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Research Article

Some Bond Incident Degree Indices of (Molecular) Graphs with Fixed Order and Number of Cut Vertices

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A bond incident degree (BID) index of a graph G is defined as $\sum_{uv\in E(G)} f(d_G(u), d_G(v))$, where $d_G(w)$ denotes the degree of a vertex w of G, $E(G)$ is the edge set of G, and f is a real-valued symmetric function. The choice $f(d_G(u), d_G(v)) = a^{d_G(u)} + a^{d_G(v)}$ in the aforementioned formula gives the variable sum exdeg index SEI_a, where $a \neq 1$ is any positive real number. A cut vertex of a graph G is a vertex whose removal results in a graph with more components than G has. A graph of maximum degree at most 4 is known as a molecular graph. Denote by $\mathbb{V}_{n,k}$ the class of all n-vertex graphs with $k \geq 1$ cut vertices and containing at least one cycle. Recently, Du and Sun [*AIMS Mathematics*, vol. 6, pp. 607–622, 2021] characterized the graphs having the maximum value of SEI_a from the set $\mathbb{V}_n^k$ for $a > 1$. In the present paper, we not only characterize the graphs with the minimum value of SEI_a from the set $\mathbb{V}_n^k$ for $a > 1$, but we also solve a more general problem concerning a special type of BID indices. As the obtained extremal graphs are molecular graphs, they remain extremal if one considers the class of all n-vertex molecular graphs with $k \geq 1$ cut vertices and containing at least one cycle.

1. Introduction

Graph invariants of the following form are known as the bond incident degree (BID) indices [1–4]:

$$\mathrm{BID}(G) = \sum_{uv\in E(G)} f(d_G(u), d_G(v)), \tag{1}$$

where $d_G(w)$ denotes the degree of a vertex w of the graph G, $E(G)$ is the edge set of G, and f is a real-valued symmetric function. In this paper, we are concerned with the following type [5] of the BID indices:

$$I_{f_i}(G) = \sum_{uv\in E(G)} \left[\frac{f_i(d_G(u))}{d_G(u)} + \frac{f_i(d_G(v))}{d_G(v)}\right] = \sum_{v\in V(G)} f_i(d_G(v)), \tag{2}$$

where $i \in \{1, 2\}$, f_1 is a strictly increasing and strictly convex function, while f_2 is a strictly decreasing and strictly concave function.

If $a \neq 1$ is a positive real number, then the variable sum exdeg index SEI_a of a graph G can be defined as

$$\mathrm{SEI}_a(G) = \sum_{v\in V(G)} d_G(v) a^{d_G(v)}. \tag{3}$$

The graph invariant SEI_a was introduced in 2011 by Vukičević [6] for predicting the octanol-water partition coefficient of chemical compounds. For detail about the mathematical results on the variable sum exdeg index, we refer the interested readers to references [7–12].

A cut vertex of a graph G is a vertex whose removal results in a graph with more components than G has. An n-vertex graph is a graph of order n. Let $\mathbb{V}_n^k$ be the set of all n-vertex graphs with $k \geq 1$ cut vertices and containing at least one cycle.

Nowadays, finding graphs with maximum or minimum values of some graph quantity from a given class of graphs is one of the popular problems in chemical graph theory.

Recently, Du and Sun [13] characterized the graphs with the maximum variable sum exdeg index SEI_a from the set $\mathbb{V}_n^k$ when $a > 1$. The main motivation of the present paper comes from [13]. In this paper, we not only characterize the graphs with the minimum variable sum exdeg index SEI_a from the set $\mathbb{V}_n^k$ for $a > 1$, but also we solve a more general problem concerning the BID indices I_{f_1} and I_{f_2}. By using the obtained general result, we also characterize the graphs with the minimum general zeroth-order Randić index ${}^0R_\alpha$ (see [14]) when $\alpha > 1$, minimum multiplicative second Zagreb index Π_2 (see [15]), and minimum sum lordeg index SL (see [16–18]) from the class $\mathbb{V}_n^k$, where

$$ {}^0R_\alpha(G) = \sum_{v \in V(G)} [d_G(v)]^\alpha, \tag{4} $$

$$ \Pi_2(G) = \prod_{v \in V(G)} [d_G(v)]^{d_G(v)}, \tag{5} $$

$$ \begin{aligned} \mathrm{SL}(G) &= \sum_{v \in V(G)} d_G(v)\sqrt{\ln[d_G(v)]} \\ &= \sum_{v \in V(G); d_G(v) \geq 2} d_G(v)\sqrt{\ln[d_G(v)]}. \end{aligned} \tag{6} $$

We note that equation (5) gives

$$ \ln[\Pi_2(G)] = \sum_{v \in V(G)} [d_G(v)] \ln[d_G(v)], \tag{7} $$

which is minimum in a given class of graphs if and only if $\Pi_2(G)$ is minimum in the considered class of graphs.

