

Article

A Complete Characterization of Bipartite Graphs with Given Diameter in Terms of the Inverse Sum Indeg Index

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Abstract: In 2010, Vukičević introduced a new graph invariant, the inverse sum indeg index of a graph, which has been studied due to its wide range of applications. Let \mathcal{B}_n^d be the class of bipartite graphs of order n and diameter d . In this paper, we mainly characterize the bipartite graphs in \mathcal{B}_n^d with the maximal inverse sum indeg index. Bipartite graphs with the largest, second-largest, and smallest inverse sum indeg indexes are also completely characterized.

Keywords: the inverse sum indeg index; bipartite graphs; diameter; extremal graphs

1. Introduction and Notation

We use [1] for terminology and notation not defined here and consider only simple graphs. Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. For any vertex $u \in V(G)$, we use $\delta_G(u)$ (or $\delta(u)$ when no confusion can arise) to denote the degree of u in G , which equals to the number of edges incident to u . The distance between two vertices x and y in G , denoted by $d(x, y)$, is the number of edges in the shortest path joining x and y . The distance between any pair of farthest vertices in G is called the diameter of G , denoted by $diam(G)$.

For $X \subset V(G)$, we use $G \setminus X$ to denote the graph obtained from G by deleting the vertices in X and the edges incident with them. For any two non-adjacent vertices x and y in G , let $G + e$ be the graph formed from G by adding a new edge $e = xy$. The union of two graphs G' and G'' , denoted by $G' \cup G''$, is the graph with the vertex set $V(G') \cup V(G'')$ and edge set $E(G') \cup E(G'')$. The join of two graphs \hat{G} and \tilde{G} , denoted by $\hat{G} + \tilde{G}$, is the graph with the vertex set $V(\hat{G}) \cup V(\tilde{G})$ and edge set $E(\hat{G}) \cup E(\tilde{G}) \cup \{uv | u \in V(\hat{G}), v \in V(\tilde{G})\}$. We use K_n to denote the complete graph of n vertices, and $K_{m,n}$ the complete bipartite graph with m and n vertices in its two partition sets, respectively. Let \mathcal{B}_n^d (resp. \mathcal{B}_n) be the set of n -vertex bipartite graphs with diameter d (resp. be the set of n -vertex bipartite graphs). Note that the bipartite graph in \mathcal{B}_n^d is isomorphic to K_2 when $d = 1$, so we always assume that $d \geq 2$ in the subsequent investigation.

The topological index (sometimes call graph descriptor) is a single real number that can be used to characterize some properties of the molecule graph. Topological indices have been used for combinatorial library design, toxicology hazard assessments, isomer discrimination, drug design, and quantitative structure versus property/activity relationships (QSPR/QSAR). In 2010, Vukičević and Gašperov [2] showed that topological indices also have very good predictive properties on the benchmark sets. In [3], Vukičević introduced the inverse sum indeg index of graph G (we call it the ISI-index for short):

$$ISI(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{\delta(u)} + \frac{1}{\delta(v)}} = \sum_{uv \in E(G)} \frac{\delta(u)\delta(v)}{\delta(u) + \delta(v)}, \quad (1)$$

which has been investigated due to its wide range of applications, especially in chemical and mathematical properties. For example, Sedlar et al. in [4] determined extremal values



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of the ISI-index for general connected graphs, chemical graphs, and trees, respectively. Two years later, Falahati-Nezhad et al. [5] showed several sharp bounds on this graph invariant in terms of some well-known graph parameters. In 2018, An et al. [6] considered the extremal problems for this graph descriptors for graphs with a given matching number, independence number, and vertex-connectivity. Almost in the same year, Chen et al. [7] derived several sharp bounds for this index in terms of graph parameters, such as vertex-connectivity, edge-connectivity, chromatic number, and vertex bipartiteness. We encourage the interested reader to consult [8–16] and references cited therein.

Motivated by the results of [17], in this paper we focus on characterizing structural properties of $G \in \mathcal{B}_n^d$ in terms of the ISI-index. Bipartite graphs with the largest, second-largest, and smallest ISI-indexes are also completely characterized, respectively.

2. Bipartite Graphs in \mathcal{B}_n^d with Maximal ISI-Index

Let G be a graph in \mathcal{B}_n^d , and there must exist a partition $\mathcal{V}_0, \mathcal{V}_1, \dots, \mathcal{V}_d$ of the vertex set $V(G)$ which satisfies the following two conditions: (i) $|\mathcal{V}_0| = 1$ and (ii) $d(u, v_i) = i$ for each vertex $v_i \in \mathcal{V}_i$ and $u \in \mathcal{V}_0$, where $i \in \{1, 2, \dots, d\}$. For simplicity, each \mathcal{V}_i is called the partition cell (P-cell for short), and $l_i = |\mathcal{V}_i|$ denotes the number of vertices in \mathcal{V}_i .

Lemma 1 ([18]). *Let $G \in \mathcal{B}_n^d$ be a graph with the above partition, then $G[\mathcal{V}_i]$ induces an empty graph for each $i \in \{1, 2, \dots, d\}$, where $G[\mathcal{V}_i]$ is the subgraph induced by \mathcal{V}_i .*

Lemma 2 ([4]). *Let $G \neq K_n$ be a connected graph, then $ISI(G + e) > ISI(G)$ for each $e \in E(\overline{G})$, where \overline{G} denotes the complement of G .*

Lemma 3. *Let $G \in \mathcal{B}_n^d$ be a graph with the maximal ISI-index, then $G[\mathcal{V}_{i-1} \cup \mathcal{V}_i]$ is a complete bipartite graph for each $i \in \{1, 2, \dots, d\}$ and $|\mathcal{V}_d| = 1$ if $d \geq 3$.*

Proof. The first part follows directly from Lemma 2. It remains to verify the correctness of the second part. Suppose that $u \in \mathcal{V}_d$ and $v \in \mathcal{V}_{d-3}$ for $d \geq 3$. If $|\mathcal{V}_d| \geq 2$, then $G + uv \in \mathcal{B}_n^d$ and $\mathcal{V}_0 \cup \mathcal{V}_1 \cup \dots \cup \mathcal{V}_{d-3} \cup (\mathcal{V}_{d-2} \cup \{u\}) \cup \mathcal{V}_{d-1} \cup (\mathcal{V}_d \setminus \{u\})$ is a partition of $G + uv$. By Lemma 2, $ISI(G + uv) > ISI(G)$, a contradiction. Hence, $|\mathcal{V}_d| = 1$ for $d \geq 3$. □

Lemma 4. *Let $G \in \mathcal{B}_n^d$ be a graph with the maximal ISI-index, then there are at most two P-cells \mathcal{V}_i and \mathcal{V}_j such that $|\mathcal{V}_i| \geq 2$, $|\mathcal{V}_j| \geq 2$ and $|i - j| = 1$.*

Proof. We always assume that $d \geq 3$ since the rest part is trivial. By contradiction, we suppose that there are at least two P-cells \mathcal{V}_i and \mathcal{V}_j with $|\mathcal{V}_i| \geq 2$ and $|\mathcal{V}_j| \geq 2$. Thus, it is sufficient to show that $|i - j| = 1$. It follows from Lemma 3 that each vertex in \mathcal{V}_l has the same degree, say δ_l , since $G[\mathcal{V}_{l-1} \cup \mathcal{V}_l]$ is a complete bipartite subgraph for $l \in \{1, 2, \dots, d\}$. To complete the proof, we begin with several auxiliary claims. □

Claim 1. Any pair of P-cells $\mathcal{V}_i, \mathcal{V}_{i+1}, \dots, \mathcal{V}_j$ with cardinality at least two are successive.

