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Research Article

The extremal Sombor index of trees with a given dissociation number φ

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Abstract: The Sombor index is a topological index in graph theory defined by Gutman in 2021. In this article, we find the maximum Sombor index of trees of order $\mathbf{n}$ with a given dissociation number φ, where $\lceil \frac{2\mathbf{n}}{3} \rceil \leq \varphi(G) \leq \mathbf{n}-1$. We also provide the unique graph among the chosen class where the maximum Sombor index is attained.

Keywords: trees, Sombor index, dissociation number.

AMS Subject Classification: 05C10, 05C35, 05C38

1. Introduction

Let $G = (V(G), E(G))$ be a finite, simple, connected graph with $V(G)$ as the set of vertices and $E(G)$ as the set of edges in G. We simply write $G = (V, E)$ if there is no scope of confusion. We write $u \sim v$ to indicate that the vertices $u, v \in V$ are adjacent in G. The degree of the vertex v, denoted by $d_G(v)$ (or simply $d(v)$), equals the number of vertices in V that are adjacent to v. A graph H is said to be a subgraph of G if $V(H) \subset V(G)$ and $E(H) \subset E(G)$. For any subset $S \subset V(G)$, a subgraph of G is said to be an induced subgraph with vertex set S, denoted by $G[S]$, if $G[S]$ is a maximal subgraph of G with vertex set $V(G[S]) = S$.
For any two vertices $u, v \in V(G)$, we will use $d(u, v)$ to denote the distance between the vertices u and v, i.e. the length of the shortest path connecting u and v. For a vertex $u \in V(G)$, we use $N(u)$ to denote the set of neighbors of u, *i.e.* the set of vertices that are adjacent to u. A vertex $u \in V(G)$ is said to be a pendant vertex if $d(u) = 1$. Since a pendant vertex $u \in V(G)$ has $d(u) = 1$ it is adjacent to exactly one vertex in G, say v and this vertex v is said to be the support vertex of u.
A graph $G = (V, E)$ is said to be bipartite if the vertex set V can be partitioned into two subsets M and N such that $E \subset M \times N$. A bipartite graph with vertex

partitions M and N is said to be a complete bipartite graph if every vertex of M is adjacent to every vertex of N and moreover, if $|M| = m$ and $|N| = n$, then the complete bipartite graph is denoted by $K_{m,n}$. Let $S_n = K_{1,n-1}$ be the star graph of order n. Set $V(S_n) = \{v_0, v_1, \cdots, v_{n-1}\}$ such that $d(v_0) = n-1$ and $d(v_i) = 1$ for all $1 \leq i \leq n-1$. The vertex v_0 is called the central vertex of S_n.

A vertex cover of a graph is a set of vertices that includes at least one endpoint of every edge of the graph. Given a graph G and a positive integer k, a subset S of the vertices of G is a vertex k-path cover if, for every path on k vertices in G, it contains a vertex from S. The minimum cardinality of a vertex k-path cover is denoted by $\psi_k(G)$. The graph invariant $\psi_k(G)$ was introduced in [3, 4] motivated by the problem of ensuring data integrity of communications in wireless sensor networks. One can see that $\psi_2(G)$ is the same as the minimum cardinality of a vertex cover of G; hence, the concept of vertex k-path cover is a generalization of vertex cover.

A set I of vertices in a graph G is an independent set if no pair of vertices of I are adjacent. The independence number of G, denoted by $\alpha(G)$, is the maximum cardinality of an independent set in G. We have a nice relation between $\psi_2(G)$ and $\alpha(G)$ as follows:

$$\psi_2(G) + \alpha(G) = |V(G)|.$$

A set D of vertices in a graph G is a dissociation set if the induced subgraph with vertex set D has maximum degree at most 1. A maximum dissociation set of G is a dissociation set with maximum cardinality. The dissociation number of G, denoted by $\varphi(G)$, is the cardinality of a maximum dissociation set. Note that $I \subset D$. Clearly one can also observe that $\psi_3(G)$ and $\varphi(G)$ are related as follows:

$$\psi_3(G) + \varphi(G) = |V(G)|.$$

In [12], Gutman defined a new topological index under the name Sombor index. For a graph G, its Sombor index is defined as

$$SO(G) = \sum_{u \sim v} \sqrt{d(u)^2 + d(v)^2}.$$

Note that, in $SO(G)$, the summation is over all edges of G. This new index attracted many researchers within a short period of time and some of them were able to show applications of the Sombor index, for example see [18]. For articles related to Sombor index the readers can refer to [1, 5, 8–14, 17–19, 24–26].

In graph theory, studying extremal graphs and indices for a class of graphs with a given parameter is a very interesting problem. For example, one may refer to [2, 8, 9, 19, 20, 23, 25, 26]. For a fixed independence number, extremal graphs have been studied for indices like the Harary index in [2], the first Zagreb index in [23] and functions like the Extremal vertex-degree function in [20].

In [26], the authors have studied the extremal Sombor index of trees and unicyclic graphs with a given matching number. In [25], the authors have studied the Sombor

index of trees and unicyclic graphs with a given maximum degree. In [19], the authors found the maximum and the minimum Sombor index of trees with fixed domination number. In [6], the author found the maximum Sombor index of trees with a given independence number.
From the definition of the dissociation number, it is clear that the dissociation number is an immediate generalization of the independence number. Several interesting results have been published related to dissociation number (for example see [7, 15, 16, 21, 22]).
In this article, we find the maximum Sombor index of trees of order $\mathbf{n}$ with a given dissociation number φ, where $\lceil \frac{2\mathbf{n}}{3} \rceil \leq \alpha \leq \mathbf{n} - 1$ and also provide the unique graph where the maximum Sombor index is attained.
This article is organized as follows: In Section 2, we state the preliminary results, state some basic inequalities and a result related to trees and its maximal independence set that will be used in the later section. In Section 3, we build up the necessary tools required to prove the main result and lastly in Theorem 1, we state and prove the main result of the article.

2. Notation and preliminaries

The next two lemmas directly follow from verifying $f'(x) > 0$ and $g'(x) < 0$ and these will be used again and again in the future proofs.

