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New lower bounds for the second variable Zagreb index

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Abstract The aim of this paper is to obtain new sharp inequalities for a large family of topological indices, including the second variable Zagreb index M_2^α, and to characterize the set of extremal graphs with respect to them. Our main results provide lower bounds on this family of topological indices involving just the minimum and the maximum degree of the graph. These inequalities are new even for the Randić, the second Zagreb and the modified Zagreb indices.

Keywords Second variable Zagreb index · Graph invariant · Vertex-degree-based graph invariant · Topological index

Mathematics Subject Classification MSC 05C07 · MSC 92E10

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1 Introduction

A topological descriptor is a single number that represents a chemical structure in graph-theoretical terms via the molecular graph, they play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. A topological descriptor is called a topological index if it correlates with a molecular property. Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener (1947).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index (R) (Randić 1975).

Two of the main successors of the Randić index are the first and second Zagreb indices, denoted by M_1 and M_2, respectively, and introduced by Gutman and Trinajstić in 1972 (see Gutman and Trinajstić 1972). They are defined as

$$M_1(G) = \sum_{u \in V(G)} d_u^2, \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u. Along the paper, we will denote by m and n, the cardinality of the sets $E(G)$ and $V(G)$, respectively.

There is a vast amount of research on the Zagreb indices. For details of their chemical applications and mathematical theory see Gutman (2013), Gutman and Das (2004), Gutman and Réti (2014), Nikolić et al. (2003), and the references therein.

In Li and Zheng (2005), Li and Zhao (2004) and Miličević and Nikolić (2004), the *first and second variable Zagreb indices* are defined as

$$M_1^\alpha(G) = \sum_{u \in V(G)} d_u^{2\alpha}, \qquad M_2^\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$$

with $\alpha \in \mathbb{R}$.

Note that M_1^0 is n, $M_1^{1/2}$ is $2m$, M_1^1 is the first Zagreb index M_1, $M_1^{-1/2}$ is the inverse index ID (Fajtlowicz 1987), $M_1^{3/2}$ is the forgotten index F, etc.; also, M_2^0 is m, $M_2^{-1/2}$ is the usual Randić index, M_2^1 is the second Zagreb index M_2, M_2^{-1} is the modified Zagreb index (Nikolić et al. 2003), etc.

The concept of variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see Randić 1991a, b), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes Randić et al. 2001). The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a particular studied property is as small as possible (see, e.g., Miličević and Nikolić 2004).

In the paper of Gutman and Tošović (2013), the correlation abilities of 20 vertex-degree-based topological indices occurring in the chemical literature were tested for the case of standard heats of formation and normal boiling points of octane isomers. It is remarkable to realize that the second variable Zagreb index M_2^α with exponent $\alpha = -1$ (and to a lesser extent with exponent $\alpha = -2$) performs significantly better than the Randić index ($R = M_2^{-0.5}$).

The second variable Zagreb index is used in the structure-boiling point modeling of benzenoid hydrocarbons (Nikolić et al. 2004). Also, variable Zagreb indices exhibit a potential applicability for deriving multi-linear regression models (Drmota 2009). Various properties and relations of these indices are discussed in several papers (see, e.g., Andova and Petrusevski 2011; Li and Zhao 2004; Liu and Liu 2010; Rodríguez and Sigarreta 2017; Sigarreta 2015; Singh et al. 2014; Zhang et al. 2006; Zhang and Zhang 2006).

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) non-trivial ($E(G) \neq \emptyset$) graph. A main topic in the study of topological indices is to find bounds of the indices involving several parameters. The aim of this paper is to obtain new sharp inequalities for a large family of topological indices and to characterize the set of extremal graphs with respect to them. Our main results provide lower bounds on this family of topological indices involving just the minimum and the maximum degree of the graph (see Theorems 1, 2, 3 and 4). This family of indices includes, among others, the second variable Zagreb index M_2^α (see Sect. 4). The inequalities obtained are new even for the Randić, the second Zagreb and the modified Zagreb indices.

2 Minimum and maximum degree

Let $\mathcal{I}$ be any topological index defined as

$$\mathcal{I}(G) = \sum_{uv \in E(G)} h(d_u, d_v),$$

where $h(x, y)$ is any positive symmetric function $h : \mathbb{Z}^+ \times \mathbb{Z}^+ \to \mathbb{R}^+$.

Definition 1 A graph G with minimum degree δ and maximum degree Δ is *minimal* for $\mathcal{I}$ if $\mathcal{I}(G) \leq \mathcal{I}(\Gamma)$ for every graph Γ with minimum degree δ and maximum degree Δ.

Given integers $1 \leq \delta \leq \Delta$, let us define $\mathcal{G}_{\delta,\Delta}$ as the set of graphs G with minimum degree δ, maximum degree Δ and such that:

(1) G is isomorphic to the complete graph with $\Delta + 1$ vertices $K_{\Delta+1}$, if $\delta = \Delta$,
(2) $|V(G)| = \Delta + 1$ and there are Δ vertices with degree δ, if $\delta < \Delta$ and $\Delta(\delta + 1)$ is even,
(3) $|V(G)| = \Delta + 1$ and there are $\Delta - 1$ vertices with degree δ and a vertex with degree $\delta + 1$, if $\delta < \Delta - 1$ and $\Delta(\delta + 1)$ is odd,
(4) $|V(G)| = \Delta + 1$ and there are $\Delta - 1$ vertices with degree δ and two vertices with degree Δ, if $\delta = \Delta - 1$ and Δ is odd (and thus $\Delta(\delta + 1)$ is odd).

