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ON THE FIRST BANHATTI-SOMBOR INDEX

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Abstract. Let d_v be the degree of the vertex v in a connected graph G. The first Banhatti-Sombor index of G is defined as

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

which is a new vertex-degree-based topological index introduced by Kulli. In this paper, the mathematical relations between the first Banhatti-Sombor index and some other well-known vertex-degree-based topological indices are established. In addition, the trees extremal with respect to the first Banhatti-Sombor index on trees and chemical trees are characterized, respectively.

1. Introduction

Let G be a simple undirected connected graph with vertex set $V(G)$ and edge set $E(G)$. The number of vertices and edges of G is called order and size, respectively. Denote by $\overline{G}$ the complement of G. For $v \in V(G)$, d_v denotes the degree of vertex v in G. The minimum and the maximum degree of G are denoted by $\delta(G)$ and $\Delta(G)$, or simply δ and Δ, respectively. A pendant vertex of G is a vertex of degree one. A graph G is called (Δ, δ)-semiregular if $\{d_u, d_v\} = \{\Delta, \delta\}$ holds for all edges $uv \in E(G)$. Denote by K_n, C_n, P_n and $K_{1,n-1}$ the complete graph, cycle, path and star with n vertices, respectively.

The study of topological indices of various graph structures has been of interest to chemists, mathematicians, and scientists from related fields due to the fact that the topological indices play a significant role in mathematical chemistry especially

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in the QSPR/QSAR modeling. In 1975, the Randić index of a graph G introduced by Randić [**16**] is the most important and widely applied. It is defined as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The modified second Zagreb index of a graph G, introduced by Nikolić et al. [**15**], is defined as

$$M_2^*(G) = \sum_{uv\in E(G)} \frac{1}{d_u d_v}.$$

The harmonic index and the inverse degree index of a graph G proposed by Fajtlowicz [**6**] are two the older vertex-degree-based topological indices. They are respectively defined as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}, \quad ID(G) = \sum_{uv\in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2}\right).$$

The symmetric division deg index, inverse sum indeg index and geometric-arithmetic index of a graph G, introduced by Vukičević [**20, 21, 22**], Gašperov [**22**] and Furtula [**21**], are respectively defined as

$$SDD(G) = \sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{2d_u d_v}, \quad ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v},$$

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The forgotten topological index, introduced by Furtula and Gutman [**7**], is defined as

$$F(G) = \sum_{uv\in E(G)} \left(d_u^2 + d_v^2\right).$$

In 2021, the Sombor index of a graph G is defined as

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

which is a novel vertex-degree-based molecular structure descriptor proposed by Gutman [**8**]. The investigation of the Sombor index of graphs has quickly received much attention. In particular, Redžepović [**18**] showed that the Sombor index may be used successfully on modeling thermodynamic properties of compounds due to the fact that the Sombor index has satisfactory prediction potential in modeling entropy and enthalpy of vaporization of alkanes. Das et al. [**3**], Milovanović et al. [**14**] and Wang et al. [**23**] gave the mathematical relations between the Sombor index and some other well-known vertex-degree-based topological indices. For other related results, one may refer to [**1, 5, 10, 13, 19**] and the references therein.

Inspired by work on Sombor index, the first Banhatti-Sombor index of a connected graph G was introduced by Kulli [**9**] very recently and is defined as

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

We find that the new index has close contact with numerous well-known vertex-degree-based topological indices. Moreover, the trees with the maximum and minimum first Banhatti-Sombor index among the set of trees with n vertices are determined, respectively. In particular, the extremal values of the first Banhatti-Sombor index for chemical trees are characterized.

2. Preliminaries

LEMMA 2.1. *For any edge $uv \in E(G)$, $d_u^2 + d_v^2$ or $\frac{1}{d_u^2} + \frac{1}{d_v^2}$ is a constant if and only if G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite).*

LEMMA 2.2. *For any positive real number a and b, we have*

$$\frac{2\sqrt{2}(a^2 + b^2 + ab)}{3(a+b)} \leqslant \sqrt{a^2 + b^2} \leqslant \frac{\sqrt{2}(a^2 + b^2)}{a+b}$$

with equality if and only if $a = b$.

LEMMA 2.3. ([**17**]) *If $a_i > 0$, $b_i > 0$, $p > 0$, $i = 1, 2, \ldots, n$, then the following inequality holds:*

$$\sum_{i=1}^{n} \frac{a_i^{p+1}}{b_i^p} \geqslant \frac{\left(\sum\limits_{i=1}^{n} a_i\right)^{p+1}}{\left(\sum\limits_{i=1}^{n} b_i\right)^{p}}$$

with equality if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_n}{b_n}$.

