - 4$. From $a_5 \geq \Delta - 6$, we get $a_3 \leq 2$. Also we have

$$|E(G)| = a_1(\Delta - 1) + a_3(\Delta - 3) + a_5(\Delta - 5) = a_0\Delta + a_2(\Delta - 2) + a_4(\Delta - 4) + a_6(\Delta - 6)$$

and an elementary calculation gives that

$$3a_0 + 2a_2 + a_4 = 2\Delta + 4 + a_3. \tag{3.10}$$

If $a_0 + a_2 \geq \Delta + 2$ then from (3.10), we have $a_0 + a_4 \leq a_3 \leq 2$. It follows that $a_0 = a_4 = 1$, $a_3 = 2$ and $a_0 + a_2 = \Delta + 2$. Then $a_5 = \Delta - 6$, $a_6 = \Delta - 5$ and it contradicts to $a_5(\Delta - 5) > a_6(\Delta - 6)$.

If $a_0 + a_2 = \Delta + 1$ then from (3.10), we have $a_0 + a_4 = a_3 + 2$. Since $a_4 + a_6 = \Delta - 3$ and $a_3 + a_5 = \Delta - 4$, we get $a_0 + a_5 = a_6 + 1$. On the other hand, we have

$$(\Delta + 1)(\Delta - 2) + 2a_0 = a_0\Delta + a_2(\Delta - 2) > a_1(\Delta - 1) = \Delta(\Delta - 1).$$

Hence, we get $a_0 \geq 2$ and $a_6 \geq a_5 + 1$. Therefore, we have

$$a_5(\Delta - 5) > a_6(\Delta - 6) \geq (a_5 + 1)(\Delta - 6).$$

It follows that $a_5 > \Delta - 6$. Since $a_3 + a_5 = \Delta - 4$, we get $a_5 = \Delta - 5$. Similarly, we get $a_6 = \Delta - 4$ and $a_3 = a_4 = 1$. Now we consider the number of edges between A_4 and A_5. This number is $a_5(\Delta - 5) - a_6(\Delta - 6) = a_4(\Delta - 4) - 1$ because there is only one edge between A_3 and A_4. Hence, we get $\Delta = 6$ and a contradiction.

If $a_0 + a_2 = \Delta$ then the inequality

$$\Delta(\Delta - 2) + 2a_0 = a_0\Delta + a_2(\Delta - 2) > a_1(\Delta - 1) = \Delta(\Delta - 1)$$

holds and hence $2a_0 \geq \Delta \geq 7$ and so $a_0 \geq 4$. Also from (3.10), we have $a_0 + a_4 = 4 + a_3$. Since $a_4 + a_6 = \Delta - 2$ and $a_3 + a_5 = \Delta - 4$, we get

$$a_6 = a_0 + a_5 - 2 \geq a_5 + 2.$$

Therefore, we have

$$a_5(\Delta - 5) > a_6(\Delta - 6) \geq (a_5 + 2)(\Delta - 6)$$

and it follows that $2\Delta - 11 \leq a_5 \leq \Delta - 5$ since $a_3 + a_5 = \Delta - 4$. Hence we get $\Delta \leq 6$ and a contradiction.

Case 2. If $|Y| \geq |X| + 2$ then $|X| \leq 2\Delta - 4$ and

$$|X| = a_0 + a_2 + a_4 + a_6 \geq \Delta + \Delta - 5 = 2\Delta - 5.$$

Thus, $|X| = 2\Delta - 4$ and $|Y| = 2\Delta - 2$ by Lemma 2.1(iii). Hence $a_0 + a_2 \leq \Delta + 1$ and $a_4 = 2\Delta - 4 - (a_0 + a_2) - a_6 \leq 2\Delta - 5 - (a_0 + a_2)$. We also have

$$2\Delta - 4 = |X| = a_0 + a_2 + a_4 + a_6 \geq a_0 + \Delta - 3 + 1$$

and we obtain $a_0 \leq \Delta - 2$. Therefore

$$\begin{aligned} |E(G)| &= a_0\Delta + a_2(\Delta - 2) + a_4(\Delta - 4) + a_6(\Delta - 6) \\ &= (a_0 + a_2 + a_4 + a_6)(\Delta - 6) + 2a_4 + 4(a_0 + a_2) + 2a_0 \\ &\leq (2\Delta - 4)(\Delta - 6) + 2(2\Delta - 5) + 2(a_0 + a_2) + 2(\Delta - 2) \\ &\leq 2\Delta^2 - 8\Delta + 12. \end{aligned} \tag{3.11}$$

