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Research Paper

The Sombor index for unicyclic and bicyclic graphs with given (total) domination number

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Abstract. The Sombor index is one of the vertex-degree-based topological indices that was introduced in 2021 by Gutman. In this paper we obtain some bounds of Sombor index of trees, unicyclic and bicyclic graphs with given (total) domination number.

Keywords. Sombor index, (total) domination number, tree, unicyclic graph, bicyclic graph.
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1 Introduction

Topological indices are numerical descriptors that are invariant under graph isomorphisms. A large number of these indices have been introduced in the chemical and mathematical graph theory, and widely have been studied. In general, they are defined as

$$TI(G) = \sum_{uv \in E(G)} f(d_u, d_v),$$

where f is a symmetric positive two-variables function.

The ordered pair (z,t), which $z = d_u$ and $t = d_v$, is named the d-coordinate (or degree-coordinate) of the edge $uv \in E(G)$. In the two dimensions coordinate system, it matches to a point named the d-point (or degree-point) of the edge uv. With the Euclidean metrics, the distance between the d-point (z,t) and the origin of the coordinate system is named the d-radius (or degree-radius) of the edge uv and this is defined as $r(z,t) = \sqrt{z^2 + t^2}$.

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From the above concept, Gutman in [6] introduced a vertex-degree-based topological index which is called Sombor index, and defined by

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

He investigated some properties of this index on some special graphs.

Recently, the Sombor index has received much attention within chemistry and mathematics specially graph theory, because trees, unicyclic and bicyclic graphs, as three great classes of chemical structures, have played an essential role in these concerns. For instance, Alidadi et al. [2] determined the minimum Sombor index for unicyclic graphs with fixed diameter. Cruz and Rada [5] obtained maximum and minimum of the Sombor index for unicyclic and bicyclic graphs, and Liu in [9] solved the extremal problem of unicyclic graphs with fixed diameter, which is inspired by the problem of trees with some parameters such as segment number, diameter, pendent vertices, matching number, and branching number.

Senthilkumar et al. in [15] characterized the first-two maximum values of the Sombor index of unicyclic graphs with given order and girth. Zhou et al. [17] studied the extremal problem of Sombor index of unicyclic graphs and trees with given maximum degree. Zhou et al. [18] attained the extremal Sombor index of trees and unicyclic graphs with given matching number. Milovanović et al. [10] determined upper and lower bounds on the Sombor indices and their relationships with other degree-based indices. The authors also proved two inequalities for the Sombor index of the Nordhaus-Gaddum type.

Redžepović [13] determined chemical applicability of Sombor indices and studied their predictive and discriminative potentials. He examined that Sombor indices have a good predictive potential. Réti et al. [14] attained some bounds on the Sombor index and showed that among all connected unicyclic graphs of order $n \geq 4$, the cycle graphs C_n have the minimal Sombor index, and showed that the maximal Sombor index is the device for determine the classes of all connected graphs with a specific cycle.

In [7], the authors confirmed a conjecture on the Sombor index, and established an upper bound for graphs, which is based on their size and the eigenvalues of the Sombor matrix. In [11], the authores presented some bounds for the Sombor index using some topological and statistical indices. Sun and Du [16] obtained the upper and lower bounds of Sombor index on trees with given domination number.

Similar investigations have also been conducted on other vertex-degree-based topological indices. Jamri et al. [8] determined the bound of the Randić index of trees with given total domination number and they characterized trees that have minimum Randić index. Mojdeh et al. [12] determined bounds of the first and second Zagreb indices for trees, unicyclic, and bicyclic graphs with given (total) domination number.

In recent years, the variety and scope of research on topological indices of graphs have been expanded. For example, in [1], the authors determined the explicit expressions of different weighted versions of edge Mostar indices of carbon nanostructures. In [3], Alidadi et al. introduced various types of topological indices, and investigated their applications in chemical graph theory extensively, and in [4], the authors computed the elliptic Sombor characteristic polynomial and the elliptic Sombor energy for some classes of graphs.

In the present paper, continuing the research on finding upper bounds on the Sombor index, some bounds on trees, unicyclic and bicyclic graphs are established in terms of (total) domination number. We start with some definitions and lemmas which are needed in the sequel.