LEMMA 2.4. ([**4**]) *Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers such that $q \leqslant \frac{a_i}{b_i} \leqslant Q$ and $a_i \neq 0$ for $i = 1, 2, \ldots, n$. Then there holds*

$$\sum_{i=1}^{n} b_i^2 + Qq \sum_{i=1}^{n} a_i^2 \leqslant (Q + q) \sum_{i=1}^{n} a_i b_i$$

with equality if and only if $b_i = q a_i$ or $b_i = Q a_i$ for at least one i, $i = 1, 2, \ldots, n$.

LEMMA 2.5. ([**2**]) *If $a = (a_1, a_2, \ldots, a_n)$, $b = (b_1, b_2, \ldots, b_n)$ are sequences of real numbers and $c = (c_1, c_2, \ldots, c_n)$, $d = (d_1, d_2, \ldots, d_n)$ are nonnegative, then*

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n} c_i a_i^2 + \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i b_i^2 \geqslant 2 \sum_{i=1}^{n} c_i a_i \sum_{i=1}^{n} d_i b_i$$

with equality if and only if $a = b = (k, k, \ldots, k)$ is a constant sequence for positive c_i and d_i, $i = 1, 2, \ldots, n$.

LEMMA 2.6. ([**12**]) *Let $a_1, a_2, \dots, a_n$ and $b_1, b_2, \dots, b_n$ be real numbers such that $a \leqslant a_i \leqslant A$ and $b \leqslant b_i \leqslant B$ for $i = 1, 2, \dots, n$. Then there holds*

$$\left| \frac{1}{n} \sum_{i=1}^{n} a_i b_i - \frac{1}{n} \sum_{i=1}^{n} a_i \frac{1}{n} \sum_{i=1}^{n} b_i \right| \leqslant \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \right) (A-a)(B-b),$$

where $\lfloor x \rfloor$ denotes the integer part of x.

3. On relations between the first Banhatti-Sombor index and other degree-based indices

3.1. Bounds in terms of order, size and degree.

THEOREM 3.1. *Let G be a connected graph of order n and size m with the minimum degree δ. Then*

$$\frac{n}{\sqrt{2}} \leqslant BSO(G) \leqslant \frac{\sqrt{2}m}{\delta}$$

with equality if and only if G is a regular graph.

PROOF. Note that

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

with equality if and only if $d_u = \delta$ for any vertex u, that is, G is a regular graph.

By the Cauchy-Schwarz inequality, we have

$$BSO(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} \geqslant \sum_{uv \in E(G)} \frac{1}{\sqrt{2}} \left(\frac{1}{d_u} + \frac{1}{d_v} \right) = \frac{1}{\sqrt{2}} n$$

with equality if and only if $d_u = d_v$ for any edge uv, that is, G is a regular graph. □

COROLLARY 3.1. *Let G be a regular connected graph with n vertices. Then*

$$BSO(G) = \frac{n}{\sqrt{2}}.$$

REMARK 3.1. This implies that $BSO(G)$ does not increase with the increase of the number of edges of G. Clearly, $BSO(K_n) = BSO(C_n)$.

COROLLARY 3.2. *Let U_n be a unicyclic graph with n vertices. Then*

$$BSO(U_n) \geqslant \frac{n}{\sqrt{2}}$$

with equality if and only if $G \cong C_n$.

COROLLARY 3.3. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$\sqrt{2}n \leqslant BSO(G) + BSO(\overline{G}) \leqslant \sqrt{2} \left(\frac{m}{\delta} + \frac{n(n-1) - 2m}{2(n-1-\Delta)} \right)$$

with equality if and only if G is a regular graph.

COROLLARY 3.4. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$\frac{n}{\sqrt{2}} \leqslant BSO(G) \leqslant \frac{n\Delta}{\sqrt{2}\delta}$$

with equality if and only if G is a regular graph.

PROOF. Since $2m \leqslant n\Delta$, we have the proof. $\square$

THEOREM 3.2. *Let G be a connected graph of order n and size m with the maximum degree Δ. Then*

$$BSO(G) \leqslant n - m(2-\sqrt{2})\frac{1}{\Delta}$$

with equality if and only if G is a regular graph.

