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Bond Incident Degree Indices of Connected (n, m)-Graphs With Fixed Maximum Degree

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Abstract

This article gives bounds on a substantial number of BID (bond incident degree) indices for connected graphs in terms of their order, size, and maximum degree. The considered BID indices include, among others, the Sombor index (together with its reduced version), atom-bond sum-connectivity index, symmetric division deg index, sum-connectivity index, harmonic index, and Randić index. All the graphs that attain the obtained bounds are also characterized. All the established bounds are valid also for molecular graphs. A graph of order n and size m is called an (n, m)-graph. The obtained bounds provide a partial solution to the problem of finding graphs with extremum (considered) BID indices over the class of all connected (n, m)-graphs with a fixed maximum degree under certain constraints.

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1 Introduction

In mathematical chemistry, particularly in the study of molecular graphs, a topological index is a numerical quantity associated with the molecular graph of a chemical compound. One of the primary goals of studying topological indices in chemistry is to encode structural information about molecules into numerical values. Particularly, such indices are useful in quantitative structure-activity relationship studies and can be employed to correlate molecular structure with various chemical and physical properties [18,41].

A molecular graph's bond incident degree index (BID index, for short [6]) is a topological index that is determined by adding up the contributions from each edge (bond), provided that each edge's contribution depends only on the degrees of its incident vertices (atoms) [44]. As far as the authors are aware, the earliest known BID index is the Platt index [35,36]. For a graph G, its Platt index is defined as

$$\mathcal{P}\ell(G) = \sum_{ab\in E} (d_a + d_b - 2),$$

where E denotes the set of edges of G and d_b represents the degree of the vertex b; other (chemical) graph theoretical terms used in this paper can be found in some stand books on (chemical) graph theory, like [13,15,41,47]. The Platt index has a significant connection with the first Zagreb index M_1 (see [14,26]), which is one of the most extensively researched BID indices:

$$\mathcal{P}\ell(G) = M_1(G) - 2|E|.$$

The set of all distinct elements in a graph G's degree sequence is known as the degree set of G. For a graph G, the general form [24,27,46] of a BID index of G is given as follows:

$$BID(G) = \sum_{ab\in E} F_{BID}(d_a, d_b), \tag{1}$$

where F_{BID} is a non-negative function defined the Cartesian square of the degree set of G such that $F_{BID}(d_a, d_b) = F_{BID}(d_b, d_a)$. The choices $F_{BID}(d_a, d_b) = d_a + d_b - 2$ and $F_{BID}(d_a, d_b) = d_a + d_b$ in (1) yield the Platt index and the first Zagreb index, respectively. Other choices for the function F_{BID} used in (1), that correspond to the certain BID indices considered in this paper, are given in Table 1.

Table 1. Some BID indices that are taken into account in this article.

The function $F_{BID}(d_a, d_b)$	Equation (1) corresponds to	Symbol
$(d_a\, d_b)^{-1/2}$	Randić index [31, 38]	R
$2(d_a + d_b)^{-1}$	harmonic index [12, 22]	H
$\sqrt{(d_a\, d_b)^{-1}(d_a + d_b - 2)}$	atom-bond connectivity index [5, 19, 21, 28]	ABC
$2\sqrt{d_a\, d_b}(d_a + d_b)^{-1}$	geometric-arithmetic index [17, 37, 45]	GA
$(d_u + d_v)^{-1/2}$	sum-connectivity index [12, 50]	SC
$\Big((d_a)^2 + (d_b)^2\Big)(d_a\, d_b)^{-1}$	symmetric division deg index [7, 46]	SDD
$\Big((d_a + d_b - 2)^{-1}(d_a\, d_b)\Big)^3$	augmented Zagreb index [10, 23]	AZI
$(d_a + d_b)^{-1}(d_a\, d_b)$	inverse sum indeg index [9, 46]	ISI
$\sqrt{(d_a)^2 + (d_b)^2}$	Sombor index [25, 33]	SO
$\sqrt{(d_a - 1)^2 + (d_b - 1)^2}$	reduced Sombor index [25, 33]	SO_{red}
$\sqrt{1 - 2(d_a + d_b)^{-1}}$	atom-bond sum-connectivity index [11]	ABS
$4\, d_a\, d_b\, (d_a + d_b)^{-2}$	harmonic-arithmetic index [2]	HA
$\sqrt{\Big((d_a)^2 + (d_b)^2\Big)(2 d_a d_b)^{-1}}$	modified symmetric division deg index [2]	SDD^*

In certain cases, mathematical properties of many BID indices are similar or the same [29, 30, 40, 42, 43]. Due to this fact, the properties of these indices are nowadays being studied in unified ways. Many attempts have already been made in this regard; for example, BID indices were studied generally in [4, 48, 49] for general graphs, [1, 8, 32] for particular classes of graphs, [3, 20, 39] for molecular graphs, where a graph having a maximum degree less than 5 is called a molecular graph.

The present article provides sharp bounds on a significant number of BID indices for connected graphs in terms of their order, size, and maximum degree. The first Zagreb index (and hence the Platt index) and the indices listed in Table 1 are particularly discussed. The graphs that attain the obtained bounds are also characterized.

A graph of order n and size m is referred to as an (n, m)-graph. In the rest of this paper, we consider only connected graphs.

2 Upper bounds

In this section, first we establish an upper bound on an arbitrary BID index under certain constraints, and then we derive upper bounds on the following BID indices: ABS, SO, SO_{red}, SDD, SDD^*, M_1 (see Table 1). If G is a graph with maximum degree Δ and if $\mathtt{m}_{a,b}$ denotes the number of elements of the set $\{xy \in E : d_x = a,\ d_y = b\}$, then Equation (1) can be rewritten as

$$BID(G) = \sum_{1 \le i \le j \le \Delta} \mathtt{m}_{i,j}\, F_{BID}(i, j) \tag{2}$$

Using (2), we derive our first result as follows.