Let $G(V,E)$ be a simple connected and undirected graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, $N_v(G)$ is the set of all neighbors of v. The degree of v is equal to the number of neighbors of v and defined by $d_v(G) = |N_v(G)|$. A pendent vertex is a vertex of degree one. The diameter of G, denoted by $D(G)$, is the maximum distance between any two vertices of G. A diametral path is a path with $D(G)$ edges between two vertices.

A unicyclic graph is a connected graph G with exactly one cycle, such that $|V(G)| = |E(G)|$. A bicyclic graph is a connected graph G containing exactly two cycles, that $|E(G)| = |V(G)| + 1$.

The set $D \subseteq V(G)$ is called a domination set of G, if for each $v \in V(G)$, $v \in D$ or there is $u \in N_v(G)$, such that $u \in D$. Minimum cardinality of D is called domination number of G and denoted by $\gamma(G)$.

The total domination set $D \subseteq V(G)$ is a domination set that the induced subgraph of D has not isolated vertex. The minimum cardinality of D is called total domination number of G and denoted by $\gamma_t(G)$.

Lemma 1.1. *[16] Let T be a tree with domination number γ, then*

$$SO(T) \leq (n-2\gamma+1)\sqrt{(n-\gamma)^2+1} + (\gamma-1)\sqrt{(n-\gamma)^2+4} + \sqrt{5}(\gamma-1).$$

Lemma 1.2. *[14] Let G be a connected unicyclic graph with $n \geq 4$ vertices, then*

$$SO(G) \geq n\sqrt{8} = SO(C_n).$$

Lemma 1.3. *[12] Let G be a connected graph with domination number $\gamma(G)$. If $e \in E(G)$, then $\gamma(G-e) \in \{\gamma(G), \gamma(G)+1\}$.*

Lemma 1.4. *[12] Let G be a connected graph with domination number $\gamma(G)$. If $e, e' \in E(G)$, then $\gamma(G - \{e, e'\}) \in \{\gamma(G), \gamma(G)+1, \gamma(G)+2\}$.*

Lemma 1.5. *Let $x \geq 2$, then*

$$\sqrt{x^2+4} + \sqrt{5} < \frac{x^2}{\sqrt{x^2+4}} + 2\sqrt{x^2+1}. \tag{1}$$

Proof. Let $f(x) = 2\sqrt{x^2+1} - \sqrt{5}$ and $g(x) = \frac{4}{\sqrt{x^2+4}}$, then f (res. g) is an increasing (res. a decreasing) function for $x \geq 2$, and

$$f(x) \geq f(2) = \sqrt{5} > \frac{4}{\sqrt{8}} = g(2) \geq g(x).$$

Therefore

$$2\sqrt{x^2+1} - \sqrt{5} > \frac{4}{\sqrt{x^2+4}}, \tag{2}$$

and (1) comes by addition the expression $\frac{x^2}{\sqrt{x^2+4}}$ to both sides of (2). □

Lemma 1.6. *Let G be a connected graph with $n \geq 3$ vertices and domination number γ. If*

$$f(n,\gamma) = (n-2\gamma+1)\sqrt{(n-\gamma)^2+1} + (\gamma-1)\sqrt{(n-\gamma)^2+4} + \sqrt{5}(\gamma-1), \tag{3}$$

then $f(n,\gamma)$ is a strictly decreasing function of γ.

Proof. We must show that

$$\frac{\partial f(n,\gamma)}{\partial \gamma} = -(n-\gamma)\left[\frac{n-2\gamma+1}{\sqrt{(n-\gamma)^2+1}} + \frac{\gamma-1}{\sqrt{(n-\gamma)^2+4}}\right] -2\sqrt{(n-\gamma)^2+1} + \sqrt{(n-\gamma)^2+4} + \sqrt{5} < 0.$$

Since $n-\gamma \geq 2$, we have

$$\frac{n-2\gamma+1}{\sqrt{(n-\gamma)^2+1}} + \frac{\gamma-1}{\sqrt{(n-\gamma)^2+4}} > \frac{n-2\gamma+1}{\sqrt{(n-\gamma)^2+4}} + \frac{\gamma-1}{\sqrt{(n-\gamma)^2+4}} = \frac{n-\gamma}{\sqrt{(n-\gamma)^2+4}} \geq 0.$$

Therefore, it suffices to show that

$$-(n-\gamma)\left[\frac{n-\gamma}{\sqrt{(n-\gamma)^2+4}}\right] - 2\sqrt{(n-\gamma)^2+1} + \sqrt{(n-\gamma)^2+4} + \sqrt{5} < 0. \tag{4}$$

Let $x = n-\gamma$, then (4) comes from Lemma 1.5. □

2 Upper bounds on the Sombor index of the unicyclic and bicyclic graphs with domination number

In this section we will obtain some upper bounds on the Sombor index of the unicyclic and bicyclic graphs with domination number γ.