If $\Delta(\delta+1)$ is odd, let us define $\mathcal{G}'_{\delta,\Delta}$ as the set of graphs G with minimum degree δ, maximum degree Δ and such that $|V(G)| = \Delta + 2$, a vertex with degree Δ has Δ neighbors with degree δ and the last vertex has degree $\delta + 1$ (note that $\delta < \Delta$ since $\Delta(\delta + 1)$ is odd).

Remark 1 Every graph $G \in \mathcal{G}_{\delta,\Delta}$ has maximum degree Δ and $|V(G)| = \Delta + 1$. Hence, every graph $G \in \mathcal{G}_{\delta,\Delta}$ is connected. Also, every graph $G \in \mathcal{G}'_{\delta,\Delta}$ is connected.

Let us recall the following proposition from Martínez-Pérez and Rodríguez (2018):

Proposition 1 *For any integers* $1 \le \delta \le \Delta$*, we have* $\mathcal{G}_{\delta,\Delta} \ne \emptyset$*. Let G be a graph with minimum degree* δ *and maximum degree* Δ*. Then*

$$|E(G)| \ge \frac{\Delta(\delta+1)}{2} \quad if\ \Delta(\delta+1)\ is\ even,$$
$$|E(G)| \ge \frac{\Delta(\delta+1)+1}{2} \quad if\ \Delta(\delta+1)\ is\ odd,$$

with equality if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

Proposition 2 *For any integers* $1 \le \delta < \Delta$ *such that* $\Delta(\delta+1)$ *is odd, we have* $\mathcal{G}'_{\delta,\Delta} \ne \emptyset$.

Proof Consider a graph G with $\Delta + 2$ vertices $v_0, \dots, v_{\Delta+1}$. Assume $d_{v_0} = \Delta$ with v_i adjacent to v_0 for every $1 \le i \le \Delta$.

Let us define for every $1 \le i, j \le \Delta$, $||i - j|| = \min\{|i - j|, \Delta - |i - j|\}$ (this is, the distance between the vertices v_i and v_j in the cycle $v_1, v_2, \dots, v_\Delta, v_1$). Consider an edge $v_i v_j$ for every pair of vertices with $||i - j|| \le \frac{\delta-2}{2}$. This is possible since $\delta - 2$ is even and $\delta - 2 < \Delta - 1$.

Consider also an edge $v_i v_j$ for every pair of vertices with $j - i = \frac{\Delta-1}{2}$ and $1 \le i \le \frac{\Delta-\delta-1}{2}$. This is well defined since $\frac{\Delta-\delta-1}{2} < \frac{\Delta-1}{2}$ and a new edge since $\frac{\delta-2}{2} < \frac{\Delta-1}{2}$. Therefore, we have $d_{v_i} = \delta$ for every $1 \le i \le \frac{\Delta-\delta-1}{2}$ and $\frac{\Delta+1}{2} \le i \le \Delta - \frac{\delta}{2} - 1$ and $d_{v_j} = \delta - 1$ for every $\frac{\Delta-\delta+1}{2} \le j \le \frac{\Delta-1}{2}$ and $\Delta - \frac{\delta}{2} \le j \le \Delta$, this is, we have $\Delta - \delta - 1$ vertices with degree δ and $\delta + 1$ vertices with degree $\delta - 1$ in $\{v_1, \dots, v_\Delta\}$. Finally, let us define an edge joining $v_{\Delta+1}$ to every vertex with degree $\delta - 1$. It is immediate to check that $G \in \mathcal{G}'_{\delta,\Delta}$. □

Notice that if $G \in \mathcal{G}_{\delta,\Delta}$ with $\Delta(\delta+1)$ even, then

$$\mathcal{I}(G) = \Delta h(\Delta,\delta) + \frac{\Delta(\delta-1)}{2} h(\delta,\delta),$$

and if $G \in \mathcal{G}_{\delta,\Delta}$ with $\Delta(\delta+1)$ odd, then

$$\mathcal{I}(G) = (\Delta-1)h(\Delta,\delta) + h(\Delta,\delta+1) + \delta h(\delta+1,\delta) + \frac{(\Delta-2)(\delta-1)-1}{2} h(\delta,\delta).$$

Also, if $G \in \mathcal{G}'_{\delta,\Delta}$, then

$$\mathcal{I}(G) = \Delta h(\Delta, \delta) + (\delta + 1)h(\delta + 1, \delta) + \frac{\Delta(\delta - 1) - (\delta + 1)}{2} h(\delta, \delta).$$

Theorem 1 *For any integers $1 \leq \delta \leq \Delta$ such that $\Delta(\delta + 1)$ is even, if h is non-decreasing in the first variable, then G is minimal for $\mathcal{I}$ if and only if $G \in \mathcal{G}_{\delta,\Delta}$. Hence,*

$$\mathcal{I}(G) \geq \Delta h(\Delta, \delta) + \frac{\Delta(\delta - 1)}{2} h(\delta, \delta)$$

for every graph G with minimum degree δ and maximum degree Δ.