Theorem 1. *Let G be an (n, m)-graph of maximum degree $\Delta \geq 2$. Consider a BID index defined via (2) and let i, j, be the integers satisfying $1 \le i \le j \le \Delta$ with $j \ge 2$ provided that $(i, j) \notin \{(1, \Delta), (\Delta, \Delta)\}$. If the function Ψ_{BID} defined by*

$$\Psi_{BID}(i, j, \Delta) = \frac{\left(2 - \frac{\Delta}{i} - \frac{\Delta}{j}\right) F_{BID}(1, \Delta) + \left(\frac{\Delta}{i} + \frac{\Delta}{j} - \Delta - 1\right) F_{BID}(\Delta, \Delta)}{\Delta - 1} + F_{BID}(i, j), \tag{3}$$

is negative valued, then

$$BID(G) \le \frac{1}{\Delta - 1}\Big((n\Delta - 2m)\, F_{BID}(1, \Delta) + \big(m(\Delta + 1) - n\Delta\big)\, F_{BID}(\Delta, \Delta)\Big), \tag{4}$$

where the equality in (4) *holds if and only if the degree set of* G *is either* $\{\Delta\}$ *or* $\{1, \Delta\}$.

Proof. For G, the following system of equations holds:

$$\begin{cases} \mathtt{m}_{1,2} + \mathtt{m}_{1,3} + \cdots + \mathtt{m}_{1,\Delta} = \eta_1 \\ \mathtt{m}_{2,1} + 2\mathtt{m}_{2,2} + \mathtt{m}_{2,3} + \cdots + \mathtt{m}_{2,\Delta} = 2\eta_2 \\ \mathtt{m}_{3,1} + \mathtt{m}_{3,2} + 2\mathtt{m}_{3,3} + \cdots + \mathtt{m}_{3,\Delta} = 3\eta_3 \\ \vdots \\ \mathtt{m}_{\Delta,1} + \mathtt{m}_{\Delta,2} + \mathtt{m}_{\Delta,3} + \cdots + 2\mathtt{m}_{\Delta,\Delta} = \Delta\eta_\Delta \\ \eta_1 + \eta_2 + \eta_3 + \cdots + \eta_\Delta = n \\ \eta_1 + 2\eta_2 + 3\eta_3 + \cdots + \Delta\eta_\Delta = 2m, \end{cases} \tag{5}$$

where η_i is the number of elements of $\{x \in V(G) : d_x = i\}$ for $i \in \{1, 2, \ldots, \Delta\}$. For every $i \in \{1, 2, \ldots, \Delta\}$, we define Θ_i as follows:

$$\begin{cases} \Theta_1 = \eta_1 - \mathtt{m}_{1,\Delta} \\ \Theta_2 = 2\eta_2 \\ \Theta_3 = 3\eta_3 \\ \vdots \\ \Theta_{\Delta-1} = (\Delta - 1)\eta_\Delta \\ \Theta_\Delta = \Delta\eta_\Delta - \mathtt{m}_{1,\Delta} - 2\mathtt{m}_{\Delta,\Delta}. \end{cases} \tag{6}$$

From Systems (5) and (6), we have

$$\sum_{i=1}^{\Delta} \Theta_i = 2(m - \mathtt{m}_{1,\Delta} - \mathtt{m}_{\Delta,\Delta}) \tag{7}$$

and

$$\sum_{i=1}^{\Delta} \frac{\Theta_i}{i} = n - \left(\frac{1}{\Delta} + 1\right) \mathtt{m}_{1,\Delta} - \frac{2}{\Delta} \mathtt{m}_{\Delta,\Delta}\,. \tag{8}$$

Solving Equations (7) and (8) for $\mathtt{m}_{1,\Delta}$ and $\mathtt{m}_{\Delta,\Delta}$, we have

$$\mathtt{m}_{1,\Delta} = \frac{1}{\Delta - 1} \left(n\Delta - 2m + \sum_{i=1}^{\Delta} \left(1 - \frac{\Delta}{i}\right) \Theta_i \right) \tag{9}$$

and

$$\mathtt{m}_{\Delta,\Delta} = \frac{1}{\Delta - 1} \left(m(\Delta + 1) - n\Delta + \sum_{i=1}^{\Delta} \left(\frac{\Delta}{i} - \frac{\Delta + 1}{2}\right) \Theta_i \right). \tag{10}$$

Define $A = \{(i,j) : 1 \le i \le j \le \Delta,\ (i,j) \ne (1,\Delta),\ (i,j) \ne (\Delta,\Delta)\}$. By utilizing (5) and (6) in (9) and (10), we have

$$\mathtt{m}_{1,\Delta} = \frac{1}{\Delta - 1} \left(n\Delta - 2m + \sum_{(i,j)\in A} \left(2 - \frac{\Delta}{i} - \frac{\Delta}{j}\right) \mathtt{m}_{i,j} \right) \tag{11}$$

and

$$\mathtt{m}_{\Delta,\Delta} = \frac{1}{\Delta - 1} \left(m(\Delta + 1) - n\Delta + \sum_{(i,j)\in A} \left(\frac{\Delta}{i} + \frac{\Delta}{j} - \Delta - 1\right) \mathtt{m}_{i,j} \right). \tag{12}$$

Now, by using (11) and (12) in (2), we have

$$BID(G) = \frac{(n\Delta - 2m)\, F_{BID}(1,\Delta) + \big(m(\Delta + 1) - n\Delta\big)\, F_{BID}(\Delta,\Delta)}{\Delta - 1} + \sum_{(i,j)\in A} \mathtt{m}_{i,j}\, \Psi_{BID}(i,j,\Delta), \tag{13}$$

where $\Psi_{BID}(i,j,\Delta)$ is defined via (3). Since $\Psi_{BID}(i,j,\Delta) < 0$, the desired result follows from Equation (13). ■

Many existing BID indices satisfy the conditions of Theorem 1. In what follows, we prove that the mentioned conditions hold for the indices:

ABS, *SO*, SO_{red}, *SDD*, M_1 (see Table 1).