Theorem 2.1. *Let G be a unicyclic graph with n vertices, domination number $\gamma(G) = \gamma$, and maximum degree Δ, then,*

$$SO(G) \leq (n-2\gamma+1)\sqrt{(n-\gamma)^2+1} + (\gamma-1)\sqrt{(n-\gamma)^2+4} + \sqrt{5}(\gamma-1) + \sqrt{2}\Delta + 2\sqrt{2}(\Delta-1)^2.$$

Proof. Let C be the unique cycle of G, and $e = xy \in E(C)$ be an edge. Considering the tree $T = G - e$ besides the Lemma 1.1, imply that

$$\begin{aligned}
SO(G) &= SO(T) + \sqrt{d_x^2 + d_y^2} + \sum_{z \in N_x, z \neq y} \left(\sqrt{d_x^2 + d_z^2} - \sqrt{(d_x - 1)^2 + d_z^2} \right) \\
&+ \sum_{w \in N_y, w \neq x} \left(\sqrt{d_y^2 + d_w^2} - \sqrt{(d_y - 1)^2 + d_w^2} \right) \\
&\leq (n - 2\gamma(T) + 1)\sqrt{(n - \gamma(T))^2 + 1} + (\gamma(T) - 1)\sqrt{(n - \gamma(T))^2 + 4} \\
&+ \sqrt{5}(\gamma(T) - 1) + \sqrt{\Delta^2 + \Delta^2} + 2\sum_{1}^{\Delta - 1} \left(\sqrt{\Delta^2 + \Delta^2} - \sqrt{2} \right) \\
&\leq (n - 2\gamma(T) + 1)\sqrt{(n - \gamma(T))^2 + 1} + (\gamma(T) - 1)\sqrt{(n - \gamma(T))^2 + 4} \\
&+ \sqrt{5}(\gamma(T) - 1) + \sqrt{2}\Delta + 2(\Delta - 1) \left(\sqrt{2}\Delta - \sqrt{2} \right) \\
&= (n - 2\gamma(T) + 1)\sqrt{(n - \gamma(T))^2 + 1} + (\gamma(T) - 1)\sqrt{(n - \gamma(T))^2 + 4} \\
&+ \sqrt{5}(\gamma(T) - 1) + \sqrt{2}\Delta + 2\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

By Lemma 1.3, we have $\gamma(T) \in \{\gamma, \gamma + 1\}$. Therefore if $\gamma(T) = \gamma$, then the theorem is true and

$$\begin{aligned}
SO(G) &\leq (n - 2\gamma + 1)\sqrt{(n - \gamma)^2 + 1} + (\gamma - 1)\sqrt{(n - \gamma)^2 + 4} \\
&+ \sqrt{5}(\gamma - 1) + \sqrt{2}\Delta + 2\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

If $\gamma(T) = \gamma + 1$, then by substitution in perivous equation, we will attain,

$$\begin{aligned}
SO(G) &\leq (n - 2\gamma - 1)\sqrt{(n - \gamma - 1)^2 + 1} + \gamma\sqrt{(n - \gamma - 1)^2 + 4} \\
&+ \sqrt{5}\gamma + \sqrt{2}\Delta + 2\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

But by Lemma 1.6, $f(n, \gamma)$ is a strictly decreasing function of γ, and the proof is complete. □

Theorem 2.2. *let G be a bicyclic graph with n vertices, domination number γ, and maximum degree Δ, then,*

$$\begin{aligned}
SO(G) &\leq (n - 2\gamma + 1)\sqrt{(n - \gamma)^2 + 1} + (\gamma - 1)\sqrt{(n - \gamma)^2 + 4} \\
&+ \sqrt{5}(\gamma - 1) + 2\sqrt{2}\Delta + 4\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

