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Research article

Extremal problems on the general Sombor index of a graph

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Abstract: In this work we obtain new lower and upper optimal bounds of general Sombor indices. Specifically, we get inequalities for these indices relating them with other indices: the first Zagreb index, the forgotten index and the first variable Zagreb index. Finally, we solve some extremal problems for general Sombor indices.

Keywords: Sombor indices; variable indices; degree-based topological indices; inequalities
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1. Introduction

Topological indices have become an important research topic associated with the study of their mathematical and computational properties and, fundamentally, for their multiple applications to various areas of knowledge (see, e.g., [1–3]). Within the study of mathematical properties, we will contribute to the study of inequalities and optimization problems associated with topological indices. Our main goals are the Sombor indices, introduced by Gutman in [4].

In what follows, $G = (V(G), E(G))$ will be a finite undirected graph, and we will assume that each vertex has at least a neighbor. We denote by d_w the degree of the vertex w, i.e., the number of neighbors of w. We denote by uv the edge joining the vertices u and v (or v and u). For each graph G, its *Sombor index* is

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}\,.$$

In the same paper is also defined the *reduced Sombor index* by

$$SO_{red}(G) = \sum_{uv\in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}.$$

In [5] it is shown that these indices have a good predictive potential.

Also, the *modified Sombor index* of G was proposed in [6] as

$$^{m}SO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u^2 + d_v^2}}. \tag{1.1}$$

In addition, two other Sombor indices have been introduced: the *first Banhatti-Sombor index* [7]

$$BSO(G) = \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} \tag{1.2}$$

and the α-*Sombor index* [8]

$$SO_\alpha(G) = \sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{1/\alpha}, \tag{1.3}$$

here $\alpha \in \mathbb{R} \setminus \{0\}$. In fact, there is a general index that includes most Sombor indices listed above: the first $(\alpha,\beta)-KA$ *index* of G which was introduced in [9] as

$$KA_{\alpha,\beta}(G) = KA^1_{\alpha,\beta}(G) = \sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^\beta, \tag{1.4}$$

with $\alpha,\beta \in \mathbb{R}$. Note that $SO(G) = KA_{2,1/2}(G)$, $^{m}SO(G) = KA_{2,-1/2}(G)$, $BSO(G) = KA_{-2,1/2}(G)$, and $SO_\alpha(G) = KA_{\alpha,1/\alpha}(G)$. Also, we note that $KA_{1,\beta}(G)$ equals the general sum-connectivity index [10] $\chi_\beta(G) = \sum_{uv\in E(G)}(d_u + d_v)^\beta$. Reduced versions of $SO(G)$, $^{m}SO(G)$ and $KA_{\alpha,\beta}(G)$ were also introduced in [4, 6, 11], e.g., the reduced $(\alpha,\beta)-KA$ index is

$$_{red}KA_{\alpha,\beta}(G) = \sum_{uv\in E(G)} ((d_u - 1)^\alpha + (d_v - 1)^\alpha)^\beta.$$

If $\alpha < 0$, then $_{red}KA_{\alpha,\beta}(G)$ is just defined for graphs without pendant vertices (recall that a vertex is said pendant if its degree is equal to 1).

Since I. Gutman initiated the study of the mathematical properties of Sombor index in [4], many papers have continued this study, see e.g., [12–18].

Our main aim is to obtain new bounds of Sombor indices, and to characterize the graphs where equality occurs. In particular, we have obtained bounds for Sombor indices relating them with the first Zagreb index, the forgotten index and the first variable Zagreb index. Also, we solve some extremal problems for Sombor indices.

2. Inequalities for the Sombor indices

The following inequalities are known for $x, y > 0$:

$$\begin{aligned} x^a + y^a < (x+y)^a &\le 2^{a-1}(x^a + y^a) && \text{if } a > 1, \\ 2^{a-1}(x^a + y^a) \le (x+y)^a &< x^a + y^a && \text{if } 0 < a < 1, \\ (x+y)^a &\le 2^{a-1}(x^a + y^a) && \text{if } a < 0, \end{aligned}$$

and the second, third or fifth equality is attained for each a if and only if $x = y$. These inequalities allow to obtain the following result relating KA indices.

Theorem 1. *Let G be any graph and $\alpha, \beta, \lambda \in \mathbb{R} \setminus \{0\}$. Then*

$$
\begin{aligned}
KA_{\alpha\beta/\lambda,\lambda}(G) < KA_{\alpha,\beta}(G) &\le 2^{\beta-\lambda} KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta > \lambda,\ \beta\lambda > 0,\\
2^{\beta-\lambda} KA_{\alpha\beta/\lambda,\lambda}(G) \le KA_{\alpha,\beta}(G) &< KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta < \lambda,\ \beta\lambda > 0,\\
KA_{\alpha,\beta}(G) &\le 2^{\beta-\lambda} KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta < 0, \lambda > 0,\\
KA_{\alpha,\beta}(G) &\ge 2^{\beta-\lambda} KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta > 0, \lambda < 0,
\end{aligned}
$$

and the second, third, fifth or sixth equality is attained for each α, β, λ if and only if all the connected components of G are regular graphs.