Corollary 1. *If G is an (n,m)-graph of maximum degree $\Delta \geq 2$, then for the atom-bond sum-connectivity (ABS) index the following inequality holds:*

$$ABS(G) \leq \frac{n\Delta - 2m}{\sqrt{\Delta^2 - 1}} + \frac{m(\Delta+1) - n\Delta}{\sqrt{\Delta(\Delta-1)}}, \tag{14}$$

where the equality in (14) *holds if and only if the degree set of G is either* $\{\Delta\}$ *or* $\{1, \Delta\}$.

Proof. The function Ψ_{BID} defined via (3) for the ABS index becomes

$$\Psi_{ABS}(i,j,\Delta) = \frac{\left(2 - \frac{\Delta}{i} - \frac{\Delta}{j}\right)\sqrt{\frac{\Delta-1}{\Delta+1}} + \left(\frac{\Delta}{i} + \frac{\Delta}{j} - \Delta - 1\right)\sqrt{\frac{\Delta-1}{\Delta}}}{\Delta - 1} + \sqrt{1 - \frac{2}{i+j}}. \tag{15}$$

We assume that $i, j, \Delta,$ are real numbers satisfying $1 \leq i \leq j \leq \Delta$ and $j \geq 2$ provided that $(i,j) \neq (1,\Delta)$ and $(i,j) \neq (\Delta,\Delta)$. Then, the partial derivative of the function Ψ_{ABS} with respect to j is given as

$$\frac{\partial}{\partial j}\Psi_{ABS}(i,j,\Delta) = \frac{1}{(i+j)^{3/2}}\sqrt{\frac{1}{i+j-2}} + \frac{\Delta - \sqrt{\Delta(\Delta+1)}}{j^2\sqrt{\Delta^2-1}}. \tag{16}$$

We note that

$$\frac{d}{d\Delta}\left(\frac{\Delta - \sqrt{\Delta(\Delta+1)}}{\sqrt{\Delta^2-1}}\right) = \frac{(\Delta+1)^{3/2} - 2\sqrt{\Delta}}{2\sqrt{\Delta}(\Delta^2-1)^{3/2}} > 0,$$

for $\Delta \geq 2$. Thus, Equation (16) implies that

$$\frac{\partial}{\partial j}\Psi_{ABS}(i,j,\Delta) \geq \frac{1}{(i+j)^{3/2}}\sqrt{\frac{1}{i+j-2}} + \frac{j - \sqrt{j(j+1)}}{j^2\sqrt{j^2-1}}. \tag{17}$$

We use $\Phi_{ABS}(i,j)$ to denote the right-hand side of (17) . Then

$$\frac{\partial}{\partial i}\Phi_{ABS}(i,j) = (3 - 2i - 2j)\left(\frac{1}{(i+j-2)(i+j)^3}\right)^{3/2}(i+j)^2 < 0$$

for $i \geq 1$ and $j \geq 2$. Hence, (17) yields

$$\frac{\partial}{\partial j}\Psi_{ABS}(i,j,\Delta) \geq \Phi_{ABS}(j,j) = \frac{1}{j\sqrt{j(j-1)}}\left(\sqrt{\frac{j}{j+1}} - \frac{3}{4}\right) > 0$$

for $1 \leq i \leq j \leq \Delta$ and $j \geq 2$. Consequently, if all the members of the set $\{i, j, \Delta\}$ are integers satisfying $1 \leq i \leq j \leq \Delta$ and $j \geq 2$ provided that $(i,j) \neq (1,\Delta)$ and $(i,j) \neq (\Delta,\Delta)$, then we have

$$\begin{aligned}\Psi_{ABS}(1,j,\Delta) &\leq \Psi_{ABS}(1,\Delta-1,\Delta)\\ &= \sqrt{\frac{\Delta-2}{\Delta}} + \frac{1}{(\Delta-1)^{3/2}}\left(\frac{1}{\sqrt{\Delta}} - \frac{\Delta(\Delta-2)+2}{\sqrt{\Delta+1}}\right) < 0,\end{aligned}$$

Also,

$$\Psi_{ABS}(i,j,\Delta) \leq \Psi_{ABS}(i,\Delta,\Delta) = \frac{1-i}{i\sqrt{\frac{\Delta-1}{\Delta}}} + \frac{i-\Delta}{i\sqrt{\Delta^2-1}} + \sqrt{1-\frac{2}{i+\Delta}} < 0$$

for $2 \leq i \leq j \leq \Delta$ with $(i,j) \neq (\Delta,\Delta)$. Now, the desired bound follows from Theorem 1. ∎

Corollary 2. *Let G be an (n,m)-graph of maximum degree $\Delta \geq 2$. Then, for the Sombor (SO) index, the following inequality holds:*

$$SO(G) \leq \frac{\sqrt{\Delta^2+1}(\Delta n - 2m) + \sqrt{2}\Delta(\Delta m + m - \Delta n)}{\Delta - 1}, \tag{18}$$

where the equality in (18) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1,\Delta\}$.*