Proof of Claim 1. For simplicity, we will distinguish the following three cases. □

Case 1. $\exists i \in \{1, 2, \dots, d\}$ such that $|\mathcal{V}_i| \geq 2, |\mathcal{V}_{i+1}| = 1$ and $|\mathcal{V}_{i+2}| = |\mathcal{V}_j| \geq 2$.

Without loss of generality, we suppose that $\mathcal{V}_{i+1} = \{v_{i+1}\}$ and $\mathcal{V}_0 = \{v_0\}$. Let G' be a graph obtained from G by the following process: (i) deleting all edges incident to vertex v_{i+1} ; (ii) joining vertex v_{i+1} to vertex v_0 ; (iii) guaranteeing $G'[\mathcal{V}_i \cup \mathcal{V}_j]$ is a complete bipartite graph. Simple calculations show that

$$\begin{aligned}
 ISI(G') - ISI(G) &= \left(\frac{\delta_{i-1}(\delta_i + l_j - 1)}{\delta_i + \delta_{i-1} + l_j - 1} l_{i-1} l_i - \frac{\delta_{i-1} \delta_i}{\delta_{i-1} + \delta_i} l_{i-1} l_i \right) \\
 &+ \left(\frac{(\delta_j + l_i - 1) \delta_{i+3}}{\delta_j + \delta_{i+3} + l_i - 1} l_j l_{i+3} - \frac{\delta_j \delta_{i+3}}{\delta_j + \delta_{i+3}} l_j l_{i+3} \right) \\
 &+ \left(\frac{(1 + \delta_0) \delta_1}{\delta_0 + \delta_1 + 1} l_1 - \frac{\delta_0 \delta_1}{\delta_0 + \delta_1} l_1 \right) + \frac{1(\delta_0 + 1)}{1 + \delta_0 + 1} \\
 &+ \left(\frac{(\delta_i + l_j - 1)(\delta_j + l_i - 1)}{\delta_i + \delta_j + l_i + l_j - 2} l_i l_j - \frac{\delta_i(l_i + l_j)}{\delta_i + l_i + l_j} l_i - \frac{\delta_j(l_i + l_j)}{\delta_j + l_i + l_j} l_j \right). \tag{1a}
 \end{aligned}$$

Note that $\frac{(x+t)y}{x+y+t} - \frac{xy}{x+y} = \frac{ty^2}{(x+y)(x+y+t)} > 0$ holds for any positive numbers x, y, z , then we have

$$\begin{cases} \frac{\delta_{i-1}(\delta_i+l_j-1)}{\delta_i+\delta_{i-1}+l_j-1} l_{i-1} l_i > \frac{\delta_{i-1} \delta_i}{\delta_{i-1} + \delta_i} l_{i-1} l_i \\ \frac{(\delta_j+l_i-1) \delta_{i+3}}{\delta_j+\delta_{i+3}+l_i-1} l_j l_{i+3} > \frac{\delta_j \delta_{i+3}}{\delta_j + \delta_{i+3}} l_j l_{i+3} \\ \frac{(1+\delta_0) \delta_1}{\delta_0+\delta_1+1} l_1 > \frac{\delta_0 \delta_1}{\delta_0 + \delta_1} l_1. \end{cases}$$

It remains to prove that the last term in (1a) is non-negative. Equivalently, we only need to verify

$$\frac{(\delta_i + l_j - 1)(\delta_j + l_i - 1)}{\delta_i + \delta_j + l_i + l_j - 2} l_i l_j \geq \frac{\delta_i(l_i + l_j)}{\delta_i + l_i + l_j} l_i + \frac{\delta_j(l_i + l_j)}{\delta_j + l_i + l_j} l_j. \tag{2}$$

For convenience, we let $l_j - 1 = a, l_i - 1 = b$ and $\delta_i \geq \delta_j \geq 2$. Thus, the left side and right side of inequality (2) can be, respectively, rewritten as

$$\mathcal{A}(\delta_i, \delta_j) = \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} (a + 1) + \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} b(a + 1),$$

and

$$\mathcal{B}(\delta_i, \delta_j) = \frac{\delta_j(a + b + 2)}{\delta_j + a + b + 2} (a + 1) + \frac{\delta_i(a + b + 2)}{\delta_i + a + b + 2} (b + 1).$$

What is left is to prove the difference of $\mathcal{A}(\delta_i, \delta_j)$ and $\mathcal{B}(\delta_i, \delta_j)$ is non-negative.

Subcase 1.1. $\delta_i \leq b + 2$.

It is routine to check that $\mathcal{B}(\delta_i, \delta_j) \leq \frac{\delta_i(a+b+2)}{\delta_i+a+b+2} (a + 1) + \frac{\delta_i(a+b+2)}{\delta_i+a+b+2} (b + 1) \doteq \mathcal{C}(\delta_i, \delta_j)$ since $\frac{(x+a)y}{x+y+a} > \frac{xy}{x+y}$. Hence, we shall prove that $\mathcal{A}(\delta_i, \delta_j) - \mathcal{C}(\delta_i, \delta_j) \geq 0$. Note that $\frac{(\delta_i+a)(\delta_j+b)}{\delta_i+\delta_j+a+b} \geq \frac{(\delta_i+a)(2+b)}{\delta_i+a+b+2}$, then we have

$$\frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} - \frac{\delta_i(a + b + 2)}{\delta_i + a + b + 2} \geq \frac{(\delta_i + a)(2 + b)}{\delta_i + a + b + 2} - \frac{\delta_i(a + b + 2)}{\delta_i + a + b + 2} = \frac{a(b + 2 - \delta_i)}{\delta_i + a + b + 2} \geq 0,$$

and consequently, we get

$$\mathcal{A}(\delta_i, \delta_j) - \mathcal{B}(\delta_i, \delta_j) \geq \mathcal{A}(\delta_i, \delta_j) - \mathcal{C}(\delta_i, \delta_j) \geq \frac{\delta_i(a + b + 2)}{\delta_i + a + b + 2} (b(a + 1) - (b + 1)) \geq 0.$$

Hence, $ISI(G') - ISI(G) > 0$, a contradiction.

Subcase 1.2. $\delta_i > b + 2$.