Proof. If $a = \beta/\lambda$, $x = d_u^\alpha$ and $y = d_v^\alpha$, then the previous inequalities give

$$
\begin{aligned}
d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda} < (d_u^\alpha + d_v^\alpha)^{\beta/\lambda} &\le 2^{\beta/\lambda-1}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda}) && \text{if } \beta/\lambda > 1,\\
2^{\beta/\lambda-1}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda}) \le (d_u^\alpha + d_v^\alpha)^{\beta/\lambda} &< d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda} && \text{if } 0 < \beta/\lambda < 1,\\
(d_u^\alpha + d_v^\alpha)^{\beta/\lambda} &\le 2^{\beta/\lambda-1}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda}) && \text{if } \beta/\lambda < 0,
\end{aligned}
$$

and the second, third or fifth equality is attained if and only if $d_u = d_v$.

Hence, we obtain

$$
\begin{aligned}
(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda < (d_u^\alpha + d_v^\alpha)^\beta &\le 2^{\beta-\lambda}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda && \text{if } \beta/\lambda > 1,\ \lambda > 0,\\
2^{\beta-\lambda}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda \le (d_u^\alpha + d_v^\alpha)^\beta &< (d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda && \text{if } \beta/\lambda > 1,\ \lambda < 0,\\
2^{\beta-\lambda}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda \le (d_u^\alpha + d_v^\alpha)^\beta &< (d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda && \text{if } 0 < \beta/\lambda < 1,\ \lambda > 0,\\
(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda < (d_u^\alpha + d_v^\alpha)^\beta &\le 2^{\beta-\lambda}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda && \text{if } 0 < \beta/\lambda < 1,\ \lambda < 0,\\
(d_u^\alpha + d_v^\alpha)^\beta &\le 2^{\beta-\lambda}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda && \text{if } \beta < 0, \lambda > 0,\\
(d_u^\alpha + d_v^\alpha)^\beta &\ge 2^{\beta-\lambda}(d_u^{\alpha\beta/\lambda} + d_v^{\alpha\beta/\lambda})^\lambda && \text{if } \beta > 0, \lambda < 0,
\end{aligned}
$$

and the equality in the non-strict inequalities is tight if and only if $d_u = d_v$.

If we sum on $uv \in E(G)$ these inequalities, then we obtain (1). □

Remark 2. *Note that the excluded case $\beta = \lambda$ in Theorem 1 is not interesting, since $KA_{\alpha\beta/\lambda,\lambda}(G) = KA_{\alpha,\beta}(G)$ if $\beta = \lambda$.*

The argument in the proof of Theorem 1 also allows to obtain the following result relating reduced KA indices.

Theorem 3. *Let G be any graph and $\alpha, \beta, \lambda \in \mathbb{R} \setminus \{0\}$. If $\alpha < 0$ or $\alpha\beta\lambda < 0$, we also assume that G does not have pendant vertices. Then*

$$
\begin{aligned}
{}_{red}KA_{\alpha\beta/\lambda,\lambda}(G) < {}_{red}KA_{\alpha,\beta}(G) &\le 2^{\beta-\lambda}\, {}_{red}KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta > \lambda,\ \beta\lambda > 0,\\
2^{\beta-\lambda}\, {}_{red}KA_{\alpha\beta/\lambda,\lambda}(G) \le {}_{red}KA_{\alpha,\beta}(G) &< {}_{red}KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta < \lambda,\ \beta\lambda > 0,\\
{}_{red}KA_{\alpha,\beta}(G) &\le 2^{\beta-\lambda}\, {}_{red}KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta < 0, \lambda > 0,\\
{}_{red}KA_{\alpha,\beta}(G) &\ge 2^{\beta-\lambda}\, {}_{red}KA_{\alpha\beta/\lambda,\lambda}(G) && \text{if } \beta > 0, \lambda < 0,
\end{aligned}
$$

and the second, third, fifth or sixth equality is attained for each α, β, λ if and only if all the connected components of G are regular graphs.

If we take $\beta = 1/\alpha$ and $\mu = 1/\lambda$ in Theorem 1, we obtain the following inequalities for the α-Sombor index.

Corollary 4. *Let G be any graph and $\alpha, \mu \in \mathbb{R} \setminus \{0\}$. Then*

$$\begin{aligned} SO_\mu(G) < SO_\alpha(G) &\le 2^{1/\alpha-1/\mu} SO_\mu(G) && \text{if } \mu > \alpha,\ \alpha\mu > 0, \\ 2^{1/\alpha-1/\mu} SO_\mu(G) \le SO_\alpha(G) &< SO_\mu(G) && \text{if } \mu < \alpha,\ \alpha\mu > 0, \\ SO_\alpha(G) &\le 2^{1/\alpha-1/\mu} SO_\mu(G) && \text{if } \alpha < 0, \mu > 0, \end{aligned}$$

and the second, third or fifth equality is attained for each α, μ if and only if all the connected components of G are regular graphs.