PROOF. Without loss of generality, we suppose that $d_u \geqslant d_v$. Then we have

$$\begin{aligned} BSO(G) &= \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2}+\frac{1}{d_v^2}} \leqslant \sum_{uv\in E(G)} \left(\frac{1}{d_v}+(\sqrt{2}-1)\frac{1}{d_u}\right) \\ &\leqslant \sum_{uv\in E(G)} \left(\frac{1}{d_v}+\frac{1}{d_u}\right) + m(\sqrt{2}-2)\frac{1}{\Delta} = n - m(2-\sqrt{2})\frac{1}{\Delta} \end{aligned}$$

with equality if and only if G is a regular graph. $\square$

COROLLARY 3.5. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$\sqrt{2}n \leqslant BSO(G) + BSO(\overline{G}) \leqslant 2n - (2-\sqrt{2})\left(\frac{m}{\Delta} + \frac{n(n-1)-2m}{2(n-1-\delta)}\right)$$

with equality if and only if G is a regular graph.

3.2. Bounds in terms of the Randić index, the modified second Zagreb index and the inverse degree index.

THEOREM 3.3. *Let G be a connected graph with the maximum degree Δ. Then*

$$\sqrt{2}R(G) \leqslant BSO(G) \leqslant \sqrt{2}\Delta M_2^*(G)$$

with equality if and only if G is a regular graph.

PROOF. By the arithmetic geometric inequality, we have

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

with equality if and only if $d_u = d_v$ for any edge uv, that is, G is a regular graph. It is easy to see that

$$BSO(G) = \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2}+\frac{1}{d_v^2}} \leqslant \sum_{uv\in E(G)} \frac{\sqrt{2\Delta^2}}{d_u d_v} = \sqrt{2}\Delta M_2^*(G)$$

with equality if and only if $d_u = d_v = \Delta$ for any edge uv, that is, G is a regular graph. $\square$

THEOREM 3.4. *Let G be a connected graph with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \sqrt{mID(G)}$$

with equality if and only if G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite).

PROOF. By the Cauchy-Schwarz inequality, we have

$$\begin{aligned} BSO(G) &= \sum_{uv \in E(G)} 1 \cdot \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} \\ &\leqslant \sqrt{\sum_{uv \in E(G)} 1^2 \sum_{uv \in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2} \right)} \\ &= \sqrt{mID(G)} \end{aligned}$$

with equality if and only if $\frac{1}{d_u^2} + \frac{1}{d_v^2}$ is a constant for any edge uv in a connected graph G. By Lemma 2.1, G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite). $\square$

3.3. Bounds in terms of the harmonic index, the symmetric division deg index and the modified second Zagreb index.

THEOREM 3.5. *Let G be a connected graph with the maximum degree Δ and the minimum degree δ. Then*

$$\sqrt{2}H(G) \leqslant BSO(G) \leqslant \frac{1}{\sqrt{2}} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right) H(G)$$

with equality if and only if G is a regular graph.

PROOF. By Lemma 2.2, we have

$$\begin{aligned} BSO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} \leqslant \sum_{uv \in E(G)} \frac{\sqrt{2} \left(\frac{d_v}{d_u} + \frac{d_u}{d_v} \right)}{d_u + d_v} \\ &\leqslant \sum_{uv \in E(G)} \frac{1}{\sqrt{2}} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right) \frac{2}{d_u + d_v} = \frac{1}{\sqrt{2}} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right) H(G) \end{aligned}$$

with equality if and only if $d_u = d_v$ for any edge uv, that is, G is a regular graph.

By Lemma 2.2, we have

$$\begin{aligned} BSO(G) &= \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2}+\frac{1}{d_v^2}} \geqslant \sum_{uv\in E(G)} \frac{2\sqrt{2}\left(\frac{d_v}{d_u}+\frac{d_u}{d_v}+1\right)}{3(d_u+d_v)} \\ &\geqslant \sum_{uv\in E(G)} \frac{2\sqrt{2}(2+1)}{3(d_u+d_v)} = \sqrt{2}H(G) \end{aligned}$$

with equality if and only if $d_u = d_v$ for any edge uv, that is, G is a regular graph. □

Theorem 3.6. *Let G be a connected graph with the maximum degree Δ and the minimum degree δ. Then*

$$\frac{2\sqrt{2}}{3\Delta}SDD(G)+\frac{\sqrt{2}}{3}H(G) \leqslant BSO(G) \leqslant \frac{\sqrt{2}}{\delta}SDD(G)$$

with equality if and only if G is a regular graph.

