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Research Article

Degree-weighted Sombor indices of trees and unicyclic graphs: An extremal approach

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Abstract: We consider two generalizations of the Sombor index, obtained by weighting the standard contribution $\sqrt{d_\Omega(\eta)^2 + d_\Omega(\eta')^2}$ of an edge $\eta\eta'$ of a graph Ω by the sum and by the product of degrees of its end-vertices, respectively. The first generalization has been considered under the name of the elliptic Sombor index, while the second one seems to be new. We consider trees and unicyclic graphs on a given number of vertices n with a given maximum degree Δ and characterize the graphs minimizing both generalizations over those classes of graphs.

Keywords: Sombor index, degree-weighted Sombor index, elliptic Sombor index, trees, unicyclic graphs.

AMS Subject classification: 05C07, 05C09, 05C92

1. Introduction

The recently introduced Sombor index belongs to the class of bond-additive topological indices, defined as the sum over all edges of contributions depending on various properties of the end-vertices. Soon after its introduction, it has been generalized in various ways. One of such generalizations, motivated by geometric considerations and known as the elliptic Sombor index, has been introduced in a recent paper by Gutman, Furtula and Oz [14]. It follows the common pattern of similar generalizations in which the original edge contributions are weighted by some function of degrees of

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the end-vertices. The two most common cases are the additive and the multiplicative weightings, in which the original contribution is multiplied by the sum, and by the product of degrees of the end-vertices, respectively. In this parlance, the elliptic Sombor index is the additively degree-weighted Sombor index. The multiplicatively weighted version has not been considered in [14], probably for the lack of a clear geometric interpretation present in the additively weighted case. Nevertheless, it might be interesting to consider both variants in a unifying context and to investigate their basic properties and potential usefulness.

In this paper we investigate the behavior of both generalizations over all trees and unicyclic graphs on a given number of vertices with a given maximum degree. The maximum degree constraint is a fairly natural one, given the chemical motivation behind the considered indices and the fact that the graphs modeling organic compounds cannot have vertices of degree exceeding four. Hence, we look at the mentioned classes of graphs and characterize their members minimizing both generalizations.

2. Definitions and preliminaries

Let Ω be a simple connected graph of order n with vertex set $V(\Omega)$ and edge set $E(\Omega)$. For $\eta \in \Omega$, we let $N_\Omega(\eta) = \{\eta' \in V(\Omega) \mid \eta\eta' \in E(\Omega)\}$ be the open neighborhood of η and $d_\Omega(\eta) = |N_\Omega(\eta)|$ be the degree of η. The maximum degree of Ω is denoted by Δ. The (shortest path) distance between the vertices $\eta, \eta' \in V(\Omega)$, denoted by $d(\eta, \eta')$, is the number of edges in any shortest path connecting η and η' in G.

A *topological index* of a graph Ω is a numerical quantity depending on some properties of Ω which remains invariant under its automorphisms. Hundreds of topological indices have been defined so far; we refer the reader to [24] for a comprehensive review of their uses in chemistry and other disciplines.

In 2021, a novel degree-based topological index, called the *Sombor index*, was introduced by Gutman [12]. The Sombor index is defined as

$$SO(\Omega) = \sum_{\eta\eta' \in E(\Omega)} \sqrt{d_\Omega(\eta)^2 + d_\Omega(\eta')^2}.$$

In [12], Gutman obtained some mathematical properties of the Sombor index. Some lower and upper bounds on Sombor index in terms of graph parameters were obtained by Das et al. [4, 6]. Réti, et al. [22] determined the maximum Sombor index among all connected k-cyclic graphs of order n, where $1 \le k \le n-2$. In [18], Ning, et al. determined the graph(s) with maximum Sombor index among all cacti with n vertices and k cut edges. For more informations about Sombor index and its variants see [2, 3, 5, 7–10, 13, 15–17, 19, 21, 25].

Recently, Gutman, Furtula and Oz [14] defined a new variant of Sombor index, called the *elliptic Sombor index*. They defined it as

$$ESO(\Omega) = \sum_{\eta\eta' \in E(\Omega)} (d_\Omega(\eta) + d_\Omega(\eta'))\sqrt{d_\Omega(\eta)^2 + d_\Omega(\eta')^2}.$$

The new invariant quickly attracted attention of researchers, and several recent papers are reporting its properties. We refer to [11, 20, 23] for some recent results on ESO index.
As mentioned in the Introduction, the elliptic Sombor index is the additively degree-weighted Sombor index. Here we consider also the multiplicatively weighted case. For a given graph Ω, its *multiplicatively degree-weighted Sombor index* $MSO(\Omega)$ is defined as

$$MSO(\Omega) = \sum_{\eta\eta' \in E(\Omega)} (d_\Omega(\eta)\, d_\Omega(\eta'))\sqrt{d_\Omega(\eta)^2 + d_\Omega(\eta')^2}.$$

It was brought to our attention during the reviewing process that the multiplicatively weighted case was introduced in a recent reference [1] under the name of *Zagreb-Sombor index*.
In this paper, we investigate behavior of both degree-weighted versions of the Sombor index over all trees and unicyclic graphs with a given maximum degree. In particular, we characterize all graphs minimizing both indices over the considered classes.

3. Trees

A *tree* is a connected graph with no cycles. A tree on n vertices has exactly $n-1$ edges. A vertex of degree one in a tree is usually called a *leaf*, while a vertex of degree greater than two is called a *branching vertex* or just a *branching*. A tree with exactly one branching is called a *spider*. By extending the zoological analogy, the paths attached to the only branching vertex in a spider are called its *legs*. A leg is *short* if it has the length one, and *long* otherwise. Hence, a star is a special spider with all legs short. Paths can be seen as degenerate spiders, but we will not need this fact.
In this section, we consider the set of all trees of order n with maximum degree Δ and denote it by $\mathcal{T}_n^\Delta$. By T we denote a rooted tree with the root ω, where $d_T(\omega) = \Delta$ and $N_T(\omega) = \{\omega_1, \omega_2, \ldots, \omega_\Delta\}$. Unless explicitly said otherwise, we will assume $\Delta > 2$.
We start by introducing three transformations of trees from $\mathcal{T}_n^\Delta$ which reduce the values of the considered indices. Our goal is to show that any tree minimizing $ESO(T)$ or $MSO(T)$ over $\mathcal{T}_n^\Delta$ must be a spider. Before considering the transformations in more detail, we make the following observation.

Proposition 1. *The functions*

$$f_a(x, y) = (x + y)\sqrt{x^2 + y^2} \qquad \text{and} \qquad f_m(x, y) = xy\sqrt{x^2 + y^2}$$

are symmetric in their arguments and both are increasing in their first argument if the second one is held constant.

The claim, playing a crucial role in subsequent proofs, is easily verified by computing the respective partial derivatives, and we omit the details.