Recall that one of the most studied topological indices is the *first Zagreb index*, defined by

$$M_1(G) = \sum_{u \in V(G)} d_u^2.$$

If we take $\mu = 1$ in Corollary 4, we obtain the following result.

Corollary 5. *Let G be any graph and $\alpha \in \mathbb{R} \setminus \{0\}$. Then*

$$\begin{aligned} M_1(G) < SO_\alpha(G) &\le 2^{1/\alpha-1} M_1(G) && \text{if } 0 < \alpha < 1, \\ 2^{1/\alpha-1} M_1(G) \le SO_\alpha(G) &< M_1(G) && \text{if } \alpha > 1, \\ SO_\alpha(G) &\le 2^{1/\alpha-1} M_1(G) && \text{if } \alpha < 0, \end{aligned}$$

and the second, third or fifth equality is attained for each α if and only if all the connected components of G are regular graphs.

If we take $\alpha = 2, \beta = -1/2$ and $\lambda = 1/2$ in Theorem 1, we obtain the following inequality relating the modified Sombor and the first Banhatti-Sombor indices.

Corollary 6. *Let G be any graph. Then*

$${}^{m}SO(G) \le \frac{1}{2} BSO(G)$$

and the bound is tight if and only if all the connected components of G are regular graphs

In [19–21], the *first variable Zagreb index* is defined by

$$M_1^\alpha(G) = \sum_{u \in V(G)} d_u^\alpha,$$

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

Note that M_1^α generalizes numerous degree–based topological indices which earlier have independently been studied. For $\alpha = 2$, $\alpha = 3$, $\alpha = -1/2$, and $\alpha = -1$, M_1^α is, respectively, the ordinary first Zagreb index M_1, the forgotten index F, the zeroth–order Randić index ${}^0R$, and the inverse index ID [2, 22].

The next result relates the $KA_{\alpha,\beta}$ and $M_1^{\alpha+1}$ indices.

Theorem 7. *Let G be any graph with maximum degree Δ, minimum degree δ and m edges, and $\alpha \in \mathbb{R} \setminus \{0\}$, $\beta > 0$. Then*

$$KA_{\alpha,\beta}(G) \geq \Big(\frac{M_1^{\alpha+1}(G) + 2\Delta^{\alpha/2}\delta^{\alpha/2} m}{\sqrt{2}\,(\Delta^{\alpha/2} + \delta^{\alpha/2})} \Big)^{2\beta} \qquad \text{if } 0 < \beta < 1/2,$$
$$KA_{\alpha,\beta}(G) \geq \Big(\frac{M_1^{\alpha+1}(G) + 2\Delta^{\alpha/2}\delta^{\alpha/2} m}{\sqrt{2}\,(\Delta^{\alpha/2} + \delta^{\alpha/2})} \Big)^{2\beta} m^{1-2\beta} \qquad \text{if } \beta \geq 1/2,$$

and the second equality is attained for some α,β if and only if G is a regular graph.

Proof. If $uv \in E(G)$ and $\alpha > 0$, then

$$\sqrt{2}\,\delta^{\alpha/2} \leq \sqrt{d_u^\alpha + d_v^\alpha} \leq \sqrt{2}\,\Delta^{\alpha/2}.$$

If $\alpha < 0$, then the converse inequalities hold. Hence,

$$\Big(\sqrt{d_u^\alpha + d_v^\alpha} - \sqrt{2}\,\delta^{\alpha/2} \Big)\Big(\sqrt{2}\,\Delta^{\alpha/2} - \sqrt{d_u^\alpha + d_v^\alpha} \Big) \geq 0,$$
$$\sqrt{2}\,(\Delta^{\alpha/2} + \delta^{\alpha/2}) \sqrt{d_u^\alpha + d_v^\alpha} \geq d_u^\alpha + d_v^\alpha + 2\Delta^{\alpha/2}\delta^{\alpha/2}.$$

Since

$$\sum_{uv \in E(G)} (d_u^\alpha + d_v^\alpha) = \sum_{u \in V(G)} d_u\, d_u^\alpha = \sum_{u \in V(G)} d_u^{\alpha+1} = M_1^{\alpha+1}(G),$$

If $0 < \beta < 1/2$, then $1/(2\beta) > 1$ and

$$\begin{aligned} \sum_{uv \in E(G)} \sqrt{d_u^\alpha + d_v^\alpha} &= \sum_{uv \in E(G)} \big((d_u^\alpha + d_v^\alpha)^\beta \big)^{1/(2\beta)} \\ &\leq \Big(\sum_{uv \in E(G)} (d_u^\alpha + d_v^\alpha)^\beta \Big)^{1/(2\beta)} = KA_{\alpha,\beta}(G)^{1/(2\beta)}. \end{aligned}$$

Consequently, we obtain

$$KA_{\alpha,\beta}(G)^{1/(2\beta)} \geq \frac{M_1^{\alpha+1}(G) + 2\Delta^{\alpha/2}\delta^{\alpha/2} m}{\sqrt{2}\,(\Delta^{\alpha/2} + \delta^{\alpha/2})}.$$