Proof. By Lemma 2.2, we have

$$\begin{aligned} BSO(G) &= \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2}+\frac{1}{d_v^2}} \leqslant \sum_{uv\in E(G)} \frac{\sqrt{2}\left(\frac{d_v}{d_u}+\frac{d_u}{d_v}\right)}{d_u+d_v} \\ &\leqslant \sum_{uv\in E(G)} \frac{\sqrt{2}\left(\frac{d_v}{d_u}+\frac{d_u}{d_v}\right)}{\delta+\delta} = \frac{\sqrt{2}}{\delta}SDD(G) \end{aligned}$$

with equality if and only if $d_u = d_v = \delta$ for any edge uv, that is, G is a regular graph.

By Lemma 2.2, we have

$$\begin{aligned} BSO(G) &= \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2}+\frac{1}{d_v^2}} \\ &\geqslant \sum_{uv\in E(G)} \frac{2\sqrt{2}\left(\frac{d_v}{d_u}+\frac{d_u}{d_v}+1\right)}{3(d_u+d_v)} \\ &= \sum_{uv\in E(G)} \frac{2\sqrt{2}\left(\frac{d_v}{d_u}+\frac{d_u}{d_v}\right)}{3(d_u+d_v)} + \sum_{uv\in E(G)} \frac{2\sqrt{2}}{3(d_u+d_v)} \\ &= \frac{2\sqrt{2}}{3\Delta}SDD(G)+\frac{\sqrt{2}}{3}H(G) \end{aligned}$$

with equality if and only if $d_u = d_v = \Delta$ for any edge uv, that is, G is a regular graph. □

Theorem 3.7. *Let G be a connected graph with n vertices. Then*

$$BSO(G) \leqslant \sqrt{2M_2^*(G)SDD(G)}$$

with equality if and only if G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite).

PROOF. Let $p = 1$, $a_i = \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}}$ and $b_i = \frac{1}{d_u d_v}$ in Lemma 2.3. Then we have

$$\frac{\left(\sum\limits_{uv\in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}}\right)^2}{\sum\limits_{uv\in E(G)} \frac{1}{d_u d_v}} \leqslant \sum_{uv\in E(G)} \frac{\frac{1}{d_u^2} + \frac{1}{d_v^2}}{\frac{1}{d_u d_v}} = \sum_{uv\in E(G)} \left(\frac{d_v}{d_u} + \frac{d_u}{d_v}\right),$$

that is,

$$BSO(G) \leqslant \sqrt{2M_2^*(G)SDD(G)}$$

with equality if and only if $\sqrt{d_u^2 + d_v^2}$ is a constant for any edge uv in G, by Lemma 2.1, G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite). □

COROLLARY 3.6. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \sqrt{mM_2^*(G)\left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)}$$

with equality if and only if G is a regular graph or a (Δ, δ)-semiregular bipartite graph.

PROOF. Without loss of generality, we assume that $d_u \geqslant d_v$. By the proof of Theorem 3.7, we have

$$\frac{\left(\sum\limits_{uv\in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}}\right)^2}{\sum\limits_{uv\in E(G)} \frac{1}{d_u d_v}} \leqslant \sum_{uv\in E(G)} \left(\frac{d_v}{d_u} + \frac{d_u}{d_v}\right) \leqslant \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right) m$$

with equality if and only if $d_u = \Delta$ and $d_v = \delta$ for any edge uv. This implies that G is a regular graph or a (Δ, δ)-semiregular bipartite graph. Conversely, it is easy to check that equality holds in Corollary 3.6 when G is a regular graph or a (Δ, δ)-semiregular bipartite graph. □

3.4. Bounds in terms of the forgotten index.

THEOREM 3.8. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \geqslant \frac{\sqrt{2}}{\Delta^3 + \delta^3} \left(\frac{m\delta^3}{\Delta} + \frac{F}{2}\right)$$

with equality if and only if G is a regular graph.

Proof. Let $a_i = \sqrt{d_u^2 + d_v^2}$ and $b_i = \frac{1}{d_u d_v}$ in Lemma 2.4. Then $q = \frac{1}{\sqrt{2}\Delta^3}$ and $Q = \frac{1}{\sqrt{2}\delta^3}$. By Lemma 2.4, we have

$$\sum_{uv\in E(G)} \frac{1}{d_u^2 d_v^2} + \frac{1}{2\Delta^3\delta^3} \sum_{uv\in E(G)} (d_u^2 + d_v^2) \leqslant \frac{1}{\sqrt{2}} \left(\frac{1}{\Delta^3} + \frac{1}{\delta^3}\right) \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}},$$

that is,

$$\frac{m}{\Delta^4} + \frac{1}{2\Delta^3\delta^3} F(G) \leqslant \frac{1}{\sqrt{2}} \left(\frac{1}{\Delta^3} + \frac{1}{\delta^3}\right) BSO(G),$$

that is,

$$BSO(G) \geqslant \frac{\sqrt{2}}{\Delta^3 + \delta^3} \left(\frac{m\delta^3}{\Delta} + \frac{F}{2}\right)$$

with equality if and only if $d_u = d_v = \Delta$ for any edge uv, that is, G is a regular graph. □