Lemma 1. *Let $T \in \mathcal{T}_n^{\Delta}$ and T has a branching vertex $\theta \neq \omega$. If θ is adjacent to at least two leaves, then there is a tree $T' \in \mathcal{T}_n^{\Delta}$ with $ESO(T) > ESO(T')$ and $MSO(T) > MSO(T')$.*

Proof. If there are several non-root branchings, we chose one farthest from the root. (If there are more than one at the maximum distance from the root, we chose any of them.) Hence, let θ be a branching with $d_T(\theta) = \alpha \geq 3$ such that $d_T(\omega, \theta)$ is maximum over all branchings. Further, let $N_T(\theta) = \{\theta_1, \theta_2, \ldots, \theta_\alpha\}$. We may assume that θ_α lies on the (ω, θ)-path and $d_T(\theta_1) = d_T(\theta_2) = 1$. Let $T' = (T - \{\theta\theta_1\}) \cup \{\theta_1\theta_2\}$. In other words, we form a new tree T' by detaching a leaf (θ_1) from the considered branching vertex and attaching it to another leaf (θ_2) adjacent to θ. This operations

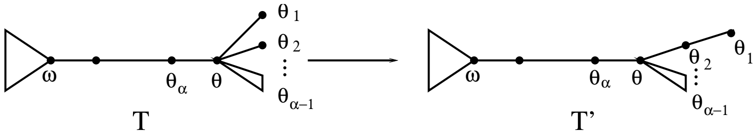

Figure 1. **With the proof of Lemma 1.**

leaves the contributions of most edges unchanged. The only ones that change are the contributions of the edges incident to θ in T and in T' and the contribution of the transplanted edge. Now we have

$$\begin{aligned}
ESO(T) - ESO(T') = & \sum_{\eta\eta' \in E(T)} (d_T(\eta) + d_T(\eta'))\sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
& - \sum_{\eta\eta' \in E(T')} (d_{T'}(\eta) + d_{T'}(\eta'))\sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
= & (d_T(\theta_1) + d_T(\theta))\sqrt{d_T^2(\theta_1) + d_T^2(\theta)} \\
& + (d_T(\theta_2) + d_T(\theta))\sqrt{d_T^2(\theta_2) + d_T^2(\theta)} \\
& + \sum_{i=3}^{\alpha}(d_T(\theta) + d_T(\theta_i))\sqrt{d_T^2(\theta) + d_T^2(\theta_i)} \\
& - (d_{T'}(\theta_1) + d_{T'}(\theta_2))\sqrt{d_{T'}^2(\theta_1) + d_{T'}^2(\theta_2)} \\
& - (d_{T'}(\theta_2) + d_{T'}(\theta))\sqrt{d_{T'}^2(\theta_2) + d_{T'}^2(\theta)} \\
& - \sum_{i=3}^{\alpha}(d_{T'}(\theta) + d_{T'}(\theta_i))\sqrt{d_{T'}^2(\theta) + d_T^2(\theta_i)} \\
= & 2(\alpha + 1)\sqrt{\alpha^2 + 1} + \sum_{i=3}^{\alpha}(\alpha + d_T(\theta_i))\sqrt{\alpha^2 + d_T^2(\theta_i)}
\end{aligned}$$

$$
\begin{aligned}
&- 3\sqrt{5} - (\alpha+1)\sqrt{(\alpha-1)^2+4} \\
&- \sum_{i=3}^{\alpha} (\alpha + d_T(\theta_i) - 1)\sqrt{(\alpha-1)^2 + d_T^2(\theta_i)} \\
>& 2(\alpha+1)\sqrt{\alpha^2+1} - 3\sqrt{5} - (\alpha+1)\sqrt{(\alpha-1)^2+4}.
\end{aligned}
$$

Here the fact that $f_a(x,y)$ is increasing in its first argument allowed us to conclude that the difference of two sums is positive, hence the inequality. It can be easily verified that the resulting final expression is an increasing function of α, and that it is positive for $\alpha = 3$. Hence, it is strictly positive for all $\alpha \geq 3$, $ESO(T) - ESO(T') > 0$, and the claim follows.
Similarly,

$$
\begin{aligned}
MSO(T) - MSO(T') =& \sum_{\eta\eta' \in E(T)} d_T(\eta)\, d_T(\eta') \sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
&- \sum_{\eta\eta' \in E(T')} d_{T'}(\eta)\, d_{T'}(\eta') \sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
=& 2\,\alpha\sqrt{\alpha^2+1} + \sum_{i=3}^{\alpha} \alpha\, d_T(\theta_i) \sqrt{\alpha^2 + d_T^2(\theta_i)} \\
&- 2\sqrt{5} - 2(\alpha-1)\sqrt{(\alpha-1)^2+4} \\
&- \sum_{i=3}^{\alpha} (\alpha-1)\, d_T(\theta_i) \sqrt{(\alpha-1)^2 + d_T^2(\theta_i)} \\
>& 2\,\alpha\sqrt{\alpha^2+1} - 2\sqrt{5} - 2(\alpha-1)\sqrt{(\alpha-1)^2+4}.
\end{aligned}
$$

Again, the inequality is a consequence of the positivity of the difference of two sums, since f_m is increasing in its first argument. The resulting expression is increasing in α and the claim follows by verifying that it is positive for $\alpha = 3$. □

Lemma 2. *Let $T \in \mathcal{T}_n^{\Delta}$ and T has a branching vertex $\theta \neq \omega$. If θ is adjacent to exactly one leaf, then there is a tree $T' \in \mathcal{T}_n^{\Delta}$ with $ESO(T) > ESO(T')$ and $MSO(T) > MSO(T')$.*

Proof. As in the previous Lemma, let $d_T(\theta) = \alpha \geq 3$ and $d_T(\omega, \theta)$ is maximum over all vertices $\theta \neq \omega$. Let $N_T(\theta) = \{\theta_1, \theta_2, \ldots, \theta_\alpha\}$. We may again assume that θ_α lies on the (ω, θ)-path and $d_T(\theta_1) = 1$. Then $d_T(\theta_i) = 2$ for $2 \leq i \leq \alpha - 1$. Let $\theta\gamma_1\gamma_2\ldots\gamma_\rho$ is a path in T such that $\rho \geq 2$ and $\theta_2 = \gamma_1$. Let T' be a tree formed by detaching θ_1 from θ and transplanting it to the leaf at the end of the path starting at θ_2. Hence,

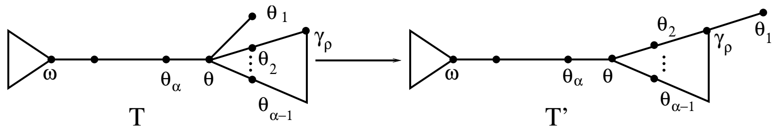

Figure 2. **With the proof of Lemma 2.**

$T' = (T - \{\theta\theta_1\}) \cup \{\theta_1\gamma_\rho\}$. Then

$$
\begin{aligned}
ESO(T) - ESO(T') = &\sum_{\eta\eta' \in E(T)} (d_T(\eta) + d_T(\eta'))\sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
&- \sum_{\eta\eta' \in E(T')} (d_{T'}(\eta) + d_{T'}(\eta'))\sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
=&(\alpha+1)\sqrt{\alpha^2+1} + 3\sqrt{5} + \sum_{i=2}^{\alpha}(\alpha + d_T(\theta_i))\sqrt{\alpha^2 + d_T^2(\theta_i)} \\
&- 3\sqrt{5} - 4\sqrt{8} - \sum_{i=2}^{\alpha}(\alpha + d_T(\theta_i) - 1)\sqrt{(\alpha-1)^2 + d_T^2(\theta_i)} \\
>&(\alpha+1)\sqrt{\alpha^2+1} - 4\sqrt{8}.
\end{aligned}
$$