Note that $\delta_i > b + 2$ and $\delta_j \geq 2$, then direct calculations yield that

$$\begin{aligned} \mathcal{A}(\delta_i, \delta_j) - \mathcal{B}(\delta_i, \delta_j) &= \left(\frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} (a + 1) + \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} b(a + 1) \right) \\ &\quad - \left(\frac{\delta_j(a + b + 2)}{\delta_j + a + b + 2} (a + 1) + \frac{\delta_i(a + b + 2)}{\delta_i + a + b + 2} (b + 1) \right) \\ &> \frac{b(a + b + 2)^2}{(\delta_j + a + 2b + 2)(\delta_j + a + b + 2)} (a + 1) \\ &\quad + \frac{(\delta_i + a)(2 + b)}{\delta_i + 2 + a + b} b(a + 1) - \frac{\delta_i(a + b + 2)}{\delta_i + a + b + 2} (b + 1) \\ &= \frac{\mathcal{D}(\delta_i, \delta_j)}{(\delta_j + a + 2b + 2)(\delta_j + a + b + 2)(\delta_i + 2 + a + b)}, \end{aligned}$$

where $\mathcal{D}(\delta_i, \delta_j) = [(\delta_i + a)(2 + b)(a + 1)b - (a + b + 2)(b + 1)\delta_i](\delta_j + a + 2b + 2)(\delta_j + a + b + 2) + b(a + b + 2)^2(a + 1)(\delta_i + \delta_j + a + b)(\delta_i + a + b + 2)$. It is routine to check that $\mathcal{D}(\delta_i, \delta_j)$ is a non-negative number for $a \neq 1, b \neq 1$ and $a \neq 2, b \neq 1$. The remains case will be verified by elementary calculations, here we omit the details. Hence, we have $\mathcal{A}(\delta_i, \delta_j) - \mathcal{B}(\delta_i, \delta_j) \geq 0$. Consequently, $ISI(G') - ISI(G) > 0$, again a contradiction.

Case 2. $\exists i \in \{1, 2, \dots, d\}$ such that $|\mathcal{Y}_i| \geq 2, |\mathcal{Y}_{i+1}| = |\mathcal{Y}_{i+2}| = 1$ and $|\mathcal{Y}_{i+3}| \geq 2$.

Without loss of generality, we suppose that $\mathcal{Y}_{i+1} = \{v_{i+1}\}$ and $\mathcal{Y}_{i+2} = \{v_{i+2}\}$. Let G' be the graph obtained from G by the following process: (i) deleting all edges incident to vertex v_{i+1} (resp. v_{i+2}); (ii) joining vertex v_{i+1} (resp. v_{i+2}) to vertex v_0 (resp. v_{i+1}); (iii) guaranteeing $G'[\mathcal{Y}_i \cup \mathcal{Y}_{i+3}]$ is a complete bipartite subgraph. Simple calculations show that

$$\begin{aligned} ISI(G') - ISI(G) &= \left(\frac{\delta_{i-1}(\delta_i + l_{i+3} - 1)}{\delta_i + \delta_{i-1} + l_{i+3} - 1} l_{i-1} l_i - \frac{\delta_{i-1} \delta_i}{\delta_{i-1} + \delta_i} l_{i-1} l_i \right) \\ &\quad + \left(\frac{(\delta_{i+3} + l_i - 1) \delta_{i+4}}{\delta_{i+3} + \delta_{i+4} + l_i - 1} l_{i+3} l_{i+4} - \frac{\delta_{i+3} \delta_{i+4}}{\delta_{i+3} + \delta_{i+4}} l_{i+3} l_{i+4} \right) \\ &\quad + \left(\frac{(1 + \delta_0) \delta_1}{\delta_0 + \delta_1 + 1} l_1 - \frac{\delta_0 \delta_1}{\delta_0 + \delta_1} l_1 \right) + \frac{1 \cdot 2}{1 + 2} + \frac{2(\delta_0 + 1)}{2 + \delta_0 + 1} \\ &\quad + \left(\frac{(\delta_i + l_{i+3} - 1)(\delta_{i+3} + l_i - 1)}{\delta_i + \delta_{i+3} + l_i + l_{i+3} - 2} l_i l_{i+3} - \frac{\delta_i(l_i + 1)}{\delta_i + l_i + 1} l_i \right) \\ &\quad - \left(\frac{(l_i + 1)(l_{i+3} + 1)}{l_i + l_{i+3} + 2} + \frac{\delta_{i+3}(l_{i+3} + 1)}{\delta_{i+3} + l_{i+3} + 1} l_{i+3} \right). \end{aligned} \tag{2a}$$

Bearing in mind that $\frac{(x+l)y}{x+y+l} > \frac{xy}{x+y}$, then we have

$$\left\{ \begin{aligned} \frac{\delta_{i-1}(\delta_i + l_{i+3} - 1)}{\delta_i + \delta_{i-1} + l_{i+3} - 1} l_{i-1} l_i &> \frac{\delta_{i-1} \delta_i}{\delta_{i-1} + \delta_i} l_{i-1} l_i \\ \frac{(\delta_{i+3} + l_i - 1) \delta_{i+4}}{\delta_{i+3} + \delta_{i+4} + l_i - 1} l_{i+3} l_{i+4} &> \frac{\delta_{i+3} \delta_{i+4}}{\delta_{i+3} + \delta_{i+4}} l_{i+3} l_{i+4} \\ \frac{(1 + \delta_0) \delta_1}{\delta_0 + \delta_1 + 1} l_1 &> \frac{\delta_0 \delta_1}{\delta_0 + \delta_1} l_1. \end{aligned} \right.$$

To complete the proof of Claim 1, it is sufficient to show the last two terms in (2a) are non-negative. In other words, we only need to prove the following

$$\frac{(\delta_i + l_{i+3} - 1)(\delta_{i+3} + l_i - 1)}{\delta_i + \delta_{i+3} + l_i + l_{i+3} - 2} l_i l_{i+3} > \frac{\delta_i(l_i + 1)}{\delta_i + l_i + 1} l_i + \frac{(l_i + 1)(l_{i+3} + 1)}{l_i + l_{i+3} + 2} + \frac{\delta_{i+3}(l_{i+3} + 1)}{\delta_{i+3} + l_{i+3} + 1} l_{i+3}. \tag{3}$$

Let $l_{i+3} - 1 = a, l_i - 1 = b$ and $\delta_i \geq \delta_{i+3} \geq 2$, then inequality (3) is equivalent to the following

$$\begin{aligned} & \left(\frac{(\delta_i + a)(\delta_{i+3} + b)}{\delta_i + \delta_{i+3} + a + b} (a + 1) - \frac{\delta_{i+3}(a + 2)}{\delta_{i+3} + a + 2} (a + 1) \right) + \left(\frac{(\delta_i + a)(\delta_{i+3} + b)}{\delta_i + \delta_{i+3} + a + b} - \frac{\delta_i(b + 2)}{\delta_i + b + 2} \right) \\ & + \left(\frac{(\delta_i + a)(\delta_{i+3} + b)}{\delta_i + \delta_{i+3} + a + b} (b - 1) - \frac{(b + 2)(a + 2)}{a + b + 4} \right) + \left(\frac{(\delta_i + a)(\delta_{i+3} + b)}{\delta_i + \delta_{i+3} + a + b} ab - \frac{\delta_i(b + 2)}{\delta_i + b + 2} b \right) > 0, \end{aligned}$$

which always holds for $b \geq 2$, as desired. If $b = 1, a \neq 1$ and $b = 1, a = 1$, it is routine to check that the result is still correct. Hence, $ISI(G') - ISI(G) > 0$, a contradiction.

Case 3. There exist $i, j \in \{1, 2, \dots, d\}$ such that $j - i > 3, |\mathcal{V}_i| \geq 2, |\mathcal{V}_{i+1}| = |\mathcal{V}_{i+2}| = \dots = |\mathcal{V}_{j-1}| = 1$ and $|\mathcal{V}_j| \geq 2$.