Lemma 1. *For $x \geq 1$, if $f(x) = \sqrt{(x+c)^2 + d^2} - \sqrt{x^2 + d^2}$, where c, d are positive integers, then $f(x)$ is a monotonically increasing function of x.*

Lemma 2. *For $x \geq 1$, if $g(x) = \sqrt{c^2 + x^2} - \sqrt{d^2 + x^2}$, where c, d are positive integers and $c > d$, then $g(x)$ is a monotonically decreasing function of x.*

A vertex is called a quasi-pendant vertex if it is adjacent to a pendant vertex. For a graph G, let $P(G)$ and $Q(G)$ denote the set of all pendant and quasi-pendant vertices, respectively. Moreover, let $Q_2(G)$ be the set of all quasi-pendant vertices of degree 2 in G. In [15], the authors showed that there exists a maximum dissociation set of G such that it contains all vertices of $P(G) \cup Q_2(G)$. The result is stated as follows:

Lemma 3. *[15] Let G be a graph with order $n \geq 5$. Then there exists a maximum dissociation set $D(G)$ such that $P(G) \cup Q_2(G) \subseteq D(G)$.*

Lemma 4. *Let T be a tree that has the maximum possible Sombor index among all trees of order $\mathbf{n}$ with dissociation number $\varphi(T)$. Then $Q_2(T) = \emptyset$.*

Proof. Suppose, to the contrary, that $Q_2(T) \neq \emptyset$ and let $v \in Q_2(T)$. Let $N(v) = \{u, w\}$, where w is a pendant vertex. Let T^* be the graph obtained from T by deleting the edge $v \sim w$ and adding the edge $u \sim w$. Then,

$$SO(T^*) - SO(T) > \left(\sqrt{(d(u)+1)^2+1^2} - \sqrt{d(u)^2+2^2}\right) + \left(\sqrt{(d(u)+1)^2+1^2} - \sqrt{2^2+1^2}\right) > 0,$$

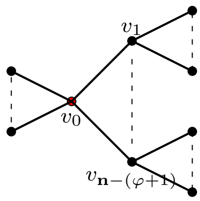
where, the last inequality follows from the fact that $d(u) \geq 2$.
By Lemma 3, there exists a maximum dissociation set D of T containing $P(T) \cup Q_2(T)$, so in particular $v, w \in D$. Since D is a dissociation set, we must have $u \notin D$, otherwise v would have degree 2 in the subgraph induced by D. Since the transformation from T to T^* only replaces the edge $v \sim w$ by $u \sim w$ and $u \notin D$, no edge inside the induced subgraph on D is added or removed. Thus D is also a dissociation set of T^*, which implies $\varphi(T^*) \geq \varphi(T)$. As the degree of u increases in T^*, no larger dissociation set can be formed in T^*, and hence $\varphi(T^*) = \varphi(T)$.
But $SO(T^*) > SO(T)$, which contradicts the assumption that T has the maximum possible Sombor index among all trees with dissociation number $\varphi(T)$. Hence $Q_2(T) = \emptyset$. □

3. Trees with a given dissociation number

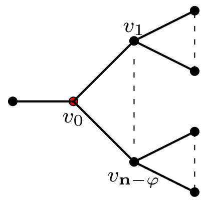
Let $T(\mathbf{n}, \varphi)$ be the collection of trees of order $\mathbf{n}$ and dissociation number φ. Observe that, if $\varphi = \mathbf{n} - 1$ then $T(\mathbf{n}, \mathbf{n}-1) = \{S_{\mathbf{n}}\}$ and $SO(S_{\mathbf{n}}) = (\mathbf{n}-1)\sqrt{(\mathbf{n}-1)^2+1} = \varphi\sqrt{\varphi^2+1}$, hence we consider the case when $\varphi \leq \mathbf{n} - 2$. It is also important to note that, for every tree in the class $T(\mathbf{n}, \varphi)$, there exists a maximal dissociation set $D(T)$, which has exactly φ elements.
Let $T_1(\mathbf{n}, \varphi)$ be a set of trees on $\mathbf{n}$ vertices obtained from $S_{\mathbf{n}-\varphi}$ by attaching at least two pendant edges to each vertex of $S_{\mathbf{n}-\varphi}$ so that the total number of pendant vertices of the trees in $S_{\mathbf{n}-\varphi}$ is φ. Let $T_2(\mathbf{n}, \varphi)$ be a set of trees on $\mathbf{n}$ vertices obtained from $S_{\mathbf{n}-(\varphi-1)}$ by attaching at least two pendant edges to each vertices in $\{v_1, \ldots, v_{\mathbf{n}-\varphi}\}$ and attaching one pendant edge to v_0 so that the total number of leaves of the trees in $T_2(\mathbf{n}, \alpha)$ is $\varphi - 1$, where $\varphi \notin \left\{\frac{2\mathbf{n}}{3}, \frac{2\mathbf{n}+1}{3}\right\}$. Let $T_3(\mathbf{n}, \varphi)$ be a set of trees on n vertices obtained from $S_{\mathbf{n}-(\varphi-1)}$ by attaching at least two pendant edges to each vertex in $\{v_1, \ldots, v_{\mathbf{n}-\varphi}\}$ so that the total number of leaves of the trees in $T_3(\mathbf{n}, \varphi)$ is $\varphi - 1$, where $\varphi \neq \frac{2\mathbf{n}}{3}$. Note that $T_1(\mathbf{n}, \varphi) \cup T_2(\mathbf{n}, \varphi) \cup T_3(\mathbf{n}, \varphi) \subset T(\mathbf{n}, \alpha)$. For reference, one can see Figure 1.
Let $T^*(\mathbf{n}, \varphi)$ be the tree of order $\mathbf{n}$ obtained from the star $S_{\mathbf{n}-\varphi}$ by attaching exactly two pendant edge to each of the vertices $\{v_1, v_2, \cdots, v_{\mathbf{n}-(\varphi+1)}\} \subset V(S_{\mathbf{n}-\alpha})$ and attaching $3\varphi - 2(\mathbf{n}-1)$ pendant vertices to the central vertex v_0 of $S_{\mathbf{n}-\alpha}$. Observe that, $T^*(\mathbf{n}, \alpha) \in T_1(\mathbf{n}, \alpha) \subset T(\mathbf{n}, \alpha)$. For reference, one can see Figure 2.