The inequality follows by the same argument as in the previous Lemma. By plugging in $\alpha = 3$ in the resulting expression, we obtain $4\sqrt{10} - 4\sqrt{8} > 0$, and the claim follows by referring once more to Proposition 1.
For $MSO(T) - MSO(T')$, we have

$$
\begin{aligned}
MSO(T) - MSO(T') = &\sum_{\eta\eta' \in E(T)} d_T(\eta)\, d_T(\eta')\, \sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
&- \sum_{\eta\eta' \in E(T')} d_{T'}(\eta)\, d_{T'}(\eta')\, \sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
=&\alpha\,\sqrt{\alpha^2+1} + 2\alpha\,\sqrt{\alpha^2+4} + 2\sqrt{5} + \sum_{i=3}^{\alpha} \alpha\, d_T(\theta_i)\,\sqrt{\alpha^2 + d_T^2(\theta_i)} \\
&- 2\sqrt{5} - 2(\alpha-1)\,\sqrt{(\alpha-1)^2+4} - 4\sqrt{8} \\
&- \sum_{i=3}^{\alpha}(\alpha-1)\, d_T(\theta_i)\,\sqrt{(\alpha-1)^2 + d_T^2(\theta_i)} \\
>&\alpha\,\sqrt{\alpha^2+1} + 2\alpha\,\sqrt{\alpha^2+4} - 2(\alpha-1)\,\sqrt{(\alpha-1)^2+4} - 4\sqrt{8}.
\end{aligned}
$$

If $\alpha \geq 4$, then $\alpha\,\sqrt{\alpha^2+1} \geq 4\sqrt{17} > 4\sqrt{8}$ and $MSO(T) - MSO(T') > 0$, and if $\alpha = 3$, then

$$MSO(T) - MSO(T') > 3\,\sqrt{10} + 6\,\sqrt{13} - 8\,\sqrt{8} \approx 8.4927 > 0.$$

Hence, the claim is established for all $\alpha \geq 3$. □

Lemma 3. *Let $T \in \mathcal{T}_n^{\Delta}$ and T has a branching vertex $\theta \neq \omega$. Then there is a tree $T' \in \mathcal{T}_n^{\Delta}$ with $ESO(T) > ESO(T')$ and $MSO(T) > MSO(T')$.*

Proof. Let $d_T(\theta) = \alpha \geq 3$ and $d_T(\omega, \theta)$ is maximum over all vertices $\theta \neq \omega$ and let $N_T(\theta) = \{\theta_1, \theta_2, \ldots, \theta_\alpha\}$. By Lemmas 1 and 2, $d_T(\theta_i) = 2$ for $1 \leq i \leq \alpha - 1$. Let $\theta\sigma_1\sigma_2\ldots\sigma_\kappa$ and $\theta\gamma_1\gamma_2\ldots\gamma_\rho$ be two paths in T for $\kappa, \rho \geq 2$ such that $\theta_1 = \sigma_1$ and $\theta_2 = \gamma_1$. Let $T' = (T - \{\theta\theta_1\}) \cup \{\theta_1\gamma_\rho\}$. Then

$$\begin{aligned}
ESO(T) - ESO(T') = &\sum_{\eta\eta' \in E(T)} (d_T(\eta) + d_T(\eta'))\sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
&- \sum_{\eta\eta' \in E(T')} (d_{T'}(\eta) + d_{T'}(\eta'))\sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
=&(\alpha + 2)\sqrt{\alpha^2 + 4} + 3\sqrt{5} + \sum_{i=2}^{\alpha}(\alpha + d_T(\theta_i))\sqrt{\alpha^2 + d_T^2(\theta_i)} \\
&- 8\sqrt{8} - \sum_{i=2}^{\alpha}(\alpha + d_T(\theta_i) - 1)\sqrt{(\alpha - 1)^2 + d_T^2(\theta_i)} \\
>&(\alpha + 2)\sqrt{\alpha^2 + 4} + 3\sqrt{5} - 8\sqrt{8} \\
\geq&5\sqrt{13} + 3\sqrt{5} - 8\sqrt{8} > 0.
\end{aligned}$$

In the same way,

$$\begin{aligned}
MSO(T) - MSO(T') = &\sum_{\eta\eta' \in E(T)} d_T(\eta)\, d_T(\eta')\, \sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
&- \sum_{\eta\eta' \in E(T')} d_{T'}(\eta)\, d_{T'}(\eta')\, \sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
=&2\,\alpha\,\sqrt{\alpha^2 + 4} + 2\sqrt{5} + \sum_{i=2}^{\alpha} \alpha\, d_T(\theta_i)\, \sqrt{\alpha^2 + d_T^2(\theta_i)} \\
&- 8\,\sqrt{8} - \sum_{i=2}^{\alpha}(\alpha - 1)\, d_T(\theta_i)\, \sqrt{(\alpha - 1)^2 + d_T^2(\theta_i)} \\
>&2\,\alpha\,\sqrt{\alpha^2 + 4} + 2\sqrt{5} - 8\,\sqrt{8} \\
\geq&6\,\sqrt{13} + 2\sqrt{5} - 8\,\sqrt{8} \approx 3.4780.
\end{aligned}$$

□

An alternative approach, yielding essentially the same results, was employed in ref. [1]. We can summarize our results so far by saying that both the additively and the multiplicatively weighted Sombor index are minimized over $\mathcal{T}_n^{\Delta}$ by spiders. Our next result offers further insight into the structure of minimizing spiders.

Proposition 2. *Let $T \in \mathcal{T}_n^{\Delta}$ be a spider with $\Delta \geq 3$ legs. If T has two legs of length at least two, then there exists a spider $T' \in \mathcal{T}_n^{\Delta}$ with $ESO(T) > ESO(T')$ and $MSO(T) > MSO(T')$.*

Proof. Let ω be the center of T and $N_T(\omega) = \{\omega_1, \ldots, \omega_\Delta\}$. We may assume that $\omega_1\theta_1\theta_2\ldots\theta_\kappa$ and $\omega_2\gamma_1\gamma_2\ldots\gamma_\rho$, $\kappa, \rho \geq 2$ are two longest legs of T. Let $T' = (T - \{\omega_1\theta_1\}) \cup \{\theta_1\gamma_\rho\}$. Then

$$\begin{aligned}
ESO(T) - ESO(T') = & \sum_{\eta\eta' \in E(T)} (d_T(\eta) + d_T(\eta'))\sqrt{d_T^2(\eta) + d_T^2(\eta')} \\
& - \sum_{\eta\eta' \in E(T')} (d_{T'}(\eta) + d_{T'}(\eta'))\sqrt{d_{T'}^2(\eta) + d_{T'}^2(\eta')} \\
= & (d_T(\omega) + d_T(\omega_1))\sqrt{d_T^2(\omega) + d_T^2(\omega_1)} \\
& + (d_T(\omega_1) + d_T(\theta_1))\sqrt{d_T^2(\omega_1) + d_T^2(\theta_1)} \\
& + (d_T(\gamma_\rho) + d_T(\gamma_{\rho-1}))\sqrt{d_T^2(\gamma_\rho) + d_T^2(\gamma_{\rho-1})} \\
& - (d_{T'}(\omega) + d_{T'}(\omega_1))\sqrt{d_{T'}^2(\omega) + d_T^2(\omega_1)} \\
& - (d_{T'}(\theta_1) + d_{T'}(\gamma_\rho))\sqrt{d_{T'}^2(\theta_1) + d_{T'}^2(\gamma_\rho)} \\
& - (d_{T'}(\gamma_\rho) + d_{T'}(\gamma_{\rho-1}))\sqrt{d_{T'}^2(\gamma_\rho) + d_{T'}^2(\gamma_{\rho-1})} \\
= & (\Delta + 2)\sqrt{\Delta^2 + 4} + 3\sqrt{5} - (\Delta + 1)\sqrt{\Delta^2 + 1} - 4\sqrt{8}.
\end{aligned}$$