Theorem 3.9. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \frac{2mSDD(G) + M_2^*(G)F(G)}{2SO(G)}$$

with equality if and only if G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite).

Proof. Let $a_i = b_i = \sqrt{d_u^2 + d_v^2}$, $c_i = \frac{1}{d_u d_v}$ and $d_i = 1$ in Lemma 2.5. Then we have

$$m \sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v} + \sum_{uv\in E(G)} \frac{1}{d_u d_v} \sum_{uv\in E(G)} (d_u^2 + d_v^2)$$
$$\geqslant 2 \sum_{uv\in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u d_v} \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2},$$

that is,

$$2mSDD(G) + M_2^*(G)F(G) \geqslant 2BSO(G)SO(G),$$

that is,

$$BSO(G) \leqslant \frac{2mSDD(G) + M_2^*(G)F(G)}{2SO(G)}$$

with equality if and only if $a_i = b_i = \sqrt{d_u^2 + d_v^2}$ for any edge uv in G, that is, $d_u^2 + d_v^2$ is a constant for any edge uv in G, by Lemma 2.1, G is a regular graph (when G is non-bipartite) or G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite). □

Corollary 3.7. *Let G be a connected graph of size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \frac{m(\Delta^2\delta + \delta^2) + \Delta F(G)}{2\sqrt{2}\Delta\delta^3}$$

with equality if and only if G is a regular graph.

COROLLARY 3.8. *Let G be a connected graph of size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \frac{m^2(2\Delta^3 + \Delta^2\delta + \delta^3)}{2\Delta\delta^2 SO(G)}$$

with equality if and only if G is a regular graph.

3.5. Bounds in terms of the inverse sum indeg index and geometric-arithmetic index.

THEOREM 3.10. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \frac{H(G)SDD(G) + 2M_2^*(G)ISI(G)}{\sqrt{2}GA(G)}$$

with equality if and only if G is a regular graph.

PROOF. Let $a_i = \sqrt{d_u^2 + d_v^2}$, $b_i = \sqrt{2d_u d_v}$, $c_i = \frac{1}{d_u d_v}$ and $d_i = \frac{1}{d_u + d_v}$ in Lemma 2.5. Then we have

$$\sum_{uv\in E(G)} \frac{1}{d_u + d_v} \sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v} + \sum_{uv\in E(G)} \frac{1}{d_u d_v} \sum_{uv\in E(G)} \frac{2d_u d_v}{d_u + d_v}$$
$$\geqslant 2 \sum_{uv\in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u d_v} \sum_{uv\in E(G)} \frac{\sqrt{2d_u d_v}}{d_u + d_v},$$

that is,

$$H(G)SDD(G) + 2M_2^*(G)ISI(G) \geqslant \sqrt{2}BSO(G)GA(G),$$

that is,

$$BSO(G) \leqslant \frac{H(G)SDD(G) + 2M_2^*(G)ISI(G)}{\sqrt{2}GA(G)}$$

with equality if and only if $\sqrt{d_u^2 + d_v^2} = \sqrt{2d_u d_v}$ for any edge uv, that is, G is a regular graph. $\square$

COROLLARY 3.9. *Let G be a connected graph of size m with the maximum degree Δ and the minimum degree δ. Then*

$$BSO(G) \leqslant \frac{m^2\Delta^2 + m^2\delta^2 + 4m\Delta ISI(G)}{2\sqrt{2}\Delta\delta^2 GA(G)}$$

with equality if and only if G is a regular graph.

3.6. Bounds in terms of the Sombor index and the modified second Zagreb index.

THEOREM 3.11. *Let G be a connected graph of size m with the maximum degree Δ and the minimum degree δ. Then*

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

with equality if and only if G is a regular graph.

PROOF. It is easy to see that

$$BSO(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} \leqslant \frac{1}{\delta^2} \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \leqslant \frac{1}{\delta^2} SO(G),$$

with equality if and only if $d_u = d_v = \Delta$ for any edge uv, that is, G is a regular graph.