Remark 1. Let $T^*(\mathbf{n}, \alpha) \in T_1(\mathbf{n}, \alpha) \subset T(\mathbf{n}, \alpha)$ be defined as above, then $d(v_0) = 2\varphi - \mathbf{n} + 1$, $d(v_i) = 3$ for all $1 \leq i \leq \mathbf{n} - (\varphi + 1)$ and all the remaining vertices have degree 1. Thus, we have

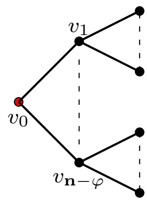
$$\begin{aligned} SO(T^*(\mathbf{n}, \alpha)) &= (3\varphi - 2(\mathbf{n}-1))\sqrt{(2\varphi - \mathbf{n} + 1)^2 + 1} \\ &\quad + (\mathbf{n} - (\varphi+1))[\sqrt{(2\varphi - \mathbf{n} + 1)^2 + 3^2} + 2\sqrt{3^2+1}], \end{aligned}$$



(a) $T \in T_1(\mathbf{n}, \varphi)$



(b) $T \in T_2(\mathbf{n}, \varphi)$



(c) $T \in T_3(\mathbf{n}, \varphi)$

Figure 1: Trees in $T_1(\mathbf{n}, \varphi)$, $T_2(\mathbf{n}, \varphi)$ and $T_3(\mathbf{n}, \varphi)$ with some labeled vertices.

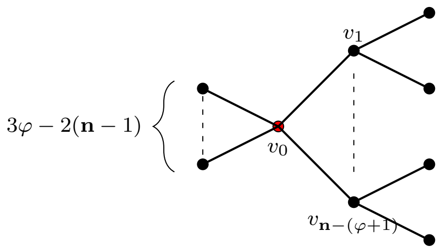


Figure 2: $T^*(\mathbf{n}, \varphi)$

and since the vertex v_0 has atleast two pendant vertices, we have $3\varphi - 2(\mathbf{n} - 1) \geq 2$, *i.e.* $\varphi \geq \lceil \frac{2\mathbf{n}}{3} \rceil$.

Lemma 5. *Let $T \in T(\mathbf{n}, \varphi)$ be a tree with maximal Sombor index, then $T \in T_1(\mathbf{n}, \varphi) \cup T_2(\mathbf{n}, \varphi) \cup T_3(\mathbf{n}, \varphi)$.*

Proof. Suppose $T \in T(\mathbf{n}, \varphi) \setminus (T_1(\mathbf{n}, \varphi) \cup T_2(\mathbf{n}, \varphi) \cup T_3(\mathbf{n}, \varphi))$ and T' be the tree obtained from T by deleting all the pendant vertices along with their edges. Then, the number of support vertices in T' is at least 2, otherwise $T \in T_1(\mathbf{n}, \varphi) \cup T_2(\mathbf{n}, \varphi) \cup T_3(\mathbf{n}, \varphi)$. Thus, we can choose two support vertices from T', u and v such that $d(u, v)$ is the maximum in T'. Since T' is a tree, there is a unique path between u and v and let $u \sim x$ and $y \sim v$ on this path.

Let $N_T(u) = \{u_1, \cdots, u_m\} \cup \{u_{m+1}, \cdots, u_{m+a}\} \cup \{x\}$, where $m \geq 1$, $d(u_i) \geq 2$ for all $1 \leq i \leq m$ and $d(u_{m+i}) = 1$ for all $1 \leq i \leq a$. Let $N_T(v) = \{v_1, \cdots, v_n\} \cup$

$\{v_{n+1}, \cdots, v_{n+b}\} \cup \{y\}$,where $n \geq 1$, $d(v_j) \geq 2$ for all $1 \leq j \leq n$ and $d(v_{n+j}) = 1$ for all $1 \leq j \leq b$. Note that we have assumed $m \geq 1$ and $n \geq 1$. If $m = 0$, then u ceases to be a support vertex in T', and a symmetric argument holds for v if $n = 0$. If we delete the edges $u \sim x$ and $v \sim y$, then T becomes disconnected into three components: one component containing the path between u and v (containing vertices x and y), one component containing u and one component containing v. Let H be the component of the tree T containing x and y. Note that $d(u) = m + a + 1$ and $d(v) = n + b + 1$. We prove the result by dividing it into multiple cases. In all cases, the graph transformation does not add or delete any edges between vertices in $D(T)$ and hence the dissociation number φ remains invariant after the transformation.

Case 1. $a > 1$ and $b > 1$.
Using Lemma 3, we can choose a maximal dissociation set $D(T)$ such that it contains all the pendant and degree 2 quasi-pendant vertices. Also, by Lemma 4, it holds that $Q_2(T) = \emptyset$. Since $a, b > 1$, $\{u, v\} \cup \{u_1, \cdots, u_m\} \cup \{v_1, \cdots, v_n\} \notin D(T)$.

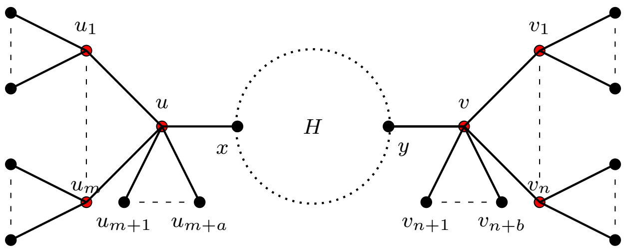


Figure 3: $a > 1$ and $b > 1$.

As pendant vertices are necessarily included in the maximum dissociation set $D(T)$, it is evident from Figure 3 that all pendant neighbors of u_i belong to $D(T)$ for each $1 \leq i \leq m$. Consequently, the set $N(u_i)$ contributes $d(u_i) - 1$ to $\varphi(T)$. By an analogous argument, $N(v_j)$ contributes $d(v_j) - 1$ to $\varphi(T)$ for each $1 \leq j \leq n$. Furthermore, the pendant vertices $\{u_{m+1}, \ldots, u_{m+a}\} \cup \{v_{n+1}, \ldots, v_{n+b}\}$ are contained in $D(T)$, contributing $a + b$ to the dissociation number.
Given that $u, v \notin D(T)$, the selection of vertices from the subgraph H for inclusion in $D(T)$ is independent of the vertices in $V(T) \setminus V(H)$. Thus, we obtain:

$$\varphi(T) = \sum_{i=1}^{m}(d(u_i) - 1) + \sum_{j=1}^{n}(d(v_j) - 1) + a + b + \varphi(H).$$

Without loss of generality, we assume $d(u) \geq d(v)$.

Subcase 1.1. $d(y) > d(x)$.
Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $v \sim v_j$ for all $1 \leq j \leq n + (b - 2)$.
- Add the edges $u \sim v_j$ for all $1 \leq j \leq n + (b - 2)$.