The final expression is positive for $\Delta = 3$, and it can be easily verified that it is an increasing function of Δ. Hence, it is positive for all $\Delta \geq 3$, and the first claim is established. By performing the analogous computations for MSO, we obtain

$$MSO(T) - MSO(T') = 2\,\Delta\,\sqrt{\Delta^2 + 4} + 2\,\sqrt{5} - \Delta\,\sqrt{\Delta^2 + 1} - 4\sqrt{8}.$$

Again, the resulting expression is an increasing function of Δ, and the second claim follows by verifying that it is positive for $\Delta = 3$. □

Hence, in both cases the minimizing spiders have at most one long leg. Such trees are sometime called *brooms*.
Now we have the first main theorem of this paper.

Theorem 1. *If $T \in \mathcal{T}_n^{\Delta}$, then*

$$ESO(T) = \Delta(\Delta + 1)\sqrt{\Delta^2 + 1},$$

and

$$MSO(T) = \Delta^2\,\sqrt{\Delta^2 + 1},$$

when $\Delta = n-1$. *Also,*

$$ESO(T) \geq (\Delta^2-1)\sqrt{\Delta^2+1}+(\Delta+2)\sqrt{\Delta^2+4}+4(n-\Delta-2)\sqrt{8}+3\sqrt{5},$$

and

$$MSO(T) \geq \Delta\,(\Delta-1)\sqrt{\Delta^2+1}+2\,\Delta\sqrt{\Delta^2+4}+4(n-\Delta-2)\sqrt{8}+2\sqrt{5},$$

when $\Delta < n-1$. *Equality holds if and only if* T *is a spider with at most one long leg.*

Proof. We prove the Theorem for the additively weighted case. The proof for the MSO index is similar and we omit the details.
Assume that $T^{'} \in \mathcal{T}_n^{\Delta}$ with $ESO(T) \geq ESO(T')$ for all trees $T \in \mathcal{T}_n^{\Delta}$. Let $d_{T'}(\omega) = \Delta$ and root T' at ω. Cases $\Delta = 0$, $\Delta = 1$, and $\Delta = 2$ are trivial and easily verified by direct computation. If $\Delta \geq 3$, then from Lemmas 1, 2 and 3, T' is a spider with center ω, and, by Proposition 2, T' must be a broom. Hence,

$$ESO(T') = ESO(S_n) = \Delta(\Delta+1)\sqrt{\Delta^2+1},$$

when $T' = S_n$ ($\Delta = n-1$), and

$$ESO(T') = (\Delta^2-1)\sqrt{\Delta^2+1}+(\Delta+2)\sqrt{\Delta^2+4}+4(n-\Delta-2)\sqrt{8}+3\sqrt{5}$$

when $\Delta < n-1$. This completes the proof. □

4. Unicyclic graphs

A *unicyclic graph* of order n is a connected graph containing exactly one cycle C_ℓ on $\ell \leq n$ vertices with, possibly, some trees whose roots lie on the cycle C_ℓ. A connected unicyclic graphs has the same number of edges and vertices. Throughout this section, $\mathcal{U}_n^{\Delta}$ stands for the set of unicyclic graphs with n vertices and maximum degree Δ. In this section, we study and characterize the unicyclic graphs minimizing $ESO(U)$ and $MSO(U)$ over $\mathcal{U}_n^{\Delta}$. The results are less elegant than in the case of trees, but nevertheless, we present the full solution of the problem. We proceed by proving a series of auxiliary results, each of them specifying some properties of the minimizing graphs.

Lemma 4. *Let* $U \in \mathcal{U}_n^{\Delta}$ *and no vertex of degree* Δ *lies on the unique cycle of* U. *Let* ω *be a vertex of degree* Δ *and let* θ *be a vertex on the cycle of* U *closest to* ω. *If* U *contains another branching vertex besides* ω *and* θ, *or if* $d_U(\theta) \geq 4$, *then there is a unicyclic graph* $U' \in \mathcal{U}_n^{\Delta}$ *such that* $ESO(U') < ESO(U)$ *and* $MSO(U') < MSO(U)$.

Proof. Since ω is not on the unique cycle C of U, it must be in some of the trees rooted in vertices of C. Moreover, the tree containing ω is rooted in θ. There must be a unique path connecting ω and θ; denote this path by P.

Let us first suppose that there is another branching vertex, say η, in U which is neither ω nor θ. Let T_η be the rooted tree such that T_η has maximum conceivable number of vertices connected to η.

If $\eta \notin V(C) \cup V(P)$, then by Lemmas 1, 2 and 3, we can convert T_η to a path P_η of the same order, $ESO(T_\eta) > ESO(P_\eta)$ and $MSO(T_\eta) > MSO(P_\eta)$. Let $U' \in \mathcal{U}_n^\Delta$ be obtained from U by removing T_η and adding P_η. Then $ESO(U) > ESO(U')$ and $MSO(U) > MSO(U')$.

Now, let $\eta \in V(C)$ (the proof of the case $\eta \in V(P)$ is similar) and let $\eta_1, \eta_2 \in N_U(\eta) - V(T_\eta)$, where η_1 and η_2 are on C. Then, by Lemmas 1, 2 and 3, we can convert T_η to a path P_η of the same order such that $ESO(T_\eta) > ESO(P_\eta)$ and $MSO(T_\eta) > MSO(P_\eta)$. Let $U' \in \mathcal{U}_n^\Delta$ be obtained from U by replacing T_η by P_η. Then $ESO(U) \geq ESO(U')$, $MSO(U) \geq MSO(U')$ and $d_{U'}(\eta) = 3$. Now let $U'' \in \mathcal{U}_n^\Delta$ be derived from U' by removing P_η and adding the path $\eta_1\, P_\eta\, \eta$. Thus $d_{U''}(\eta_1) = d_{U'}(\eta_1)$ and $d_{U''}(\eta_2) = d_{U'}(\eta_2)$. If the length of P_η is at least two, then

$$\begin{aligned} ESO(U') - ESO(U'') =& (d_{U'}(\eta_1) + 3)\sqrt{d_{U'}^2(\eta_1) + 9} \\ &+ (d_{U'}(\eta_2) + 3)\sqrt{d_{U'}^2(\eta_2) + 9} + 5\sqrt{13} + 3\sqrt{5} \\ &- (d_{U''}(\eta_1) + 2)\sqrt{d_{U''}^2(\eta_1) + 4} \\ &- (d_{U''}(\eta_2) + 2)\sqrt{d_{U''}^2(\eta_2) + 4} - 8\sqrt{8} \\ >& 5\sqrt{13} + 3\sqrt{5} - 8\sqrt{8} > 0, \end{aligned}$$

and

$$\begin{aligned} MSO(U') - MSO(U'') =& 3\, d_{U'}(\eta_1)\sqrt{d_{U'}^2(\eta_1) + 9} \\ &+ 3\, d_{U'}(\eta_2)\sqrt{d_{U'}^2(\eta_2) + 9} + 6\sqrt{13} + 2\sqrt{5} \\ &- 2\, d_{U''}(\eta_1)\sqrt{d_{U''}^2(\eta_1) + 4} \\ &- 2\, d_{U''}(\eta_2)\sqrt{d_{U''}^2(\eta_2) + 4} - 8\sqrt{8} \\ >& 6\sqrt{13} + 2\sqrt{5} - 8\sqrt{8} > 0. \end{aligned}$$