Proof. The function Ψ_{BID} defined via (3) for the SO index becomes

$$\begin{aligned}\Psi_{SO}(i,j,\Delta) = \sqrt{i^2+j^2} &+ \frac{\sqrt{\Delta^2+1}\,(2ij - \Delta(i+j))}{ij(\Delta-1)}\\ &+ \frac{\sqrt{2}\Delta\left(\Delta\left(\frac{1}{i}+\frac{1}{j}-1\right)-1\right)}{\Delta-1}.\end{aligned} \tag{19}$$

Assume that i, j, Δ are real numbers satisfying $1 \leq i \leq j \leq \Delta$ and $j \geq 2$ provided that $(i,j) \neq (1,\Delta)$ and $(i,j) \neq (\Delta,\Delta)$. The partial derivative of the function Ψ_{SO} with respect to Δ is given as

$$\frac{\partial}{\partial \Delta}\Psi_{SO}(i,j,\Delta) = \frac{\Phi_{SO}(i,j,\Delta)}{ij(\Delta-1)^2\sqrt{\Delta^2+1}}, \tag{20}$$

where

$$\begin{aligned}\Phi_{SO}(i,j,\Delta) = \Big[i \Big\{ & \Delta(\Delta-2)\left(\sqrt{2}\sqrt{\Delta^2+1}-\Delta\right) \\ & + \Big(-\Delta\left(\sqrt{2}\Delta\sqrt{\Delta^2+1}-2\sqrt{2}\sqrt{\Delta^2+1}+2\right) \\ & + \sqrt{2}\sqrt{\Delta^2+1}-2\Big) j + 1 \Big\} \\ & + \Delta\,(\Delta-2)\left(\sqrt{2}\sqrt{\Delta^2+1}-\Delta\right) j + j \Big].\end{aligned}$$

After some lengthy (but elementary) calculations, it is verified that

$$\Phi_{SO}(i,j,\Delta) < 0$$

under the considered constraints. Thus, from (20), we have

$$\frac{\partial}{\partial \Delta}\Psi_{SO}(i,j,\Delta) < 0$$

and thereby

$$\Psi_{SO}(i,j,\Delta) \leq \Psi_{SO}(i,j,j) = \sqrt{i^2+j^2} + \frac{(i-j)\sqrt{j^2+1} - \sqrt{2}(i-1)j^2}{i(j-1)} < 0$$

under the considered constraints. Therefore, by Theorem 1, we have the required result. ■

Corollary 3. *If G is an (n,m)-graph of maximum degree $\Delta \geq 2$, then for the reduced Sombor index SO_{red} the following inequality holds:*

$$SO_{red}(G) \leq \left(\sqrt{2}\Delta + \sqrt{2} - 2\right) m - \left(\sqrt{2}-1\right)\Delta n, \tag{21}$$

where the equality in (21) holds if and only if the degree set of G is either

$\{\Delta\}$ *or* $\{1, \Delta\}$.

Proof. The function Ψ_{BID} defined via (3) for the reduced Sombor index SO_{red} becomes

$$\Psi_{SO_{red}}(i,j,\Delta) = \frac{1}{ij}\Big[\left(\sqrt{2}-1\right)\Delta i - \left(\sqrt{2}\Delta + \sqrt{2} - 2\right) ij + ij\sqrt{(i-2)i+(j-2)j+2} + \left(\sqrt{2}-1\right) j\Delta\Big]. \quad (22)$$

Assume that i, j, Δ are real numbers satisfying $1 \le i \le j \le \Delta$ and $j \ge 2$ provided that $(i,j) \ne (1,\Delta)$ and $(i,j) \ne (\Delta,\Delta)$. The partial derivative of the function $\Psi_{SO_{red}}$ with respect to Δ satisfies

$$\frac{\partial}{\partial \Delta}\Psi_{SO_{red}}(i,j,\Delta) = \left(\sqrt{2}-1\right)\left(\frac{1}{i}+\frac{1}{j}\right) - \sqrt{2} < 0 \quad (23)$$

and thereby

$$\Psi_{SO_{red}}(i,j,\Delta) \le \Psi_{SO_{red}}(i,j,j) = \frac{i\left(\sqrt{(i-2)i+(j-2)j+2} - \sqrt{2}j + 1\right) + \left(\sqrt{2}-1\right)j}{i} < 0$$

under the considered constraints. Now, the desired result follows from Theorem 1. ■

Corollary 4. *Let G be an (n,m)-graph of maximum degree $\Delta \ge 2$. Then, for the symmetric division deg (SDD) index, the following inequality holds:*

$$SDD(G) \le \frac{2m}{\Delta} + (\Delta - 1)n, \quad (24)$$

where the equality in (24) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1, \Delta\}$.*

Proof. The function Ψ_{BID} defined via (3) for the SDD index becomes

$$\Psi_{SDD}(i,j,\Delta) = \frac{\Delta\left(i^2+i+j^2+j\right) - \Delta^2(i+j) - 2ij}{ij\Delta}. \quad (25)$$

We assume that i, j, Δ are real numbers satisfying $1 \le i \le j \le \Delta$ and $j \ge 2$ provided that $(i,j) \ne (1,\Delta)$ and $(i,j) \ne (\Delta,\Delta)$. Denote by $\Phi_{SDD}(i,j,\Delta)$ the expression present in the numerator of the right-hand side of (25). The partial derivative of the function Φ_{SDD} with respect to Δ satisfies

$$\frac{\partial}{\partial \Delta}\Phi_{SDD}(i,j,\Delta) = i^2 - 2\Delta(i+j) + i + j^2 + j < 0$$

and thus $\Phi_{SDD}(i,j,\Delta) \le \Phi_{SDD}(i,j,j) = j(i-j)(i-1) \le 0$ for $1 \le i \le j \le \Delta$ and $j \ge 2$, where the equation $\Phi_{SDD}(i,j,\Delta) = 0$ holds if and only if either $(i,j,\Delta) = (1,\Delta,\Delta)$ or $(i,j,\Delta) = (\Delta,\Delta,\Delta)$; but, neither of these two cases is possible because of the assumption $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$. Therefore, under our constraints, $\Phi_{SDD}(i,j,\Delta) < 0$ and hence from (25) we have $\Psi_{SDD}(i,j,\Delta) < 0$. Now, the required result follows from Theorem 1. ■