Let $a_i = b_i = \frac{1}{\sqrt{d_u d_v}}$ and $c_i = d_i = \sqrt{d_u^2 + d_v^2}$ in Lemma 2.5. Then

$$2 \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} \geqslant 2 \left(\sum_{uv \in E(G)} \sqrt{\frac{d_u^2 + d_v^2}{d_u d_v}} \right)^2 \geqslant 4m^2,$$

that is,

$$2SO(G)BSO(G) \geqslant 4m^2,$$

that is,

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

with equality if and only if G is a regular graph. □

THEOREM 3.12. *Let G be a connected graph of order n and size m with the maximum degree Δ and the minimum degree δ. Then*

$$\left| \frac{1}{m} BSO(G) - \frac{1}{m^2} SO(G) M_2^*(G) \right| \leqslant \xi(m) \frac{\sqrt{2}(\Delta + \delta)(\Delta - \delta)^2}{\Delta^2 \delta^2},$$

where

$$\xi(m) = \frac{1}{4} \left(1 - \frac{1 + (-1)^{m+1}}{2m^2} \right).$$

PROOF. Let $a_i = \sqrt{d_u^2 + d_v^2}$ and $b_i = \frac{1}{d_u d_v}$ in Lemma 2.6. Then $a = \sqrt{2}\delta$, $A = \sqrt{2}\Delta$, $b = \frac{1}{\Delta^2}$ and $B = \frac{1}{\delta^2}$. By Lemma 2.6, we have

$$\left| \frac{1}{m} \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}} - \frac{1}{m^2} \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \sum_{uv \in E(G)} \frac{1}{d_u d_v} \right|$$
$$\leqslant \frac{1}{m} \left\lfloor \frac{m}{2} \right\rfloor \left(1 - \frac{1}{m} \left\lfloor \frac{m}{2} \right\rfloor \right) \sqrt{2}(\Delta - \delta)(\frac{1}{\delta^2} - \frac{1}{\Delta^2}),$$

that is,

$$\left|\frac{1}{m}BSO(G) - \frac{1}{m^2}SO(G)M_2^*(G)\right| \leqslant \xi(m)\frac{\sqrt{2}(\Delta+\delta)(\Delta-\delta)^2}{\Delta^2\delta^2},$$

where

$$\xi(m) = \frac{1}{m}\left\lfloor\frac{m}{2}\right\rfloor\left(1-\frac{1}{m}\left\lfloor\frac{m}{2}\right\rfloor\right) = \frac{1}{4}\left(1-\frac{1+(-1)^{m+1}}{2m^2}\right).$$

□

4. The first Banhatti-Sombor index of trees

In this section, we determine the trees with the maximum and minimum first Banhatti-Sombor index among the set of trees of order n, respectively. For a tree T_n of order n with maximum degree Δ, denote by n_i the number of vertices with degree i in T_n for $1 \leqslant i \leqslant \Delta$, and $m_{i,j}$ the number of edges of T_n connecting vertices of degree i and j, where $1 \leqslant i \leqslant j \leqslant \Delta$. Note that T_n is connected, so $m_{1,1} = 0$ for $n \geqslant 3$. Let $N = \{(i,j) \in \mathbb{N} \times \mathbb{N} : 1 \leqslant i \leqslant j \leqslant \Delta\}$. Then clearly the following relations hold:

$$|V(T_n)| = n = \sum_{i=1}^{\Delta} n_i, \tag{4.1}$$

$$|E(T_n)| = n-1 = \sum_{(i,j)\in N} m_{i,j}, \tag{4.2}$$

and

$$\begin{cases} 2m_{1,1} + m_{1,2} + \ldots + m_{1,\Delta} = n_1, \\ m_{1,2} + 2m_{2,2} + \ldots + m_{2,\Delta} = 2n_2, \\ \ldots \\ m_{1,\Delta} + m_{2,\Delta} + \ldots + 2m_{\Delta,\Delta} = \Delta n_\Delta. \end{cases} \tag{4.3}$$

It follows easily from (4.1) and (4.3) that

$$n = \sum_{(i,j)\in N} \frac{i+j}{ij} m_{i,j}. \tag{4.4}$$

And the definition of the first Banhatti-Sombor index is equivalent to

$$SO(T_n) = \sum_{(i,j)\in N} \sqrt{\frac{1}{i^2}+\frac{1}{j^2}}\, m_{i,j}. \tag{4.5}$$

THEOREM 4.1. *Let T_n be a tree with n-vertex. Then*

$$\frac{\sqrt{2}(n-3)}{2} + \sqrt{5} \leqslant BSO(T_n) \leqslant \sqrt{1+(n-1)^2}.$$

The equality in the left-hand side holds if and only if $T_n \cong P_n$, and the equality in the right-hand side holds if and only if $T_n \cong K_{1,\,n-1}$.

