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Sombor Index on Trees – A Review

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Abstract

The recently developed Sombor Index has garnered significant attention in the research community. Numerous studies have been published based on the Sombor index, about various versions of the Sombor index, studies on different properties of graphs, operations on graphs, chemical applications, and applications to trees. This paper reviews the major research works on the Sombor index in the perspective of trees.

1 Introduction

Graph theory, a remarkable field in mathematics and computer science, is concerned with the study of graphs, which are mathematical structures used to model pairwise associations between objects or different parts within the same object. Among various types of graphs, trees hold a significant place due to their primary attributes and clarity. Trees, defined as connected acyclic graphs, are broadly applied in various applications, including chemical graph theory.

Degree-based topological indices have gained substantial recognition in graph theory research for their ability to condense structural properties of graphs into a single numeric value. Such a topological based index, the

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Sombor (SO) index, was introduced by Gutman in 2021 [19] and it has materialized as an important tool in this area. Defined for a simple graph $G = (V, E)$, with vertices V and edges E, the SO index is calculated using the degrees of adjacent vertices. Its mathematical formulation is given by:

$$\mathrm{SO}(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$$

where $d(u)$ and $d(v)$ denote the degrees of vertices u and v, respectively.

The SO index has exhibited extreme potential in various fields, especially in chemical graph theory, where it is used to predict molecular properties. Trees, representing molecular structures, put forward a simple and natural model for studying these attributes. Therefore, surveying the SO index in the context of trees not only enhances our understanding of this topological index but also give insight on to its pragmatic applications.

This research aims to survey the major research studies on the SO index of trees. In this study, different versions of the SO index are explored, investigated its properties in relation to various tree structures, and discussed its significance in chemical applications. By consolidating existing knowledge and highlighting significant findings, this review seeks to provide a comprehensive overview of the SO index on trees and identify potential directions for future research.

2 Bounds and extremal tree graphs

In this section, the bounds and extremal properties of the Sombor index in the context of tree graphs are surveyed . The extremal tree graphs that maximize or minimize the Sombor index are explored and provided insights into their structural characteristics. Furthermore, various bounds on the Sombor index for trees of a given order and independence number, highlighting key results and their implications are reviewed. Notable research findings are summarized here.

Authors explored the extremal trees with given degree sequence that minimize and maximize the Sombor index in [33] and they characterized the extremal trees with maximum Sombor index among the trees with given degree sequence. The authors proposed 3 algorithms to construct these trees. The first algorithm is to construct a subtree, second algorithm describe the method to merge these subtrees and the third is a Greedy algorithm for constructing a minimum optimal tree.

Let $T_{n,m}$ and $U_{n,m}$ are two unicyclic graphs on n vertices with fixed matching number m. In [46] the authors studied about the above graphs and determined the tree and the unicyclic graph with the maximum Sombor index among $T_{n,m}$ and $U_{n,m}$, respectively.

The authors characterized the extremal graphs with regard to the Sombor index among all the trees with order n and a given diameter in [29]. In the same study, initially the authors ordered the trees based on the Sombor index among the n-vertex trees with diameter 3. Then, the largest and the second largest Sombor indices of n-vertex trees with a given diameter $d \geq 4$ are determined and characterized the corresponding trees. Additionally, characterized the extremal trees with order n which reach from the third to the fourth (resp. the sixth, the seventh) largest Sombor indices with $d = 4$ (resp. $d = 5, d \geq 6$) for $n - d = 3$. Also characterized the extremal n-order trees which reach from the third to the fifth (resp. the eighth, the ninth) largest Sombor indices with $d = 4$ (resp. $d = 5, d \geq 6$) for $n - d \geq 4$. The top four trees with order n with respect to the Sombor index are also categorized. Few results are derived based on the concept [29].

A study of Sombor index among trees with a maximum of three branch vertices is done and determined the extremal values of Sombor Index [7].

In another study, General Sombor index is explored and obtained its bounds for trees. The authors also determined the trees with the extremal general Sombor index [34].

3 Special graph classes

This section provide a survey of research work, which focused on Sombor index in specific graph classes.