Corollary 5. *Let G be an (n,m)-graph of maximum degree $\Delta \ge 2$. Then, for the first Zagreb index M_1, the following inequality holds:*

$$M_1(G) \le 2(\Delta+1)m - \Delta n, \tag{26}$$

where the equality in (26) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1,\Delta\}$.*

Proof. The function Ψ_{BID} defined via (3) for M_1 satisfies

$$\Psi_{M_1}(i,j,\Delta) = -2(\Delta+1) + \frac{\Delta}{i} + i + \frac{\Delta}{j} + j < 0$$

for the integers i, j, Δ, satisfying $1 \le i \le j \le \Delta$ and $j \ge 2$ provided that $(i,j) \ne (1,\Delta)$ and $(i,j) \ne (\Delta,\Delta)$. Hence, by Theorem 1 we have the required result. ■

Here we remark that Corollary 5 follows also from Theorem 4.3 of [16]. Also, several bounds of the type (26) exist in literature; here, we compare briefly them with (26) without giving detail. The bound presented in Theorem 23 of [14] and the one given in Corollary 5 are incomparable. The bound reported in Corollary 4 of [14] is weaker than the one given in Corollary 5. For the case of trees, although the bound presented in Corollary 5 is better than the one given in Theorem 95 of [14]; however, both of these bounds are weaker than the bound mentioned after Theorem 96 on Page 57 in [14].

Corollary 6. *Let G be a molecular (n,m)-graph of maximum degree $\Delta \geq 2$. Then, for the modified symmetric division deg index SDD^*, the following inequality holds:*

$$SDD^*(G) \leq \frac{\sqrt{2\Delta}(\Delta m + m - \Delta n) + \sqrt{\Delta^2+1}(\Delta n - 2m)}{\sqrt{2\Delta}(\Delta - 1)}, \tag{27}$$

where the equality in (27) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1,\Delta\}$.*

Proof. The function Ψ_{BID} defined via (3) for SDD^* becomes

$$\Psi_{SDD^*}(i,j,\Delta) = \frac{\Delta\left(\frac{1}{i}+\frac{1}{j}-1\right)-1}{\Delta-1} + \frac{\sqrt{\Delta+\frac{1}{\Delta}}\left(2-\frac{\Delta(i+j)}{ij}\right)}{\sqrt{2}(\Delta-1)} + \frac{\sqrt{\frac{i}{j}+\frac{j}{i}}}{\sqrt{2}}.$$

However, $\Psi_{SDD^*}(i,j,\Delta) < 0$ for every $(i,j,\Delta) \in \{(1,2,3),(1,2,4),(1,3,4),(2,2,3),(2,2,4),(2,3,3),(2,3,4),(2,4,4),(3,3,4),(3,4,4)\}$. Therefore, the desired result follows from Theorem 1. ■

As $\Psi_{SDD^*}(2,7,7) > 0$, we remark here that we cannot utilize Theorem 1 when we consider general graphs in Corollary 6 instead of molecular graphs.

3 Lower bounds

In the current section, we present first a lower bound on an arbitrary BID index under certain constraints and then we derive lower bounds on the following BID indices: H, SC, R, GA, HA (see Table 1).

Theorem 2. *Let G be an (n,m)-graph of maximum degree $\Delta \geq 2$. Consider a BID index defined via* (2) *and let i,j, be the integers satisfying $1 \leq i \leq j \leq \Delta$ with $j \geq 2$ provided that $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$. If the* *function* $\Psi_{BID}(i,j,\Delta)$ *defined via* (3) *is positive valued then*

$$BID(G) \geq \frac{1}{\Delta-1}\Big((n\Delta-2m)\,F_{BID}(1,\Delta)+\big(m(\Delta+1)-n\Delta\big)\,F_{BID}(\Delta,\Delta)\Big). \tag{28}$$

where the equality in (28) *holds if and only if the degree set of* G *is either* $\{\Delta\}$ *or* $\{1,\Delta\}$.

Proof. The proof is completely analogous to the proof of Theorem 1. ■

Many existing BID indices satisfy the conditions of Theorem 2. In what follows, we prove that the mentioned conditions hold for the indices: H, SC, R (see Table 1).

Corollary 7. *Let* G *be an* (n,m)*-graph of maximum degree* $\Delta \geq 2$*. Then, for the harmonic index* H*, the following inequality holds:*

$$H(G) \geq \frac{m(\Delta-1)+n\Delta}{\Delta(\Delta+1)}, \tag{29}$$

where the equality in (29) *holds if and only if the degree set of* G *is either* $\{\Delta\}$ *or* $\{1,\Delta\}$.