Now if the length of P_η is one, then

$$\begin{aligned} ESO(U') - ESO(U'') =& (d_{U'}(\eta_1) + 3)\sqrt{d_{U'}^2(\eta_1) + 9} \\ &+ (d_{U'}(\eta_2) + 3)\sqrt{d_{U'}^2(\eta_2) + 9} + 4\sqrt{10} \end{aligned}$$

$$
\begin{aligned}
&- (d_{U''}(\eta_1)+2)\sqrt{d^2_{U''}(\eta_1)+4} - (d_{U''}(\eta_2)+2)\sqrt{d^2_{U''}(\eta_2)+4} - 4\sqrt{8}\\
&> 4\sqrt{10} - 4\sqrt{8} > 0,
\end{aligned}
$$

and

$$
\begin{aligned}
MSO(U') - MSO(U'') =& 3\, d_{U'}(\eta_1)\sqrt{d^2_{U'}(\eta_1)+9}\\
&+ 3\, d_{U'}(\eta_2)\sqrt{d^2_{U'}(\eta_2)+9} + 3\sqrt{10}\\
&- 2\, d_{U''}(\eta_1)\sqrt{d^2_{U''}(\eta_1)+4}\\
&- 2\, d_{U''}(\eta_2)\sqrt{d^2_{U''}(\eta_2)+4} - 4\sqrt{8}\\
>& d_{U'}(\eta_1)\sqrt{d^2_{U'}(\eta_1)+9} + d_{U'}(\eta_2)\sqrt{d^2_{U'}(\eta_2)+9} + 3\sqrt{10} - 4\sqrt{8}\\
\geq& 4\sqrt{13} + 3\sqrt{10} - 4\sqrt{8} > 0.
\end{aligned}
$$

This settles the case of branching vertices different from ω and θ. It remains to consider the case of $d_U(\theta) \geq 4$.
So, assume that $d_U(\theta) \geq 4$, $\theta_1, \theta_2, \theta_3 \in N_U(\theta)$, where θ_1 and θ_2 are on C and θ_3 is on P. Let T_θ be the rooted tree such that T_θ has maximum conceivable number of vertices connected to θ and $\theta_1, \theta_2, \theta_3 \notin V(T_\theta)$. Then, by Lemmas 1, 2 and 3, we can convert T_θ to a path P_θ of the same order such that $ESO(T_\theta) \geq ESO(P_\theta)$ and $MSO(T_\theta) \geq MSO(P_\theta)$. Let $U' \in \mathcal{U}_n^\Delta$ be obtained from U by removing T_θ and adding P_θ. Then $ESO(U) \geq ESO(U')$, $MSO(U) \geq MSO(U')$ and $d_{U'}(\theta) = 4$. Now let $U'' \in \mathcal{U}_n^\Delta$ be derived from U' by removing P_θ and adding the path $\theta_1\, P_\theta\, \theta$. Thus $d_{U''}(\theta_1) = d_{U'}(\theta_1)$, $d_{U''}(\theta_2) = d_{U'}(\theta_2)$ and $d_{U''}(\theta_3) = d_{U'}(\theta_3)$. If the length of P_θ is at least two, then

$$
\begin{aligned}
ESO(U') - ESO(U'') =& (d_{U'}(\theta_1)+4)\sqrt{d^2_{U'}(\theta_1)+16}\\
&+ (d_{U'}(\theta_2)+4)\sqrt{d^2_{U'}(\theta_2)+16}\\
&+ (d_{U'}(\theta_3)+4)\sqrt{d^2_{U'}(\theta_3)+16} + 6\sqrt{20} + 3\sqrt{5}\\
&- (d_{U''}(\theta_1)+2)\sqrt{d^2_{U''}(\theta_1)+4}\\
&- (d_{U''}(\theta_2)+3)\sqrt{d^2_{U''}(\theta_2)+9}\\
&- (d_{U''}(\theta_3)+3)\sqrt{d^2_{U''}(\theta_3)+9} - 5\sqrt{13} - 4\sqrt{8}\\
>& 6\sqrt{20} + 3\sqrt{5} - 5\sqrt{13} - 4\sqrt{8} > 0,
\end{aligned}
$$

and

$$\begin{aligned}
MSO(U') - MSO(U'') =& 4\, d_{U'}(\theta_1)\sqrt{d^2_{U'}(\theta_1) + 16} \\
&+ 4\, d_{U'}(\theta_2)\sqrt{d^2_{U'}(\theta_2) + 16} \\
&+ 4\, d_{U'}(\theta_3)\sqrt{d^2_{U'}(\theta_3) + 16} + 8\sqrt{20} + 2\sqrt{5} \\
&- 2\, d_{U''}(\theta_1)\sqrt{d^2_{U''}(\theta_1) + 4} \\
&- 3\, d_{U''}(\theta_2)\sqrt{d^2_{U''}(\theta_2) + 9} \\
&- 3\, d_{U''}(\theta_3)\sqrt{d^2_{U''}(\theta_3) + 9} - 6\sqrt{13} - 4\sqrt{8} \\
>& 8\sqrt{20} + 2\sqrt{5} - 6\sqrt{13} - 4\sqrt{8} > 0,
\end{aligned}$$

If the length of P_θ is one, then

$$\begin{aligned}
ESO(U') - ESO(U'') =& (d_{U'}(\theta_1) + 4)\sqrt{d^2_{U'}(\theta_1) + 16} \\
&+ (d_{U'}(\theta_2) + 4)\sqrt{d^2_{U'}(\theta_2) + 16} \\
&+ (d_{U'}(\theta_3) + 4)\sqrt{d^2_{U'}(\theta_3) + 16} + 5\sqrt{17} \\
&- (d_{U''}(\theta_1) + 2)\sqrt{d^2_{U''}(\theta_1) + 4} \\
&- (d_{U''}(\theta_2) + 3)\sqrt{d^2_{U''}(\theta_2) + 9} \\
&- (d_{U''}(\theta_3) + 3)\sqrt{d^2_{U''}(\theta_3) + 9} - 5\sqrt{13} \\
>& 5\sqrt{17} - 5\sqrt{13} > 0,
\end{aligned}$$

and

$$\begin{aligned}
MSO(U') - MSO(U'') =& 4\, d_{U'}(\theta_1)\sqrt{d^2_{U'}(\theta_1) + 16} \\
&+ 4\, d_{U'}(\theta_2)\sqrt{d^2_{U'}(\theta_2) + 16} \\
&+ 4\, d_{U'}(\theta_3)\sqrt{d^2_{U'}(\theta_3) + 16} + 4\sqrt{17} \\
&- 2\, d_{U''}(\theta_1)\sqrt{d^2_{U''}(\theta_1) + 4} \\
&- 3\, d_{U''}(\theta_2)\sqrt{d^2_{U''}(\theta_2) + 9} \\
&- 3\, d_{U''}(\theta_3)\sqrt{d^2_{U''}(\theta_3) + 9} - 6\sqrt{13} \\
>& 2\, d_{U'}(\theta_1)\sqrt{d^2_{U'}(\theta_1) + 16} + 4\sqrt{17} - 6\sqrt{13} \\
\geq& 4\sqrt{20} + 4\sqrt{17} - 6\sqrt{13} > 0.
\end{aligned}$$

This settles the case of $d_U(\theta) \geq 4$, and hence the Lemma. □

The proof of the next lemma follows along the same line and is therefore omitted.