A cactus is defined as a connected graph in which each block is either an edge or a cycle. Let $T(n, k)$ be the set of cacti of order n and with number of cycles equal to$k$. Evidently, $T(n, 0)$ is the set of all trees and

$T(n,1)$ is the set of all unicyclic graphs, then the cacti of order n and with k ($k \geq 2$) cycles is a generalization of cycle number k. In [18], the authors established an acute upper bound for the Sombor index of a cactus in $G(n,k)$ and the corresponding extremal graphs are characterized. Additionally,a sharp lower bound for the Sombor index of a cactus in $G(n,k)$ is computed and characterized the corresponding extremal graphs for the case when $n \geq 6k-3$ as well. In the study, a conjecture is also proposed about the minimum value of the Sombor index among $G(n,k)$ when $n \geq 3k$.

A Quasi tree is called a connected graph $G = (V,E)$ if there exists $u \in V(G)$ such that $G-u$ is a tree. It is denoted as follows.

$Q(n,k) = \{G : G$ is a quasi-tree graph of order n with $G-u$ being a tree and $d_G(u) = k\}$.

The minimum and the second minimum Sombor indices of all quasi-trees in $Q(n,k)$ are determined, and the corresponding extremal graphs are characterized in [28].

The authors disproved the conjecture posed by Liu et al. [30] and derived and proved the corrected version [23].

The new theorem is given below.

Theorem 1. *[23] For $n \geq 7$, if T is a chemical tree of order n, then*

$$eSO_{red}(T) \leq \frac{1}{3}\left(2e^3 + e^3\sqrt{2}\right)n + \frac{1}{3}\left(2e^3 - 5e^3\sqrt{2}\right) + \begin{cases} \frac{1}{3}\left(3e - 5e^3 - e^3\sqrt{2} + 3e\sqrt{10}\right), & \text{if } n \equiv 0\,(mod\ 3) \\ \frac{1}{3}\left(6e^2 - 7e^3 - 2e^3\sqrt{2} + 3e\sqrt{13}\right), & \text{if } n \equiv 1\,(mod\ 3) \\ 0, & \text{if } n \equiv 2\,(mod\ 3). \end{cases}$$

In the same work the authors derived the following results also.

Lemma 1. *[23] Let T be a chemical tree of order n, where $n \geq 7$. The inequality*

$$\Gamma(T) < \frac{1}{3}\left(6e^2 - 7e^3 - 2e^3\sqrt{2} + 3e\sqrt{13}\right) (\approx -41.6804),$$

holds if any of the following conditions is satisfied:

1. $\max\{m_{3,3}, m_{2,2}, m_{2,3}\} \geq 1$,
2. $\max\{m_{3,4}, m_{2,4}\} \geq 2$,
3. $n_2 + n_3 \geq 2$.

Theorem 2. *[23] Among all chemical trees of a fixed order n, the members of the class T_n are the only trees possessing the maximum value of the multiplicative (reduced) Sombor index for every $n \geq 11$.*

Theorem 3. *[23] For every $n \geq 7$, the trees of the class T_n^* uniquely attain the maximum value of the exponential Sombor index among all chemical trees of a fixed order n.*

Let $G_1(n, k)$ is the set of all quasi-tree graphs of order$n$ with $G - u$ being a tree and the degree of u in G being k. Top three values of the Sombor indices of all quasi tree graphs in $G_1(n, k)$ is studied and their corresponding extremal graphs are characterized [45].

A greedy tree was defined as the unique tree from the set of all trees that have a specified degree sequence such that its breadth first traversal yields the sequence$(1, 2, 3, ...)$. In a study based on greedy trees, it is proved that the greedy tree provides the minimum value of Sombor index in the set of all trees that have a specified degree sequence [10].

An alternative proof for the same theorem is provided in [9] by constructing an auxiliary graph invariant named Pseudo Sombor index.

Alternating greedy tree which provides the maximum Sombor index has explored in [8].

Banana tree graphs and fractal tree type Dendrimers are measured using Sombor index using graph theory based edge partition method [32]. Shannon's entropy model is used to determine the graph based entropy of these graphs.

Another interesting study was carried out among k apex unicyclic graphs and k apex trees [44]. The authors determined the extremal values and extremal graphs of Sombor index among k apex unicyclic graphs and k apex trees respectively.

Another important work is the computation of the maximum Sombor index of trees of order n with a given independence number α, where $\frac{n}{2} \leq \alpha(G) \leq n-1$ [11]. They also identified the single graph among the chosen class where the maximum Sombor index is attained.