If $\beta \geq 1/2$, then $2\beta \geq 1$ and Hölder inequality gives

$$\begin{aligned} \sum_{uv \in E(G)} \sqrt{d_u^\alpha + d_v^\alpha} &= \sum_{uv \in E(G)} \big((d_u^\alpha + d_v^\alpha)^\beta \big)^{1/(2\beta)} \\ &\leq \Big(\sum_{uv \in E(G)} (d_u^\alpha + d_v^\alpha)^\beta \Big)^{1/(2\beta)} \Big(\sum_{uv \in E(G)} 1^{2\beta/(2\beta-1)} \Big)^{(2\beta-1)/(2\beta)} \\ &= m^{(2\beta-1)/(2\beta)} KA_{\alpha,\beta}(G)^{1/(2\beta)}. \end{aligned}$$

Consequently, we obtain

$$KA_{\alpha,\beta}(G)^{1/(2\beta)} \geq \frac{M_1^{\alpha+1}(G) + 2\Delta^{\alpha/2}\delta^{\alpha/2} m}{\sqrt{2}\,(\Delta^{\alpha/2} + \delta^{\alpha/2})}\, m^{(1-2\beta)/(2\beta)}.$$

If G is regular, then

$$\begin{aligned}\Big(\frac{M_1^{\alpha+1}(G)+2\Delta^{\alpha/2}\delta^{\alpha/2}m}{\sqrt{2}\,(\Delta^{\alpha/2}+\delta^{\alpha/2})}\Big)^{2\beta}m^{1-2\beta} &= \Big(\frac{2\Delta^{\alpha}m+2\Delta^{\alpha}m}{\sqrt{2}\,2\Delta^{\alpha/2}}\Big)^{2\beta}m^{1-2\beta}\\ &= \Big(\sqrt{2}\,\Delta^{\alpha/2}m\Big)^{2\beta}m^{1-2\beta}\\ &= (2\Delta^{\alpha})^{\beta}m = KA_{\alpha,\beta}(G).\end{aligned}$$

If the second equality is attained for some α,β, then we have $d_u^\alpha + d_v^\alpha = 2\delta^\alpha$ or $d_u^\alpha + d_v^\alpha = 2\Delta^\alpha$ for each $uv \in E(G)$. Also, the equality in Hölder inequality gives that there exists a constant c such that $d_u^\alpha + d_v^\alpha = c$ for every $uv \in E(G)$. Hence, we have either $d_u^\alpha + d_v^\alpha = 2\delta^\alpha$ for each edge uv or $d_u^\alpha + d_v^\alpha = 2\Delta^\alpha$ for each edge uv, and hence, G is regular. □

If we take $\alpha = 2$ and $\beta = 1/2$ in Theorem 7 we obtain:

Corollary 8. *Let G be any graph with maximum degree Δ and minimum degree δ, and m edges. Then*

$$SO(G) \geq \frac{F(G)+2\Delta\delta m}{\sqrt{2}\,(\Delta+\delta)},$$

and the bound is tight if and only if G is regular.

In order to prove Theorem 10 below we need an additional technical result. A converse of Hölder inequality appears in [23, Theorem 3], which, in the discrete case, can be stated as follows [23, Corollay 2].

Proposition 9. *Consider constants $0 < \alpha \leq \beta$ and $1 < p, q < \infty$ with $1/p + 1/q = 1$. If $w_k, z_k \geq 0$ satisfy $\alpha z_k^q \leq w_k^p \leq \beta z_k^q$ for $1 \leq k \leq n$, then*

$$\Big(\sum_{k=1}^{n} w_k^p\Big)^{1/p}\Big(\sum_{k=1}^{n} z_k^q\Big)^{1/q} \leq C_p(\alpha,\beta)\sum_{k=1}^{n} w_k z_k,$$

where

$$C_p(\alpha,\beta) = \begin{cases} \dfrac{1}{p}\Big(\dfrac{\alpha}{\beta}\Big)^{1/(2q)} + \dfrac{1}{q}\Big(\dfrac{\beta}{\alpha}\Big)^{1/(2p)}, & \text{when } 1 < p < 2,\\[2ex] \dfrac{1}{p}\Big(\dfrac{\beta}{\alpha}\Big)^{1/(2q)} + \dfrac{1}{q}\Big(\dfrac{\alpha}{\beta}\Big)^{1/(2p)}, & \text{when } p \geq 2.\end{cases}$$

If $(w_1, \dots, w_n) \neq 0$, then the bound is tight if and only if $w_k^p = \alpha z_k^q$ for each $1 \leq k \leq n$ and $\alpha = \beta$.

Recall that a bipartite graph with X and Y partitions is called (a, b)-biregular if all vertices of X have degree a and all vertices of Y have degree b.

The next result relates several KA indices.