Lemma 5. *Let $U \in \mathcal{U}_n^{\Delta}$ have the vertex ω of degree Δ on its cycle. If there is another branching vertex $\eta \in V(U) - \{\omega\}$ with $d_U(\eta) \geq 3$, then $\mathcal{U}_n^{\Delta}$ contains a unicyclic graph U' with $ESO(U') < ESO(U)$ and $MSO(U') < MSO(U)$.*

Hence, a minimizing graph in $\mathcal{U}_n^{\Delta}$ for both considered indices can have at most two branchings. Moreover, if a vertex of maximum degree Δ is on the unique cycle, then it is the only branching of any minimizing graph. Now we proceed by investigating the neighborhood of the branching vertices.

Lemma 6. *Let $U \in \mathcal{U}_n^{\Delta}$ have the vertex ω of degree Δ which is not on its unique cycle. If ω is adjacent to at least two vertices of degree more than one, then $\mathcal{U}_n^{\Delta}$ contains an unicyclic graph U' with $ESO(U) > ESO(U')$ and $MSO(U) > MSO(U')$.*

Proof. As before, let θ be a vertex on the cycle of U in which the tree containing ω is rooted and let P be the (ω, θ)-path. Assume that T_ω is the rooted tree such that T_ω has the maximum conceivable number of vertices connected to ω. By Lemmas 1, 2 and 3, we can convert T_ω to the tree T'_ω of the same order and $ESO(T_\omega) \geq ESO(T'_\omega)$. Let $U' \in \mathcal{U}_n^{\Delta}$ be obtained from U by removing T_ω and adding T'_ω. Then $ESO(U) \geq ESO(U')$ and $MSO(U) \geq MSO(U')$.
If ω is adjacent with at least two vertices of degree more than one, then, by Theorem 1, T'_ω is a spider with at most one long leg. Denote this leg by $P' =: \eta_1\,\eta_2\,\ldots\eta_k$. Assume that $\eta_1 \in N_{U'}(\omega) \cap V(P')$ and $\gamma \in N_{U'}(\omega) - \{\eta_1\}$ lies on the P. Let $U'' \in \mathcal{U}_n^{\Delta}$ be derived from U' by removing the vertices $\eta_2, \ldots, \eta_k$ and adding the paths $\gamma\,\eta_2\,\ldots\eta_k\,\omega$. By Lemma 4, we can assume that $d_{U''}(\gamma) = d_{U'}(\gamma) = 2$.
Then

$$\begin{aligned} ESO(U') - ESO(U'') =& 2(\Delta+2)\sqrt{\Delta^2+4} + 3\sqrt{5} \\ & - (\Delta+2)\sqrt{\Delta^2+4} - (\Delta+1)\sqrt{\Delta^2+1} - 4\sqrt{8} \\ =& (\Delta+2)\sqrt{\Delta^2+4} + 3\sqrt{5} - (\Delta+1)\sqrt{\Delta^2+1} - 4\sqrt{8} > 0, \end{aligned}$$

and

$$\begin{aligned} MSO(U') - MSO(U'') =& 4\,\Delta\sqrt{\Delta^2+4} + 2\sqrt{5} \\ & - 2\,\Delta\sqrt{\Delta^2+4} - \Delta\sqrt{\Delta^2+1} - 4\sqrt{8} \\ =& 2\,\Delta\sqrt{\Delta^2+4} + 2\sqrt{5} - \Delta\sqrt{\Delta^2+1} - 4\sqrt{8} > 0. \end{aligned}$$

By the same arguments as in the proof of Proposition 2, $MSO(U') - MSO(U'') > 0$. □

The proof of the next lemma is very similar, and is therefore omitted.

Lemma 7. *Let $U \in \mathcal{U}_n^{\Delta}$ has the vertex ω of degree Δ on its cycle. If ω is adjacent with at least three vertices of degree more than one, then $\mathcal{U}_n^{\Delta}$ contains a unicyclic graph U' with $ESO(U) > ESO(U')$ and $MSO(U) > MSO(U')$.*

Now we consider the following three sets:

- Let $\mathcal{U}_1$ be the set of unicyclic graphs from $\mathcal{U}_n^{\Delta}$ such that every unicyclic graph $U \in \mathcal{U}_1$ has a vertex ω of degree Δ, ω is adjacent with $\Delta - 1$ leaves and ω is not on the cycle of U. Also, θ is a vertex on cycle of U such that $d_U(\omega, \theta)$ is the minimum, $d_U(\omega, \theta) = 1$, $d_U(\theta) = 3$, and for every vertex $\eta \in V(U) - \{\omega, \theta\}$, $d_U(\eta) \leq 2$. Therefore, for every unicyclic graph $U \in \mathcal{U}_1$,

$$ESO(U) = (\Delta-1)(\Delta+1)\sqrt{\Delta^2+1} + (\Delta+3)\sqrt{\Delta^2+9} + 10\sqrt{13} + 4\sqrt{8}(n-\Delta-2),$$

  and

$$MSO(U) = \Delta(\Delta-1)\sqrt{\Delta^2+1} + 3\,\Delta\sqrt{\Delta^2+9} + 12\sqrt{13} + 4\sqrt{8}(n-\Delta-2).$$

- Let $\mathcal{U}_2$ be the set of unicyclic graphs from $\mathcal{U}_n^{\Delta}$ such that every unicyclic graph $U \in \mathcal{U}_2$ has a vertex ω of degree Δ, ω is adjacent with $\Delta - 1$ leaves and ω is not on the cycle of U. Also, θ is a vertex on cycle of U such that $d_U(\omega, \theta)$ is the minimum, $d_U(\omega, \theta) \geq 2$, $d_U(\theta) = 3$ and for every vertex $\eta \in V(U) - \{\omega, \theta\}$, $d_U(\eta) \leq 2$. Therefore, for every unicyclic graph $U \in \mathcal{U}_2$,

$$ESO(U) = (\Delta-1)(\Delta+1)\sqrt{\Delta^2+1} + (\Delta+2)\sqrt{\Delta^2+4} + 15\sqrt{13} + 4\sqrt{8}(n-\Delta-3),$$

  and

$$MSO(U) = \Delta(\Delta-1)\sqrt{\Delta^2+1} + 2\,\Delta\sqrt{\Delta^2+4} + 18\sqrt{13} + 4\sqrt{8}(n-\Delta-3).$$