Without loss of generality, we suppose that $\mathcal{V}_{i+1} = \{v_{i+1}\}, \mathcal{V}_{i+2} = \{v_{i+2}\}, \dots, \mathcal{V}_{j-1} = \{v_{j-1}\}$. Let G' be the graph obtained from G by the following process: (i) moving the $\{v_{i+1}, v_{i+2}, \dots, v_{j-1}\}$ -segment to the position ahead of vertex v_0 ; (ii) joining vertex v_{j-1} to vertex v_0 ; (iii) guaranteeing $G'[\mathcal{V}_i \cup \mathcal{V}_j]$ is a complete bipartite subgraph. It is straightforward to check that

$$\begin{aligned} ISI(G') - ISI(G) &= \left(\frac{\delta_{i-1}(\delta_i + l_j - 1)}{\delta_i + \delta_{i-1} + l_j - 1} l_{i-1} l_i - \frac{\delta_{i-1} \delta_i}{\delta_{i-1} + \delta_i} l_{i-1} l_i \right) \\ &+ \left(\frac{(\delta_j + l_i - 1) \delta_{j+1}}{\delta_j + \delta_{j+1} + l_i - 1} l_j l_{j+1} - \frac{\delta_j \delta_{j+1}}{\delta_j + \delta_{j+1}} l_j l_{j+1} \right) \\ &+ \left(\frac{(1 + \delta_0) \delta_1}{\delta_0 + \delta_1 + 1} l_1 - \frac{\delta_0 \delta_1}{\delta_0 + \delta_1} l_1 \right) \\ &+ \left(\frac{1 \cdot 2}{1 + 2} + \frac{2 \cdot 2}{2 + 2} + \frac{2(\delta_0 + 1)}{2 + \delta_0 + 1} \right) \\ &+ \left(\frac{(\delta_i + l_j - 1)(\delta_j + l_i - 1)}{\delta_i + \delta_j + l_i + l_j - 2} l_i l_j + \frac{\delta_i(l_i + 1)}{\delta_i + l_i + 1} l_i \right) \\ &+ \left(\frac{2(l_i + 1)}{l_i + 3} + \frac{2(l_j + 1)}{l_j + 3} + \frac{\delta_j(l_j + 1)}{\delta_j + l_j + 1} l_j \right) > 0, \end{aligned}$$

which is because

$$\left\{ \begin{aligned} \frac{\delta_{i-1}(\delta_i + l_j - 1)}{\delta_i + \delta_{i-1} + l_j - 1} l_{i-1} l_i &> \frac{\delta_{i-1} \delta_i}{\delta_{i-1} + \delta_i} l_{i-1} l_i \\ \frac{(\delta_j + l_i - 1) \delta_{j+1}}{\delta_j + \delta_{j+1} + l_i - 1} l_j l_{j+1} &> \frac{\delta_j \delta_{j+1}}{\delta_j + \delta_{j+1}} l_j l_{j+1} \\ \frac{(1 + \delta_0) \delta_1}{\delta_0 + \delta_1 + 1} l_1 &> \frac{\delta_0 \delta_1}{\delta_0 + \delta_1} l_1 \end{aligned} \right.$$

and

$$\frac{(\delta_i + l_j - 1)(\delta_j + l_i - 1)}{\delta_i + \delta_j + l_i + l_j - 2} l_i l_j \geq \frac{\delta_i(l_i + 1)}{\delta_i + l_i + 1} l_i + \frac{(l_i + 1)2}{l_i + 3} + \frac{2(l_j + 1)}{l_j + 3} + \frac{\delta_j(l_j + 1)}{\delta_j + l_j + 1} l_j. \tag{4}$$

Next, we need to show that the inequality (4) holds. Let $l_j - 1 = a, l_i - 1 = b$ and $\delta_i \geq \delta_j \geq 2$, then the left side of inequality (4) can be rewritten as

$$\begin{aligned} \mathcal{P}(\delta_i, \delta_j) &= \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} a + \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} ab \\ &+ \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} (b - 1) + \frac{(\delta_i + a)(\delta_j + b)}{\delta_i + \delta_j + a + b} \cdot 2, \end{aligned}$$

and the right side of inequality (4) can be given by

$$\mathcal{H}(\delta_i, \delta_j) = \frac{\delta_i(b+2)}{\delta_i+b+2}(b+1) + \frac{2(b+2)}{b+4} + \frac{2(a+2)}{a+4} + \frac{\delta_j(a+2)}{\delta_j+a+2}(a+1),$$

which is less than or equal to

$$\mathcal{R}(\delta_i, \delta_j) = \frac{\delta_i(b+2)}{\delta_i+b+2}b + \frac{\delta_j(a+2)}{\delta_j+a+2}a + \frac{\delta_i(b+2)}{\delta_i+b+2} \cdot 2 + \frac{\delta_j(a+2)}{\delta_j+a+2} \cdot 2.$$

To complete the verification of the correctness of inequality (4), we need consider the following six possibilities illustrated in Table 1. If $b \geq 3$, then we have $\mathcal{P}(\delta_i, \delta_j) - \mathcal{H}(\delta_i, \delta_j) \geq \mathcal{P}(\delta_i, \delta_j) - \mathcal{R}(\delta_i, \delta_j) \geq 0$, as desired. If $b = 2, a \geq 2$, we have $\frac{(d_i+a)(d_j+b)}{d_i+d_j+a+b}ab > \frac{d_i(b+2)}{d_i+b+2}b + \frac{d_j(a+2)}{d_j+a+2} \cdot 2$, as desired. The left cases will be shown by direct computations. Here we omit the details.

Table 1. Non-negativity of $\mathcal{P}(\delta_i, \delta_j) - \mathcal{H}(\delta_i, \delta_j)$.

≥ 0	≥ 0	≥ 0	≥ 0	≥ 0	≥ 0
$b \geq 3$	$a \geq 2, b = 2$	$a \geq 3, b = 1$	$a = 1, b = 2$	$a = 2, b = 1$	$a = 1, b = 1$

Hence, $ISI(G') - ISI(G) > 0$, which contradicts our initial hypothesis.

This completes the proof of Claim 1.

Claim 2. There are at most two P-cells \mathcal{V}_i and \mathcal{V}_j such that $|\mathcal{V}_i| \geq 2$ and $|\mathcal{V}_j| \geq 2$.

Proof of Claim 2. Without loss of generality, we assume that there are at least three such P-cells, say $\mathcal{V}_i, \mathcal{V}_{i+1}, \dots, \mathcal{V}_{j-1}, \mathcal{V}_j$, which are successive and with cardinality at least two. We choose a vertex $u \in \mathcal{V}_i$ (resp. $u \in \mathcal{V}_j$) and let G' (resp. G'') be the graph obtained from G by the following process: (i) deleting all edges incident to vertex u ; (ii) joining vertex u to each vertex in $\mathcal{V}_{j-1} \cup \mathcal{V}_{j+1}$ (resp. $\mathcal{V}_{i-1} \cup \mathcal{V}_{i+1}$) of G . It is routine to check that $G' \in \mathcal{B}_n^d$ (resp. $G'' \in \mathcal{B}_n^d$). Hence, we have