Proof Suppose Γ is a graph with minimum degree δ and maximum degree Δ and $G \in \mathcal{G}_{\delta,\Delta}$. Then, by Proposition 1, $|E(\Gamma)| \geq |E(G)|$. The graph Γ has a vertex v_0 with degree Δ and Δ vertices, $v_1, \ldots, v_\Delta$, adjacent to it with degree at least δ. Thus, v_0 has Δ edges with one endpoint with degree Δ and $v_1, \ldots, v_\Delta$, are endpoints of at least $\delta - 1$ new edges where the endpoints have degree at least δ. Therefore, by Handshaking Lemma, and since h is non-decreasing in the first variable,

$$\mathcal{I}(\Gamma) \geq \Delta h(\Delta, \delta) + \frac{\Delta(\delta - 1)}{2} h(\delta, \delta) = \mathcal{I}(G),$$

for every $G \in \mathcal{G}_{\delta,\Delta}$. Hence, every $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for $\mathcal{I}$.

Assume that $\Gamma \notin \mathcal{G}_{\delta,\Delta}$. The graph Γ has a vertex v_0 with degree Δ and Δ vertices, $v_1, \ldots, v_\Delta$, adjacent to it with degree at least δ and, since $\Gamma \notin \mathcal{G}_{\delta,\Delta}$, we have that one of them has degree greater than δ or there is some other vertex $v_{\Delta+1}$. If one of them has degree greater than δ, then there are $\Delta - 1$ edges joining a vertex with degree Δ to a vertex with degree at least δ, one edge joining a vertex with degree Δ to a vertex with degree at least $\delta + 1$, at least δ edges joining a vertex with degree $\delta + 1$ to a vertex with degree at least δ and, finally, at least $\frac{(\Delta-1)(\delta-1)-\delta}{2}$ edges joining two vertices with degree at least δ. Thus,

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq (\Delta - 1)h(\Delta, \delta) + h(\Delta, \delta + 1) + \delta h(\delta, \delta+1) + \frac{(\Delta - 1)(\delta - 1) - \delta}{2} h(\delta, \delta) \\ &\geq \Delta h(\Delta, \delta) + \frac{(\Delta - 1)(\delta - 1) + \delta}{2} h(\delta, \delta) > \Delta h(\Delta, \delta) \\ &\quad + \frac{\Delta(\delta - 1)}{2} h(\delta, \delta) = \mathcal{I}(G),\end{aligned}$$

for every $G \in \mathcal{G}_{\delta,\Delta}$.

If there is a vertex $v_{\Delta+1}$, there are at least $\frac{\Delta(\delta-1)+\delta}{2}$ edges where the endpoints have at least degree δ and, since h is positive, $\mathcal{I}(\Gamma) \geq \Delta h(\Delta, \delta) + \frac{\Delta(\delta-1)+\delta}{2} h(\delta, \delta) > \Delta h(\Delta, \delta) + \frac{\Delta(\delta-1)}{2} h(\delta, \delta) = \mathcal{I}(G)$, for every $G \in \mathcal{G}_{\delta,\Delta}$. □

Theorem 2 *Consider any integers $1 \le \delta \le \Delta$ such that $\Delta(\delta+1)$ is odd, and assume that h is non-decreasing in the first variable. The following inequalities hold:*

(1) *If*

$$h(\Delta, \delta) + h(\delta+1, \delta) + \frac{\delta-2}{2} h(\delta, \delta) \ge h(\Delta, \delta+1), \tag{1}$$

then $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for $\mathcal{I}$, and thus

$$\mathcal{I}(G) \ge (\Delta-1)h(\Delta, \delta) + h(\Delta, \delta+1) + \delta h(\delta+1, \delta) + \frac{(\Delta-2)(\delta-1)-1}{2} h(\delta, \delta)$$

for every graph G with minimum degree δ and maximum degree Δ. Moreover, if the inequality (1) is strict, then G is minimal for $\mathcal{I}$ if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

(2) *If*

$$h(\Delta, \delta) + h(\delta+1, \delta) + \frac{\delta-2}{2} h(\delta, \delta) \le h(\Delta, \delta+1), \tag{2}$$

then $G \in \mathcal{G}'_{\delta,\Delta}$ is minimal for $\mathcal{I}$, and thus

$$\mathcal{I}(G) \ge \Delta h(\Delta, \delta) + (\delta+1)h(\delta+1, \delta) + \frac{\Delta(\delta-1)-(\delta+1)}{2} h(\delta, \delta)$$

for every graph G with minimum degree δ and maximum degree Δ. Moreover, if the inequality (2) is strict, then G is minimal for $\mathcal{I}$ if and only if $G \in \mathcal{G}'_{\delta,\Delta}$.

Proof Suppose Γ has minimum degree δ and maximum degree Δ. Then, by Proposition 1, $|E(\Gamma)| \ge |E(G)|$ for every $G \in \mathcal{G}_{\delta,\Delta}$. The graph Γ has a vertex v_0 with degree Δ and Δ vertices, $v_1, \ldots, v_\Delta$, adjacent to it with degree at least δ. Thus, v_0 has Δ edges with one endpoint with degree Δ, $v_1, \ldots, v_\Delta$, and are endpoints of at least $\delta - 1$ new edges where the endpoints have degree at least δ. Note that there is a vertex different from v_0 with degree at least $\delta+1$; otherwise, if Γ has n vertices and m edges, then Handshaking Lemma gives $2m = \sum_{u \in V(G)} d_u = \Delta + (n-1)\delta$, which is a contradiction since Δ is odd and δ is even. Hence, one of the vertices in $\{v_1, \ldots, v_\Delta\}$ has degree at least $\delta+1$ or there is some other vertex $v_{\Delta+1}$ with (odd) degree at least $\delta+1$. If there is a vertex in $\{v_1, \ldots, v_\Delta\}$ with degree at least $\delta+1$, then it is immediate to check that