A graph of maximum degree at most 4 is known as a molecular graph. As the obtained extremal graphs are molecular graphs, they remain extremal if one considers the class of all n-vertex molecular graphs with $k \geq 1$ cut vertices and containing at least one cycle.

All the graphs considered in this paper are connected. The notation and terminology that are used in this paper but not defined here can be found in some standard graph-theoretical books, like [19, 20].

2. Lemmas

A cut vertex of G is a vertex whose removal increases the number of components of G. Denote by $\mathbb{V}_n^k$ the class of all connected n-vertex graphs with k cut vertices and containing at least one cycle. In this section, in order to obtain the main result, we establish some preliminary lemmas.

Lemma 1. *If v_1 and v_2 are adjacent vertices of a graph G, then it holds that*

$$ \begin{aligned} I_{f_1}(G - v_1v_2) &< I_{f_1}(G), \\ I_{f_2}(G - v_1v_2) &> I_{f_2}(G). \end{aligned} \tag{8} $$

Proof. The proof follows directly from the definitions of I_{f_1} and I_{f_2}. □

A cactus graph is a connected graph in which every pair of cycles has at most one vertex in common.

Lemma 2. *If G is a graph having the minimum (maximum) I_{f_1} (I_{f_2}, respectively) value among all graphs of the class $\mathbb{V}_n^k$, then G is a cactus graph.*

Proof. If G is not a cactus graph, then there exists at least one edge, say $uv \in E(G)$, lying on at least two cycles of G. Thus, the number of cut vertices of $G - uv$ and G is the same, that is, $G - uv \in \mathbb{V}_n^k$. But Lemma 1 forces that $I_{f_1}(G - uv) < I_{f_1}(G)$ and $I_{f_2}(G - uv) > I_{f_2}(G)$, which is a contradiction. □

A nontrivial connected graph containing no cut vertex is known as a nonseparable graph. A nonseparable subgraph B of a connected graph is said to be maximal nonseparable subgraph if B is not a proper subgraph of any other nonseparable subgraph of G. A block in a graph G is defined as a maximal nonseparable subgraph of G. The next corollary follows directly from Lemma 2.

Corollary 1. *If G is a graph having the minimum (maximum) I_{f_1} (I_{f_2}, respectively) value among all graphs of the class $\mathbb{V}_n^k$, then every block of G is either a cycle or K_2 (complete graph of order 2).*

Lemma 3. *If G is a graph having the minimum (maximum) I_{f_1} (I_{f_2}, respectively) value among all graphs of the class $\mathbb{V}_n^k$, then G contains exactly one cycle.*

Proof. Suppose to the contrary that G has at least two cycles, say C and C'. By Lemma 2, G is a cactus graph.

We claim that each of the cycles C and C' has length at least 4. Contrarily, suppose that at least one of C and C' has length 3. Without loss of generality, we assume that C has length 3. Then, there exists at least one edge, say xy, on C such that $G - xy \in \mathbb{V}_n^k$ (if all the three vertices of C are cut vertices, then xy may be chosen arbitrarily; if exactly two vertices of C are cut vertices, then xy may be chosen in such a way that exactly one of x and y is a cut vertex; if exactly one vertex of C is a cut vertex, then xy may be chosen in such a way that neither of x and y is a cut vertex), and hence, by using Lemma 1, we have $I_{f_1}(G - uv) < I_{f_1}(G)$ and $I_{f_2}(G - uv) > I_{f_2}(G)$, a contradiction.