Theorem 10. *Let G be any graph, $\alpha,\beta,\mu \in \mathbb{R}$ and $p > 1$. Then*

$$D_p^p\, KA_{\alpha,p(\beta-\mu)}(G) KA_{\alpha,p\mu/(p-1)}(G)^{p-1} \leq KA_{\alpha,\beta}(G)^p \leq KA_{\alpha,p(\beta-\mu)}(G)\, KA_{\alpha,p\mu/(p-1)}(G)^{p-1}$$

where

$$D_p = \begin{cases} C_p((2\delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})}, (2\Delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})})^{-1}, & \text{if } \alpha(\beta-\mu\frac{p}{p-1}) \geq 0, \\ \\ C_p((2\Delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})}, (2\delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})})^{-1}, & \text{if } \alpha(\beta-\mu\frac{p}{p-1}) < 0, \end{cases}$$

and C_p is the constant in Proposition 9. The equality in the upper(lower) bound is tight for each α, β, μ, p if G is a biregular graph (with $\alpha(\beta-\mu\frac{p}{p-1}) \neq 0$ if and only if G is a regular graph.)

Proof. Hölder inequality gives

$$\begin{aligned} KA_{\alpha,\beta}(G) &= \sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{\beta-\mu}(d_u^\alpha + d_v^\alpha)^\mu \\ &\leq \Big(\sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{p(\beta-\mu)}\Big)^{1/p}\Big(\sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{p\mu/(p-1)}\Big)^{(p-1)/p}, \\ KA_{\alpha,\beta}(G)^p &\leq KA_{\alpha,p(\beta-\mu)}(G)\, KA_{\alpha,p\mu/(p-1)}(G)^{p-1}. \end{aligned}$$

If G is a biregular graph with m edges, we obtain

$$\begin{aligned} &KA_{\alpha,p(\beta-\mu)}(G)\, KA_{\alpha,p\mu/(p-1)}(G)^{p-1} = (\Delta^\alpha + \delta^\alpha)^{p(\beta-\mu)} m((\Delta^\alpha + \delta^\alpha)^{p\mu/(p-1)} m)^{p-1} \\ &= (\Delta^\alpha + \delta^\alpha)^{p(\beta-\mu)}(\Delta^\alpha + \delta^\alpha)^{p\mu} m^p = ((\Delta^\alpha + \delta^\alpha)^\beta m)^p = KA_{\alpha,\beta}(G)^p. \end{aligned}$$

Since

$$\frac{(d_u^\alpha + d_v^\alpha)^{p(\beta-\mu)}}{(d_u^\alpha + d_v^\alpha)^{p\mu/(p-1)}} = (d_u^\alpha + d_v^\alpha)^{p(\beta-\mu\frac{p}{p-1})},$$

if $\alpha p(\beta-\mu\frac{p}{p-1}) \geq 0$, then

$$(2\delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})} \leq \frac{(d_u^\alpha + d_v^\alpha)^{p(\beta-\mu)}}{(d_u^\alpha + d_v^\alpha)^{p\mu/(p-1)}} \leq (2\Delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})},$$

and if $\alpha p(\beta-\mu\frac{p}{p-1}) < 0$, then

$$(2\Delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})} \leq \frac{(d_u^\alpha + d_v^\alpha)^{p(\beta-\mu)}}{(d_u^\alpha + d_v^\alpha)^{p\mu/(p-1)}} \leq (2\delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})}.$$

Proposition 9 gives

$$\begin{aligned} KA_{\alpha,\beta}(G) &= \sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{\beta-\mu}(d_u^\alpha + d_v^\alpha)^\mu \\ &\geq D_p\Big(\sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{p(\beta-\mu)}\Big)^{1/p}\Big(\sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha)^{p\mu/(p-1)}\Big)^{(p-1)/p}, \\ KA_{\alpha,\beta}(G)^p &\geq D_p^p\, KA_{\alpha,p(\beta-\mu)}(G)\, KA_{\alpha,p\mu/(p-1)}(G)^{p-1}. \end{aligned}$$

Proposition 9 gives that the equality is tight in this last bound for some α, β, μ, p with $\alpha(\beta-\mu\frac{p}{p-1}) \neq 0$ if and only if

$$(2\delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})} = (2\Delta^\alpha)^{p(\beta-\mu\frac{p}{p-1})} \quad\Leftrightarrow\quad \delta = \Delta,$$

i.e., G is regular. □

If we take $\beta = 0$ in Theorem 10 we obtain the following result.

Corollary 11. *Let G be any graph with m edges, $\alpha, \mu \in \mathbb{R}$ and $p > 1$. Then*

$$KA_{\alpha,-p\mu}(G)\, KA_{\alpha,p\mu/(p-1)}(G)^{p-1} \geq m^p.$$

The equality in the bound is tight for each α, μ, p if G is a biregular graph.

If we take $\alpha = 2, \beta = 0$, $p = 2$ and $\mu = 1/4$ in Theorem 10 we obtain the following result.

Corollary 12. *Let G be any graph with maximum degree Δ, minimum degree δ and m edges, then*

$$m^2 \leq {}^{m}SO(G)\, SO(G) \leq \frac{(\Delta+\delta)^2}{4\Delta\delta}\, m^2.$$

The equality in the upper bound is tight if and only if G is regular. The equality in the lower bound is tight if G is a biregular graph.

Note that the following result improves the upper bound in Corollary 5 when $\alpha > 1$.