$$\begin{aligned} \mathcal{I}(\Gamma) \ge\ & (\Delta-1)h(\Delta, \delta) + h(\Delta, \delta+1) + \delta h(\delta+1, \delta) \\ & + \frac{(\Delta-2)(\delta-1)-1}{2} h(\delta, \delta) = \mathcal{I}(G), \end{aligned}$$

for every $G \in \mathcal{G}_{\delta,\Delta}$. If every vertex in $\{v_1, \ldots, v_\Delta\}$ has degree δ, then there is a vertex $v_{\Delta+1}$ with (odd) degree at least $\delta+1$. Thus, $|E(\Gamma)| \ge \Delta + \frac{\Delta(\delta-1)+(\delta+1)}{2}$. Moreover,

$$\mathcal{I}(\Gamma) \ge \Delta h(\Delta, \delta) + (\delta+1)h(\delta+1, \delta) + \frac{\Delta(\delta-1)-(\delta+1)}{2} h(\delta, \delta).$$

If inequality (1) holds, then

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)\\ &\quad+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta)=\mathcal{I}(G),\end{aligned}$$

for every $G \in \mathcal{G}_{\delta,\Delta}$. Hence, every $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for $\mathcal{I}$.

We have proved that if one of the vertices in $\{v_1,\dots,v_\Delta\}$ has degree at least $\delta+1$, then

$$\mathcal{I}(\Gamma)\geq(\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta).$$

Therefore, if inequality (2) holds, then

$$\mathcal{I}(\Gamma)\geq\Delta h(\Delta,\delta)+(\delta+1)h(\delta+1,\delta)+\frac{\Delta(\delta-1)-(\delta+1)}{2}h(\delta,\delta)=\mathcal{I}(G),$$

for every $G \in \mathcal{G}'_{\delta,\Delta}$. If every vertex in $\{v_1,\dots,v_\Delta\}$ has degree δ, then there is a vertex $v_{\Delta+1}$ with degree at least $\delta+1$. Hence,

$$\mathcal{I}(\Gamma)\geq\Delta h(\Delta,\delta)+(\delta+1)h(\delta+1,\delta)+\frac{\Delta(\delta-1)-(\delta+1)}{2}h(\delta,\delta)=\mathcal{I}(G),$$

for every $G \in \mathcal{G}'_{\delta,\Delta}$. Hence, every $G \in \mathcal{G}'_{\delta,\Delta}$ is minimal for $\mathcal{I}$.

Assume now that the inequality in (1) is strict and $\Gamma \notin \mathcal{G}_{\delta,\Delta}$. The graph Γ has a vertex v_0 with degree Δ and Δ vertices, $v_1,\dots,v_\Delta$, adjacent to it with degree at least δ and, since $\Gamma \notin \mathcal{G}_{\delta,\Delta}$, we are in one of the following cases:

Case 1: One of them has degree greater than $\delta+1$.
Case 2: Two of them have degree greater than δ.
Case 3: There is some vertex $v_{\Delta+1}$ with degree δ and one of the vertices in $\{v_1,\dots,v_\Delta\}$ has degree at least $\delta+1$.
Case 4: There is some vertex $v_{\Delta+1}$ with degree greater than δ.

In Case 1, one can check that

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+2)+(\delta+1)h(\delta+2,\delta)\\ &\quad+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta)\\ &> (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)\\ &\quad+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta).\end{aligned}$$

In Case 2, also one can check that

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq (\Delta-2)h(\Delta,\delta)+2h(\Delta,\delta+1)+2\delta h(\delta+1,\delta)\\ &\quad+\frac{(\Delta-2)(\delta-1)-2\delta}{2}h(\delta,\delta)\\ &> (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)\\ &\quad+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta).\end{aligned}$$

In Case 3, there are at least $\Delta+\frac{(\Delta-1)(\delta-1)}{2}+\delta$ edges, where $\Delta-1$ join a vertex with degree Δ to a vertex with degree at least δ, one joins a vertex with degree Δ to a vertex with degree at least $\delta+1$, δ join a vertex with degree at least $\delta+1$ to a vertex with degree at least δ, and $\frac{(\Delta-1)(\delta-1)}{2}$ join two vertices with degree at least δ. Therefore,

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)+\frac{(\Delta-1)(\delta-1)}{2}h(\delta,\delta)\\ &> (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta).\end{aligned}$$

In Case 4, there are at least $\Delta+\frac{\Delta(\delta-1)+\delta+1}{2}$ edges, where Δ join a vertex with degree Δ to a vertex with degree at least δ, $\delta+1$ join a vertex with degree at least $\delta+1$ to a vertex with degree at least δ, and $\frac{\Delta(\delta-1)-(\delta+1)}{2}$ join two vertices with degree at least δ. Therefore,

$$\mathcal{I}(\Gamma) \geq \Delta h(\Delta,\delta)+(\delta+1)h(\delta+1,\delta)+\frac{\Delta(\delta-1)-(\delta+1)}{2}h(\delta,\delta)$$

and, since inequality (1) is strict, we have

$$\mathcal{I}(\Gamma) > (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta).$$

Assume now that the inequality in (2) is strict and $\Gamma\notin\mathcal{G}'_{\delta,\Delta}$. The graph Γ has a vertex v_0 with degree Δ and Δ vertices, $v_1,\dots,v_\Delta$, adjacent to it with degree at least δ and, since $\Gamma\notin\mathcal{G}'_{\delta,\Delta}$, we are in one of the following cases:

Case 1: One of the vertices in $\{v_1,\dots,v_\Delta\}$ has degree at least $\delta+1$.
Case 2: Every vertex in $\{v_1,\dots,v_\Delta\}$ has degree δ and there is some vertex $v_{\Delta+1}$ with degree at least $\delta+2$.
Case 3: Every vertex in $\{v_1,\dots,v_\Delta\}$ has degree δ, there is some vertex $v_{\Delta+1}$ with degree $\delta+1$, and there is some vertex $v_{\Delta+2}$ with degree at least δ.

