MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **87** (2022) 89-96
ISSN: 0340-6253
doi: 10.46793/match.87-1.089A

On Bond Incident Degree Indices of (n, m)-Graphs

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(Received July 30, 2021)

Abstract

A bond incident degree (BID) index of a graph G is defined as $\sum f(d_G(u), d_G(v))$, with summation ranging over all pairs of adjacent vertices u, v of G, where $d_G(w)$ denotes the degree of the vertex w of G, and f is a real-valued symmetric function. This paper reports extremal results for BID indices of the type $I_{f_i}(G) = \sum [f_i(d_G(u))/d_G(u) + f_i(d_G(v))/d_G(v)]$, where $i \in \{1, 2\}$, f_1 is strictly convex, and f_2 is strictly concave. Graphs attaining minimum I_{f_1} and maximum I_{f_2} are characterized from the class of connected (n, m)-graphs and chemical (n, m)-graphs, where n and m satisfy the conditions $3n \geq 2m$, $n \geq 4$, $m \geq n+1$. By this, we extend and complement the recent result by Tomescu [*MATCH Commun. Math. Comput. Chem.* **85** (2021) 285–294], and cover several well-known indices, including general zeroth-order Randić index, multiplicative first and second Zagreb indices, variable sum exdeg index, and Lanzhou index.

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Its order (= number of vertices) and size (= number of edges) are denoted by n and m, respectively. By $d_G(w)$

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we denote the degree (= number of first neighbors) of the vertex $w \in V(G)$. The graphs considered in this paper are assumed to be connected. The notation and terminology used in this paper, but not defined, can be found in standard graph-theoretical books, such as [4, 5].

Graph invariants of the following form are called *bond incident degree (BID) indices* [3]:

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

where f is a real-valued symmetric function, for which $f(x, y) = f(y, x)$.

In this paper, we examine the following type of the BID indices [1]:

$$I_{f_i}(G) = \sum_{uv \in E(G)} \left[\frac{f_i(d_G(u))}{d_G(u)} + \frac{f_i(d_G(v))}{d_G(v)} \right] = \sum_{u \in V(G)} f_i(d_G(u)) \qquad (1)$$

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

Note that Eq. (1) is a special case of the identity [6]

$$\sum_{uv \in E(G)} \left[\psi(u) + \psi(v) \right] = \sum_{u \in V(G)} \psi(u)\, d_G(u)$$

which holds for any function $\psi(u)$ defined for the vertices u of the considered graph G.

A connected graph whose maximum vertex degree is at most 4 is known as a *chemical graph* [13, 17]. An (n, m)-graph is a graph of order n and size m.

The motivation for the present work comes from the recent publication by Tomescu [12], in which the extremal (n, m)-graphs with respect to the graph invariants I_{f_i} were determined, namely, the graphs attaining maximum I_{f_1}-value and minimum I_{f_2}-value. Here, by continuing Tomescu's researches, we characterize the (n, m)-graph(s) attaining minimum I_{f_1}-value and maximum I_{f_2}-value. By using our main result, we characterize the graphs attaining the minimum general zeroth-order Randić index ${}^0R_\alpha$ for $\alpha > 1$ or $\alpha < 0$ and maximum for $0 < \alpha < 1$ (see [2]), minimum variable sum exdeg index SEI_a for $a > 1$ (see [14]), minimum multiplicative second Zagreb index Π_2 (see [8, 10]), maximum multiplicative first Zagreb index Π_1 (see [8]), and minimum sum lordeg index SL (see [12, 15]). These results hold provided the parameters n and m satisfy the conditions $3n \geq 2m$, $n \geq 4$, and $m \geq n + 1$.

The above mentioned BID indices are defined as:

$${}^0R_\alpha(G) = \sum_{v \in V(G)} d_G(v)^\alpha$$

$$
\begin{aligned}
SEI_a(G) &= \sum_{v \in V(G)} d_G(v)\, a^{d_G(v)} \\
\Pi_2(G) &= \prod_{uv \in E(G)} d_G(u)\, d_G(v) = \prod_{v \in V(G)} d_G(v)^{d_G(v)} \\
SL(G) &= \sum_{v \in V(G)} d_G(v) \sqrt{\ln d_G(v)} = \sum_{v \in V(G);\ d_G(v) \geq 2} d_G(v) \sqrt{\ln d_G(v)} \\
\Pi_1(G) &= \prod_{v \in V(G)} d_G(v)^2 \,.
\end{aligned}
$$

Recall that the special cases of ${}^0R_\alpha(G)$ for $\alpha = 2$ and $\alpha = 3$ are, respectively, the first Zagreb index M_1 [9] and the forgotten topological index F [7].

The obtained extremal graphs have maximum degree 3 and minimum degree at least 2. Thus, they remain extremal also if one restricts the consideration to the class of chemical (n, m)-graphs.