$$ISI(G) - ISI(G') = \mathcal{H}_1(i) - \mathcal{H}_1(j), \text{ where}$$

$$\begin{aligned} \mathcal{H}_1(i) = & \left(\frac{2(l_i+1)}{l_i+3} - \frac{2l_i}{l_i+2} \right) + \left(\frac{(l_i+1)(l_{i+1}+1)}{l_i+l_{i+1}+2} - \frac{l_i(l_{i+1}+1)}{l_i+l_{i+1}+1} \right) l_i \\ & + \left(\frac{(l_{i+1}+1)(l_i+l_{i+2})}{l_i+l_{i+1}+l_{i+2}+1} - \frac{(l_{i+1}+1)(l_i+l_{i+2}-1)}{l_i+l_{i+1}+l_{i+2}} \right) l_i l_{i+1} \\ & + \left(\frac{(l_i+l_{i+2})(l_{i+1}+l_{i+3})}{l_i+l_{i+1}+l_{i+2}+l_{i+3}} - \frac{(l_i+l_{i+2}-1)(l_{i+1}+l_{i+3})}{l_i+l_{i+1}+l_{i+2}+l_{i+3}-1} \right) l_{i+1} l_{i+2} \\ & + \left(\frac{l_i(l_{i+1}+1)}{l_i+l_{i+1}+1} + \frac{(l_{i+1}+1)(l_i+l_{i+2}-1)}{l_i+l_{i+1}+l_{i+2}} \right) l_{i+1} \end{aligned}$$

and

$$\begin{aligned} \mathcal{H}_1(j) = & \left(\frac{(l_{j-3}+l_{j-1})(l_{j-2}+l_j+1)}{l_{j-3}+l_{j-2}+l_{j-1}+l_j+1} - \frac{(l_{j-3}+l_{j-1})(l_{j-2}+l_j)}{l_{j-3}+l_{j-2}+l_{j-1}+l_j} \right) l_{j-2} l_{j-1} \\ & + \left(\frac{(l_{j-2}+l_j+1)(l_{j-1}+1)}{l_{j-2}+l_{j-1}+l_j+2} - \frac{(l_{j-2}+l_j)(l_{j-1}+1)}{l_{j-2}+l_{j-1}+l_j+1} \right) l_{j-1} l_j \\ & + \left(\frac{(l_{j-1}+1)(l_j+2)}{l_{j-1}+l_j+3} - \frac{(l_{j-1}+1)(l_j+1)}{l_{j-1}+l_j+2} \right) l_j - \left(\frac{2(l_j+2)}{l_j+4} - \frac{2(l_j+1)}{l_j+3} \right) \\ & + \frac{(l_{j-1}+1)(l_j+2)}{l_{j-1}+l_j+3} - \frac{(l_{j-2}+l_j+1)(l_{j-1}+1)}{l_{j-2}+l_{j-1}+l_j+2} l_{j-1}. \end{aligned}$$

If $ISI(G) - ISI(G') < 0$, then we get the required result. Hence, in what follows we assume that $ISI(G) - ISI(G') \geq 0$. By direct calculations, we get $ISI(G'') - ISI(G') = \mathcal{H}_2(i) - \mathcal{H}_2(j)$, where

$$\begin{aligned} \mathcal{H}_2(i) = & \left(\frac{2(l_i + 2)}{l_i + 4} - \frac{2l_i}{l_i + 2} \right) + \left(\frac{(l_i + 2)(l_{i+1} + 1)}{l_i + l_{i+1} + 3} - \frac{l_i(l_{i+1} + 1)}{l_i + l_{i+1} + 1} \right) l_i \\ & + \left(\frac{(l_i + 2)(l_{i+1} + 1)}{l_i + l_{i+1} + 3} + \frac{l_i(l_{i+1} + 1)}{l_i + l_{i+1} + 1} \right) \\ & + \left(\frac{(l_{i+1} + 1)(l_i + l_{i+2} + 1)}{l_i + l_{i+1} + l_{i+2} + 2} - \frac{(l_{i+1} + 1)(l_i + l_{i+2} - 1)}{l_i + l_{i+1} + l_{i+2}} \right) l_i l_{i+1} \\ & + \left(\frac{(l_{i+1} + 1)(l_i + l_{i+2} + 1)}{l_i + l_{i+1} + l_{i+2} + 2} - \frac{(l_{i+1} + 1)(l_i + l_{i+2} - 1)}{l_i + l_{i+1} + l_{i+2}} \right) l_{i+1} \\ & + \left(\frac{(l_i + l_{i+2} + 1)(l_{i+1} + l_{i+3})}{l_i + l_{i+1} + l_{i+2} + l_{i+3} + 1} - \frac{(l_i + l_{i+2} - 1)(l_{i+1} + l_{i+3})}{l_i + l_{i+1} + l_{i+2} + l_{i+3} - 1} \right) l_{i+1} l_{i+2} \end{aligned}$$

and

$$\begin{aligned} \mathcal{H}_2(j) = & \left(\frac{(l_{j-3} + l_{j-1})(l_{j-2} + l_j + 1)}{l_{j-3} + l_{j-2} + l_{j-1} + l_j + 1} - \frac{(l_{j-3} + l_{j-1})(l_{j-2} + l_j - 1)}{l_{j-3} + l_{j-2} + l_{j-1} + l_j - 1} \right) l_{j-2} l_{j-1} \\ & + \left(\frac{(l_{j-2} + l_j + 1)(l_{j-1} + 1)}{l_{j-2} + l_{j-1} + l_j + 2} - \frac{(l_{j-2} + l_j - 1)(l_{j-1} + 1)}{l_{j-2} + l_{j-1} + l_j} \right) l_{j-1} l_j \\ & + \left(\frac{(l_{j-2} + l_j + 1)(l_{j-1} + 1)}{l_{j-2} + l_{j-1} + l_j + 2} + \frac{(l_{j-2} + l_j - 1)(l_{j-1} + 1)}{l_{j-2} + l_{j-1} + l_j} \right) l_{j-1} \\ & + \left(\frac{(l_{j-1} + 1)(l_j + 2)}{l_{j-1} + l_j + 3} - \frac{(l_{j-1} + 1)l_j}{l_{j-1} + l_j + 1} \right) l_j \\ & + \left(\frac{(l_{j-1} + 1)(l_j + 2)}{l_{j-1} + l_j + 3} + \frac{(l_{j-1} + 1)l_j}{l_{j-1} + l_j + 1} \right) - \left(\frac{2(l_j + 2)}{l_j + 4} - \frac{2l_j}{l_j + 2} \right), \end{aligned}$$

It is routine to check that $ISI(G'') - ISI(G') > ISI(G) - ISI(G') \geq 0$, which contradicts our hypothesis. As desired, we get the proof of Claim 2.

This completes the proof of Lemma 4. \square

Let $G \in \mathcal{B}_n^d$ be a graph with maximal ISI-index and P-cells $\mathcal{V}_0, \mathcal{V}_1, \dots, \mathcal{V}_d$. By Lemma 4, we know $|\mathcal{V}_a| \geq 2$ and $|\mathcal{V}_{a+1}| \geq 2$, and $|\mathcal{V}_j| = 1$ for all $j \in \{1, 2, \dots, d\} \setminus \{a, a + 1\}$. By Lemma 3, $G[\mathcal{V}_{i-1} \cup \mathcal{V}_i]$ induces a complete bipartite subgraph for each $i \in \{1, 2, \dots, d\}$. Thus, $G \in \mathcal{B}_n^d$ can be represented as $\overrightarrow{G[a, s, t, b]}$ such that

$$\begin{cases} s = l_a = |\mathcal{V}_a| \\ t = l_{a+1} = |\mathcal{V}_{a+1}| \\ a + b = d - 1 \\ s + t = n - d + 1. \end{cases}$$

Without loss of generality, we assume that $a \leq b$ for the graph $\overrightarrow{G[a, s, t, b]}$ throughout this paper.