From $a_1 \geq \Delta$ and $a_3 \geq 1$, we obtain

$$\begin{aligned} |E(G)| = a_1(\Delta - 1) + a_3(\Delta - 3) + a_5(\Delta - 5) &= (a_1 + a_3 + a_5)(\Delta - 5) + 4a_1 + 2a_3 \\ &= (2\Delta - 2)(\Delta - 5) + 4a_1 + 2a_3 \geq 2\Delta^2 - 8\Delta + 12. \end{aligned} \tag{3.12}$$

From (3.11) and (3.12), we obtain $a_0 = \Delta - 2, a_1 = \Delta, a_2 = 3, a_3 = 1, a_4 = \Delta - 6, a_5 = \Delta - 4, a_6 = 1$ which contradicts to $a_4(\Delta - 4) + a_6(\Delta - 6) > a_5(\Delta - 5)$.

The above two cases, the proof is finished. □

Lemma 3.4. *Let G be a SI graph of order $n \equiv 2 \pmod 4$ with the maximum degree Δ and the minimum degree δ. If $\delta = \Delta - 5$ then*

$$\Delta < \frac{n+6}{4}.$$

Proof. Conversely, suppose $\Delta = (n + 6)/4$. Then $n = 4\Delta - 6$. Since $\delta = \Delta - 5$, clearly $a_5 \geq 1, a_6 = 0$. Then $|Y| = a_1 + a_3 + a_5 \geq 2\Delta - 4$ by (2.1) and (2.3).

If $|X| \geq |Y| + 2$ then $|X| \geq 2\Delta - 2$. It follows from $|X| + |Y| = 4\Delta - 6$ that

$$|X| = 2\Delta - 2 \text{ and } |Y| = 2\Delta - 4.$$

Thus, $a_1 = \Delta, a_3 + a_5 = \Delta - 4$ and $a_3 \leq \Delta - 5$. Hence, we get

$$\begin{aligned} |E(G)| &= a_1(\Delta - 1) + (a_3 + a_5)(\Delta - 5) + 2a_3 \\ &\leq \Delta(\Delta - 1) + (\Delta - 4)(\Delta - 5) + 2(\Delta - 5) \\ &= 2\Delta^2 - 8\Delta + 10 \end{aligned} \tag{3.13}$$

and

$$\begin{aligned} |E(G)| &= a_0\Delta + a_2(\Delta - 2) + a_4(\Delta - 4) \\ &= (a_0 + a_2 + a_4)(\Delta - 4) + 2(a_0 + a_2) + 2a_0 \\ &\geq (2\Delta - 2)(\Delta - 4) + 2\Delta + 2 \\ &= 2\Delta^2 - 8\Delta + 10. \end{aligned} \tag{3.14}$$

From inequalities (3.13) and (3.14), it follows that $a_5 = 1, a_3 = \Delta - 5, a_2 = \Delta - 1, a_0 = 1$. But it contradicts to the inequalities $a_0\Delta + a_2(\Delta - 2) > a_1(\Delta - 1)$ and $\Delta \geq 6$.

If $|Y| \geq |X| + 2$ then from $|X| + |Y| = 4\Delta - 6$, we have $|X| \leq 2\Delta - 4$ and other hand

$$|X| = a_0 + a_2 + a_4 \geq \Delta + \Delta - 5 = 2\Delta - 5.$$

Hence we have $|X| = 2\Delta - 4$ by Lemma 2.1(iii). Moreover, one can see that $a_4 = \Delta - 4$ or $a_4 = \Delta - 5$. Since $a_0\Delta < a_1(\Delta - 1)$, we get $(a_1 - a_0)\Delta > a_1 \geq \Delta$ and it follows that $a_1 - a_0 \geq 2$. Also we have

$$|E(G)| = a_1(\Delta - 1) + a_3(\Delta - 3) + a_5(\Delta - 5) = a_0\Delta + a_2(\Delta - 2) + a_4(\Delta - 4)$$