Proof. Suppose that $e = xy$ and $e' = zw$ be two edges of G. Applying the Lemma 1.1 to the tree $T = G - \{e, e'\}$ implies that:

$$\begin{aligned}
SO(G) &= SO(T) + \sqrt{d_x^2 + d_y^2} + \sqrt{d_z^2 + d_w^2} \\
&\quad + \sum_{u \in N_x, u \neq y} \left(\sqrt{d_x^2 + d_u^2} - \sqrt{(d_x - 1)^2 + d_u^2} \right) \\
&\quad + \sum_{v \in N_y, v \neq x} \left(\sqrt{d_y^2 + d_v^2} - \sqrt{(d_y - 1)^2 + d_v^2} \right) \\
&\quad + \sum_{t \in N_z, t \neq w} \left(\sqrt{d_z^2 + d_t^2} - \sqrt{(d_z - 1)^2 + d_t^2} \right) \\
&\quad + \sum_{r \in N_w, r \neq z} \left(\sqrt{d_w^2 + d_r^2} - \sqrt{(d_w - 1)^2 + d_r^2} \right) \\
&\leq (n - 2\gamma(T) + 1)\sqrt{(n - \gamma(T))^2 + 1} + (\gamma(T) - 1)\sqrt{(n - \gamma(T))^2 + 4} \\
&\quad + \sqrt{5}(\gamma(T) - 1) + 2\sqrt{\Delta^2 + \Delta^2} + 4\sum_{1}^{\Delta - 1} \left(\sqrt{\Delta^2 + \Delta^2} - \sqrt{2} \right) \\
&\leq (n - 2\gamma(T) + 1)\sqrt{(n - \gamma(T))^2 + 1} + (\gamma(T) - 1)\sqrt{(n - \gamma(T))^2 + 4} \\
&\quad + \sqrt{5}(\gamma(T) - 1) + 2\sqrt{2}\Delta + 4(\Delta - 1)\left(\sqrt{2}\Delta - \sqrt{2} \right) \\
&\leq (n - 2\gamma(T) + 1)\sqrt{(n - \gamma(T))^2 + 1} + (\gamma(T) - 1)\sqrt{(n - \gamma(T))^2 + 4} \\
&\quad + \sqrt{5}(\gamma(T) - 1) + 2\sqrt{2}\Delta + 4\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

Now, according to Lemma 1.4, if $\gamma(T) = \gamma$ then,

$$\begin{aligned}
SO(G) \leq &(n - 2\gamma + 1)\sqrt{(n - \gamma)^2 + 1} + (\gamma - 1)\sqrt{(n - \gamma)^2 + 4} \\
&+ \sqrt{5}(\gamma - 1) + 2\sqrt{2}\Delta + 4\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

and if $\gamma(T) = \gamma + 1$ or $\gamma(T) = \gamma + 2$, then by Lemma 1.6, $f(n, \gamma)$ is a strictly decreasing function of γ, so we have,

$$\begin{aligned}
SO(G) \leq &(n - 2\gamma + 1)\sqrt{(n - \gamma)^2 + 1} + (\gamma - 1)\sqrt{(n - \gamma)^2 + 4} \\
&+ \sqrt{5}(\gamma - 1) + 2\sqrt{2}\Delta + 4\sqrt{2}(\Delta - 1)^2.
\end{aligned}$$

□

3 Upper bounds on Sombor index of trees, unicyclic and bicyclic graphs with total domination number

In this section we would obtain an upper bound on the Sombor index of trees, unicyclic and bicyclic graphs with given total domination number.

Theorem 3.1. *Let T be a tree with n vertices and total domination number γ_t, then*

$$\begin{aligned} SO(T) \leq & (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1}+(\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4} \\ & +(\gamma_t-2)\sqrt{5}+2(n-\gamma_t)^2+(\gamma_t+3)(n+\gamma_t). \end{aligned}$$

Proof. Let

$$\begin{aligned} g(n,\gamma_t) = & (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1}+(\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4} \\ & +(\gamma_t-2)\sqrt{5}+2(n-\gamma_t)^2+(\gamma_t+3)(n+\gamma_t). \end{aligned}$$