- Let $\mathcal{U}_3$ be the set of unicyclic graphs from $\mathcal{U}_n^{\Delta}$ such that every unicyclic graph $U \in \mathcal{U}_3$ has a vertex ω of degree Δ, ω is adjacent with $\Delta - 2$ leaves and ω is on the cycle of U. Also, for every vertex $\eta \in V(U) - \{\omega, \theta\}$, $d_U(\eta) \leq 2$. Therefore, for every unicyclic graph $U \in \mathcal{U}_3$,

$$ESO(U) = (\Delta-2)(\Delta+1)\sqrt{\Delta^2+1} + 2(\Delta+2)\sqrt{\Delta^2+4} + 4\sqrt{8}(n-\Delta),$$

  and

$$MSO(U) = \Delta(\Delta-2)\sqrt{\Delta^2+1} + 4\,\Delta\sqrt{\Delta^2+4} + 4\sqrt{8}(n-\Delta).$$

The examples are shown in Figure 3

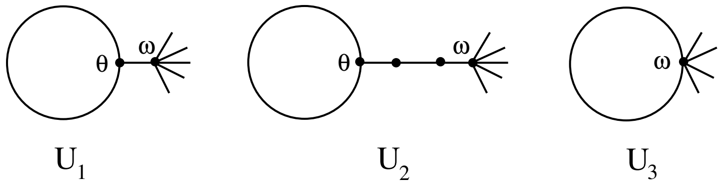

Figure 3. **Examples of unicyclic graphs U_i from $\mathcal{U}_i$ for $i = 1, 2, 3$ and $\Delta = 6$.**

Lemma 8. *Let $U_1 \in \mathcal{U}_1$ and $U_2 \in \mathcal{U}_2$ be two unicyclic graphs from $\mathcal{U}_n^\Delta$ with $\Delta < n-3$. Then $ESO(U_1) > ESO(U_2)$ and $MSO(U_1) > MSO(U_2)$.*

Proof.

$$\begin{aligned} ESO(U_1) - ESO(U_2) =& (\Delta-1)(\Delta+1)\sqrt{\Delta^2+1} + (\Delta+3)\sqrt{\Delta^2+9} \\ &+ 10\sqrt{13} + 4\sqrt{8}(n-\Delta-2) \\ &- (\Delta-1)(\Delta+1)\sqrt{\Delta^2+1} - (\Delta+2)\sqrt{\Delta^2+4} \\ &- 15\sqrt{13} - 4\sqrt{8}(n-\Delta-3) \\ =& (\Delta+3)\sqrt{\Delta^2+9} + 4\sqrt{8} - (\Delta+2)\sqrt{\Delta^2+4} - 5\sqrt{13}. \end{aligned}$$

It can be easily verified that the resulting expression is an increasing function of Δ and that it is nonnegative for $\Delta = 3$. This establishes the first claim. Similarly,

$$\begin{aligned} MSO(U_1) - MSO(U_2) =& \Delta(\Delta-1)\sqrt{\Delta^2+1} + 3\,\Delta\sqrt{\Delta^2+9} \\ &+ 12\sqrt{13} + 4\sqrt{8}(n-\Delta-2) \\ &- \Delta(\Delta-1)\sqrt{\Delta^2+1} - 2\,\Delta\sqrt{\Delta^2+4} \\ &- 18\sqrt{13} - 4\sqrt{8}(n-\Delta-3) \\ =& 3\,\Delta\sqrt{\Delta^2+9} + 4\sqrt{8} - 2\,\Delta\sqrt{\Delta^2+4} - 6\sqrt{13}, \end{aligned}$$

and the claim follows by similar arguments. □

Lemma 9. *Let $U_2 \in \mathcal{U}_2$ and $U_3 \in \mathcal{U}_3$ be two unicyclic graphs of $\mathcal{U}_n^\Delta$.*
a) If $\Delta \geq 19$, then $ESO(U_3) > ESO(U_2)$ and if $\Delta < 19$, then $ESO(U_2) > ESO(U_3)$.
b) If $\Delta \geq 6$, then $MSO(U_3) > MSO(U_2)$ and if $\Delta < 6$, then $MSO(U_2) > MSO(U_3)$.

Proof. Proof of case (a):

$$\begin{aligned}ESO(U_3)-ESO(U_2)=&(\Delta-2)(\Delta+1)\sqrt{\Delta^2+1}+2(\Delta+2)\sqrt{\Delta^2+4}\\&+4\sqrt{8}(n-\Delta)\\&-(\Delta-1)(\Delta+1)\sqrt{\Delta^2+1}-(\Delta+2)\sqrt{\Delta^2+4}\\&-15\sqrt{13}-4\sqrt{8}(n-\Delta-3)\\=&(\Delta+2)\sqrt{\Delta^2+4}+12\sqrt{8}-(\Delta+1)\sqrt{\Delta^2+1}-15\sqrt{13}.\end{aligned}$$

The resulting expression is an increasing function on Δ for all nonnegative values of its argument. Moreover, its only zero on $[0,\infty)$ lies between 18 and 19. Hence, the expression changes its sign there and is negative for $\Delta\le 18$ and positive for $\Delta\ge 19$, as claimed in the statement of the Lemma.
Proof of case (b):

$$\begin{aligned}MSO(U_3)-MSO(U_2)=&\Delta(\Delta-2)\sqrt{\Delta^2+1}+4\,\Delta\sqrt{\Delta^2+4}\\&+4\sqrt{8}(n-\Delta)\\&-\Delta(\Delta-1)\sqrt{\Delta^2+1}-2\,\Delta\sqrt{\Delta^2+4}\\&-18\sqrt{13}-4\sqrt{8}(n-\Delta-3)\\=&2\,\Delta\sqrt{\Delta^2+4}+12\sqrt{8}-\Delta\sqrt{\Delta^2+1}-18\sqrt{13}.\end{aligned}$$

Again, the resulting expression is an increasing function in Δ changing its sign from negative to positive between 5 and 6, and the claim follows. □

Now we can formulate our second main result.

Theorem 2. *If $U\in\mathcal{U}_n^{\Delta}$, then*

- $$ESO(U)=n(n-3)\sqrt{(n-1)^2+1}+2(n+1)\sqrt{(n-1)^2+4}+4\sqrt{8},$$

  and

  $$MSO(U)=(n-1)(n-3)\sqrt{(n-1)^2+1}+4\,(n-1)\sqrt{(n-1)^2+4}+4\sqrt{8},$$

  when $\Delta=n-1$.

- $$ESO(U)\ge(n-1)(n-4)\sqrt{(n-2)^2+1}+2n\sqrt{(n-2)^2+4}+8\sqrt{8},$$

  and

  $$MSO(U)\ge(n-2)(n-4)\sqrt{(n-2)^2+1}+4\,(n-2)\sqrt{(n-2)^2+4}+8\sqrt{8},$$

  when $\Delta=n-2$, with equality if and only if $U\in\mathcal{U}_3$.