and an elementary calculation gives that $1 + a_0 - a_4 = a_1 - a_5$. Hence, we get

$$a_5 = a_4 + a_1 - a_0 - 1 \geq a_4 + 1.$$

Therefore, $a_4(\Delta - 4) > a_5(\Delta - 5) \geq (a_4 + 1)(\Delta - 5)$ and it is equivalent to $a_4 > \Delta - 5$, i.e., $a_4 = \Delta - 4$. If $a_5 \geq \Delta - 2$ then it contradicts to the inequality $a_4(\Delta - 4) > a_5(\Delta - 5)$ and $\Delta \geq 6$. Hence, we have $a_5 = \Delta - 3$, $a_1 - a_0 = 2$ and $a_1 + a_3 = \Delta + 1$. Moreover, $a_1 = \Delta$, $a_3 = 1$, $a_0 = \Delta - 2$ and $a_2 = 2$.

Since $a_4(\Delta - 4) - a_5(\Delta - 5) = 1$ and $a_2 = 2$, we have $\Delta - 3 = 3$. Therefore $\Delta = 6$ and one can easily see that the graph is disconnected. This completes the proof. □

Lemma 3.5. *Let G be a SI graph of order $n \equiv 2(\mathrm{mod}\ 4)$ with the maximum degree Δ and the minimum degree δ. If $\delta = \Delta - 4$ then*

$$\Delta < \frac{n + 6}{4}.$$

Proof. Conversely, suppose $\Delta = (n + 6)/4$. Then $n = 4\Delta - 6$. Since $\delta = \Delta - 4$, clearly $a_4 \geq 1$ and $a_5 = 0$. From (2.1) and (2.2), it follows that $|Y| = a_1 + a_3 \geq 2\Delta - 4$.

If $|X| \geq |Y| + 2$ then $|X| \geq 2\Delta - 2$. Therefore, by $|X| + |Y| = 4\Delta - 6$,

$$|X| = 2\Delta - 2 \ \text{ and } \ |Y| = 2\Delta - 4.$$

Thus, $a_1 = \Delta, a_3 = \Delta - 4$. We have

$$|E(G)| = a_1(\Delta - 1) + a_3(\Delta - 3) = 2\Delta^2 - 8\Delta + 12. \tag{3.15}$$

Since $a_4(\Delta - 4) < a_3(\Delta - 3) = (\Delta - 4)(\Delta - 3)$, we can easily see that $a_4 \leq \Delta - 4$ and $a_0 + a_2 \geq \Delta + 2$. Thus,

$$\begin{aligned} |E(G)| &= (a_0 + a_2 + a_4)(\Delta - 4) + 2(a_0 + a_2) + 2a_0 \\ &\geq (2\Delta - 2)(\Delta - 4) + 2(\Delta + 2) + 2 \\ &= 2\Delta^2 - 8\Delta + 14 \end{aligned}$$

and it contradicts to (3.15).

If $|Y| \geq |X| + 2$ then $|X| \leq 2\Delta - 4$. Therefore, by $|X| + |Y| = 4\Delta - 6$, we can see that $|Y| \geq 2\Delta - 2$. Using (2.1) and $|Y| \geq 2\Delta - 2$, we obtain

$$\begin{aligned} |E(G)| &= a_1(\Delta - 1) + a_3(\Delta - 3) = (a_1 + a_3)(\Delta - 3) + 2a_1 \\ &\geq (2\Delta - 2)(\Delta - 3) + 2\Delta = 2\Delta^2 - 6\Delta + 6. \end{aligned} \tag{3.16}$$

Also, using $|X| \leq 2\Delta - 4$, (2.3) and $a_4 \geq 1$, we obtain

$$\begin{aligned} |E(G)| &= a_0\Delta + a_2(\Delta - 2) + a_4(\Delta - 4) = (a_0 + a_2 + a_4)\Delta - 2(a_2 + a_4) - 2a_4 \\ &\leq (2\Delta - 4)\Delta - 2(\Delta - 3) - 2 = 2\Delta^2 - 6\Delta + 4 \end{aligned}$$

and it contradicts to (3.16). □

In this section, our purpose is provided by the next theorem.