In Case 1, we have seen that

$$\mathcal{I}(\Gamma) \geq (\Delta-1)h(\Delta,\delta)+h(\Delta,\delta+1)+\delta h(\delta+1,\delta)+\frac{(\Delta-2)(\delta-1)-1}{2}h(\delta,\delta).$$

Since the inequality in (2) is strict, we have

$$\mathcal{I}(\Gamma) > \Delta h(\Delta,\delta) + (\delta+1)h(\delta+1,\delta) + \frac{\Delta(\delta-1)-(\delta+1)}{2}h(\delta,\delta) = \mathcal{I}(G),$$

for every $G \in \mathcal{G}'_{\delta,\Delta}$.

In Case 2, one can check that

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq \Delta h(\Delta,\delta) + (\delta+2)h(\delta+2,\delta) + \frac{\Delta(\delta-1)-(\delta+2)}{2}h(\delta,\delta)\\ &> \Delta h(\Delta,\delta) + (\delta+1)h(\delta+1,\delta) + \frac{\Delta(\delta-1)-(\delta+1)}{2}h(\delta,\delta).\end{aligned}$$

In Case 3, we have

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq \Delta h(\Delta,\delta) + (\delta+1)h(\delta+1,\delta) + \frac{\Delta(\delta-1)-(\delta+1)+\delta}{2}h(\delta,\delta)\\ &> \Delta h(\Delta,\delta) + (\delta+1)h(\delta+1,\delta) + \frac{\Delta(\delta-1)-(\delta+1)}{2}h(\delta,\delta).\end{aligned}$$

□

Remark 2 Let $\mathcal{I}'(G) := \prod_{uv\in E(G)} h'(d_u, d_v)$, where h' is any positive symmetric function $h' : \mathbb{Z}^+ \times \mathbb{Z}^+ \to (1,\infty)$. Since $\log \mathcal{I}'(G) = \sum_{uv\in E(G)} \log h'(d_u, d_v)$ and the logarithm is an strictly increasing function, Theorems 1 and 2 can be applied to $\mathcal{I}'$.

3 Other bounds

We have obtained sharp inequalities involving a broad family of topological indices, when h is non-decreasing in the first variable. In this section we obtain some lower bounds if h is non-increasing in the first variable.

Theorem 3 *For any integers $1 \leq \delta \leq \Delta$, if h is non-increasing in the first variable, then*

$$\begin{aligned}\mathcal{I}(G) &\geq \delta h(\Delta,\delta) + \frac{\Delta(\delta+1)-2\delta}{2}h(\Delta,\Delta) \quad \text{if } \Delta(\delta+1) \text{ is even},\\ \mathcal{I}(G) &\geq \delta h(\Delta,\delta) + \frac{\Delta(\delta+1)+1-2\delta}{2}h(\Delta,\Delta) \quad \text{if } \Delta(\delta+1) \text{ is odd},\end{aligned}$$

for every graph G with minimum degree δ and maximum degree Δ.

Proof Let G be a graph with minimum degree δ and maximum degree Δ. Thus, G has a vertex with degree δ and δ edges joining it and vertices with degree at most Δ. By Proposition 1,

$$|E(G)| \geq \frac{\Delta(\delta+1)}{2} \quad \text{if } \Delta(\delta+1) \text{ is even}, \quad |E(G)| \geq \frac{\Delta(\delta+1)+1}{2} \quad \text{if } \Delta(\delta+1) \text{ is odd}.$$

Therefore, there are at least $|E(G)| - \delta$ additional edges, joining vertices with degree at most Δ. Hence, since h is a non-increasing function in the first variable, we obtain the desired inequalities.

Theorem 4 *Consider any integers $1 \leq \delta \leq \Delta$, and assume that h is non-increasing in the first variable.*

(1) *If $\Delta(\delta+1)$ is even and*

$$h(\Delta,\Delta) \geq (\Delta-\delta)\,[h(\Delta,\delta)-h(\Delta,\Delta)] + \frac{\Delta(\delta-1)}{2}\,[h(\delta,\delta)-h(\Delta,\Delta)], \qquad (3)$$

then $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for $\mathcal{I}$ and thus,

$$\mathcal{I}(\Gamma) \geq \Delta\, h(\Delta,\delta) + \frac{\Delta(\delta-1)}{2}\, h(\delta,\delta)$$

for every graph Γ with minimum degree δ and maximum degree Δ. Moreover, if the inequality (3) is strict, then G is minimal for $\mathcal{I}$ if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

(2) *If $\Delta(\delta+1)$ is odd and*

$$\begin{aligned} h(\Delta,\Delta) \geq{} & (\Delta-\delta-1)\,[h(\Delta,\delta)-h(\Delta,\Delta)] + [h(\Delta,\delta+1)-h(\Delta,\Delta)] \\ & + \delta\,[h(\delta+1,\delta)-h(\Delta,\Delta)] + \frac{(\Delta-2)(\delta-1)-1}{2}\,[h(\delta,\delta)-h(\Delta,\Delta), \end{aligned} \qquad (4)$$

then $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for $\mathcal{I}$ and thus,

$$\mathcal{I}(\Gamma) \geq (\Delta-1)\, h(\Delta,\delta) + h(\Delta,\delta+1) + \delta\, h(\delta+1,\delta) + \frac{(\Delta-2)(\delta-1)-1}{2}\, h(\delta,\delta)$$

for every graph Γ with minimum degree δ and maximum degree Δ. Moreover, if the inequality (4) is strict, then G is minimal for $\mathcal{I}$ if and only if $G \in \mathcal{G}_{\delta,\Delta}$. □