Now, observe that after the transformation we have $\varphi(T) = \varphi(T^*)$ and

$$\begin{aligned} SO(T^*) - SO(T) &= \sqrt{d_{T^*}(u)^2 + d_{T^*}(x)^2} - \sqrt{d_T(u)^2 + d_T(x)^2} \\ &+ \sqrt{d_{T^*}(v)^2 + d_{T^*}(y)^2} - \sqrt{d_T(v)^2 + d_T(y)^2} \\ &+ \sum_{i=1}^{m+a} \left(\sqrt{d_{T^*}(u)^2 + d_{T^*}(u_i)^2} - \sqrt{d_T(u)^2 + d_T(u_i)^2} \right) \\ &+ \sum_{j=1}^{n+b-2} \left(\sqrt{d_{T^*}(u)^2 + d_{T^*}(v_j)^2} - \sqrt{d_T(v)^2 + d_T(v_j)^2} \right) \\ &+ \sqrt{d_{T^*}(v)^2 + d_{T^*}(v_{n+b-1})^2} - \sqrt{d_T(v)^2 + d_T(v_{n+b-1})^2} \\ &+ \sqrt{d_{T^*}(v)^2 + d_{T^*}(v_{n+b})^2} - \sqrt{d_T(v)^2 + d_T(v_{n+b})^2}. \end{aligned}$$

Note that, after the transformation only the degree of vertices u and v are changed, where $d_{T^*}(u) = m + n + a + b - 1$ and $d_{T^*}(v) = 3$. Thus, substituting the values of degree we have

$$\begin{aligned} SO(T^*) - SO(T) &= \sqrt{(m+n+a+b-1)^2 + d(x)^2} - \sqrt{(m+a+1)^2 + d(x)^2} \\ &+ \sqrt{3^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2} \\ &+ \sum_{i=1}^{m+a} \left(\sqrt{(m+n+a+b-1)^2 + d(u_i)^2} - \sqrt{(m+a+1)^2 + d(u_i)^2} \right) \\ &+ \sum_{j=1}^{n+b-2} \left(\sqrt{(m+n+a+b-1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2} \right) \\ &+ 2(\sqrt{3^2 + 1^2} - \sqrt{(n+b+1)^2 + 1^2}). \end{aligned}$$

Since $a > 1$, we have at least two pendant vertices attached to u, say u_{m+1} and u_{m+2}. Also, since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$ we have

$$\sqrt{(m+n+a+b-1)^2 + d(u_i)^2} - \sqrt{(m+a+1)^2 + d(u_i)^2} > 0,$$

for $1 \leq i \leq m + a$ and

$$\sqrt{(m+n+a+b-1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2} > 0,$$

for $1 \leq j \leq n + b - 1$. Thus, combining we have

$$\begin{aligned} SO(T^*) - SO(T) &> \sqrt{(m+n+a+b-1)^2 + d(x)^2} - \sqrt{(m+a+1)^2 + d(x)^2} \\ &+ \sqrt{3^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2} \\ &+ 2(\sqrt{(m+n+a+b-1)^2 + 1} - \sqrt{(m+a+1)^2 + 1}) \\ &+ 2(\sqrt{3^2 + 1} - \sqrt{(n+b+1)^2 + 1}). \end{aligned}$$

Note that, in the previous step, while calculating the change of Sombor index, we have omitted the sums $\sum_{i=1}^{m+a}\left(\sqrt{(m+n+a+b-1)^2+d(u_i)^2}-\sqrt{(m+a+1)^2+d(u_i)^2}\right)$ and $\sum_{j=1}^{n+b-2}\left(\sqrt{(m+n+a+b-1)^2+d(v_j)^2}-\sqrt{(n+b+1)^2+d(v_j)^2}\right)$ except for the terms corresponding to the edges $u\sim u_{m+1}$ and $u\sim u_{m+2}$, using the fact that $h(x)=\sqrt{x^2+a^2}$ is monotonically increasing for $x>0$.

Using Lemma 1 and substituting $c=n+b-2$ and $d=1$, we have

$$\sqrt{(m+n+a+b-1)^2+1}-\sqrt{(m+a+1)^2+1}>\sqrt{(n+b+1)^2+1}-\sqrt{3^2+1},$$

since $f(m+a+1)>f(3)$, which holds true since $m+a\geq 3$. Next, again using Lemma 1 and substituting $c=n+b-2$ and $d=d(x)$, we have

$$\sqrt{(m+n+a+b-1)^2+d(x)^2}-\sqrt{(m+a+1)^2+d(x)^2}>\sqrt{(n+b+1)^2+d(x)^2}-\sqrt{3^2+d(x)^2},$$

since $f(m+a+1)>f(3)$, which holds true since $m+a\geq 3$. Finally, using Lemma 2 and $c=n+b+1$ and $d=3$, we have

$$\sqrt{(n+b+1)^2+d(x)^2}-\sqrt{3^2+d(x)^2}\geq\sqrt{(n+b+1)^2+d(y)^2}-\sqrt{3^2+d(y)^2},$$

since $d(y)>d(x)$ and hence $g(d(x))>g(d(y))$. Thus, combining the above inequalities we have $SO(T^*)-SO(T)>0$, which is a contradiction.

Subcase 1.2. $d(x)\geq d(y)$.

Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $u\sim x$ and $v\sim y$.
- Add the edges $u\sim y$ and $v\sim x$.
- Delete the edges $v\sim v_j$ for all $1\leq j\leq n+(b-2)$.
- Add the edges $u\sim v_j$ for all $1\leq j\leq n+(b-2)$.

Note that, after the transformation we have $\varphi(T)=\varphi(T^*)$ and

$$\begin{aligned}
SO(T^*)-SO(T)=&\sqrt{d_{T^*}(u)^2+d_{T^*}(y)^2}-\sqrt{d_T(v)^2+d_T(y)^2}\\
&+\sqrt{d_{T^*}(v)^2+d_{T^*}(x)^2}-\sqrt{d_T(u)^2+d_T(x)^2}\\
&+\sum_{i=1}^{m+a}\left(\sqrt{d_{T^*}(u)^2+d_{T^*}(u_i)^2}-\sqrt{d_T(u)^2+d_T(u_i)^2}\right)\\
&+\sum_{j=1}^{n+b-2}\left(\sqrt{d_{T^*}(u)^2+d_{T^*}(v_j)^2}-\sqrt{d_T(v)^2+d_T(v_j)^2}\right)\\
&+\sqrt{d_{T^*}(v)^2+d_{T^*}(v_{n+b-1})^2}-\sqrt{d_T(v)^2+d_T(v_{n+b-1})^2}\\
&+\sqrt{d_{T^*}(v)^2+d_{T^*}(v_{n+b})^2}-\sqrt{d_T(v)^2+d_T(v_{n+b})^2}.
\end{aligned}$$