Although our considerations are not directly applicable to the Lanzhou index Lz [16]

$$
Lz(G) = \sum_{v \in V(G)} \big[n - d_G(v) - 1\big]\, d_G(v)^2 \,,
$$

we still are able to utilize our main result for characterizing the graphs having minimum Lz-value among chemical (n, m)-graphs satisfying $3n \geq 2m$, $n \geq 4$, and $m \geq n + 1$.

At this point, it needs to be mentioned that the Lanzhou index obeys the identity

$$
Lz(G) = (n-1)M_1(G) + F(G) \qquad \text{i.e.,} \qquad Lz(G) = (n-1)\ {}^0R_2(G) + {}^0R_3(G)
$$

and is same as the coindex of the forgotten topological index F [11].

2 Auxiliary lemmas

In this section, we prove two lemmas that will be used to obtain the main result of this paper.

A vertex $u \in V(G)$ of degree one is said to be pendent. A path $P : u_1 u_2 \cdots u_k$ in a graph G is said to be a pendent path if one of u_1 and u_k is pendent and the other is of degree at least three, and every other vertex (if it exists) of P is of degree two.

Lemma 1. *Let n and m be fixed integers satisfying the conditions $3n \geq 2m$, $n \geq 4$, and $m \geq n$. If G attains the minimum I_{f_1}-value or maximum I_{f_2}-value among all connected (n, m)-graphs, then the minimum degree of G is at least two.*

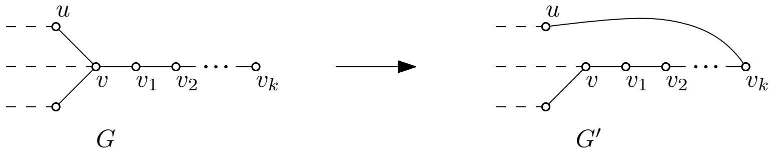

Figure 1: The graph transformation used in the proof of Lemma 1.

Proof. Contrarily, suppose that the minimum degree of G is one. Since $m \geq n$, G contains at least one pendent path. Let $vv_1v_2\cdots v_k$ be a pendent path of G, where v_k is the pendent vertex and v has degree at least three. Let u be a neighbor of v different from v_1. If G' is the graph formed by removing the edge uv from G and adding the edge uv_k (see Figure 1) then one has

$$\begin{aligned} I_{f_i}(G) - I_{f_i}(G') &= f_i(d_G(v)) - f_i(d_G(v)-1) + f_i(d_G(v_k)) - f_i(d_G(v_k)+1) \\ &= f_i(d_G(v)) - f_i(d_G(v)-1) - \big[f_i(2) - f_i(1)\big]. \end{aligned}$$

Note that both graphs G and G' have the same order and size.

By Lagrange's mean value theorem, there exist numbers c_1 and c_2 such that

$$c_1 \in (d_G(v)-1, d_G(v)) \quad \text{and} \quad c_2 \in (1,2),$$

and

$$I_{f_i}(G) - I_{f_i}(G') = f_i'(c_1) - f_i'(c_2)\,. \tag{2}$$

Note that $c_1 > c_2$ (because $d_G(v) \geq 3$), which implies that the right-hand side of Eq. (2) is positive for $i = 1$ and negative for $i = 2$, because f_1 is strictly convex and f_2 is strictly concave. Therefore, we have $I_{f_1}(G) > I_{f_1}(G')$ and $I_{f_2}(G) < I_{f_2}(G')$, a contradiction to the minimality of $I_{f_1}(G)$ and to the maximality of $I_{f_2}(G)$. ■

Lemma 2. *Let n and m be fixed integers satisfying the conditions $3n \geq 2m$, $n \geq 4$, and $m \geq n+1$. If G attains the minimum I_{f_1}-value or maximum I_{f_2}-value among all connected (n,m)-graphs, then the maximum degree of G is three,*

Proof. The assumption $m \geq n+1$ implies that the maximum degree of G must be at least three. Contrarily, suppose that the maximum degree of G is at least four.

By Lemma 1, the minimum degree of G is at least 2. If n_i denotes the number of vertices of G having degree i, then the inequality $3n \geq 2m$ yields

$$\sum_{2\leq i\leq \Delta} n_i \geq 2(m-n) = 2\left(\sum_{2\leq i\leq \Delta} \frac{i\,n_i}{2} - \sum_{2\leq i\leq \Delta} n_i\right) = 2\left(\sum_{3\leq i\leq \Delta} \frac{i\,n_i}{2} - \sum_{3\leq i\leq \Delta} n_i\right),$$

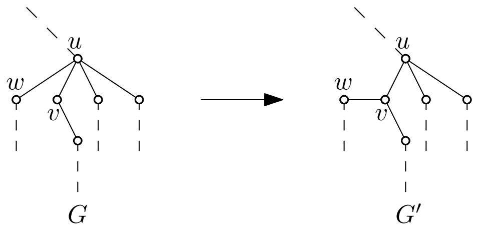

Figure 2: An example of the graph transformation used in the proof of Lemma 2.

which implies that

$$n_2 \geq \sum_{4 \leq i \leq \Delta} (i-3) n_i \, .$$

Thus, we conclude that G has at least one vertex of degree two.