Let $w \in V(G)$ be a cut vertex lying on C such that w_1 and w_2 are the neighbors of w that also lie on C. Let u (different from w) be a neighbor of w_1. Let $xy \in E(G)$ be an edge lying on the cycle C'. Let us take $G' = G - \{w_1u, w_2w, xy\} + \{ux, w_2y\}$. Then, we have

$$ \begin{aligned} I_{f_i}(G) - I_{f_i}(G') = {} & f_i(d_G(w)) - f_i(d_G(w) - 1) \\ & + f_i(d_G(w_1)) - f_i(d_G(w_1) - 1). \end{aligned} \tag{9} $$

Since f_1 is strictly increasing and f_2 is strictly decreasing, from equation (9), it follows that

$$ I_{f_i}(G) - I_{f_i}(G') \begin{cases} > 0, & \text{if } i = 1, \\ < 0, & \text{if } i = 2, \end{cases} \tag{10} $$

which is a contradiction. □

A graph containing exactly one cycle is known as a unicyclic graph. Since the cycle graph C_n of order n has no cut vertex and it is the only unicyclic graph of minimum degree at least 2, the next result is an immediate consequence of Lemma 3.

Corollary 2. *If G is a graph having the minimum (maximum) I_{f_1}(, respectively) value among all graphs of the class $\mathbb{V}_n^k$, then the minimum degree of G is one.*

Lemma 4. *Let G be a unicyclic graph. Let $v \in V(G)$ be a pendent vertex having a neighbor w of degree at least 3 such that w remains a cut vertex in $G - v$. Let $xy \in E(G)$ be an edge lying on the unique cycle of G. It holds that*

$$I_{f_i}(G) - I_{f_i}(G - \{wv, xy\} + \{xv, vy\}) \begin{cases} > 0, & \text{if } i = 1, \\ < 0, & \text{if } i = 2. \end{cases} \tag{11}$$

Proof. We have

$$\begin{aligned} I_{f_i}(G) - I_{f_i}(G - \{wv, xy\} + \{xv, vy\}) &= f_i(d_G(w)) - f_i(d_G(w) - 1) + f_i(d_G(v)) - f_i(d_G(v) + 1) \\ &= f_i(d_G(w)) - f_i(d_G(w) - 1) - [f_i(2) - f_i(1)]. \end{aligned} \tag{12}$$

Due to Lagrange's mean value theorem, there exist numbers θ_1 and θ_2 such that

$$\begin{aligned} &\theta_1 \in (d_G(w) - 1, d_G(w)), \\ &\theta_2 \in (1, 2), \end{aligned} \tag{13}$$

$$I_{f_i}(G) - I_{f_i}(G - \{wv, xy\} + \{xv, vy\}) = f_i'(\theta_1) - f_i'(\theta_2). \tag{14}$$

We recall that $d_G(w) \geq 3$, which implies that $\theta_1 > \theta_2$, and hence, the right-hand side of equation (14) is positive for $i = 1$ and negative for $i = 2$ because f_1 is strictly convex and f_2 is strictly concave. □

A path P: $v_1 v_2 \dots v_r$ in a graph G is called a pendent path if one of the two vertices v_1, v_r, is pendent and the other has degree greater than 2, and every other vertex (if exists) of P has degree 2. If P: $v_1 v_2 \dots v_r$ is a pendent path in which v_1 has degree greater than 2, then v_1 is known as the branching vertex. Two pendent paths are said to be adjacent if they have the same branching vertex.

Lemma 5. *Let G be a unicyclic graph. Let P: $wv_1v_2 \dots v_r$ and P': $wu_1u_2 \dots u_q$ be two adjacent pendent paths in G, where $r, q \geq 2$. Let $xy \in E(G)$ be an edge lying on the unique cycle of G. It holds that*

$$I_{f_i}(G) - I_{f_i}\left(G - \{v_1v_2, v_1w, xy\} + \{v_1x, v_1y, u_qv_2\}\right) \begin{cases} > 0, & \text{if } i = 1, \\ < 0, & \text{if } i = 2. \end{cases} \tag{15}$$

Proof. For simplicity, we take $G' = G - \{v_1v_2, v_1w, xy\} + \{v_1x, v_1y, u_qv_2\}$. Now, we have

$$I_{f_i}(G) - I_{f_i}(G') = f_i(d_G(w)) - f_i(d_G(w) - 1) - [f_i(2) - f_i(1)], \tag{16}$$

which is positive for $i = 1$ and negative for $i = 2$ (see the proof of Lemma 4). □

Lemma 6. *Let G be a unicyclic graph. Let P: $wv_1v_2 \dots v_r$ and P': $w'u_1u_2 \dots u_q$ be two nonadjacent pendent paths in G, where each of the vertices w and w' has degree greater than 2. It holds that*

$$I_{f_i}(G) - I_{f_i}\left(G - wv_1 + v_1u_q\right) \begin{cases} > 0, & \text{if } i = 1, \\ < 0, & \text{if } i = 2. \end{cases} \tag{17}$$

Proof. The proof is analogous to that of Lemma 4 and hence omitted. □

3. Main Result

In this section, we state and prove the lower bound on I_{f_1} and upper bound on I_{f_2} for the graphs belonging to $\mathbb{V}_n^k$. The graphs attaining these bounds are characterized as well.