Theorem 13. *Let G be any graph with minimum degree δ, and $\alpha \geq 1$. Then*

$$2^{1/\alpha-1} M_1(G) \leq SO_\alpha(G) \leq M_1(G) - (2 - 2^{1/\alpha})\delta,$$

and the equality holds for some $\alpha > 1$ in each bound if and only if G is regular.

Proof. The lower bound follows from Corollary 5. Let us prove the upper bound.

First of all, we are going to prove that

$$(x^\alpha + y^\alpha)^{1/\alpha} \leq x + (2^{1/\alpha} - 1)y \tag{2.1}$$

for every $\alpha \geq 1$ and $x \geq y \geq 0$. Since (2.1) is direct for $\alpha = 1$, it suffices to consider the case $\alpha > 1$.

We want to compute the minimum value of the function

$$f(x,y) = x + (2^{1/\alpha} - 1)y$$

with the restrictions $g(x,y) = x^\alpha + y^\alpha = 1$, $x \geq y \geq 0$. If (x,y) is a critical point, then there exists $\lambda \in \mathbb{R}$ such that

$$\begin{aligned} 1 &= \lambda\, \alpha\, x^{\alpha-1}, \\ 2^{1/\alpha} - 1 &= \lambda\, \alpha\, y^{\alpha-1}, \end{aligned}$$

and so, $(y/x)^{\alpha-1} = 2^{1/\alpha} - 1$ and $y = (2^{1/\alpha} - 1)^{1/(\alpha-1)} x$; this fact and the equality $x^\alpha + y^\alpha = 1$ imply

$$\begin{aligned} &(1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})\, x^\alpha = 1, \\ &x = (1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{-1/\alpha}, \\ &y = (2^{1/\alpha} - 1)^{1/(\alpha-1)}(1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{-1/\alpha}, \\ f(x,y) &= (1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{-1/\alpha} \\ &\quad + (2^{1/\alpha} - 1)(2^{1/\alpha} - 1)^{1/(\alpha-1)}(1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{-1/\alpha} \\ &= (1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{-1/\alpha} \\ &\quad + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)}(1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{-1/\alpha} \\ &= (1 + (2^{1/\alpha} - 1)^{\alpha/(\alpha-1)})^{(\alpha-1)/\alpha} > 1. \end{aligned}$$

If $y = 0$, then $x = 1$ and $f(x, y) = 1$.
If $y = x$, then $x = 2^{-1/\alpha} = y$ and

$$f(x, y) = 2^{-1/\alpha} + (2^{1/\alpha} - 1)2^{-1/\alpha} = 1.$$

Hence, $f(x, y) \geq 1$ and the bound is tight if and only if $y = 0$ or $y = x$. By homogeneity, we have $f(x, y) \geq 1$ for every $x \geq y \geq 0$ and the bound is tight if and only if $y = 0$ or $y = x$. This finishes the proof of (2.1).

Consequently,

$$(d_u^\alpha + d_v^\alpha)^{1/\alpha} \leq d_u + (2^{1/\alpha} - 1)d_v = d_u + d_v - (2 - 2^{1/\alpha})d_v$$

for each $\alpha \geq 1$ and $d_u \geq d_v$. Thus,

$$(d_u^\alpha + d_v^\alpha)^{1/\alpha} \leq d_u + d_v - (2 - 2^{1/\alpha})\delta$$

for each $\alpha \geq 1$ and $uv \in E(G)$, and the equality holds for some $\alpha > 1$ if and only if $d_u = d_v = \delta$. Therefore,

$$SO_\alpha(G) \leq M_1(G) - (2 - 2^{1/\alpha})\delta,$$

and the equality holds for some $\alpha > 1$ if and only if $d_u = d_v = \delta$ for every $uv \in E(G)$, i.e., G is regular. □

Corollary 14. *Let G be any graph with minimum degree δ. Then*

$$2^{-1/2} M_1(G) \leq SO(G) \leq M_1(G) - (2 - \sqrt{2})\delta,$$

and the equality holds in each bound if and only if G is regular.

The upper bound in Corollary 14 appears in [14, Theorem 2.7]. Hence, Theorem 13 generalizes [14, Theorem 2.7].

A family of topological indices, named *Adriatic indices*, was put forward in [24, 25]. Twenty of them were selected as significant predictors in Mathematical Chemistry. One of them, the *inverse sum indeg* index, *ISI*, was singled out in [25] as a significant predictor of total surface area of octane isomers. This index is defined as

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u\, d_v}{d_u + d_v} = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}}.$$

In the last years there has been an increasing interest in the mathematical properties of this index. We finish this section with two inequalities relating the Sombor, the first Zagreb and the inverse sum indeg indices.

Theorem 15. *Let G be any graph, then*

$$\sqrt{2}\,(M_1(G) - 2ISI(G)) \geq SO(G) > M_1(G) - 2ISI(G)$$

and the upper bound is tight if and only if all the connected components of G are regular graphs.