Theorem 3.6. *Let G be a SI graph of order $n \equiv 2 (\bmod\ 4)$ with the maximum degree Δ. Then $\Delta \le (n+2)/4$. If $G \in \mathcal{G}_n$ then $\Delta = (n+2)/4$.*

Proof. Let δ be the minimum degree in G. If $\delta > \Delta - 4$ then by Lemma 2.2(iii), we get the required result. If $\delta \le \Delta - 4$ then by Lemmas 3.1–3.5, we get the required result. Therefore, this completes the proof. □

4. Maximum value of BID index over SI graphs

In this section, we obtain some sharp upper bounds on BID index with a function f over the class of SI graphs of the given order. For the convenience, we denote $\bar{f}(x) = f(x, x-1)$. Then BID index of a SI graph G can be written as

$$BID_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)) = \sum_{uv \in E(G),\, d(u) > d(v)} \bar{f}(d(u)).$$

Lemma 4.1. *Let G be a SI graph of order n with the maximum degree Δ. If the function $\bar{f}$ is increasing then*

$$BID_f(G) \le \frac{\Delta(\Delta-1)n}{2\Delta - 1} \cdot \bar{f}(\Delta)$$

with equality if and only if $\delta = \Delta - 1$

Proof. Since $\bar{f}$ is an increasing function, we have

$$BID_f(G) = \sum_{uv \in E(G),\, d(u) > d(v)} \bar{f}(d(u)) \le \sum_{uv \in E(G),\, d(u) > d(v)} \bar{f}(\Delta) = |E(G)| \bar{f}(\Delta).$$

By Lemma 2.3, we get the desired inequality with equality if and only if $\delta = \Delta - 1$. □

Lemma 4.2. *Let G be a SI graph of order n with the maximum degree Δ. If $\bar{f}$ is an increasing function then*

$$BID(G) \le \frac{(n-1)\Delta}{2} \cdot \bar{f}(\Delta)$$

with equality if and only if $G \cong K_{\Delta,\Delta-1}$

Proof. Since $\bar{f}$ is an increasing function, we have

$$BID(G) = \sum_{uv \in E(G),\, d(u) > d(v)} \bar{f}(d(u)) \le \sum_{uv \in E(G),\, d(u) > d(v)} \bar{f}(\Delta) = |E(G)| \bar{f}(\Delta).$$

By Lemma 2.4, we get the desired inequality with equality if and only if $G \cong K_{\Delta,\Delta-1}$. □

Lemma 4.3. *Let G be a SI graph of order n with the maximum degree Δ which is different from $K_{\Delta,\Delta-1}$. If $\bar{f}$ is an increasing function then*

$$BID_f(G) \le \frac{(n+3)\Delta^2 - 2\Delta^3 - n\Delta}{2} \cdot \bar{f}(\Delta) + \frac{2\Delta^3 - (n+5)\Delta^2 + (3n+2)\Delta - 2n}{2} \cdot \bar{f}(\Delta - 1)$$

with equality if and only if $G \cong G_n$ when $n \equiv 0 (\bmod\ 4)$.

Proof. From $\Delta - 2i - 1 \le \Delta - 1$, we have

$$|E(G)| = \sum_{i\ge 0} a_{2i+1}(\Delta - 2i - 1) \le (\Delta - 1)\left(\sum_{i\ge 0} a_{2i+1}\right) = (\Delta - 1)\left(n - \sum_{i\ge 0} a_{2i}\right)$$

by using $\sum_{i\ge 0} a_i = n$. From the above inequality, we get

$$a_0\Delta + a_2(\Delta - 2) \le |E(G)| \le (\Delta - 1)(n - a_0 - a_2). \tag{4.1}$$

Hence, we have

$$2a_0 \le (\Delta - 1)n - (2\Delta - 3)(a_0 + a_2) \le (\Delta - 1)n - (2\Delta - 3)\Delta.$$

since $a_0 + a_2 \ge \Delta$.