Let $T(n, \alpha)$ be the group of trees of order n and independence number α. If $\alpha = n-1$, then $T(n, n-1) = \{S_n\}$ and $SO(S_n) = (n-1)\sqrt{(n-1)^2+1} = \alpha\sqrt{\alpha^2+1}$. Here the case is when $\alpha \leq n-2$.

Let $T_1(n, \alpha)$ and $T_2(n, \alpha)$ be subsets of $T(n, \alpha)$. Define $T^*(n, \alpha)$ as the tree of order n obtained from the star $S_{n-\alpha}$ by attaching exactly one pendant edge to each of the vertices $\{v_1, v_2, \ldots, v_{n-(\alpha+1)}\} \subseteq V(S_{n-\alpha})$ and attaching $2\alpha-(n-1)$ pendant vertices to the central vertex v_0 of $S_{n-\alpha}$.

The main results of the study are given below.

Lemma 2. *[11] Let $T^*(n, \alpha) \in T_1(n, \alpha) \subset T(n, \alpha)$ be defined as above, then*

$$SO(T^*(n, \alpha)) = (2\alpha-(n-1))\sqrt{\alpha^2+1} + (n-(\alpha+1))\left(\sqrt{\alpha^2+22} + \frac{\sqrt{2}}{2} + 1\right).$$

Lemma 3. *[11] Let $T \in T(n, \alpha)$ be a tree with maximal Sombor index, then $T \in T_1(n, \alpha) \cup T_2(n, \alpha)$.*

4 Studies on molecular trees

The very first study about the chemical applicability of Sombor indices are published in [35]. The predictive and discriminating potentials of the Sombor index, the reduced Sombor index, and the average Sombor index were examined in the same study.

In [1] , the authors calculated the best possible upper bounds on Sombor index and reduced Sombor indices for molecular trees with respect to order and number of branching vertices or vertices of degree 2. The optimal molecular trees having the derived bounds are also completely distinguished in the same work. The main results are given below.

Theorem 4. *[1] If $n \geq 6$ and $C \in \mathcal{C}_{n,1}$, then*

(i) $SO(C) \leq 2\sqrt{2(n-6)} + 3\sqrt{5} + 3\sqrt{17}$,

(ii) $SO_{red}(C) \leq \sqrt{2(n-6)} + 10 + \sqrt{10}$.

The equalities occur if and only if $C \cong B_0$.

Theorem 5. *[1] If $C \in \mathcal{C}_{n,n_b}$ and $1 < n_b < \frac{n-1}{4}$, then*

(i) $SO(C) \leq 2\sqrt{2(n-1)} + 2\sqrt{17(n_b+1)} + 4\sqrt{5(n_b-1)} - 8\sqrt{2n_b}$,

(ii) $SO_{red}(C) \leq \sqrt{2(n-4n_b-1)} + 2\sqrt{10(n_b-1)} + 6(n_b+1)$,

and the equalities occur if and only if $C \cong B_1$.

Theorem 6. *[1] If $C \in \mathcal{C}_{n,n_b}$ such that $\frac{n-1}{4} \leq n_b < \frac{n-2}{3}$, then*

(i) $SO(C) \leq 4\sqrt{5(n-3n_b-2)} - 4\sqrt{2(n-4n_b-1)} + 2\sqrt{17(n_b+1)}$,

(ii) $SO_{red}(C) \leq 2\sqrt{10(n-3n_b-2)} - 3\sqrt{2(n-4n_b-1)} + 6(n_b+1)$,

and the equalities occur if and only if $C \cong B_2$.

Theorem 7. *[1] For the molecular tree $C \in \mathcal{C}^*_{n,q}$, where $n \geq 5$, the following results hold:*

(a) If $C \in \mathcal{C}^*_{n,n-4} \setminus \mathcal{C}_3$, then $SO(C) < SO(C_3)$.

(b) If $C \in \mathcal{C}^*_{n,n-5} \setminus \mathcal{C}_4$, then $SO(C) < SO(C_4)$.