Note that, after the transformation only the degree of vertices u and v are changed, where $d_{T^*}(u) = m+n+a+b-1$ and $d_{T^*}(v) = 3$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned}SO(T^*) - SO(T) &= \sqrt{(m+n+a+b-1)^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2} \\ &+ \sqrt{3^2 + d(x)^2} - \sqrt{(m+a+1)^2 + d(x)^2} \\ &+ \sum_{i=1}^{m+a} \left(\sqrt{(m+n+a+b-1)^2 + d(u_i)^2} - \sqrt{(m+a+1)^2 + d(u_i)^2} \right) \\ &+ \sum_{j=1}^{n+b-2} \left(\sqrt{(m+n+a+b-1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2} \right) \\ &+ 2(\sqrt{3^2+1^2} - \sqrt{(n+b+1)^2+1^2}).\end{aligned}$$

Since $a > 1$, we have at least two pendant vertices attached to u, say u_{m+1} and u_{m+2}. Since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$, we have omitted the sums $\sum_{i=1}^{m+a} \left(\sqrt{(m+n+a+b-1)^2 + d(u_i)^2} - \sqrt{(m+a+1)^2 + d(u_i)^2} \right)$ and $\sum_{j=1}^{n+b-2} \left(\sqrt{(m+n+a+b-1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2} \right)$ except for the terms corresponding to the edges $u \sim u_{m+1}$ and $u \sim u_{m+2}$, while calculating the change of Sombor index in the next step. Thus, we have

$$\begin{aligned}SO(T^*) - SO(T) &> \sqrt{(m+n+a+b-1)^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2} \\ &+ \sqrt{3^2 + d(x)^2} - \sqrt{(m+a+1)^2 + d(x)^2} \\ &+ 2(\sqrt{(m+n+a+b-1)^2+1} - \sqrt{(m+a+1)^2+1}) \\ &+ 2(\sqrt{3^2+1} - \sqrt{(n+b+1)^2+1}).\end{aligned}$$

From the previous subcase, we have

$$\sqrt{(m+n+a+b-1)^2+1} - \sqrt{(m+a+1)^2+1} > \sqrt{(n+b+1)^2+1} - \sqrt{3^2+1}.$$

Now, using Lemma 1 and substituting $c = m+a-2$ and $d = d(y)$, we have

$$\sqrt{(m+n+a+b-1)^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2} > \sqrt{(m+a+1)^2 + d(y)^2} - \sqrt{3^2 + d(y)^2},$$

since $f(n+b+1) > f(3)$. Finally, using Lemma 2 and $c = m+a+1$ and $d = d(y)$, we have

$$\sqrt{(m+a+1)^2 + d(y)^2} - \sqrt{3^2 + d(y)^2} \geq \sqrt{(m+a+1)^2 + d(x)^2} - \sqrt{3^2 + d(x)^2},$$

since $d(x) \geq d(y)$ and hence $g(d(y)) \geq g(d(x))$. Thus, combining the above inequalities we have $SO(T^*) - SO(T) > 0$, which is a contradiction.

Case 2. $a = 1$ but $b > 1$ or $a > 1$ but $b = 1$.
Without loss of generality, we can assume that $a = 1$ but $b > 1$. Using Lemma 3 we can choose a maximal dissociation set $D(T)$ such that it contains all the pendant and the degree 2 quasi-pendant vertices. Since $a = 1$ but $b > 1$, $\{v\} \cup \{u_1, \cdots, u_m\} \cup \{v_1, \cdots, v_n\} \notin D(T)$.

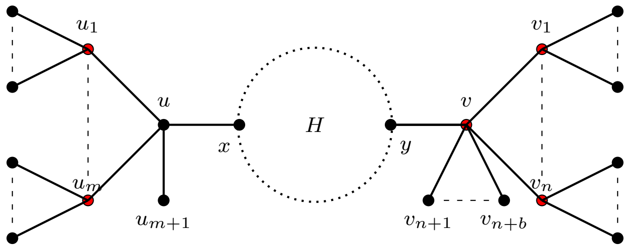


Figure 4: $a = 1$ and $b > 1$.

Since pendant vertices are necessarily contained in the maximum dissociation set $D(T)$, it follows from Figure 4 that all pendant neighbors of u_i belong to $D(T)$ for each $1 \leq i \leq m$. Consequently, the set $N(u_i) \setminus \{u\}$ contributes $d(u_i) - 1$ to the dissociation number $\varphi(T)$. By a similar argument, $N(v_j) \setminus \{v\}$ contributes $d(v_j) - 1$ to $\varphi(T)$ for $1 \leq j \leq n$. Additionally, the pendant vertices $\{v_{n+1}, \ldots, v_{n+b}\}$ are elements of $D(T)$, contributing exactly b to $\varphi(T)$. Given that $\{v\} \cup \{u_1, \ldots, u_m\} \notin D(T)$, the selection of vertices from the subgraph $G[V(H) \cup \{u, u_{m+1}\}]$ for inclusion in $D(T)$ is independent of the remaining structure of the graph. Therefore, the dissociation number of T can be expressed as:

$$\varphi(T) = \sum_{i=1}^{m}(d(u_i) - 1) + \sum_{j=1}^{n}(d(v_j) - 1) + b + \varphi(G[V(H) \cup \{u, u_{m+1}\}]).$$

Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $u \sim u_i$ for all $1 \leq i \leq m$.
- Add the edges $v \sim u_i$ for all $1 \leq i \leq m$.

Note that, after the transformation we have $\varphi(T) = \varphi(T^*)$ and we have

$$\begin{aligned} SO(T^*) - SO(T) = &\sqrt{d_{T^*}(u)^2 + d_{T^*}(x)^2} - \sqrt{d_T(u)^2 + d_T(x)^2} \\ &+ \sqrt{d_{T^*}(v)^2 + d_{T^*}(y)^2} - \sqrt{d_T(v)^2 + d_T(y)^2} \\ &+ \sum_{i=1}^{m}\left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(u_i)^2} - \sqrt{d_T(u)^2 + d_T(u_i)^2}\right) \\ &+ \sqrt{d_{T^*}(u)^2 + d_{T^*}(u_{m+1})^2} - \sqrt{d_T(u)^2 + d_T(u_{m+1})^2} \\ &+ \sum_{j=1}^{n+b}\left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(v_j)^2} - \sqrt{d_T(v)^2 + d_T(v_j)^2}\right). \end{aligned}$$