Proof. It is well-known that for $x, y > 0$, we have

$$x^2 + y^2 < (x+y)^2 \leq 2(x^2 + y^2),$$
$$\sqrt{x^2 + y^2} < x + y \leq \sqrt{2}\sqrt{x^2 + y^2},$$

and the equality

$$\sqrt{d_u^2 + d_v^2}\sqrt{d_u^2 + d_v^2} + 2d_u d_v = (d_u + d_v)^2$$

give

$$(d_u + d_v)\sqrt{d_u^2 + d_v^2} + 2d_u d_v > (d_u + d_v)^2,$$
$$\sqrt{d_u^2 + d_v^2} + \frac{2d_u d_v}{d_u + d_v} > d_u + d_v,$$
$$SO(G) + 2ISI(G) > M_1(G).$$

In a similar way, we obtain

$$\frac{1}{\sqrt{2}}(d_u + d_v)\sqrt{d_u^2 + d_v^2} + 2d_u d_v \leq (d_u + d_v)^2,$$
$$\sqrt{d_u^2 + d_v^2} + \sqrt{2}\,\frac{2d_u d_v}{d_u + d_v} \leq \sqrt{2}\,(d_u + d_v),$$
$$SO(G) + 2\sqrt{2}\,ISI(G) \leq \sqrt{2}\,M_1(G).$$

The equality in this last inequality is tight if and only if $2(d_u^2 + d_v^2) = (d_u + d_v)^2$ for each edge uv, i.e., $d_u = d_v$ for every $uv \in E(G)$, and this happens if and only if all the connected components of G are regular graphs. □

3. Optimization problems

We start this section with a technical result.

Proposition 16. *Let G be any graph, $u, v \in V(G)$ with $uv \notin E(G)$, and $\alpha, \beta \in \mathbb{R} \setminus \{0\}$ with $\alpha\beta > 0$. Then $KA_{\alpha,\beta}(G \cup \{uv\}) > KA_{\alpha,\beta}(G)$. If $\alpha > 0$, then ${}_{red}KA_{\alpha,\beta}(G \cup \{uv\}) > {}_{red}KA_{\alpha,\beta}(G)$. Furthermore, if $\alpha < 0$ and G does not have pendant vertices, then ${}_{red}KA_{\alpha,\beta}(G \cup \{uv\}) > {}_{red}KA_{\alpha,\beta}(G)$.*

Proof. Let $\{w_1, \ldots, w_{d_u}\}$ and $\{w^1, \ldots, w^{d_v}\}$ be the sets of neighbors of u and v in G, respectively. Since $\alpha\beta > 0$, the function

$$U(x, y) = (x^\alpha + y^\alpha)^\beta$$

is strictly increasing in each variable if $x, y > 0$. Hence,

$$\begin{aligned} KA_{\alpha,\beta}(G \cup \{uv\}) - KA_{\alpha,\beta}(G) &= ((d_u+1)^\alpha + (d_v+1)^\alpha)^\beta + \\ &+ \sum_{j=1}^{d_u}\Big(((d_u+1)^\alpha + d_{w_j}^\alpha)^\beta - (d_u^\alpha + d_{w_j}^\alpha)^\beta\Big) \\ &+ \sum_{k=1}^{d_v}\Big(((d_v+1)^\alpha + d_{w^k}^\alpha)^\beta - (d_v^\alpha + d_{w^k}^\alpha)^\beta\Big) \\ &> ((d_u+1)^\alpha + (d_v+1)^\alpha)^\beta > 0. \end{aligned}$$

The same argument gives the results for the ${}_{red}KA_{\alpha,\beta}$ index. □

Given an integer number $n \geq 2$, let $\Gamma(n)$ (respectively, $\Gamma_c(n)$) be the set of graphs (respectively, connected graphs) with n vertices.

We study in this section the extremal graphs for the $KA_{\alpha,\beta}$ index on $\Gamma_c(n)$ and $\Gamma(n)$.

Theorem 17. *Consider $\alpha, \beta \in \mathbb{R} \setminus \{0\}$ with $\alpha\beta > 0$, and an integer $n \geq 2$.*

(1) *The complete graph K_n is the unique graph that maximizes $KA_{\alpha,\beta}$ on $\Gamma_c(n)$ or $\Gamma(n)$.*

(2) *Any graph that minimizes $KA_{\alpha,\beta}$ on $\Gamma_c(n)$ is a path.*

(3) *If n is even, then the union of $n/2$ paths P_2 is the unique graph that minimizes $KA_{\alpha,\beta}$ on $\Gamma(n)$. If n is odd, then the union of $(n-3)/2$ paths P_2 with a path P_3 is the unique graph that minimizes $KA_{\alpha,\beta}$ on $\Gamma(n)$.*

(4) *Furthermore, if $\alpha, \beta > 0$, then the three previous statements hold if we replace $KA_{\alpha,\beta}$ with ${}_{red}KA_{\alpha,\beta}$.*