Let $u \in V(G)$ be a vertex having a maximum degree and $v \in V(G)$ be a vertex of degree two. Since $d_G(u) \geq 4$, there are at least two neighbors of u not adjacent to v; from those neighbors of u, we choose the one, say w, in such a way that the graph G' formed by removing the edge uw from G and adding the edge vw (see Figure 2) remains connected. (The case when v is also a neighbor of u is shown in Figure 2.) Then, one has

$$\begin{aligned} I_{f_i}(G) - I_{f_i}(G') &= f_i(d_G(u)) - f_i(d_G(u)-1) + f_i(d_G(v)) - f_i(d_G(v)+1) \\ &= f_i(d_G(u)) - f_i(d_G(u)-1) - [f_i(3) - f_i(2)] \begin{cases} > 0 & \text{if } \ i = 1, \\ < 0 & \text{if } \ i = 2, \end{cases} \end{aligned}$$

a contradiction, where the last inequality follows from the fact that f_1 is strictly convex, f_2 is strictly concave, and $d_G(u) \geq 4$. ■

3 Main Result

We now state and prove our main result, as well as its several direct consequences.

Theorem 1. *Let n and m be fixed integers satisfying the conditions $3n \geq 2m$, $n \geq 4$, and $m \geq n+1$. Then among all connected (n,m)-graphs, those with maximum degree 3 and minimum degree at least 2 attain the minimum I_{f_1}-value and the maximum I_{f_2}-value.*

Proof. We prove the theorem for the invariant I_{f_1}. The result concerning the other invariant can be proven in a fully analogous way. Let G be a graph attaining the minimum

I_{f_1}-value among all connected (n,m)-graphs, where n and m satisfy $3n \geq 2m$, $n \geq 4$, and $m \geq n+1$.

By Lemmas 1 and 2, the maximum degree of G is 3 and its minimum degree is at least 2. Hence

$$n_2 + n_3 = n \tag{3}$$

and

$$2n_2 + 3n_3 = 2m\,. \tag{4}$$

From Eqs. (3) and (4), it follows that $n_2 = 3n - 2m$ and $n_3 = 2(m-n)$. Thus,

$$I_{f_1}(G) = (3n-2m)\, f_1(2) + 2(m-n)\, f_1(3)\,.$$

■

Corollary 3. *Let n and m be same as in Theorem 1. Then among all connected (n,m)-graphs, those with maximum degree 3 and minimum degree at least 2 (which necessarily are chemical graphs), attain the minimum general zeroth-order Randić index ${}^0R_\alpha$ for $\alpha > 1$ or $\alpha < 0$, minimum variable sum exdeg index SEI_a for $a > 1$, minimum multiplicative second Zagreb index Π_2, minimum sum lordeg index SL, maximum general zeroth-order Randić index ${}^0R_\alpha$ for $0 < \alpha < 1$, and maximum multiplicative first Zagreb index Π_1.*

Proof. Observe that a graph G attains its minimum Π_2 value or maximum Π_1 value in a class of graphs if and only if G attains its minimum $\ln \Pi_2$ value or maximum $\ln \Pi_1$ value, respectively, in the considered class of graphs. We define $\phi_1(x) = xa^x$ with $a > 1$ and $x \geq 1$; $\phi_2(x) = x^\alpha$ with $x \geq 1$ and $\alpha > 1$ or $\alpha < 0$; $\phi_3(x) = x \ln x$ with $x \geq 1$; $\phi_4(x) = x\sqrt{\ln x}$ with $x \geq 2$; $\phi_5(x) = 2\ln x$ with $x \geq 1$; and $\phi_6(x) = x^\alpha$ with $x \geq 1$ and $0 < \alpha < 1$. It can be easily verified that for each $i \in \{1,2,3,4\}$, ϕ_i is strictly convex and for each $j \in \{5,6\}$, ϕ_j is strictly concave. Thus, the required conclusions follow from Theorem 1 . ■

Remark 4. *Since the extremal graphs specified in Theorem 1 and Corollary 3 are chemical graphs, these results determine also the respective extremal chemical graphs.*

We observe that the function $\phi(x) = (n-1-x)x^2$ is strictly convex for $x < (n-1)/3$. Thus, we have the next corollary regarding the Lanzhou index of chemical (n,m)-graphs.

Corollary 5. *Let n and m be same as in Theorem 1. Then among all chemical (n, m)-graphs, those with maximum degree 3 and minimum degree at least 2 attain the minimum Lanzhou index.*

Acknowledgment: This research was funded by the Scientific Research Deanship at the University of Ha'il – Saudi Arabia through the project RG-20 031.

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