Proof Suppose $\Delta(\delta+1)$ is even. By Proposition 1, if Γ is a graph with minimum degree δ and maximum degree Δ, then

$$|E(\Gamma)| \geq \frac{\Delta(\delta+1)}{2}$$

and the equality is attained if and only if $\Gamma \in \mathcal{G}_{\delta,\Delta}$. Suppose Γ has minimum degree δ and maximum degree Δ and $\Gamma \notin \mathcal{G}_{\delta,\Delta}$. Then,

$$|E(\Gamma)| \geq \frac{\Delta(\delta+1)}{2} + 1$$

and, since Γ has a vertex with degree δ and maximum degree Δ, then

$$\mathcal{I}(\Gamma) \geq \delta h(\Delta, \delta) + \frac{\Delta(\delta+1) - 2\delta + 2}{2} h(\Delta, \Delta).$$

If inequality (3) holds, then

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq \delta\, h(\Delta, \delta) + \frac{\Delta(\delta+1) - 2\delta + 2}{2} h(\Delta, \Delta) \\ &\geq \Delta\, h(\Delta, \delta) + \frac{\Delta(\delta-1)}{2} h(\delta, \delta) = \mathcal{I}(G),\end{aligned}$$

for any $G \in \mathcal{G}_{\delta,\Delta}$. Moreover, if inequality (3) is strict, then

$$\mathcal{I}(\Gamma) > \mathcal{I}(G).$$

Suppose $\Delta(\delta+1)$ is odd. By Proposition 1, if Γ is a graph with minimum degree δ and maximum degree Δ, then

$$|E(\Gamma)| \geq \frac{\Delta(\delta+1)+1}{2}$$

and the equality is attained if and only if $\Gamma \in \mathcal{G}_{\delta,\Delta}$. Suppose Γ has minimum degree δ and maximum degree Δ and $\Gamma \notin \mathcal{G}_{\delta,\Delta}$. Then,

$$|E(\Gamma)| \geq \frac{\Delta(\delta+1)+1}{2} + 1$$

and, since Γ has a vertex with degree δ and maximum degree Δ, then

$$\mathcal{I}(\Gamma) \geq \delta h(\Delta, \delta) + \frac{\Delta(\delta+1) - 2\delta + 3}{2} h(\Delta, \Delta).$$

If inequality (4) holds, then

$$\begin{aligned}\mathcal{I}(\Gamma) &\geq \delta h(\Delta, \delta) + \frac{\Delta(\delta+1) - 2\delta + 3}{2} h(\Delta, \Delta) \\ &\geq (\Delta-1)\, h(\Delta, \delta) + h(\Delta, \delta+1) + \delta\, h(\delta+1, \delta) \\ &\quad + \frac{(\Delta-2)(\delta-1)-1}{2} h(\delta, \delta) = \mathcal{I}(G),\end{aligned}$$

for any $G \in \mathcal{G}_{\delta,\Delta}$. Moreover, if inequality (4) is strict then

$$\mathcal{I}(\Gamma) > \mathcal{I}(G).$$

□

Corollary 1 *For any integers $1 \leq \delta \leq \Delta$, if h is non-increasing in the first variable and $h(\Delta, \Delta) = h(\delta, \delta)$, then a graph G with minimum degree δ and maximum degree Δ is minimal for $\mathcal{I}$ if and only if $G \in \mathcal{G}_{\delta,\Delta}$.*

4 Inequalities for some particular indices

In this last section, we want to apply the previous results to some particular indices.

First of all, Theorems 1 and 2 have the following consequence for the second variable Zagreb index.

Theorem 5 *Let us consider $\alpha \in \mathbb{R}$ with $\alpha > 0$, any integers $1 \leq \delta \leq \Delta$, and a graph G with minimum degree δ and maximum degree Δ. The following sharp inequalities hold:*

If $\Delta(\delta + 1)$ is even, then

$$M_2^\alpha(G) \geq \Delta^{\alpha+1}\delta^\alpha + \frac{\Delta(\delta - 1)}{2}\,\delta^{2\alpha}.$$

If $\Delta(\delta + 1)$ is odd and

$$\delta^{2\alpha+1} \geq 2\big(\Delta^\alpha - \delta^\alpha\big)\big((\delta + 1)^\alpha - \delta^\alpha\big), \tag{5}$$

then

$$M_2^\alpha(G) \geq (\Delta - 1)\Delta^\alpha\delta^\alpha + \Delta^\alpha(\delta + 1)^\alpha + \delta^{\alpha+1}(\delta + 1)^\alpha + \frac{(\Delta - 2)(\delta - 1) - 1}{2}\,\delta^{2\alpha}.$$

If $\Delta(\delta + 1)$ is odd and (5) does not hold, then

$$M_2^\alpha(G) \geq \Delta^{\alpha+1}\delta^\alpha + \delta^\alpha(\delta + 1)^{\alpha+1} + \frac{\Delta(\delta - 1) - (\delta + 1)}{2}\,\delta^{2\alpha}.$$

Note that (5) is equivalent to $2\Delta \leq 2\delta + \delta^3$ for the second Zagreb index ($\alpha = 1$).