Proof. Let G be a graph with order n, minimum degree δ and m edges.
Items (1) and (2) follow directly from Proposition 16.
(3) Assume that n is even. It is well known that the sum of the degrees of a graph is equal to twice the number of edges of the graph (handshaking lemma). Thus, $2m \geq n\delta \geq n$. Since $\alpha\beta > 0$, the function

$$U(x, y) = (x^\alpha + y^\alpha)^\beta$$

is strictly increasing in each variable if $x, y > 0$. Hence, for any graph $G \in \Gamma(n)$, we have

$$\begin{aligned} KA_{\alpha,\beta}(G) &= \sum_{uv \in E(G)} (d_u^\alpha + d_v^\alpha)^\beta \geq \sum_{uv \in E(G)} (1^\alpha + 1^\alpha)^\beta \\ &= 2^\beta m \geq 2^\beta \frac{n}{2} = 2^{\beta-1} n, \end{aligned}$$

and the equality is tight in the inequality if and only if $d_u = 1$ for all $u \in V(G)$, i.e., G is the union of $n/2$ path graphs P_2.

Finally, assume that n is odd. Fix a graph $G \in \Gamma(n)$. If $d_u = 1$ for every $u \in V(G)$, then handshaking lemma gives $2m = n$, a contradiction (recall that n is odd). Therefore, there exists a vertex w with $d_w \geq 2$. By handshaking lemma we have $2m \geq (n-1)\delta + 2 \geq n + 1$. Recall that the set of neighbors of the vertex w is denoted by $N(w)$. Since $U(x, y)$ is a strictly increasing function in each variable, we obtain

$$\begin{aligned} KA_{\alpha,\beta}(G) &= \sum_{u \in N(w)} (d_u^\alpha + d_w^\alpha)^\beta + \sum_{uv \in E(G), u,v \neq w} (d_u^\alpha + d_v^\alpha)^\beta \\ &\geq \sum_{u \in N(w)} (1^\alpha + 2^\alpha)^\beta + \sum_{uv \in E(G), u,v \neq w} (1^\alpha + 1^\alpha)^\beta \\ &\geq 2(1 + 2^\alpha)^\beta + 2^\beta (m - 2) \\ &\geq 2(1 + 2^\alpha)^\beta + 2^\beta \Big(\frac{n+1}{2} - 2 \Big) \\ &= 2(1 + 2^\alpha)^\beta + 2^\beta \frac{n-3}{2}, \end{aligned}$$

and the bound is tight if and only if $d_u = 1$ for all $u \in V(G) \setminus \{w\}$, and $d_w = 2$. Hence, G is the union of $(n-3)/2$ path graphs P_2 and a path graph P_3.

(4) If $\alpha, \beta > 0$, then the same argument gives the results for the ${}_{red}KA_{\alpha,\beta}$ index. □

We deal now with the optimization problem for ${}_{red}KA_{\alpha,\beta}$ when $\alpha, \beta < 0$.

Given an integer number $n \geq 3$, we denote by $\Gamma^{wp}(n)$ (respectively, $\Gamma_c^{wp}(n)$) the set of graphs (respectively, connected graphs) with n vertices and without pendant vertices.

Theorem 18. *Consider $\alpha, \beta < 0$, and an integer $n \geq 3$.*

(1) *The cycle graph C_n is the unique graph that minimizes ${}_{red}KA_{\alpha,\beta}$ on $\Gamma_c^{wp}(n)$.*

(2) *The union of cycle graphs are the only graphs that minimize ${}_{red}KA_{\alpha,\beta}$ on $\Gamma^{wp}(n)$.*

(3) *The complete graph K_n is the unique graph that maximizes ${}_{red}KA_{\alpha,\beta}$ on $\Gamma_c^{wp}(n)$ or $\Gamma^{wp}(n)$.*

Proof. Let G be a graph with order n, minimum degree δ and m edges. Since a graph without pendant vertices satisfies $\delta \geq 2$, handshaking lemma gives $2m \geq n\delta \geq 2n$. Since $\alpha, \beta < 0$, the function

$$U(x, y) = (x^\alpha + y^\alpha)^\beta$$

is strictly increasing in each variable if $x, y > 0$. Hence, for any graph $G \in \Gamma^{wp}(n)$, we have

$$\begin{aligned} KA_{\alpha,\beta}(G) &= \sum_{uv \in E(G)} (d_u^\alpha + d_v^\alpha)^\beta \geq \sum_{uv \in E(G)} (2^\alpha + 2^\alpha)^\beta \\ &= 2^{(\alpha+1)\beta} m \geq 2^{(\alpha+1)\beta} n, \end{aligned}$$

and the inequality is tight if and only if $d_u = 2$ for all $u \in V(G)$, i.e., the graph G is the union of cycle graphs. If G is connected, then it is the cycle graph C_n.

Item (3) follows from Proposition 16. □

4. Conclusions

In this paper, we contributed to the study of inequalities and optimization problems associated with topological indices. In particular, we obtained new lower and upper optimal bounds of general Sombor indices, and we characterized the graphs where equality occurs.

Specifically, we have obtained inequalities for these indices relating them with other indices: the first Zagreb index, the forgotten index and the first variable Zagreb index. Finally, we solve some extremal problems for general Sombor indices

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Conflict of interest

All authors declare no conflicts of interest in this paper.

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