Note that, after the transformation only the degree of vertices u and v are changed, where $d_{T^*}(u) = 2$ and $d_{T^*}(v) = m+n+b+1$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned} SO(T^*) - SO(T) = &\sqrt{2^2 + d(x)^2} - \sqrt{(m+2)^2 + d(x)^2} \\ &+ \sqrt{(m+n+b+1)^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2} \\ &+ \sum_{i=1}^{m} \left(\sqrt{(m+n+b+1)^2 + d(u_i)^2} - \sqrt{(m+2)^2 + d(u_i)^2} \right) \\ &+ \sqrt{2^2 + 1^2} - \sqrt{(m+2)^2 + 1^2} \\ &+ \sum_{j=1}^{n+b} \left(\sqrt{(m+n+b+1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2} \right). \end{aligned}$$

Since $b > 1$, we have at least two pendant vertices attached to v, say v_{n+1} and v_{n+2}. In the next step, while calculating the change of Sombor index we omit the term $\sqrt{(m+n+b+1)^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2}$ along with the sums $\sum_{i=1}^{m} \left(\sqrt{(m+n+b+1)^2 + d(u_i)^2} - \sqrt{(m+2)^2 + d(u_i)^2} \right)$ and $\sum_{j=1}^{n+b} \left(\sqrt{(m+n+b+1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2} \right)$, except for the terms corresponding to the edges $v \sim v_{n+1}$ and $v \sim v_{n+2}$, since $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$. Thus, we have

$$\begin{aligned} SO(T^*) - SO(T) > &\sqrt{2^2 + d(x)^2} - \sqrt{(m+2)^2 + d(x)^2} \\ &+ \sqrt{2^2 + 1^2} - \sqrt{(m+2)^2 + 1^2} \\ &+ 2(\sqrt{(m+n+b+1)^2 + 1} - \sqrt{(n+b+1)^2 + 1}). \end{aligned}$$

Using Lemma 1 and substituting $c = m$ and $d = 1$, we have

$$\sqrt{(m+n+b+1)^2 + 1} - \sqrt{(n+b+1)^2 + 1} > \sqrt{(m+2)^2 + 1} - \sqrt{2^2 + 1},$$

since $f(n+b+1) > f(2)$, which holds true since $n+b \geq 3$. Now using Lemma 2 and substituting $c = m+2$ and $d = 2$, we have

$$\sqrt{(m+2)^2 + 1} - \sqrt{2^2 + 1} > \sqrt{(m+2)^2 + d(x)^2} - \sqrt{2^2 + d(x)^2},$$

since $d(x) > 1$ and hence $g(1) > g(d(x))$. Thus, combining the above inequalities we have $SO(T^*) - SO(T) > 0$, which is a contradiction.

Case 3. $a = 1$ and $b = 1$.

Without loss of generality we assume that $d(x) \geq d(y)$. Using Lemma 3 we can choose

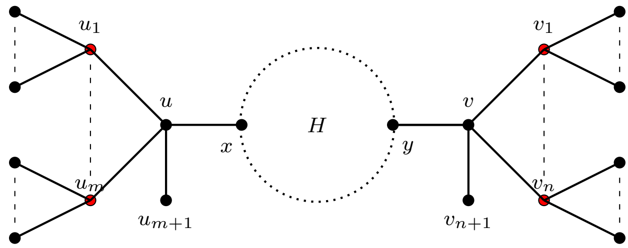


Figure 5: $a = 1$ and $b = 1$.

a maximal dissociation set $D(T)$ such that it contains all the pendant and the degree 2 quasi-pendant vertices. Since $a = 1$ and $b = 1$, $\{u_1, \cdots, u_m\} \cup \{v_1, \cdots, v_n\} \notin D(T)$. By an argument analogous to the preceding cases, it follows from Figure 5 that for each $1 \leq i \leq m$, the set $N(u_i) \setminus \{u\}$ contributes $d(u_i) - 1$ to the dissociation number $\varphi(T)$. Similarly, for each $1 \leq j \leq n$, the set $N(v_j) \setminus \{v\}$ contributes $d(v_j) - 1$. Given that the vertices in $\{u_1, \ldots, u_m\} \cup \{v_1, \ldots, v_n\}$ are excluded from the maximum dissociation set $D(T)$, the selection of vertices from the induced subgraph $G[V(H) \cup \{u, u_{m+1}, v, v_{n+1}\}]$ to be included in $D(T)$ is independent of the remaining vertices in the graph. Thus, we have

$$\varphi(T) = \sum_{i=1}^{m}(d(u_i) - 1) + \sum_{j=1}^{n}(d(v_j) - 1) + \varphi(G[V(H) \cup \{u, u_{m+1}, v, v_{n+1}\}]).$$

Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $u \sim u_i$ for all $1 \leq i \leq m$.
- Add the edges $v \sim u_i$ for all $1 \leq i \leq m$.

Note that after the transformation we have $\varphi(T) = \varphi(T^*)$ and we have

$$\begin{aligned}
SO(T^*) - SO(T) = & \sqrt{d_{T^*}(u)^2 + d_{T^*}(x)^2} - \sqrt{d_T(u)^2 + d_T(x)^2} \\
& + \sqrt{d_{T^*}(v)^2 + d_{T^*}(y)^2} - \sqrt{d_T(v)^2 + d_T(y)^2} \\
& + \sum_{i=1}^{m}\left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(u_i)^2} - \sqrt{d_T(u)^2 + d_T(u_i)^2}\right) \\
& + \sqrt{d_{T^*}(u)^2 + d_{T^*}(u_{m+1})^2} - \sqrt{d_T(u)^2 + d_T(u_{m+1})^2} \\
& + \sum_{j=1}^{n+1}\left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(v_j)^2} - \sqrt{d_T(v)^2 + d_T(v_j)^2}\right).
\end{aligned}$$

Note that, after the transformation only the degree of vertices u and v is changed, where $d_{T^*}(u) = 2$ and $d_{T^*}(v) = m + n + 2$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned}SO(T^*) - SO(T) &= \sqrt{2^2 + d(x)^2} - \sqrt{(m+2)^2 + d(x)^2} \\ &+ \sqrt{(m+n+2)^2 + d(y)^2} - \sqrt{(n+2)^2 + d(y)^2} \\ &+ \sum_{i=1}^{m} \left(\sqrt{(m+n+2)^2 + d(u_i)^2} - \sqrt{(m+2)^2 + d(u_i)^2} \right) \\ &+ \sqrt{2^2 + d(u_{m+1})^2} - \sqrt{(m+2)^2 + d(u_{m+1})^2} \\ &+ \sum_{j=1}^{n+1} \left(\sqrt{(m+n+2)^2 + d(v_j)^2} - \sqrt{(n+2)^2 + d(v_j)^2} \right).\end{aligned}$$