PROOF. First, we consider the inequality in the left-hand side. Let

$$N_1 = \Big\{(i,j) \in N : (i,j) \neq (1,1), (i,j) \neq (1,2), (i,j) \neq (2,2)\Big\}.$$

By equation (4.4), we have

$$3m_{1,2} + 2m_{2,2} = 2n - \sum_{(i,j)\in N_1} \frac{2(i+j)}{ij} m_{i,j},$$

and by equation (4.2), we have

$$m_{1,2} + m_{2,2} = n - 1 - \sum_{(i,j)\in N_1} m_{i,j}.$$

Then we obtain the following expression for $m_{1,2}$ and $m_{2,2}$:

$$m_{1,2} = 2 + \sum_{(i,j)\in N_1} \Big[2 - \frac{2(i+j)}{ij}\Big] m_{i,j},$$

$$m_{2,2} = n - 3 + \sum_{(i,j)\in N_1} \Big[\frac{2(i+j)}{ij} - 3\Big] m_{i,j}.$$

According to the expression (4.5), we have

$$\begin{aligned} BSO(T_n) &= m_{1,2}\sqrt{\frac{1}{4}+1} + m_{2,2}\sqrt{\frac{1}{4}+\frac{1}{4}} + \sum_{(i,j)\in N_1} \sqrt{\frac{1}{i^2}+\frac{1}{j^2}} m_{i,j} \\ &= \sqrt{5}\Big[1 + \sum_{(i,j)\in N_1} \Big(1 - \frac{i+j}{ij}\Big) m_{i,j}\Big] + \frac{\sqrt{2}}{2}\Big\{n - 3 \\ &\quad + \sum_{(i,j)\in N_1} \Big[\frac{2(i+j)}{ij} - 3\Big] m_{i,j}\Big\} + \sum_{(i,j)\in N_1} \sqrt{\frac{1}{i^2}+\frac{1}{j^2}} m_{i,j} \\ &= \frac{\sqrt{2}}{2}(n-3) + \sqrt{5} + \sum_{(i,j)\in N_1} \Big[\sqrt{\frac{1}{i^2}+\frac{1}{j^2}} + (\sqrt{2}-\sqrt{5})\frac{i+j}{ij} \\ &\quad + \sqrt{5} - \frac{3\sqrt{2}}{2}\Big] m_{i,j}. \end{aligned}$$

Let

$$f(x,y) = \sqrt{\frac{1}{x^2}+\frac{1}{y^2}} + (\sqrt{2}-\sqrt{5})\frac{x+y}{xy} + \sqrt{5} - \frac{3\sqrt{2}}{2},$$

where $(x,y) \in N$, it is easy to see that $f(1,2) = 0$, $f(2,2) = 0$ and $f(x,y) > 0$ for $(x,y) \in N_1$. Therefore, $BSO(T_n) = \frac{\sqrt{2}}{2}(n-3) + \sqrt{5}$ if and only if $m_{i,j} = 0$ for all $(i,j) \in N_1$. And this occurs if and only if $T_n \cong P_n$. Conversely, if $T_n \cong P_n$, by (4.5), we obtain

$$BSO(P_n) = 2\sqrt{\frac{1}{4}+1} + (n-3)\sqrt{\frac{1}{4}+\frac{1}{4}} = \frac{\sqrt{2}}{2}(n-3) + \sqrt{5}.$$

Thus, we have $BSO(T_n) \geqslant BSO(P_n)$ with equality if and only if $T_n \cong P_n$.