Theorem 8. *Let $C \in \mathcal{C}^*_{n,q}$ for $q < n-5$ such that $n_3(C) = 0$. Then*

$$SO(C) \leq \begin{cases} \frac{2\sqrt{17}}{3}(n-q+1) + \frac{4\sqrt{2}}{3}(n-4q-5) & \\ \quad +4\sqrt{5}q, & \text{if } q < \frac{n-5}{4}, \\ & \\ \frac{2\sqrt{17}}{3}(n-q+1) + \frac{4\sqrt{5}}{3}(n-q-5) & \\ \quad -\frac{2\sqrt{2}}{3}(n-4q-5), & \text{if } q \geq \frac{n-5}{4}. \end{cases}$$

and

$$SO_{red}(C) \leq \begin{cases} \sqrt{2}(n-4q-5) + 2(n-q+1) & \\ \quad +2\sqrt{10}q, & \text{if } q < \frac{n-5}{4}, \\ & \\ 2(n-q+1) + \frac{2\sqrt{10}}{3}(n-q-5) & \\ \quad -\frac{\sqrt{2}}{3}(n-4q-5), & \text{if } q \geq \frac{n-5}{4}. \end{cases}$$

Equalities hold if and only if $C \in Q_0$.

In [16], Deng et al. investigated the chemical characteristics of the Sombor Index and it is shown that the new index is powerful in estimating the physico-chemical properties with high accuracy compared to some well-established and commonly used indices. The authors obtained a sharp upper bound for the Sombor index among all molecular trees with fixed numbers of vertices, and characterized those molecular trees achieving the extremal value. Also, they computed the extremal values of the reduced Sombor index for molecular trees.

In [21], Gutman et.al. is concerned with the Sombor index (SO) of Kragujevac trees (Kg) and a slightly more general definition of Kg is offered. In the same work, a general combinatorial expression for SO(Kg) is established and determined the graphs with minimum and maximum SO(Kg) values.

The same authors also studied about the KG-Sombor index (KG) [26] and applied it to Kragujevac trees (Kg) [22]. They have also established a general combinatorial expression for KG(Kg) index and the species with minimum and maximum KG(Kg)-values are determined. Motivated by these works,recently, the Sombor and KG-Sombor indices of Kragujevac trees were studied also by Selenge et al. [36] and they determined the extremal Kragujevac trees based on these indices. The authors also provided the analytical proof of the results in their work. Kosari et al. also studied about KG Sombor index and established lower bound and determined the extremal trees that achieved this bound [24].

Sharp bound on the Sombor index of chemical trees are studied and characterized the cases of the equalities [25]. Conjectures regarding the second maximal chemical trees of order n with respect to Sombor index when $n = 0(mod3)$ and $n = 1mod(3)$ [25].

5 New variants and extensions

In this section, we review new variants and extensions of the Sombor index for trees.

In [40], the authors, Tang et al. proposed a novel geometric method for constructing vertex-degree-based molecular structure descriptors, which is the perimeter of an ellipse whose focal points represent the degree-point and its dual-point of a pair of adjacent vertices in a graph. This new index is named as Elliptic Sombor index. The authors analyzed the chemical applicability of this index, established its mathematical properties and determined the extremal values for this index among all molecular trees and characterized the corresponding extremal graphs.

Let $G = G(V, E)$ be a simple connected graph with vertex set V and edge set E. The elliptic Sombor index of G is defined as

$$ESO(G) = \sum_{uv \in E} (d(u) + d(v))\sqrt{d^2(u) + d^2(v)},$$

where $d(u)$ denotes the degree of vertex u. In [39], the authors determined the maximal value of the elliptic Sombor index of trees with a given diameter or matching number or number of pendent vertices and the extremal values of the elliptic Sombor index of unicyclic graphs are also identified. Furthermore, they characterized those trees and unicyclic graphs that achieve the obtained extremal values.

Let $T_{n,\Delta}$ and $U_{n,\Delta}$ be the set of trees and unicyclic graphs with n vertices and maximum degree Δ, respectively. Zhou et al., in their work [47], characterized the tree and the unicyclic graph with minimum Sombor index among $T_{n,\Delta}$ and $U_{n,\Delta}$.

Few years ago, in 2011, Kulli introduced a variant of the Sombor index called the first irregularity Sombor index [27]. The first irregularity Sombor index of a graph G, denoted by $ISO_1(G)$, is defined as the sum of weights $\left|d_G^2(v) - d_G^2(w)\right|$ of all edges vw of $E(G)$, where $d_G(v)$ denotes the degree of a node v in G. In [15], authors proved that for any tree T of order n with maximum degree Δ,

$$ISO_1(T) \geq \begin{cases} \sqrt{(\Delta-1)\Delta^2 - 1} + \sqrt{\Delta^2 - 4} + \sqrt{3} & \text{if } \Delta < n-1, \\ \Delta\sqrt{\Delta^2 - 1} & \text{if } \Delta = n-1. \end{cases}$$

Characterization of the extremal trees were also done in the same work.