Let $C_{n,k}$ be the graph deduced from the cycle graph C_{n-k} of order $n - k$ and path graph P_{k+1} of order $k + 1$ by identifying a vertex of C_{n-k} with an end-vertex of P_{k+1} (see Figure 1).

Theorem 1. *If $G \in \mathbb{V}_n^k$, then*

$$I_{f_i} \begin{cases} \geq (n-2) f_1(2) + f_1(3) + f_1(1), & \text{if } i = 1, \\ \leq (n-2) f_2(2) + f_2(3) + f_2(1), & \text{if } i = 2, \end{cases} \tag{18}$$

where the equality sign in any of these inequalities holds if and only if G is isomorphic to $C_{n,k}$ (see Figure 1).

Proof. Simple calculations yield

$$I_{f_i}\left(C_{n,k}\right) = (n-2) f_i(2) + f_i(3) + f_i(1). \tag{19}$$

We prove the inequality involving I_{f_1} and the other inequality can be proven in a fully analogous way. Let $G_{\min}$ be a graph having the minimum I_{f_1} value among all graphs of the class $\mathbb{V}_n^k$. From Lemma 3, it follows that $G_{\min}$ contains exactly one cycle. Lemma 4 guaranties that $G_{\min}$ does not contain a pendent vertex having a neighbor w of degree greater than 2 such that w remains a cut vertex in $G_{\min} - v$. Also, Lemma 5 forces that $G_{\min}$ does not contain any pair of adjacent pendent paths of lengths at least 2. Finally, from Lemma 6, it follows that $G_{\min}$ cannot have nonadjacent pendent paths. Thus, $G_{\min}$ is isomorphic to the graph $C_{n,k}$. □

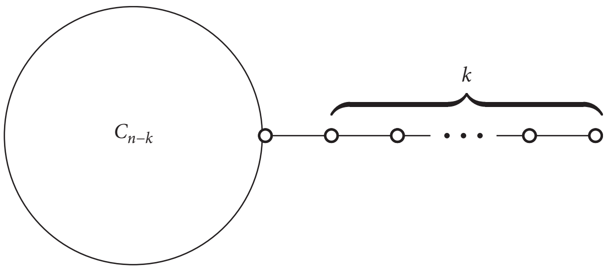

Figure 1: The graph $C_{n,k}$.

Corollary 3. *Among all the members of $\mathbb{V}_n^k$, $C_{n,k}$ is the unique graph attaining the minimum variable sum exdeg index SEI_a for $a > 1$, minimum general zeroth-order Randić index $^0R_\alpha$ for $\alpha > 1$, minimum multiplicative second Zagreb index Π_2, and minimum sum lordeg index SL.*

Proof. We note that a graph G has the minimum Π_2 value in $\mathbb{V}_n^k$ if and only if G has the minimum $\ln \Pi_2$ value in $\mathbb{V}_n^k$. Define $g_1(x) = xa^x$ with $a > 1$ and $x \geq 1$; $g_2(x) = x^\alpha$ with $\alpha > 1$ and $x \geq 1$; $g_3(x) = x \ln x$ with $x \geq 1$; and $g_4(x) = x\sqrt{\ln x}$ with $x \geq 2$. For every $i \in \{1, 2, 3, 4\}$, the function g_i is strictly increasing and strictly convex, and hence, from Theorem 1, the desired result follows. □

Remark 1. As the extremal graph $C_{n,k}$ mentioned in Theorem 1 and Corollary 3 is a molecular graph, $C_{n,k}$ remains extremal if one considers the class of all n-vertex molecular graphs with $k \geq 1$ cut vertices and containing at least one cycle instead of $\mathbb{V}_n^k$ in Theorem 1 and Corollary 3.

Data Availability

Data about this study may be requested from the authors.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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