Since $b = 1$, the vertex v has exactly one pendant vertex, say v_{n+1}. While calculating the change in the Sombor index in the next step, we have omitted the terms $\sum_{i=1}^{m} \left(\sqrt{(m+n+2)^2 + d(u_i)^2} - \sqrt{(m+2)^2 + d(u_i)^2} \right)$ and $\sum_{j=1}^{n+1} \left(\sqrt{(m+n+2)^2 + d(v_j)^2} - \sqrt{(n+2)^2 + d(v_j)^2} \right)$, except the term for the edge $v \sim v_{n+1}$, since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$. Thus, we have

$$\begin{aligned}SO(T^*) - SO(T) &> \sqrt{2^2 + d(x)^2} - \sqrt{(m+2)^2 + d(x)^2} \\ &+ \sqrt{(m+n+2)^2 + d(y)^2} - \sqrt{(n+2)^2 + d(y)^2} \\ &+ \sqrt{2^2 + 1^2} - \sqrt{(m+2)^2 + 1^2} \\ &+ \sqrt{(m+n+2)^2 + 1^2} - \sqrt{(n+2)^2 + 1^2}.\end{aligned}$$

Using Lemma 1 and substituting $c = m$ and $d = d(y)$, we have

$$\sqrt{(m+n+2)^2 + d(y)^2} - \sqrt{(n+2)^2 + d(y)^2} > \sqrt{(m+2)^2 + d(y)^2} - \sqrt{2^2 + d(y)^2},$$

since $f(n+2) > f(2)$, which holds true since $n \geq 1$. Now using Lemma 2 and substituting $c = m+2$ and $d = 2$, we have

$$\sqrt{(m+2)^2 + d(y)^2} - \sqrt{2^2 + d(y)^2} \geq \sqrt{(m+2)^2 + d(x)^2} - \sqrt{2^2 + d(x)^2},$$

since $d(x) \geq d(y)$ and hence $g(d(y)) \geq g(d(x))$. Again, using Lemma 1 and substituting $c = m$ and $d = 1$, we have

$$\sqrt{(m+n+2)^2 + 1^2} - \sqrt{(n+2)^2 + 1^2} > \sqrt{(m+2)^2 + 1^2} - \sqrt{2^2 + 1^2},$$

since $f(n+2) > f(2)$, which holds true since $n \geq 1$. Thus, combining the above inequalities we have $SO(T^*) - SO(T) > 0$, which is a contradiction.

Case 4. $a = 0$ but $b \geq 1$ or $a \geq 1$ but $b = 0$.
Without loss of generality, we can assume that $a = 0$ but $b \geq 1$. Using Lemma 3 we can choose a maximal dissociation set $D(T)$ such that it contains all the pendant and the degree 2 quasi-pendant vertices.

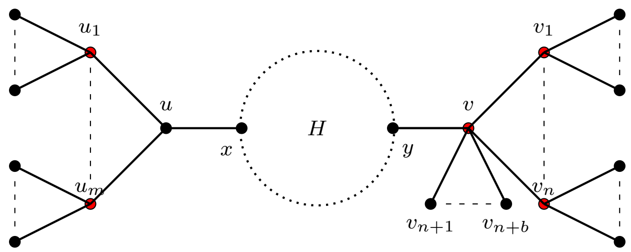


Figure 6: $a = 0$ and $b > 1$.

On one hand, if $a = 0$ and $b > 1$, then $\{v\} \cup \{u_1, \ldots, u_m\} \cup \{v_1, \ldots, v_n\} \notin D(T)$. Following an argument analogous to the previous cases and referring to Figure 6, we observe that for each $1 \leq i \leq m$, the set $N(u_i) \setminus \{u\}$ contributes $d(u_i) - 1$ to $\varphi(T)$, and for each $1 \leq j \leq n$, the set $N(v_j)$ contributes $d(v_j) - 1$. Given that $\{u_1, \ldots, u_m\} \cup \{v\}$ are excluded from $D(T)$, the selection of vertices from the induced subgraph $G[V(H) \cup \{u\}]$ for $D(T)$ is independent of the remainder of the graph. Consequently, for $a = 0$ and $b > 1$, we have:

$$\varphi(T) = \sum_{i=1}^{m} (d(u_i) - 1) + \sum_{j=1}^{n} (d(v_j) - 1) + b + \varphi(G[V(H) \cup \{u\}]).$$

On the other hand, if $a = 0$ and $b = 1$, then $\{u_1, \ldots, u_m\} \cup \{v_1, \ldots, v_n\} \cap D(T) = \emptyset$. By a similar reasoning, the dissociation number is given by:

$$\varphi(T) = \sum_{i=1}^{m} (d(u_i) - 1) + \sum_{j=1}^{n} (d(v_j) - 1) + \varphi(G[V(H) \cup \{u, v, v_{n+1}\}]).$$

Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $u \sim u_i$ for all $1 \leq i \leq m$.
- Add the edges $v \sim u_i$ for all $1 \leq i \leq m$.

Note that, after the transformation for the both cases, where $b > 1$ or $b = 1$, we have

$\varphi(T) = \varphi(T^*)$ and

$$\begin{aligned}SO(T^*) - SO(T) &= \sqrt{d_{T^*}(u)^2 + d_{T^*}(x)^2} - \sqrt{d_T(u)^2 + d_T(x)^2}\\ &+ \sqrt{d_{T^*}(v)^2 + d_{T^*}(y)^2} - \sqrt{d_T(v)^2 + d_T(y)^2}\\ &+ \sum_{i=1}^{m} \left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(u_i)^2} - \sqrt{d_T(u)^2 + d_T(u_i)^2}\right)\\ &+ \sum_{j=1}^{n+b} \left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(v_j)^2} - \sqrt{d_T(v)^2 + d_T(v_j)^2}\right).\end{aligned}$$

Note that, after the transformation only the degree of vertices u and v are changed, where $d_{T^*}(u) = 1$ and $d_{T^*}(v) = m+n+b+1$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned}SO(T^*) - SO(T) &= \sqrt{1^2 + d(x)^2} - \sqrt{(m+1)^2 + d(x)^2}\\ &+ \sqrt{(m+n+b+1)^2 + d(y)^2} - \sqrt{(n+b+1)^2 + d(y)^2}\\ &+ \sum_{i=1}^{m} \left(\sqrt{(m+n+b+1)^2 + d(u_i)^2} - \sqrt{(m+1)^2 + d(u_i)^2}\right)\\ &+ \sum_{j=1}^{n+b} \left(\sqrt{(m+n+b+1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2}\right).\end{aligned}$$