Lemma 5. Let $\overrightarrow{G[a, s, t, b]} \in \mathcal{B}_n^d$ be a graph with the maximal ISI-index, then $|s - t| \leq 1$.

Proof. We always assume that $d \geq 3$ since the case is trivial when $d \leq 2$. It follows from Lemma 1 that $a \geq 1$ and $b \geq 1$. Without loss of generality, we assume that $t > 2$ such that

$|s - t| > 1$, and consequently $t - s \geq 2$. Note that $s = |\mathcal{V}_a|$ and $t = |\mathcal{V}_{a+1}|$, it is routine to check that $\delta_a = t + 1$, $\delta_{a+1} = s + 1$ and $\delta_{a-2}, \delta_{a+3} \in \{0, 1, 2\}$. For simplicity, in what follows we let $x = \delta_{a-2}$ and $y = \delta_{a+3}$. Hence, $|x - y| \leq 2$.

For any vertex $u \in \mathcal{V}_{a+1}$, we use G' to denote the graph obtained from G by the following process: (i) deleting all edges incident to vertex u ; (ii) joining vertex u to each vertex in $(\mathcal{V}_{a-1} \cup \mathcal{V}_{a+1}) \setminus \{u\}$. It is routine to check that $G' \in \mathcal{B}_n^d$ and

$$\begin{aligned}
 ISI(G') - ISI(G) &= \left(\frac{x(s+2)}{x+s+2} - \frac{y(t+1)}{y+t+1} \right) + \left(\frac{ty}{y+t} - \frac{x(s+1)}{x+s+1} \right) \\
 &\quad + \frac{1}{s+t+2} (2t^2s - 2ts^2 + 3t^2 - s^2 - 4ts - 3t - s) > 0,
 \end{aligned}$$

which can be proved as follows. In fact

$$\begin{aligned}
 \mathcal{A}(s, t) &= \frac{x(s+2)}{x+s+2} - \frac{y(t+1)}{y+t+1} \\
 &= \frac{1}{(y+t+1)(x+s+2)} (xys + xst + xs + 2xy + 2xt + 2x) \\
 &\quad - \frac{1}{(y+t+1)(x+s+2)} (xyt + yst + 2yt + ys + 2y)
 \end{aligned}$$

and

$$\begin{aligned}
 \mathcal{B}(s, t) &= \frac{ty}{y+t} - \frac{x(s+1)}{x+s+1} \\
 &= \frac{1}{(y+t)(x+s+1)} (xyt + yst + yt - xys - xst - xy - t) \\
 &> \frac{1}{(y+t+1)(x+s+2)} (xyt + yst + yt - xys - xst - xy - t).
 \end{aligned}$$

Hence, we get

$$\begin{aligned}
 \mathcal{A}(s, t) + \mathcal{B}(s, t) &> \frac{1}{(y+t+1)(x+s+2)} ((x-y)s + 2(x-y) + (2x-1)t) \\
 &> \frac{1}{(y+t+1)(x+s+2)} ((x-y)s + 2(x-y) + (2x-1)(s+2)) \\
 &> 0.
 \end{aligned}$$

Note that $\mathcal{C}(s, t) = \frac{1}{s+t+2} (2t^2s - 2ts^2 + 3t^2 - s^2 - 4ts - 3t - s) > 0$ for $t > s \geq 1$. Hence,

$$ISI(G') - ISI(G) = \mathcal{A}(s, t) + \mathcal{B}(s, t) + \mathcal{C}(s, t) > 0,$$

as desired, we get the required result. \square

Let x be a real number, we use $\lfloor x \rfloor$ to denote the largest integer not greater than x and $\lceil x \rceil$ to represent the smallest integer not less than x . By the above lemmas and elementary calculations, we have:

Theorem 1. *Among all graphs in \mathcal{B}_n^d , $G[a, \lfloor \frac{n-d+1}{2} \rfloor, \lceil \frac{n-d+1}{2} \rceil, b]$ attains the maximal ISI-index. Furthermore, a, b satisfy the following conditions illustrated in Table 2 with respect to the diameter d :*

Table 2. Diameter determined by the values of a and b .

$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d \geq 7$
$a = 0, b = 1$	$a = 1, b = 1$	$a = 1, b = 2$	$a = 2, b = 2$	$a = 2, b = 3$	$a \geq 3, b \geq 3$

3. Ordering the Extremal Graphs according to Their Diameters

In this section, we shall explore the structural properties of graphs in \mathcal{B}_n with the largest, second-largest, and smallest ISI-indexes.

Theorem 2. Among all graphs in \mathcal{B}_n ($n \geq 2$), $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ attains the largest ISI-index, and P_n attains the smallest ISI-index.

Proof. It follows from Theorem 1 that $G[a, \lfloor \frac{n-d+1}{2} \rfloor, \lceil \frac{n-d+1}{2} \rceil, b]$ has the maximal ISI-index. Let $\mathcal{F}(d) = ISI(G[a, \lfloor \frac{n-d+1}{2} \rfloor, \lceil \frac{n-d+1}{2} \rceil, b])$. To complete the proof, it suffices to show the following claim.

Claim 3. $\mathcal{F}(d)$ is a decreasing function for $d \in [2, n - 1]$.

To complete the proof, we distinguish the following two cases.

Case 1. $d > 7$.

Note that $x = \lceil \frac{n-d}{2} \rceil \geq 1$ for $d \leq n - 1$, then we have $\delta_{a-2}, \delta_{a+3} \in \{0, 1, 2\}$. If $\delta_{a-2} = \delta_{a+3} = 2$, elementary calculations yields

$$\begin{aligned} \mathcal{F}(d) &= \frac{2\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right)}{2 + \left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right)} + \frac{2\left(\lceil \frac{n-d+1}{2} \rceil + 1\right)}{2 + \left(\lceil \frac{n-d+1}{2} \rceil + 1\right)} \\ &+ \frac{\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right)\left(\lceil \frac{n-d+1}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right) + \left(\lceil \frac{n-d+1}{2} \rceil + 1\right)} \left\lfloor \frac{n-d+1}{2} \right\rfloor \\ &+ \frac{\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right)\left(\lceil \frac{n-d+1}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right) + \left(\lceil \frac{n-d+1}{2} \rceil + 1\right)} \left\lceil \frac{n-d+1}{2} \right\rceil \\ &+ \frac{\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right)\left(\lceil \frac{n-d+1}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-d+1}{2} \rfloor + 1\right) + \left(\lceil \frac{n-d+1}{2} \rceil + 1\right)} \left\lfloor \frac{n-d+1}{2} \right\rfloor \left\lceil \frac{n-d+1}{2} \right\rceil \\ &+ \frac{1 \cdot 2}{1+2} + \frac{2 \cdot 2}{2+2}(d-7). \end{aligned}$$

The other cases could be dealt with in a similar way, here omit the details. In what follows, we shall distinguish the following two cases.