By Lemma 2.5 and $\bar{f}$ is increasing, we get

$$\begin{aligned} BID_f(G) = & \sum_{uv\in E(G),\, d(u)>d(v)} \bar{f}(d(u)) \le a_0\Delta\bar{f}(\Delta) + (|E(G)| - a_0\Delta)\bar{f}(\Delta - 1) \\ =& a_0\Delta(\bar{f}(\Delta) - \bar{f}(\Delta - 1)) + |E(G)|\bar{f}(\Delta - 1) \\ \le& a_0\Delta(\bar{f}(\Delta) - \bar{f}(\Delta - 1)) + (\Delta - 1)(n - \Delta)\bar{f}(\Delta - 1) \\ \le& \frac{(n+3)\Delta - 2\Delta^2 - n}{2} \cdot \Delta(\bar{f}(\Delta) - \bar{f}(\Delta - 1)) + (\Delta - 1)(n - \Delta)\bar{f}(\Delta - 1) \\ =& \frac{(n+3)\Delta^2 - 2\Delta^3 - n\Delta}{2} \cdot \bar{f}(\Delta) + \frac{2\Delta^3 - (n+5)\Delta^2 + (3n+2)\Delta - 2n}{2} \cdot \bar{f}(\Delta - 1) \end{aligned}$$

which is the required inequality.

Suppose now that the equality holds. Then from (4.1) and Lemma 2.5, we have $\delta = \Delta - 2$, $a_0 + a_2 = \Delta$ and $a_0 + a_1 + a_2 = n$. Hence, we have $a_1 = n - \Delta$, $a_0 = \frac{(n+3)\Delta - 2\Delta^2 - n}{2}$ and $a_2 = \frac{2\Delta^2 + n - \Delta(n+1)}{2}$. One can easily see that $n \ge 7$ and $\Delta \ge 3$ because $G \not\cong K_{\Delta,\Delta-1}$. If $n = 7$ then there exist the unique SI graph which is different from $K_{4,3}$ and it is easy to see that the strict inequality holds. Therefore, we have $n \ge 8$.

If $\Delta \le (2n - 3)/4$ then

$$\begin{aligned} a_2 =& \Delta^2 + \frac{n}{2} - \frac{\Delta(n+1)}{2} \\ \le& \max\left\{9 + \frac{n}{2} - \frac{3(n+1)}{2}, \left(\frac{2n-3}{4}\right)^2 + \frac{n}{2} - \frac{(2n-3)(n+1)}{8}\right\} \\ =& \max\left\{\frac{15-2n}{2}, \frac{15-2n}{16}\right\} < 0 \end{aligned}$$

which is a contradiction. Hence, we have $\Delta > (2n-3)/4$ and moreover $\Delta \ge (n-1)/2$. By Lemma 2.2(i), we get $\Delta = (n-1)/2$ or $\Delta = n/2$. If $\Delta = (n-1)/2$ then a_0 is not integer by an elementary calculation. If $\Delta = n/2$ then $G \cong G_n$ by Lemma 2.2(i). □

Theorem 4.4. *Let G be a SI graph of order n and $\bar{f}$ be an increasing function.*

(i) *If n is odd then* $BID_f(G) \le \frac{n^2-1}{4} \cdot \bar{f}\left(\frac{n+1}{2}\right)$ *with equality if and only if*

$G \cong K_{(n+1)/2,(n-1)/2}$.

(ii) *If* $n \equiv 2(\mathrm{mod}\ 4)$ *then* $BID_f(G) \le \frac{n^2-4}{8} \cdot \bar{f}\left(\frac{n+2}{4}\right)$ *with equality if and only if* $G \in \mathcal{G}_n$.

(iii) *If* $n \equiv 0(\mathrm{mod}\ 4)$ *then* $BID_f(G) \le \frac{n^2}{8} \cdot \bar{f}\left(\frac{n}{2}\right) + \frac{n(n-4)}{8} \cdot \bar{f}\left(\frac{n-2}{2}\right)$ *with equality if and only if* $G \cong G_n$.