From Theorem 3 we obtain the following inequalities, that are not sharp, as the ones in Theorem 5, but are simpler.

Theorem 6 *Let us consider $\alpha \in \mathbb{R}$ with $\alpha < 0$, any integers $1 \leq \delta \leq \Delta$, and a graph G with minimum degree δ and maximum degree Δ.*

If $\Delta(\delta + 1)$ is even, then

$$M_2^\alpha(G) \geq \Delta^\alpha\delta^{\alpha+1} + \frac{\Delta(\delta + 1) - 2\delta}{2}\,\Delta^{2\alpha}.$$

If $\Delta(\delta + 1)$ is odd, then

$$M_2^\alpha(G) \geq \Delta^\alpha\delta^{\alpha+1} + \frac{\Delta(\delta + 1) + 1 - 2\delta}{2}\,\Delta^{2\alpha}.$$

□

Also, Theorem 4 yields the following.

Theorem 7 *Let us consider* $\alpha \in \mathbb{R}$ *with* $\alpha < 0$*, any integers* $1 \le \delta \le \Delta$*, and a graph* G *with minimum degree* δ *and maximum degree* Δ*. The following inequalities hold:*

If $\Delta(\delta+1)$ *is even and*

$$\Delta^{2\alpha} \ge \Big[(\Delta-\delta)\Delta^{\alpha} + \frac{\Delta(\delta-1)}{2}\,(\delta^{\alpha}+\Delta^{\alpha})\Big](\delta^{\alpha}-\Delta^{\alpha}),$$

then $G \in \mathcal{G}_{\delta,\Delta}$ *is minimal for* $\mathcal{I}$ *and thus,*

$$M_2^{\alpha}(G) \ge \Delta^{\alpha+1}\delta^{\alpha} + \frac{\Delta(\delta-1)}{2}\,\delta^{2\alpha}.$$

Moreover, if the inequality is strict, then G is minimal for $\mathcal{I}$ *if and only if* $G \in \mathcal{G}_{\delta,\Delta}$*.*

If $\Delta(\delta+1)$ *is odd and*

$$\Delta^{2\alpha} \ge (\Delta-\delta-1)\Delta^{\alpha}(\delta^{\alpha}-\Delta^{\alpha}) + \Delta^{\alpha}[(\delta+1)^{\alpha}-\Delta^{\alpha}] + \delta^{\alpha+1}(\delta+1)^{\alpha} - \delta\Delta^{2\alpha} + \frac{(\Delta-2)(\delta-1)-1}{2}\,(\delta^{2\alpha}-\Delta^{2\alpha}),$$

then $G \in \mathcal{G}_{\delta,\Delta}$ *is minimal for* $\mathcal{I}$ *and thus,*

$$M_2^{\alpha}(G) \ge (\Delta-1)\Delta^{\alpha}\delta^{\alpha} + \Delta^{\alpha}(\delta+1)^{\alpha} + \delta^{\alpha+1}(\delta+1)^{\alpha} + \frac{(\Delta-2)(\delta-1)-1}{2}\,\delta^{2\alpha}.$$

Moreover, if the inequality is strict, then G is minimal for $\mathcal{I}$ *if and only if* $G \in \mathcal{G}_{\delta,\Delta}$*.* □

Theorems 1 and 2 can be applied to the *general sum-connectivity index*, defined by Zhou and Trinajstić (2010) as

$$\chi_{\alpha}(G) = \sum_{uv\in E(G)} (d_u + d_v)^{\alpha}.$$

Note that χ_1 is the first Zagreb index M_1, $2\chi_{-1}$ is the harmonic index H, $\chi_{-1/2}$ is the sum-connectivity index χ, etc.

Theorem 8 *Let us consider* $\alpha \in \mathbb{R}$ *with* $\alpha > 0$*, any integers* $1 \le \delta \le \Delta$*, and a graph* G *with minimum degree* δ *and maximum degree* Δ*. The following sharp inequalities hold:*

If $\Delta(\delta+1)$ *is even, then*

$$\chi_{\alpha}(G) \ge \Delta(\Delta+\delta)^{\alpha} + \Delta(\delta-1)\,2^{\alpha-1}\delta^{\alpha}.$$

If $\Delta(\delta+1)$ *is odd and*

$$(\Delta+\delta)^{\alpha} + (2\delta+1)^{\alpha} + (\delta-2)\,2^{\alpha-1}\delta^{\alpha} \ge (\Delta+\delta+1)^{\alpha}, \tag{6}$$

then

$$\chi_\alpha(G) \geq (\Delta - 1)(\Delta + \delta)^\alpha + (\Delta + \delta + 1)^\alpha + \delta(2\delta + 1)^\alpha \\ + \big((\Delta - 2)(\delta - 1) - 1\big)\, 2^{\alpha-1}\delta^\alpha.$$

If $\Delta(\delta + 1)$ *is odd and* (6) *does not hold, then*

$$\chi_\alpha(G) \geq \Delta(\Delta + \delta)^\alpha + (\delta + 1)(2\delta + 1)^\alpha + \big(\Delta(\delta - 1) - (\delta + 1)\big)\, 2^{\alpha-1}\delta^\alpha.$$

Notice that in the case of the first Zagreb index ($M_1 = \chi_1$) (6) is trivially satisfied and therefore:

Corollary 2 *Given any integers* $1 \leq \delta \leq \Delta$*, and a graph* G *with minimum degree* δ *and maximum degree* Δ*, the following sharp inequalities hold:*

If $\Delta(\delta + 1)$ *is even, then*

$$M_1(G) \geq \Delta(\Delta + \delta^2).$$

If $\Delta(\delta + 1)$ *is odd then*

$$M_1(G) \geq \Delta(\Delta + \delta^2) + 2\delta + 1.$$

From Theorem 3 we obtain the following inequalities.