If $n=2$, $T\cong K_2$ and $SO(K_2)=\sqrt{2}<g(2,2)$, If $n=3$, $T\cong P_3$ and $SO(P_3)=2\sqrt{5}<g(3,2)$, If $n=4$, then $T\cong S_4$ *or* P_4, $SO(S_4)=3\sqrt{10}<g(4,2)$ and $SO(P_4)=2\sqrt{5}+\sqrt{8}<g(4,2)$ and the result is true. Therefore let $n\geq 5$ and let us to continue the argument by induction on n. Let $s_1,s_2,\cdots,s_{D+1}$ be a diametral path in T, such that D is diameter of T. If $D=2$, then $T\cong S_n$, $\gamma_t(S_n)=2$, and

$$SO(S_n)=(n-1)\sqrt{(n-1)^2+1}<g(n,2)$$

so, theorem is true. Therefore let $D\geq 3$, $\gamma_t\geq 2$ and the result is true for any tree with $n-1$ vertices. Let $d_{s_2}=t\geq 2$, $N_{s_2}=\{s_1,s_3,z_1,z_2,\cdots,z_{t-2}\}$ and $d_{s_3}=k\geq 2$, $N_{s_3}=\{s_2,s_4,w_1,w_2,\cdots,w_{k-2}\}$. Since $\gamma_t(T)-1\leq\gamma_t(T-s_1)\leq\gamma_t(T)$, the following two cases hold:
Case1: $\gamma_t(T-s_1)=\gamma_t(T)$. We have,

$$\begin{aligned} SO(T) \leq & SO(T-s_1)+\sqrt{t^2+1}+\sqrt{t^2+k^2}-\sqrt{(t-1)^2+k^2} \\ & +\sum_{1}^{t-2}\left(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\right) \\ \leq & g(n-1,\gamma_t)+\sqrt{t^2+1}+\sqrt{t^2+k^2}-\sqrt{(t-1)^2+k^2} \\ & +\sum_{1}^{t-2}\left(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\right) \\ \leq & (n-2\gamma_t+2)\sqrt{(n-\gamma_t)^2+1}+(\gamma_t-2)\sqrt{(n-\gamma_t)^2+4}+(\gamma_t-2)\sqrt{5} \\ & +2(n-\gamma_t-1)^2+(\gamma_t+3)(n+\gamma_t-1)+\sqrt{t^2+1}+\sqrt{t^2+k^2} \\ & -\sqrt{(t-1)^2+k^2}+(t-2)(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}) \\ = & g(n,\gamma_t)+(n-2\gamma_t+3)\left(\sqrt{(n-\gamma_t)^2+1}-\sqrt{(n-\gamma_t+1)^2+1}\right) \\ & +(\gamma_t-2)\left(\sqrt{(n-\gamma_t)^2+4}-\sqrt{(n-\gamma_t+1)^2+4}\right) \\ & -\sqrt{(n-\gamma_t)^2+1}+\sqrt{t^2+1}+\sqrt{t^2+4} \\ & -\sqrt{(t-1)^2+4}+(t-2)\left(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\right) \\ & +2(n-\gamma_t-1)^2+(\gamma_t+3)(n+\gamma_t-1)-2(n-\gamma_t)^2-(\gamma_t+3)(n+\gamma_t). \end{aligned}$$

Thus, we must show that

$$\begin{aligned}
&(n-2\gamma_t+3)\sqrt{(n-\gamma_t)^2+1}+(\gamma_t-2)\sqrt{(n-\gamma_t)^2+4}+\sqrt{t^2+1}\\
&\quad+\sqrt{t^2+4}+(t-2)\sqrt{t^2+1}+2(n-\gamma_t-1)^2+(\gamma_t+3)(n+\gamma_t-1)\\
&\leq (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1}+\sqrt{(n-\gamma_t)^2+1}\\
&\quad+(\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4}+\sqrt{(t-1)^2+4}\\
&\quad+(t-2)\sqrt{(t-1)^2+1}+2(n-\gamma_t)^2+(\gamma_t+3)(n+\gamma_t).
\end{aligned}$$