If $n - d$ is odd, then $\lceil \frac{n-d}{2} \rceil = \lceil \frac{n-d+1}{2} \rceil = \lfloor \frac{n-d+1}{2} \rfloor = \lfloor \frac{n-d}{2} \rfloor + 1$. It yields that

$$\mathcal{F}(d) = \frac{1}{2} \left(\left\lfloor \frac{n-d}{2} \right\rfloor \right)^3 + \frac{3}{2} \left(\left\lfloor \frac{n-d}{2} \right\rfloor \right)^2 + \left\lfloor \frac{n-d}{2} \right\rfloor - \frac{8}{\left\lfloor \frac{n-d}{2} \right\rfloor + 3} + d - \frac{5}{3}$$

and

$$\begin{aligned} \mathcal{F}(d+1) &= \frac{1}{2} \left(\left\lfloor \frac{n-d}{2} \right\rfloor \right)^3 + \frac{3}{4} \left(\left\lfloor \frac{n-d}{2} \right\rfloor \right)^2 - \frac{3}{8} \left\lfloor \frac{n-d}{2} \right\rfloor \\ &- \frac{4}{\left\lfloor \frac{n-d}{2} \right\rfloor + 2} - \frac{4}{\left\lfloor \frac{n-d}{2} \right\rfloor + 3} + \frac{5}{32 \left\lfloor \frac{n-d}{2} \right\rfloor + 16} + d - \frac{47}{48}. \end{aligned}$$

After subtraction, we get

$$\begin{aligned} \mathcal{F}(d+1) - \mathcal{F}(d) &= -\frac{3}{4} \left(\left\lceil \frac{n-d}{2} \right\rceil \right)^2 - \frac{11}{8} \left(\left\lceil \frac{n-d}{2} \right\rceil \right) \\ &\quad + \left(\frac{4}{\left\lceil \frac{n-d}{2} \right\rceil + 3} - \frac{4}{\left\lceil \frac{n-d}{2} \right\rceil + 2} \right) + \frac{5}{32 \left(\left\lceil \frac{n-d}{2} \right\rceil \right) + 16} + \frac{11}{16} < 0. \end{aligned}$$

The last inequality follows from the fact that $\lceil \frac{n-d}{2} \rceil \geq 1$.

If $n - d$ is even, then $\lceil \frac{n-d}{2} \rceil = \lceil \frac{n-d+1}{2} \rceil - 1 = \lfloor \frac{n-d+1}{2} \rfloor = \lfloor \frac{n-d}{2} \rfloor$. Hence,

$$\begin{aligned} \mathcal{F}(d+1) - \mathcal{F}(d) &= -\frac{3}{4} \left(\left\lfloor \frac{n-d}{2} \right\rfloor \right)^2 - \frac{13}{8} \left(\left\lfloor \frac{n-d}{2} \right\rfloor \right) - \frac{5}{16 \left\lfloor \frac{n-d}{2} \right\rfloor + 48} \\ &\quad + \left(\frac{4}{\left\lfloor \frac{n-d}{2} \right\rfloor + 4} - \frac{4}{\left\lfloor \frac{n-d}{2} \right\rfloor + 3} \right) - \frac{251}{48} < 0 \end{aligned}$$

since $\lceil \frac{n-d}{2} \rceil \geq 1$.

Hence, $\mathcal{F}(n-1) < \mathcal{F}(n-2) < \dots < \mathcal{F}(8) < \mathcal{F}(7)$, as desired.

Next, we shall consider the case for $2 \leq d \leq 7$.

Case 2. $d \leq 7$.

We only deal with the case when n is odd, the rest part can be verified in a similar way. By direct calculations, we have

$$\mathcal{F}(2) = \frac{\left(\left\lfloor \frac{n-1}{2} \right\rfloor + 1 \right)^2 \left(\left\lceil \frac{n-1}{2} \right\rceil \right)^2}{\left(\left\lfloor \frac{n-1}{2} \right\rfloor + 1 \right) + \left\lceil \frac{n-1}{2} \right\rceil} = \frac{1}{16} \left(n^3 - 2n + \frac{1}{n} \right).$$

Note that $\lfloor \frac{n-2}{2} \rfloor = \frac{n-3}{2}$ and $\lceil \frac{n-2}{2} \rceil = \frac{n-1}{2}$, hence

$$\begin{aligned} \mathcal{F}(3) &= \frac{\lfloor \frac{n-2}{2} \rfloor \left(\lceil \frac{n-2}{2} \rceil + 1 \right) \lfloor \frac{n-2}{2} \rfloor}{\lfloor \frac{n-2}{2} \rfloor + \left(\lceil \frac{n-2}{2} \rceil + 1 \right) \lfloor \frac{n-2}{2} \rfloor} \\ &\quad + \frac{\left(\lfloor \frac{n-2}{2} \rfloor + 1 \right) \left(\lceil \frac{n-2}{2} \rceil + 1 \right) \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil}{\left(\lfloor \frac{n-2}{2} \rfloor + 1 \right) + \left(\lceil \frac{n-2}{2} \rceil + 1 \right) \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil} \\ &\quad + \frac{\left(\lfloor \frac{n-2}{2} \rfloor + 1 \right) \lceil \frac{n-2}{2} \rceil \lfloor \frac{n-2}{2} \rfloor}{\left(\lfloor \frac{n-2}{2} \rfloor + 1 \right) + \lceil \frac{n-2}{2} \rceil \lfloor \frac{n-2}{2} \rfloor} \\ &= \frac{1}{16} \left(n^3 - 10n + 4 + \frac{16}{n-1} - \frac{3}{n} \right). \end{aligned}$$

Obviously, $\frac{1}{16} \left(n^3 - 10n - 2 + \frac{16}{n-1} - \frac{3}{n} \right) < \frac{1}{16} \left(n^3 - 2n + \frac{1}{n} \right)$, which implies that $\mathcal{F}(3) < \mathcal{F}(2)$. Bearing in mind the initial fact $\lfloor \frac{n-3}{2} \rfloor = \lceil \frac{n-3}{2} \rceil = \frac{n-3}{2}$, we get

$$\begin{aligned} \mathcal{F}(4) &= \frac{\lfloor \frac{n-3}{2} \rfloor \left(\lceil \frac{n-3}{2} \rceil + 1 \right) \lfloor \frac{n-3}{2} \rfloor}{\lfloor \frac{n-3}{2} \rfloor + \left(\lceil \frac{n-3}{2} \rceil + 1 \right) \lfloor \frac{n-3}{2} \rfloor} \\ &\quad + \frac{\left(\lfloor \frac{n-3}{2} \rfloor + 1 \right) \left(\lceil \frac{n-3}{2} \rceil + 1 \right) \lfloor \frac{n-3}{2} \rfloor \lceil \frac{n-3}{2} \rceil}{\left(\lfloor \frac{n-3}{2} \rfloor + 1 \right) + \left(\lceil \frac{n-3}{2} \rceil + 1 \right) \lfloor \frac{n-3}{2} \rfloor \lceil \frac{n-3}{2} \rceil} \\ &\quad + \frac{\left(\lfloor \frac{n-3}{2} \rfloor + 1 \right) \lceil \frac{n-3}{2} \rceil \lfloor \frac{n-3}{2} \rfloor}{\left(\lfloor \frac{n-3}{2} \rfloor + 1 \right) + \lceil \frac{n-3}{2} \rceil \lfloor \frac{n-3}{2} \rfloor} + \frac{\lceil \frac{n-3}{2} \rceil \cdot 1}{\lceil \frac{n-3}{2} \rceil + 1} \\ &= \frac{1}{16} \left(n^3 - 3n^2 - 5n + 4 + \frac{5}{n-2} + \frac{n-3}{16n-16} + \frac{n-1}{16n+16} \right). \end{aligned}$$

Hence, we have $\mathcal{F}(4) < \mathcal{F}(3)$ after simple computations.