Now, we consider the inequality in the right-hand side. Let

$$N_2 = \Big\{(i,j) \in N : (i,j) \neq (1,1), (i,j) \neq (1,\Delta), (i,j) \neq (\Delta,\Delta)\Big\}.$$

Similar to the proof of the above, by equation (4.4), we have

$$(\Delta+1)m_{1,\Delta} + 2m_{\Delta,\Delta} = \Delta n - \sum_{(i,j)\in N_2} \Delta \frac{i+j}{ij} m_{i,j},$$

and by equation (4.2), we have

$$m_{1,\Delta} + m_{\Delta,\Delta} = n - 1 - \sum_{(i,j)\in N_2} m_{i,j}.$$

Then we obtain the following expression for $m_{1,\Delta}$ and $m_{\Delta,\Delta}$:

$$(\Delta-1)m_{1,\Delta} = (\Delta-2)n + 2 - \sum_{(i,j)\in N_2} \Big(\Delta\frac{i+j}{ij} - 2\Big) m_{i,j},$$

$$(\Delta-1)m_{\Delta,\Delta} = n - (\Delta+1) + \sum_{(i,j)\in N_2} \Big(\Delta\frac{i+j}{ij} - (\Delta+1)\Big) m_{i,j}.$$

According to the expression (4.5), we have

$$\begin{aligned}
BSO(T_n) &= m_{1,\Delta}\sqrt{\frac{1}{\Delta^2}+1} + m_{\Delta,\Delta}\sqrt{\frac{1}{\Delta^2}+\frac{1}{\Delta^2}} + \sum_{(i,j)\in N_2}\sqrt{\frac{1}{i^2}+\frac{1}{j^2}}m_{i,j} \\
&= \frac{\sqrt{\Delta^2+1}}{\Delta(\Delta-1)}\Big[(\Delta-2)n + 2 - \sum_{(i,j)\in N_2}\Big(\Delta\frac{i+j}{ij}-2\Big)m_{i,j}\Big] \\
&\quad + \frac{\sqrt{1+\Delta^2}}{\Delta(\Delta-1)}\Big[n-(\Delta+1) + \sum_{(i,j)\in N_2}\Big(\Delta\frac{i+j}{ij}-(\Delta+1)\Big)m_{i,j}\Big] \\
&\quad + \sum_{(i,j)\in N_2}\sqrt{\frac{1}{i^2}+\frac{1}{j^2}}m_{i,j} \\
&= \frac{(\Delta-2)n\sqrt{\Delta^2+1} + \sqrt{2}(n-\Delta-1) + 2\sqrt{\Delta^2+1}}{\Delta(\Delta-1)} \\
&\quad + \sum_{(i,j)\in N_2}\Big[\sqrt{\frac{1}{i^2}+\frac{1}{j^2}} + \frac{\sqrt{2}-\sqrt{\Delta^2+1}}{\Delta-1}\frac{i+j}{ij} \\
&\quad + \frac{2\sqrt{\Delta^2+1}-\sqrt{2}(\Delta+1)}{\Delta(\Delta-1)}\Big]m_{i,j}.
\end{aligned}$$

Let

$$g(x,y) = \sqrt{\frac{1}{x^2}+\frac{1}{y^2}} + \frac{\sqrt{2}-\sqrt{\Delta^2+1}}{\Delta-1}\frac{x+y}{xy} + \frac{2\sqrt{\Delta^2+1}-\sqrt{2}(\Delta+1)}{\Delta(\Delta-1)},$$

where $(x,y) \in N$, it is easy to see that $f(1,\Delta)=0$, $f(\Delta,\Delta)=0$ and $f(x,y)<0$ for $(x,y) \in N_2$. Therefore,

$$BSO(T_n) = \frac{(\Delta-2)n\sqrt{\Delta^2+1}+\sqrt{2}(n-\Delta-1)+2\sqrt{\Delta^2+1}}{\Delta(\Delta-1)}$$

if and only if $m_{i,j}=0$ for all $(i,j) \in N_2$. And this occurs if and only if $n_2 = n_3 = \ldots = n_{\Delta-1} = 0$.

Let

$$h(x) = \frac{(x-2)n\sqrt{x^2+1}+\sqrt{2}(n-x-1)+2\sqrt{x^2+1}}{x(x-1)}.$$

By derivative, we know that $h(x)$ is an increasing function for $[2,+\infty)$. Thus

$$h(\Delta) \leqslant h(n-1) = \sqrt{1+(n-1)^2}.$$

Conversely, $BSO(K_{1,\,n-1}) = \sqrt{1+(n-1)^2}$. Thus, we have

$$BSO(T_n) \leqslant BSO(K_{1,\,n-1})$$

with equality if and only if $T_n \cong K_{1,\,n-1}$. □

Similar to the method used in Theorem 4.1, we now give an upper bound on chemical trees without its proof.

THEOREM 4.2. *Let T_n be a chemical tree with n vertices. If $n-2=0(mod\ 3)$, then*

$$BSO(T_n) \leqslant \frac{2\sqrt{17}(n+1)+\sqrt{2}(n-5)}{12}$$

with equality if and only if $n_2 = n_3 = 0$.

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