- $$ESO(U) \geq 2(n-1)\sqrt{(n-3)^2+4}+(n-5)(n-2)\sqrt{(n-3)^2+1}+12\sqrt{8},$$

  and

  $$MSO(U) \geq 4\,(n-3)\sqrt{(n-3)^2+4}+(n-5)(n-3)\sqrt{(n-3)^2+1}+12\sqrt{8},$$

  when $\Delta = n-3$*, with equality if and only if* $U \in \mathcal{U}_3$*.*

- $$ESO(U) \geq (\Delta-2)(\Delta+1)\sqrt{\Delta^2+1}+2(\Delta+2)\sqrt{\Delta^2+4}+4\sqrt{8}(n-\Delta),$$

  when $\Delta < n-3$ *and* $3 \leq \Delta \leq 18$*, with equality if and only if* $U \in \mathcal{U}_3$*, and*

  $$ESO(U) \geq (\Delta-1)(\Delta+1)\sqrt{\Delta^2+1}+(\Delta+3)\sqrt{\Delta^2+9}+4\sqrt{8}(n-\Delta-3),$$

  when $19 \leq \Delta < n-3$*, with equality if and only if* $U \in \mathcal{U}_2$*.*

- $$MSO(U) \geq \Delta(\Delta-2)\sqrt{\Delta^2+1}+4\,\Delta\sqrt{\Delta^2+4}+4\sqrt{8}(n-\Delta),$$

  when $\Delta < n-3$ *and* $3 \leq \Delta \leq 5$*, with equality if and only if* $U \in \mathcal{U}_3$*, and*

  $$MSO(U) \geq \Delta(\Delta-1)\sqrt{\Delta^2+1}+2\,\Delta\sqrt{\Delta^2+4}+18\sqrt{13}+4\sqrt{8}(n-\Delta-3),$$

  when $6 \leq \Delta < n-3$*, with equality if and only if* $U \in \mathcal{U}_2$*.*

Proof. Assume that $U' \in \mathcal{U}_n^{\Delta}$ with $ESO(U) \geq ESO(U')$ (and $MSO(U) \geq MSO(U')$) for each $U \in \mathcal{U}_n^{\Delta}$. By Lemmas 4, 5, 6, 7, 8 and 9, U' must satisfy one of the following cases:

Case 1. If $\Delta = n-1$, then $U' \in \mathcal{U}_3$,

$$ESO(U') = n(n-3)\sqrt{(n-1)^2+1}+2(n+1)\sqrt{(n-1)^2+4}+4\sqrt{8},$$

and

$$MSO(U') = (n-1)(n-3)\sqrt{(n-1)^2+1}+4\,(n-1)\sqrt{(n-1)^2+4}+4\sqrt{8}.$$

Case 2. If $\Delta = n-2$, then $U' \in \mathcal{U}_3$,

$$ESO(U') = (n-1)(n-4)\sqrt{(n-2)^2+1}+2n\sqrt{(n-2)^2+4}+8\sqrt{8}.$$

and

$$MSO(U) \geq (n-2)(n-4)\sqrt{(n-2)^2+1}+4\,(n-2)\sqrt{(n-2)^2+4}+8\sqrt{8}.$$

Case 3. If $\Delta = n-3$, then $U' \in \mathcal{U}_1 \cup \mathcal{U}_3$. Let $U' = U_1 \in \mathcal{U}_1$ and $U' = U_3 \in \mathcal{U}_3$. Then

$$\begin{aligned}
ESO(U_1) - ESO(U_3) =& n\sqrt{(n-3)^2+9} + (n-4)(n-2)\sqrt{(n-3)^2+1} + 10\sqrt{13} + 4\sqrt{8} \\
& - 2(n-1)\sqrt{(n-3)^2+4} - (n-5)(n-2)\sqrt{(n-3)^2+1} - 12\sqrt{8} \\
=& n\sqrt{(n-3)^2+9} + (n-2)\sqrt{(n-3)^2+1} + 10\sqrt{13} \\
& - 2(n-1)\sqrt{(n-3)^2+4} - 8\sqrt{8} \\
=& n[\sqrt{(n-3)^2+9} + \sqrt{(n-3)^2+1} - 2\sqrt{(n-3)^2+4}] \\
& + 2[\sqrt{(n-3)^2+4} - \sqrt{(n-3)^2+1}] + [10\sqrt{13} - 8\sqrt{8}] > 0,
\end{aligned}$$

and

$$\begin{aligned}
MSO(U_1) - MSO(U_3) =& 3\,(n-3)\sqrt{(n-3)^2+9} + (n-4)(n-3)\sqrt{(n-3)^2+1} \\
& + 12\sqrt{13} + 4\sqrt{8} \\
& - 4\,(n-3)\sqrt{(n-3)^2+4} - (n-5)(n-3)\sqrt{(n-3)^2+1} - 12\sqrt{8} \\
=& 3\,(n-3)\sqrt{(n-3)^2+9} + (n-3)\sqrt{(n-3)^2+1} + 12\sqrt{13} \\
& - 4\,(n-3)\sqrt{(n-3)^2+4} - 8\sqrt{8} \\
=& (n-3)[3\sqrt{(n-3)^2+9} + \sqrt{(n-3)^2+1} - 4\sqrt{(n-3)^2+4}] \\
& + [12\sqrt{13} - 8\sqrt{8}] > 0.
\end{aligned}$$

Therefore, if $\Delta = n-3$, then $U' = U_3$ and

$$ESO(U') = 2(n-1)\sqrt{(n-3)^2+4} + (n-5)(n-2)\sqrt{(n-3)^2+1} + 12\sqrt{8},$$

and

$$MSO(U') = 4\,(n-3)\sqrt{(n-3)^2+4} + (n-5)(n-3)\sqrt{(n-3)^2+1} + 12\sqrt{8},$$

Case 4. If $\Delta < n-3$ and $3 \le \Delta \le 18$, then $U' \in \mathcal{U}_3$,

$$ESO(U') = (\Delta-2)(\Delta+1)\sqrt{\Delta^2+1} + 2(\Delta+2)\sqrt{\Delta^2+4} + 4\sqrt{8}(n-\Delta).$$

Also, if $19 \le \Delta < n-3$, then $U' \in \mathcal{U}_2$, and

$$ESO(U') = (\Delta-1)(\Delta+1)\sqrt{\Delta^2+1} + (\Delta+3)\sqrt{\Delta^2+9} + 4\sqrt{8}(n-\Delta-3).$$

Case 5. If $\Delta < n-3$ and $3 \le \Delta \le 5$, then $U' \in \mathcal{U}_3$,

$$MSO(U') = \Delta(\Delta-2)\sqrt{\Delta^2+1} + 4\,\Delta\sqrt{\Delta^2+4} + 4\sqrt{8}(n-\Delta).$$

Also, if $6 \le \Delta < n-3$, then $U' \in \mathcal{U}_2$, and

$$MSO(U') = \Delta(\Delta-1)\sqrt{\Delta^2+1} + 2\,\Delta\sqrt{\Delta^2+4} + 18\sqrt{13} + 4\sqrt{8}(n-\Delta-3).$$

This completes the proof. □

Hence, we have completely characterized all graphs minimizing the additively and the multiplicatively degree-weighted Sombor indices over all unicyclic graphs with a given number of vertices and a given maximum degree.

5. Concluding remarks

In this paper we have considered two generalizations of the Sombor index, both obtained by suitably chosen degree-based weightings of the basic edge contributions to the Sombor index. We have found that, for a given number of vertices and a given maximum degree, the minimizing trees for both indices must be brooms. We have also characterized the minimizing unicyclic graphs under the same set of constraints. We are convinced that the methods employed in this paper could also yield minimizing graphs for wider classes of graphs. For example, they could be employed to obtain the minimizing bicyclic graphs, at the price of having to analyze more special cases. Also, it would be interesting to investigate whether similar arguments could be applied to characterize the maximizing structures in the considered classes of graphs. Some work on those questions is underway and we hope to be able to report on it soon.

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