It is easily seen that $\lfloor \frac{n-4}{2} \rfloor = \frac{n-5}{2}$ and $\lceil \frac{n-4}{2} \rceil = \frac{n-3}{2}$ for any odd n , then we have

$$\begin{aligned} \mathcal{F}(5) &= \frac{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) \left(\lceil \frac{n-4}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) + \left(\lceil \frac{n-4}{2} \rceil + 1\right)} \left\lfloor \frac{n-4}{2} \right\rfloor \\ &+ \frac{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) \left(\lceil \frac{n-4}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) + \left(\lceil \frac{n-4}{2} \rceil + 1\right)} \left\lfloor \frac{n-4}{2} \right\rfloor \left\lceil \frac{n-4}{2} \right\rceil \\ &+ \frac{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) \left(\lceil \frac{n-4}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) + \left(\lceil \frac{n-4}{2} \rceil + 1\right)} \left\lceil \frac{n-4}{2} \right\rceil \\ &+ \frac{\left(\lceil \frac{n-4}{2} \rceil + 1\right) \cdot 1}{\left(\lceil \frac{n-4}{2} \rceil + 1\right) + 1} + \frac{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) \cdot 1}{\left(\lfloor \frac{n-4}{2} \rfloor + 1\right) + 1} \\ &= \frac{1}{16} \left(n^3 - 6n^2 + 6n + 4 + \frac{5}{n-2} + \frac{n-3}{16n-16} + \frac{n-1}{16n+16} \right), \end{aligned}$$

implying that $\mathcal{F}(5) < \mathcal{F}(4)$ holds.

Since $\lfloor \frac{n-5}{2} \rfloor = \lceil \frac{n-5}{2} \rceil = \frac{n-5}{2}$, then we have

$$\begin{aligned} \mathcal{F}(6) &= \frac{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) \left(\lceil \frac{n-5}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) + \left(\lceil \frac{n-5}{2} \rceil + 1\right)} \left\lfloor \frac{n-5}{2} \right\rfloor \\ &+ \frac{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) \left(\lceil \frac{n-5}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) + \left(\lceil \frac{n-5}{2} \rceil + 1\right)} \left\lfloor \frac{n-5}{2} \right\rfloor \left\lceil \frac{n-5}{2} \right\rceil \\ &+ \frac{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) \left(\lceil \frac{n-5}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) + \left(\lceil \frac{n-5}{2} \rceil + 1\right)} \left\lceil \frac{n-5}{2} \right\rceil \\ &+ \frac{\left(\lceil \frac{n-5}{2} \rceil + 1\right) \cdot 2}{\left(\lceil \frac{n-5}{2} \rceil + 1\right) + 2} + \frac{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) \cdot 1}{\left(\lfloor \frac{n-5}{2} \rfloor + 1\right) + 1} + \frac{2 \cdot 1}{2 + 1} \\ &= \frac{1}{16} \left(n^3 - 9n^2 + 23n - \frac{148}{3} + \frac{n-3}{16n-16} + \frac{n-3}{8n+8} \right). \end{aligned}$$

It follows from simple calculations that $\mathcal{F}(6) < \mathcal{F}(5)$.

We observe that $\lfloor \frac{n-6}{2} \rfloor = \frac{n-7}{2}$ and $\lceil \frac{n-6}{2} \rceil = \frac{n-5}{2}$, hence

$$\begin{aligned} \mathcal{F}(7) &= \frac{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) \left(\lceil \frac{n-6}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) + \left(\lceil \frac{n-6}{2} \rceil + 1\right)} \left\lfloor \frac{n-6}{2} \right\rfloor \\ &+ \frac{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) \left(\lceil \frac{n-6}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) + \left(\lceil \frac{n-6}{2} \rceil + 1\right)} \left\lfloor \frac{n-6}{2} \right\rfloor \left\lceil \frac{n-6}{2} \right\rceil \\ &+ \frac{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) \left(\lceil \frac{n-6}{2} \rceil + 1\right)}{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) + \left(\lceil \frac{n-6}{2} \rceil + 1\right)} \left\lceil \frac{n-6}{2} \right\rceil \\ &+ \frac{\left(\lceil \frac{n-6}{2} \rceil + 1\right) \cdot 2}{\left(\lceil \frac{n-6}{2} \rceil + 1\right) + 2} + \frac{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) \cdot 2}{\left(\lfloor \frac{n-6}{2} \rfloor + 1\right) + 2} + \frac{2 \cdot 2 \cdot 1}{2 + 1} \\ &= \frac{1}{16} \left(n^3 - 12n^2 + 42n - \frac{124}{3} + \frac{n-3}{8n+8} + \frac{n-5}{8n-8} \right), \end{aligned}$$

which will not exceed the value of $\mathcal{F}(6)$.

Hence, $\mathcal{F}(7) < \mathcal{F}(6) < \mathcal{F}(5) < \mathcal{F}(4) < \mathcal{F}(3) < \mathcal{F}(2)$.

This completes the proof of Theorem 2. \square

Theorem 3. Among all graphs in \mathcal{B}_n ($n \geq 3$), $K_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n+2}{2} \rceil}$ attains the second-largest ISI-index for even n , whereas $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} \setminus \{e\}$ attains the second-largest ISI-index for odd n .

Proof. Note that $ISI(K_{s,t}) = \frac{(st)^2}{s+t}$, then we have

$$ISI\left(K_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n+2}{2} \rceil}\right) = \frac{\left(\lfloor \frac{n-2}{2} \rfloor \lceil \frac{n+2}{2} \rceil\right)^2}{\lfloor \frac{n-2}{2} \rfloor + \lceil \frac{n+2}{2} \rceil}$$

and

$$ISI\left(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} \setminus \{e\}\right) = \frac{\lfloor \frac{n}{2} \rfloor \left(\lceil \frac{n}{2} \rceil - 1\right)^2}{\lfloor \frac{n}{2} \rfloor + \left(\lceil \frac{n}{2} \rceil - 1\right)} + \frac{\left(\lfloor \frac{n}{2} \rfloor - 1\right)^2 \lceil \frac{n}{2} \rceil}{\left(\lfloor \frac{n}{2} \rfloor - 1\right) + \lceil \frac{n}{2} \rceil} + \frac{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}{\lfloor \frac{n}{2} \rfloor + \lceil \frac{n}{2} \rceil} \left(\lceil \frac{n}{2} \rceil - 1\right) \left(\lfloor \frac{n}{2} \rfloor - 1\right).$$

If n is odd, then $ISI\left(K_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n+2}{2} \rceil}\right) = \frac{1}{16}(n^3 - 18n + \frac{81}{n})$, and

$$ISI\left(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} \setminus \{e\}\right) = \frac{1}{16}\left(n^3 - 2n^2 - 2n + 6 - \frac{3}{n}\right) + \frac{1}{16}\left(2n^2 - 12n + 18\right)\left(1 + \frac{2}{n-1}\right) > \frac{1}{16}\left(n^3 - 14n + 24 - \frac{3}{n}\right).$$

Hence

$$ISI\left(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} \setminus \{e\}\right) > ISI\left(K_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n+2}{2} \rceil}\right).$$

We could deal with the case when n is even, here omit the details.

This completes the proof of Theorem 3. \square

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