In the study [37], the authors presented the maximum and minimum Sombor indices of trees with fixed domination number and they have also identified the corresponding extremal trees.

An upper bound on the Sombor index of unicyclic and bicyclic graphs of order p was obtained by Cruz and Rada in [6] but characterization of the extremal graphs were not performed. In the same study, they communicated that the maximal graphs over the set of unicyclic and bicyclic graphs with respect to Sombor index, is an open problem. Motivated by this, in [12], Das and Gutman perfectly solved these problems.

In their research [43], Wang and Wu, studied about the maximum value of the Reduced Sombor index among all molecular trees of order n with perfect matching and they characterized the corresponding extremal trees. They also proved that the maximum molecular trees of exponential reduced Sombor index and reduced Sombor index are the same, which was conjectured by Liu, You, Tang and Liu (2021) [42].

For a positive real number k, the k-Sombor index of a graph G, introduced by Réti et al., is defined as

$$SO_k(G) = \sum_{uv \in E(G)} \frac{d(u)^k + d(v)^k}{d(u)d(v)}.$$

where $d(u)$ denotes the degree of the vertex u in G. By definition, $SO_2(G)$ is exactly the Sombor index of G, while $SO_1(G)$ is the first Zagreb index of G. In [42], authors presented the extremal values of the k-Sombor index of trees with parameters such as matching number, number of pendant vertices, and diameter for $k \geq 1$. This generalizes the relevant results on Sombor index due to Chen, Li, and Wang [4]. Handling $SO_k(G)$ appears to be different for $k < 1$ in contrast to the case when $k \geq 1$. To exemplify this, authors also characterized the extremal trees with respect to $SO_2(G)$ with matching number, number of pendant vertices, and diameter. Three relevant conjectures are also proposed in the same study.

The authors determined the minimum Sombor index of trees of order $n \geq 7$ with $p \geq 3$ pendant vertices in [31]. They also extended the study and determined the minimum value of the Sombor index of chemical trees of order n with p pendant vertices.

In another study, Sombor index and Co-index are studied and the maximum and second maximum of Sombor index and the minimum and second minimum Sombor co-index in two-trees are determined [17].

Two new variants of Sombor index such as reduced and increased Sombor indices are studied [13] and authors established sharp lower bounds on the reduced and increased Sombor index of trees in terms of their order and maximum vertex degree. They also characterized the extremal trees that attained the bounds.

A modified version of Sombor index named as X index is studied [3] and extremal trees with respect to this index are determined.

Recently, studies based on total domination number of trees has received attention. In one study, lower bound on Sombor index of trees with a given order and total domination number is obtained and the authors characterized the trees achieving the bound [38].

Chemical application of different variants of Sombor indices are investigated and found that all most all studied invariants are useful in predicting physicochemical properties with high accuracy [20]. The invariants are studied on molecular trees with fixed number of vertices and trees achieving the extremal value are characterized [41].

Sombor index of trees with various degree restrictions are studied and characterized all trees that have maximum and minimum Sombor index values [2]. in the same study, comparison of trees with different degree sequences are carried out and few corollaries are deduced [2].

Basic mathematical properties of Geometric Sombor index is studied [14] and proved that for any tree with fixed order and maximum degree Δ, the Geometric index is bounded below by $(\Delta^3 - \Delta)/2$. Characterization of extremal trees and unicyclic graphs that has the lower bound are also done in the same work [14].

6 Conclusion

This review on Sombor index on trees contribute an extensive survey of the published research work on Sombor index on trees, concentrating on various features such as bounds and extremal tree graphs, special graph classes, and studies on molecular trees. This discussion emphasizes the significant role of the Sombor index in understanding the structural properties and chemical characteristics of molecular graphs. Furthermore, novel variants and versions of the Sombor index have been surveyed, exemplifying its inventiveness and potential for further research. The insights acquired from these studies offer valuable contributions to the field of mathematical chemistry and graph theory, paving the way for future research inquiries and applications of the Sombor index in diverse scientific domains.

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