Proof. Note that if i,j, are integers satisfying $1 \leq i \leq j \leq \Delta$ with $j \geq 2$ provided that $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$, then $\Delta \geq 3$. The function Ψ_{BID} defined via (3) for the index H becomes

$$\Psi_H(i,j,\Delta) = \frac{2}{i+j} + \frac{1}{\Delta} - \frac{i+j+2ij}{ij(\Delta+1)}\,.$$

Assume that i,j,Δ are real numbers satisfying $1 \leq i \leq j \leq \Delta$ with $\Delta \geq 3$ and $j \geq 2$ provided that $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$. Then, the partial derivative of the function Ψ_H with respect to Δ is given as

$$\frac{\partial}{\partial\Delta}\Psi_H(i,j,\Delta) = \frac{i+j}{ij(1+\Delta)^2} + \frac{2}{(1+\Delta)^2} - \frac{1}{\Delta^2}. \tag{30}$$

For $\Delta \geq 3$, it holds that

$$\frac{2}{(1+\Delta)^2} - \frac{1}{\Delta^2} > 0$$

and hence from (30) we conclude that

$$\frac{\partial}{\partial \Delta}\Psi_H(i,j,\Delta) > 0.$$

Thus,

$$\Psi_H(i,j,\Delta) \geq \Psi_H(i,j,j) = \frac{2}{i+j} - \frac{i+1}{i(j+1)} \geq 0$$

for $1 \leq i \leq j \leq \Delta$ with $\Delta \geq 3$ and $j \geq 2$, where the equation $\Psi_H(i,j,\Delta) = 0$ holds if and only if either $(i,j,\Delta) = (1,\Delta,\Delta)$ or $(i,j,\Delta) = (\Delta,\Delta,\Delta)$; but, neither of these two cases holds because of our assumption $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$. Therefore, $\Psi_H(i,j,\Delta) > 0$ and hence the required result follows from Theorem 2. ■

Corollary 8. *If G is an (n,m)-graph of maximum degree $\Delta \geq 2$, then for the sum-connectivity (SC) index the following inequality holds:*

$$SC(G) \geq \frac{m + (m-n)\Delta}{(\Delta-1)\sqrt{2\Delta}} + \frac{n\Delta - 2m}{(\Delta-1)\sqrt{\Delta+1}}, \tag{31}$$

where the equality in (31) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1,\Delta\}$.*

Proof. The function Ψ_{BID} defined via (3) for the sum-connectivity (SC) index becomes

$$\Psi_{SC}(i,j,\Delta) = \frac{1}{\sqrt{i+j}} + \frac{\left(\frac{1}{i}+\frac{1}{j}-1\right)\Delta - 1}{(\Delta-1)\sqrt{2\Delta}} + \frac{2 - \frac{(i+j)\Delta}{ij}}{(\Delta-1)\sqrt{\Delta+1}}.$$

Assume that i, j, Δ are real numbers satisfying $1 \leq i \leq j \leq \Delta$ and $j \geq 2$ provided that $(i,j) \neq (1,\Delta)$ and $(i,j) \neq (\Delta,\Delta)$. The partial derivative of the function Ψ_{SC} with respect to j is given as

$$\frac{\partial}{\partial j}\Psi_{SC}(i,j,\Delta) = \frac{1}{\left(\frac{\sqrt{2}(\Delta+1)}{\sqrt{\Delta}} + 2\sqrt{\Delta+1}\right) j^2} - \frac{1}{2(i+j)^{3/2}}. \tag{32}$$

Note that

$$\frac{d}{d\Delta}\left(\frac{1}{\frac{\sqrt{2}(\Delta+1)}{\sqrt{\Delta}} + 2\sqrt{\Delta+1}}\right) < 0$$

and thus Equation (32) implies that

$$\frac{\partial}{\partial j}\Psi_{SC}(i,j,\Delta) \le \frac{1}{j^2\left(\frac{\sqrt{2}(j+1)}{\sqrt{j}}+2\sqrt{j+1}\right)} - \frac{1}{2(i+j)^{3/2}}\,. \tag{33}$$

Denote by $\Phi_{SC}(i,j)$ the right-hand side of (33). Since $\frac{\partial}{\partial i}\Phi_{SC}(i,j) > 0$, it holds that

$$\Phi_{SC}(i,j) \le \Phi_{SC}(j,j) = -\frac{\sqrt{2j(j+1)}+j-3}{4j^{3/2}\left(\sqrt{2}j+2\sqrt{j(j+1)}+\sqrt{2}\right)} < 0.$$

Hence, (33) implies that the function Ψ_{SC} is strictly decreasing in j and thereby we have

$$\Psi_{SC}(i,j,\Delta) \ge \Psi_{SC}(i,\Delta,\Delta) = \frac{1}{\sqrt{\Delta+i}} - \frac{(i-1)\sqrt{\Delta}+\frac{\sqrt{2}(\Delta-i)}{\sqrt{\Delta+1}}}{\sqrt{2}\,i(\Delta-1)} \ge 0$$

for $1 \le i \le j \le \Delta$ with $j \ge 2$, where the equation $\Psi_{SC}(i,j,\Delta) = 0$ holds if and only if either $(i,j,\Delta) = (1,\Delta,\Delta)$ or $(i,j,\Delta) = (\Delta,\Delta,\Delta)$; but, neither of these two cases (for the equality) holds because of our assumption $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$. Therefore, $\Psi_{SC}(i,j,\Delta) > 0$, and hence Theorem 2 yields the desired result. ■

Corollary 9. *Let G be an (n,m)-graph of maximum degree $\Delta \ge 2$. Then, for the Randić index R, the following inequality holds:*

$$R(G) \ge \frac{\left(\sqrt{\Delta}-1\right)m+\Delta n}{\Delta\left(\sqrt{\Delta}+1\right)}, \tag{34}$$

where the equality in (34) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1,\Delta\}$.*

Proof. The function Ψ_{BID} defined via (3) for the Randić index R becomes

$$\Psi_R(i,j,\Delta) = \frac{\sqrt{\Delta^3 ij}-\sqrt{\Delta}ij-\Delta(i+j)+\Delta\sqrt{ij}+ij}{\left(\sqrt{\Delta}+1\right)\Delta ij}\,. \tag{35}$$