Since

$$\begin{aligned}
&(n-2\gamma_t+3)\sqrt{(n-\gamma_t)^2+1}+(\gamma_t-2)\sqrt{(n-\gamma_t)^2+4}+\sqrt{t^2+1}\\
&\quad+\sqrt{t^2+4}+(t-2)\sqrt{t^2+1}+2(n-\gamma_t-1)^2+(\gamma_t+3)(n+\gamma_t-1)\\
&\leq (n-2\gamma_t+3)(n-\gamma_t+1)+(\gamma_t-2)(n-\gamma_t+2)+(t+1)\\
&\quad+(t+2)+(t-2)(t+1)+2(n-\gamma_t-1)^2+(\gamma_t+3)(n+\gamma_t-1),
\end{aligned}$$

and

$$\begin{aligned}
&(n-2\gamma_t+3)(n-\gamma_t+1)+(n-\gamma_t)+(\gamma_t-2)(n-\gamma_t+1)+(t-1)\\
&\quad+(t-2)(t-1)+2(n-\gamma_t)^2+(\gamma_t+3)(n+\gamma_t)\\
&\leq (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1}+\sqrt{(n-\gamma_t)^2+1}\\
&\quad+(\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4}+\sqrt{(t-1)^2+4}\\
&\quad+(t-2)\sqrt{(t-1)^2+1}+2(n-\gamma_t)^2+(\gamma_t+3)(n+\gamma_t),
\end{aligned}$$

it suffices to show that

$$\begin{aligned}
&(n-2\gamma_t+3)(n-\gamma_t+1)+(\gamma_t-2)(n-\gamma_t+2)+(t+1)\\
&\quad+(t+2)+(t-2)(t+1)+2(n-\gamma_t-1)^2+(\gamma_t+3)(n+\gamma_t-1)\\
&\leq (n-2\gamma_t+3)(n-\gamma_t+1)+(n-\gamma_t)+(\gamma_t-2)(n-\gamma_t+1)+(t-1)\\
&\quad+(t-2)(t-1)+2(n-\gamma_t)^2+(\gamma_t+3)(n+\gamma_t),
\end{aligned}$$

or $3t-5n+5\gamma_t-3\leq 0$. By definition of total domination number $t\leq\Delta\leq n-\gamma_t+1$, therefore the last inequality changes into $\gamma_t-n\leq 0$, which is correct.
Case2: $\gamma_t(T-s_1)=\gamma_t(T)-1$.

In this case we have $t=2$, because otherwise each total domination set contains s_2. Therefore $\gamma_t(T-s_1)=\gamma_t(T)$, and there is a minimum total domination set D of T such that $s_3\in D$. Moreover,

$$\begin{aligned}
SO(T) &\le SO(T-s_1)+\sqrt{t^2+1}+\sqrt{t^2+k^2}-\sqrt{(t-1)^2+k^2}\\
&\quad+\sum_{1}^{t-2}\left(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\right)\\
&\le g(n-1,\gamma_t-1)+\sqrt{t^2+1}+\sqrt{t^2+k^2}-\sqrt{(t-1)^2+k^2}\\
&\quad+\sum_{1}^{t-2}\left(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\right)\\
&\le (n-2\gamma_t+4)\sqrt{(n-\gamma_t+1)^2+1}+(\gamma_t-3)\sqrt{(n-\gamma_t+1)^2+4}+(\gamma_t-3)\sqrt{5}\\
&\quad+2(n-\gamma_t)^2+(\gamma_t+2)(n+\gamma_t-2)+\sqrt{5}+\sqrt{k^2+4}-\sqrt{k^2+1}\\
&= g(n,\gamma_t)+\sqrt{(n-\gamma_t+1)^2+1}-\sqrt{(n-\gamma_t+1)^2+4}\\
&\quad-n-3\gamma_t-4+\sqrt{k^2+4}-\sqrt{k^2+1}
\end{aligned}$$

Thus, we must show that

$$\begin{aligned}
&\sqrt{(n-\gamma_t+1)^2+1}+\sqrt{k^2+4}-\sqrt{k^2+1}\\
&\le\sqrt{(n-\gamma_t+1)^2+4}+n+3\gamma_t+4.
\end{aligned}$$

But since $k\ge 2$, we have

$$\begin{aligned}
&\sqrt{(n-\gamma_t+1)^2+1}+\sqrt{k^2+4}-\sqrt{k^2+1}\\
&\le n-\gamma_t+\frac{13}{5},
\end{aligned}$$

and

$$\begin{aligned}
&(n-\gamma_t+1)+n+3\gamma_t+4\\
&\le\sqrt{(n-\gamma_t+1)^2+4}+n+3\gamma_t+4,
\end{aligned}$$

it suffices to show that

$$n-\gamma_t+\frac{13}{5}\le(n-\gamma_t+1)+n+3\gamma_t+4,$$

which is obvious. □

The following Lemma is needed in the next theorems.