Theorem 9 *Let us consider* $\alpha \in \mathbb{R}$ *with* $\alpha < 0$*, any integers* $1 \leq \delta < \Delta$*, and a graph* G *with minimum degree* δ *and maximum degree* Δ*.*

If $\Delta(\delta + 1)$ *is even, then*

$$\chi_\alpha(G) \geq \delta(\Delta + \delta)^\alpha + \big(\Delta(\delta + 1) - 2\delta\big)\, 2^{\alpha-1}\Delta^\alpha.$$

If $\Delta(\delta + 1)$ *is odd, then*

$$\chi_\alpha(G) \geq \delta(\Delta + \delta)^\alpha + \big(\Delta(\delta + 1) + 1 - 2\delta\big)\, 2^{\alpha-1}\Delta^\alpha.$$

Theorem 4 yields the following.

Theorem 10 *Let us consider* $\alpha \in \mathbb{R}$ *with* $\alpha < 0$*, any integers* $1 \leq \delta \leq \Delta$*, and a graph* G *with minimum degree* δ *and maximum degree* Δ*. The following inequalities hold:*

If $\Delta(\delta + 1)$ *is even and*

$$(2\Delta)^\alpha \geq (\Delta - \delta)[(\Delta + \delta)^\alpha - (2\Delta)^\alpha] + 2^{\alpha-1}\Delta(\delta - 1)(\delta^\alpha - \Delta^\alpha), \tag{7}$$

then $G \in \mathcal{G}_{\delta,\Delta}$ *is minimal for* $\mathcal{I}$ *and thus,*

$$\chi_\alpha(G) \geq \Delta(\Delta + \delta)^\alpha + 2^{\alpha-1}\Delta(\delta - 1)\delta^\alpha.$$

Moreover, if the inequality (7) *is strict, then* G *is minimal for* $\mathcal{I}$ *if and only if* $G \in \mathcal{G}_{\delta,\Delta}$.

If $\Delta(\delta+1)$ *is odd and*

$$(2\Delta)^\alpha \geq (\Delta-\delta-1)[(\Delta+\delta)^\alpha-(2\Delta)^\alpha]+(\Delta+\delta+1)^\alpha-(2\Delta)^\alpha \\ +\delta[(2\delta+1)^\alpha-(2\Delta)^\alpha]+2^{\alpha-1}[(\Delta-2)(\delta-1)-1](\delta^\alpha-\Delta^\alpha), \tag{8}$$

then $G \in \mathcal{G}_{\delta,\Delta}$ *is minimal for* $\mathcal{I}$ *and thus,*

$$\chi_\alpha(G) \geq (\Delta-1)(\Delta+\delta)^\alpha+(\Delta+\delta+1)^\alpha+\delta(2\delta+1)^\alpha \\ +2^{\alpha-1}[(\Delta-2)(\delta-1)-1]\delta^\alpha.$$

Moreover, if the inequality (8) *is strict, then* G *is minimal for* $\mathcal{I}$ *if and only if* $G \in \mathcal{G}_{\delta,\Delta}$.

Also, these results can be applied to many other indices, such as the *redefined third Zagreb index*, ReZ_3, defined in Ranjini et al. (2013) as

$$ReZ_3(G) = \sum_{uv\in E(G)} d_u d_v(d_u+d_v),$$

the *inverse indeg index*, ISI, defined in Vukičević (2010) as

$$ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u+d_v},$$

the reformulated Zagreb Index defined in Miličević et al. (2004) (see Milovanović et al. 2016 for other upper and lower bounds on this index) as

$$\sum_{uv\in E(G)} (d_u+d_v-2)^2,$$

and the general index

$$\sum_{uv\in E(G)} \left(\frac{d_u+d_v-2}{d_u d_v}\right)^\alpha,$$

(if the minimum degree δ satisfies $\delta \geq 2$) which generalizes the atom-bond connectivity (ABC) and the augmented Zagreb indices (Gutman and Tošović 2013).

Besides, by Remark 2, our results can be applied to the following multiplicative indices (if $\delta \geq 2$): the *modified first multiplicative Zagreb index* (Π_1^*) and the *second multiplicative Zagreb index* (Π_2) (Gutman and Tošović 2013) or *modified Narumi–Katayama index* (NK^*) (Ghorbani et al. 2012), defined respectively as

$$\Pi_1^*(G) = \prod_{uv\in E(G)} (d_u+d_v), \quad \Pi_2(G) = NK^*(G) = \prod_{uv\in E(G)} d_u d_v,$$

Note that Π_1^* verifies the hypothesis in Remark 2; in order to verify this hypothesis for $\Pi_2 = NK^*$, we need to consider graphs G without isolated edges, i.e., with $d_u + d_v > 2$ for every $uv \in E(G)$; this holds, in particular, if $\delta \geq 2$.

As a variant of the ABC index, the *first multiplicative atom-bond connectivity index* is defined in Kulli (2016) by

$$ABC\Pi(G) = \prod_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{9}$$

If $\delta \geq 2$, then we can apply our results to $(ABC\Pi)^{-1}$, obtaining an upper bound of $ABC\Pi$ (since each factor in the product (9) is positive and less than 1).

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