Assume that i, j, Δ are real numbers satisfying $1 \leq i \leq j \leq \Delta$ and $j \geq 2$ provided that $(i,j) \neq (1,\Delta)$ and $(i,j) \neq (\Delta,\Delta)$. Denote by $\Phi_R(i,j,\Delta)$ the expression present in the numerator of the right-hand side of (35). Then

$$\frac{\partial}{\partial \Delta}\Phi_R(i,j,\Delta) = \frac{3}{2}\sqrt{\Delta i j} - i\left(\frac{j}{2\sqrt{\Delta}} + 1\right) + \sqrt{ij} - j > 0,$$

and thereby we have

$$\Phi_R(i,j,\Delta) \geq \Phi_R(i,j,j) = j^{3/2}\left(\sqrt{i} - 1\right)\left(\sqrt{j} - \sqrt{i}\right),$$

which gives $\Phi_R(i,j,\Delta) > 0$ because $(i,j) \notin \{(1,\Delta),(\Delta,\Delta)\}$. Therefore, from (35) we have $\Psi_R(i,j,\Delta) > 0$, and hence by Theorem 2, we have the required result. ■

Corollary 10. *Let G be a molecular (n,m)-graph of maximum degree $\Delta \geq 2$. Then, for the geometric-arithmetic index GA, the following inequality holds:*

$$GA(G) \geq \frac{(\Delta+1)(m + m\Delta - n\Delta) + 2(n\Delta - 2m)\sqrt{\Delta}}{\Delta^2 - 1}, \tag{36}$$

where the equality in (36) holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1,\Delta\}$.

Proof. The function Ψ_{BID} defined via (3) for GA becomes

$$\Psi_{GA}(i,j,\Delta) = \frac{\left(2 - \frac{\Delta}{i} - \frac{\Delta}{j}\right)\frac{2\sqrt{\Delta}}{\Delta+1} + \left(\frac{\Delta}{i} + \frac{\Delta}{j} - \Delta - 1\right)}{\Delta - 1} + \frac{2\sqrt{i\,j}}{i+j}.$$

However, $\Psi_{GA}(i,j,\Delta) > 0$ for every $(i,j,\Delta) \in \{(1,2,3), (1,2,4), (1,3,4), (2,2,3), (2,2,4), (2,3,3), (2,3,4), (2,4,4), (3,3,4), (3,4,4)\}$. Therefore, the desired result follows from Theorem 2. ■

Palacios [34] proved that for any n-order connected graph G with size m and maximum degree $\Delta \geq 2$, the following inequality holds

$$GA(G) \geq \frac{2m^2}{n\,\Delta} \tag{37}$$

with equality if G is regular. Note that the size of a molecular graph of order n belongs to the interval

- $[n-1, 2n]$ if the maximum degree is 4,
- $\left[n-1, \frac{3}{2}n\right]$ if the maximum degree is 3,
- $[n-1, n]$ if the maximum degree is 2;

in all three cases, the bound (36) is better than (37).

Corollary 11. *Let G be a molecular graph (n, m)-graph of maximum degree $\Delta \geq 2$. Then, for the harmonic-arithmetic (HA) index, the following inequality holds:*

$$HA(G) \geq \frac{(\Delta(\Delta+4)-1)m - (\Delta-1)\Delta n}{(\Delta+1)^2}, \tag{38}$$

where the equality in (38) *holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1, \Delta\}$.*

Proof. The proof is similar to the proof of Corollary 10. ■

As $\Psi_{GA}(2,5,5) < 0$ and $\Psi_{HA}(2,5,5) < 0$, we remark here that we cannot utilize Theorem 2 when we consider general graphs in Corollaries 10 and 11 instead of molecular graphs.

4 Concluding remarks

In the previous two sections, we see that either Theorem 1 or Theorem 2 is applicable to several well-known BID indices. However, there are some renowned BID indices to which we cannot apply either of the aforementioned theorems. For instance, the function Ψ_{BID} defined via (3) for the atom-bond connectivity (ABC) index, inverse sum index (ISI) index and augmented Zagreb index (AZI) becomes

$$\Psi_{ABC}(i,j,\Delta) = \frac{\sqrt{2}\left(\Delta\left(\frac{1}{i}+\frac{1}{j}-1\right)-1\right)}{\Delta\sqrt{\Delta-1}} + \frac{2ij-\Delta(i+j)}{ij\sqrt{\Delta(\Delta-1)}} + \sqrt{\frac{i+j-2}{ij}},$$

$$\Psi_{ISI}(i,j,\Delta)=\frac{(2ij-\Delta(i+j))\big(i(\Delta(j-1)+j)-\Delta j\big)}{2(\Delta+1)ij(i+j)},$$

$$\Psi_{AZI}(i,j,\Delta)=\frac{i^3j^3}{(i+j-2)^3}+\frac{\Delta^6\left(\Delta\left(\frac{1}{i}+\frac{1}{j}-1\right)-1\right)}{8(\Delta-1)^4}+\frac{\Delta^3\left(2-\frac{\Delta(i+j)}{ij}\right)}{(\Delta-1)^4}.$$

Since

$$\Psi_{ABC}(2,4,4)>0,\ \ \Psi_{ABC}(1,3,4)<0,\ \ \Psi_{ABC}(2,7,7)>0;$$

$$\Psi_{ISI}(2,4,4)<0,\ \ \Psi_{ISI}(1,3,4)>0,\ \ \Psi_{ISI}(2,7,7)<0;$$

$$\Psi_{AZI}(2,4,4)<0,\ \ \Psi_{AZI}(1,3,4)>0,\ \ \Psi_{AZI}(2,7,7)<0;$$

neither Theorem 1 nor Theorem 2 is applicable to the indices ABC, ISI and AZI (even for molecular graphs).