Proof. (i) Let n be an odd integer. Then $\Delta \le \frac{n+1}{2}$ by Lemma 2.2(i). Hence, by Lemma 4.1 we obtain

$$BID(G) \le \frac{\Delta(\Delta-1)n}{2\Delta-1} \cdot \bar{f}(\Delta) \le \frac{n^2-1}{4} \cdot \bar{f}\left(\frac{n+1}{2}\right) \tag{4.2}$$

since $\bar{f}(t)$ and $F(t) = (t(t-1))/(2t-1)$ are increasing for $t \ge 2$. Equalities in (4.2) hold if and only if $\delta = \Delta - 1$, $\Delta = \frac{n+1}{2}$. Therefore $G \cong K_{(n+1)/2,(n-1)/2}$ by Lemma 2.2(i).

(ii) Let n be an integer such that $n \equiv 2(\mathrm{mod}\ 4)$. Then $\Delta \le (n+2)/4$ by Theorem 3.6(ii). Hence, by Lemma 4.1, we obtain

$$BID(G) \le \frac{\Delta(\Delta-1)n}{2\Delta-1} \cdot \bar{f}(\Delta) \le \frac{n^2-4}{8} \cdot \bar{f}\left(\frac{n+2}{4}\right) \tag{4.3}$$

since $\bar{f}(t)$ and $F(t) = (t(t-1))/(2t-1)$ are increasing for $t \ge 2$. Equalities in (4.3) hold if and only if $\delta = \Delta - 1$ and $\Delta = (n+2)/4$. Then $|E(G)| = a_0\Delta = a_1(\Delta-1)$ and $a_0 + a_1 = n$. Hence we get $G \in \mathcal{G}_n$.

(iii) From $n \equiv 0(\mathrm{mod}\ 4)$, we get $\Delta \le n/2$ by Lemma 2.2(i). If $\Delta = n/2$ then $G \cong G_n$ by Lemma 2.2(i) and

$$\begin{aligned} BID_f(G) = BID_f(G_n) &= a_0\Delta\bar{f}(\Delta) + a_2(\Delta-2)\bar{f}(\Delta-1) \\ &= \frac{n^2}{8} \cdot \bar{f}\left(\frac{n}{2}\right) + \frac{n(n-4)}{8} \cdot \bar{f}\left(\frac{n-2}{2}\right). \end{aligned}$$

If $\Delta \le n/2 - 1$ then by $\bar{f}(x)$ is increasing and Lemma 2.6(ii), we get

$$\begin{aligned} BID_f(G) &= \sum_{uv \in E(G),\, d(u)>d(v)} \bar{f}(d(u)) \le |E(G)|\bar{f}(\Delta) \\ &\le \frac{n^2-2n}{4} \cdot \bar{f}(\Delta) \le \frac{n^2-2n}{4} \cdot \bar{f}\left(\frac{n}{2}-1\right) \\ &= \frac{n^2}{8} \cdot \bar{f}\left(\frac{n}{2}-1\right) + \frac{n^2-4n}{8} \cdot \bar{f}\left(\frac{n}{2}-1\right) \\ &\le \frac{n^2}{8} \cdot \bar{f}\left(\frac{n}{2}\right) + \frac{n^2-4n}{8} \cdot \bar{f}\left(\frac{n}{2}-1\right). \end{aligned} \tag{4.4}$$

If the equalities in (4.4) hold then $|E(G)| = \frac{n^2-2n}{4}$ and it follows that $G \cong G_n$ by Lemma 2.6(ii). But this contradicts to $\Delta \le n/2 - 1$. Therefore, the inequality (4.4) is strict. □

5. Conclusions

In this work, we have established a sharp upper bound on on the maximum degree of SI graphs of order n when $n \equiv 2 (\bmod\ 4)$. We utilize our upper bound and several sharp upper bounds given in [6] to study BID_f indices over the class of SI graphs. Then we give upper bounds on BID_f index in terms of the order n and the maximum degree Δ. Moreover, we completely characterize the extremal SI graphs of order n with respect to BID_f when $\bar{f}$ is increasing. Hence, we conclude that for a SI graph G of the given order, $BID_f(G)$ is maximum if and only if the size of G is maximum.

In the end, we pose the following open problems.

- Determine the maximum size of SI graphs of order n with maximum degree Δ and minimum degree one, and characterize the corresponding extremal SI graphs.
- Characterize the extremal SI graphs of order n with maximum degree Δ and minimum degree one with respect to BID_f when $\bar{f}$ is increasing.

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Conflict of interest

All authors declare that there is no conflict of interest.

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