Lemma 3.2. *Let G be a connected graph with $n\ge 3$ vertices and total domination number γ_t. Then $h(n,\gamma_t)$ defined as following, is a strictly decreasing function of γ_t.*

$$\begin{aligned}
h(n,\gamma_t) &= (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1}+(\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4}\\
&\quad+\sqrt{5}(\gamma_t-2)+2n^2+3n
\end{aligned}$$

Proof. It suffices to show that

$$\frac{\partial h(n,\gamma_t)}{\partial \gamma_t} = -(n-\gamma_t+1)\left[\frac{n-2\gamma_t+3}{\sqrt{(n-\gamma_t+1)^2+1}} + \frac{\gamma_t-2}{\sqrt{(n-\gamma_t+1)^2+4}}\right]$$
$$-2\sqrt{(n-\gamma_t+1)^2+1} + \sqrt{(n-\gamma_t+1)^2+4} + \sqrt{5} < 0$$

Since $n-\gamma_t+1 \geq 2$, as in the proof of Lemma 1.6 we have

$$\frac{n-2\gamma_t+3}{\sqrt{(n-\gamma_t+1)^2+1}} + \frac{\gamma_t-2}{\sqrt{(n-\gamma_t+1)^2+4}} \geq \frac{n-2\gamma_t+3}{\sqrt{(n-\gamma_t+1)^2+4}}$$
$$+\frac{\gamma_t-2}{\sqrt{(n-\gamma_t+1)^2+4}} = \frac{n-\gamma_t+1}{\sqrt{(n-\gamma_t+1)^2+4}} > 0.$$

Therefore, we must show,

$$\sqrt{(n-\gamma_t+1)^2+4} + \sqrt{5} < \frac{(n-\gamma_t+1)^2}{\sqrt{(n-\gamma_t+1)^2+4}} + 2\sqrt{(n-\gamma_t+1)^2+1},$$

whitch is obvious by Lemma 1.6. □

Theorem 3.3. *Let G be a unicyclic graph with n vertices, total domination number* $\gamma_t(G) = \gamma_t$*, and maximum degree* Δ*, then,*

$$SO(G) \leq (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1} + (\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4}$$
$$+\sqrt{5}(\gamma_t-2) + 2n^2 + 3n + \sqrt{2}\Delta + 2\sqrt{2}(\Delta-1)^2.$$

Proof. It is similar to the proof of Theorem 2.1. □

Theorem 3.4. *let G be a bicyclic graph with n vertices, total domination number* γ_t*, and maximum degree* Δ*, then,*

$$SO(G) \leq (n-2\gamma_t+3)\sqrt{(n-\gamma_t+1)^2+1} + (\gamma_t-2)\sqrt{(n-\gamma_t+1)^2+4}$$
$$+\sqrt{5}(\gamma_t-2) + 2n^2 + 3n + 2\sqrt{2}\Delta + 4\sqrt{2}(\Delta-1)^2.$$

Proof. The proof of this theorem is similar to Theorem 2.2. □

Open Problem: In this paper, we did not establish the sharpness of the bounds presented in Theorems 2.1, 2.2, 3.3 and 3.4. A natural question that arises is "whether there exist specific classes of graphs for which these bounds are attained exactly?" More generally, "can we characterize or classify all graphs that achieve equality in these bounds?" Identifying such extremal graph families would not only validate the tightness of the established inequalities, but also provide deeper structural insights into the parameters involved.

4 Conclusion

In this paper, we investigated the Sombor index, a recently introduced vertex-degree-based topological index, in the context of trees, unicyclic, and bicyclic graphs. We derived several bounds for the Sombor index in terms of the domination and total domination numbers. These results highlight meaningful relationships between structural graph parameters and topological indices. Our findings contribute to the growing literature on the Sombor index and its behavior under domination constraints. Further research could explore similar bounds for more complex graph classes or under other domination-related parameters.

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Data is contained within the article.

Conflicts of Interests

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