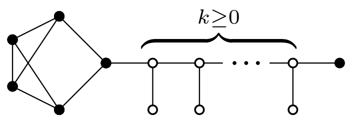

Figure 1. A graph with $2k+6$ vertices, referred in Corollary 12.

We remark that the results obtained in the previous two sections provide a partial solution to the problem of finding graphs with extremum (considered) BID indices over the class of all (n,m)-graphs with a fixed maximum degree under certain constraints. For example, Corollary 11 implies the next result.

Corollary 12. *Among all $(n,n+2)$-graphs of maximum degree 3, only the graph(s) with degree set $\{1,3\}$ attain(s) the minimum HA index, where $n=2k+6$ with $k\geq 0$; for example, see Figure 1.*

In (6), we define Θ_i by keeping in mind the quantities $\mathtt{m}_{1,\Delta}$ and $\mathtt{m}_{\Delta,\Delta}$. One may think about other possibilities; for instance,

(i) $\mathtt{m}_{2,2}$ and $\mathtt{m}_{2,3}$, or

(ii) $\mathtt{m}_{\delta,\Delta}$ and $\mathtt{m}_{\Delta,\Delta}$, or

(iii) $\mathtt{m}_{1,n-1}$ and $\mathtt{m}_{n-1,n-1}$, or

(iv) $\mathtt{m}_{1,2}$ and $\mathtt{m}_{2,2}$.

The derivation of the result for any of the above-mentioned cases is fully analogous to that of Theorem 1. We end this paper by reporting a result that corresponds to the first case in the above-mentioned four possibilities.

Theorem 3. *Let G be an (n,m)-graph with maximum degree of at least 2. Consider a BID index defined via* (2) *and let i, j, be the integers satisfying $1 \le i \le j \le n-1$ with $j \ge 2$ provided that $(i,j) \notin \{(2,2),(2,3)\}$. If the function Ψ_{BID} defined by*

$$\Psi_{BID}(i,j) = \left(5 - \frac{6}{i} - \frac{6}{j}\right) F_{BID}(2,2) + 6\left(\frac{1}{i} + \frac{1}{j} - 1\right) F_{BID}(2,3) + F_{BID}(i,j), \tag{39}$$

is negative valued, then

$$BID(G) \le 6\Big[F_{BID}(2,2) - F_{BID}(2,3)\Big]n + \Big[6F_{BID}(2,3) - 5F_{BID}(2,2)\Big]m, \tag{40}$$

where the equality in (40) *holds if and only if the degree set of G is either either $\{2\}$ or $\{2,3\}$ such that no two vertices of degree 3 are adjacent. If the function Ψ_{BID} defined via* (39) *is positive valued, then the inequality* (40) *is reversed.*

Proof. Define Θ_i for every $i \in \{1, 2, \ldots, n-1\}$ as follows:

$$\begin{cases} \Theta_1 = \eta_1 \\ \Theta_2 = 2\eta_2 - 2\mathtt{m}_{2,2} - \mathtt{m}_{2,3} \\ \Theta_3 = 3\eta_3 - \mathtt{m}_{2,3} \\ \Theta_j = j \cdot \eta_j \text{ when } 4 \le j \le n-1, \end{cases} \tag{41}$$

where η_a is defined just after (5) and $\mathtt{m}_{a,b}$ is defined just before (2). Here, we have

$$\sum_{i=1}^{n-1} \Theta_i = 2(m - \mathtt{m}_{2,2} - \mathtt{m}_{2,3}) \tag{42}$$

and

$$\sum_{i=1}^{n-1} \frac{\Theta_i}{i} = n - \mathtt{m}_{2,2} - \frac{5}{6}\mathtt{m}_{2,3}\,. \tag{43}$$

Solving Equations (42) and (43) for $\mathtt{m}_{2,2}$ and $\mathtt{m}_{2,3}$, we have

$$\mathtt{m}_{2,2} = 6n - 5m + \sum_{i=1}^{n-1} \left(\frac{5}{2} - \frac{6}{i}\right) \Theta_i \tag{44}$$

and

$$\mathtt{m}_{2,3} = 6m - 6n + 3\sum_{i=1}^{n-1} \left(\frac{2}{i} - 1\right) \Theta_i. \tag{45}$$

Define $A = \{(i,j) : 1 \le i \le j \le n-1,\ (i,j) \ne (2,2),\ (i,j) \ne (2,3)\}$. Then, Equations (44) and (45) can be rewritten as

$$\mathtt{m}_{2,2} = 6n - 5m + \sum_{(i,j)\in A} \left(5 - \frac{6}{i} - \frac{6}{j}\right) \mathtt{m}_{i,j} \tag{46}$$

and

$$\mathtt{m}_{2,3} = 6\left(m - n + \sum_{(i,j)\in A} \left(\frac{1}{i} + \frac{1}{j} - 1\right) \mathtt{m}_{i,j}\right). \tag{47}$$

By utilizing (46) and (47) in (2), we have

$$\begin{aligned} BID(G) &= \mathtt{m}_{2,2}F_{BID}(2,2) + \mathtt{m}_{2,3}F_{BID}(2,3) + \sum_{(i,j)\in A} \mathtt{m}_{i,j}F_{BID}(i,j) \\ &= 6\Big[F_{BID}(2,2) - F_{BID}(2,3)\Big]n + \Big[6F_{BID}(2,3) - 5F_{BID}(2,2)\Big]m \\ &\quad + \sum_{(i,j)\in A} \mathtt{m}_{i,j}\,\Psi_{BID}(i,j), \end{aligned} \tag{48}$$

where $\Psi_{BID}(i,j)$ is defined via (39). Now, the desired conclusion follows from (48). ■

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