Since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$, we have omitted the terms $\sum_{i=1}^{m} \left(\sqrt{(m+n+b+1)^2 + d(u_i)^2} - \sqrt{(m+1)^2 + d(u_i)^2}\right)$ and $\sum_{j=1}^{n+b} \left(\sqrt{(m+n+b+1)^2 + d(v_j)^2} - \sqrt{(n+b+1)^2 + d(v_j)^2}\right)$, while calculating the change in the Sombor index in the next step. Thus, we have

$$\begin{aligned}SO(T^*) - SO(T) &> \sqrt{1^2 + d(x)^2} - \sqrt{(m+1)^2 + d(x)^2}\\ &+ \sqrt{(m+n+b+1)^2 + 1} - \sqrt{(n+b+1)^2 + 1}.\end{aligned}$$

Using Lemma 1 and substituting $c = m$ and $d = 1$, we have

$$\sqrt{(m+n+b+1)^2 + 1} - \sqrt{(n+b+1)^2 + 1} > \sqrt{(m+1)^2 + 1} - \sqrt{1^2 + 1},$$

since $f(n+b+1) > f(1)$, which holds true since $n+b \geq 2$. Now using Lemma 2 and substituting $c = m+1$ and $d = 1$, we have

$$\sqrt{(m+1)^2 + 1} - \sqrt{1^2 + 1} > \sqrt{(m+1)^2 + d(x)^2} - \sqrt{1^2 + d(x)^2},$$

since $d(x) > 1$ and hence $g(1) > g(d(x))$. Thus, combining the above inequalities we have $SO(T^*) - SO(T) > 0$, which is a contradiction.

Case 5. $a = 0$ and $b = 0$.
Without loss of generality we assume that $d(x) \geq d(y)$. Using Lemma 3 we can choose a maximal dissociation set $D(T)$ such that it contains all the pendant and degree 2 quasi-pendant vertices. Since $a = 0$ and $b = 0$, $\{u_1, \cdots, u_m\} \cup \{v_1, \cdots, v_n\} \notin D(T)$.

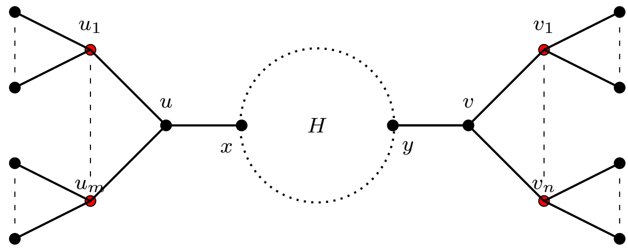


Figure 7: $a = 0$ and $b = 0$.

By referring to the structural configuration in Figure 7, it is evident that for each $1 \leq i \leq m$, the set $N(u_i) \setminus \{u\}$ contributes $d(u_i) - 1$ to the dissociation number $\varphi(T)$. Similarly, for each $1 \leq j \leq n$, the set $N(v_j) \setminus \{v\}$ contributes $d(v_j) - 1$. Given that $\{u_1, \ldots, u_m\} \cup \{v_1, \ldots, v_n\} \notin D(T)$, the selection of vertices from the induced subgraph $G[V(H) \cup \{u, v\}]$ for inclusion in $D(T)$ is independent of the remaining vertices of T. Consequently, the dissociation number is given by:

$$\varphi(T) = \sum_{i=1}^{m}(d(u_i) - 1) + \sum_{j=1}^{n}(d(v_j) - 1) + \varphi(G[V(H) \cup \{u, v\}]).$$

Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $u \sim u_i$ for all $1 \leq i \leq m$.
- Add the edges $v \sim u_i$ for all $1 \leq i \leq m$.

Note that after the transformation we have $\varphi(T) = \varphi(T^*)$ and we have

$$\begin{aligned} SO(T^*) - SO(T) &= \sqrt{d_{T^*}(u)^2 + d_{T^*}(x)^2} - \sqrt{d_T(u)^2 + d_T(x)^2} \\ &+ \sqrt{d_{T^*}(v)^2 + d_{T^*}(y)^2} - \sqrt{d_T(v)^2 + d_T(y)^2} \\ &+ \sum_{i=1}^{m}\left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(u_i)^2} - \sqrt{d_T(u)^2 + d_T(u_i)^2}\right) \\ &+ \sum_{j=1}^{n+b}\left(\sqrt{d_{T^*}(v)^2 + d_{T^*}(v_j)^2} - \sqrt{d_T(v)^2 + d_T(v_j)^2}\right). \end{aligned}$$

Note that, after the transformation only the degree of vertices u and v is changed, where $d_{T^*}(u) = 1$ and $d_{T^*}(v) = m + n + 1$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned}
SO(T^*) - SO(T) = & \sqrt{1^2 + d(x)^2} - \sqrt{(m+1)^2 + d(x)^2} \\
& + \sqrt{(m+n+1)^2 + d(y)^2} - \sqrt{(n+1)^2 + d(y)^2} \\
& + \sum_{i=1}^{m} \left(\sqrt{(m+n+1)^2 + d(u_i)^2} - \sqrt{(m+1)^2 + d(u_i)^2} \right) \\
& + \sum_{j=1}^{n+b} \left(\sqrt{(m+n+1)^2 + d(v_j)^2} - \sqrt{(n+1)^2 + d(v_j)^2} \right).
\end{aligned}$$

Since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$, we have omitted the terms $\sum_{i=1}^{m} \left(\sqrt{(m+n+1)^2 + d(u_i)^2} - \sqrt{(m+1)^2 + d(u_i)^2} \right)$ and $\sum_{j=1}^{n+b} \left(\sqrt{(m+n+1)^2 + d(v_j)^2} - \sqrt{(n+1)^2 + d(v_j)^2} \right)$, while calculating the change in the Sombor index in the next step. Thus, we have

$$\begin{aligned}
SO(T^*) - SO(T) > & \sqrt{1^2 + d(x)^2} - \sqrt{(m+1)^2 + d(x)^2} \\
& + \sqrt{(m+n+1)^2 + d(y)^2} - \sqrt{(n+1)^2 + d(y)^2}.
\end{aligned}$$

Using Lemma 1 and substituting $c = m$ and $d = d(y)$, we have

$$\sqrt{(m+n+1)^2 + d(y)^2} - \sqrt{(n+1)^2 + d(y)^2} > \sqrt{(m+1)^2 + d(y)^2} - \sqrt{1^2 + d(y)^2},$$

since $f(n+1) > f(1)$, which holds true since $n \geq 1$. Now using Lemma 2 and substituting $c = m+1$ and $d = 1$, we have

$$\sqrt{(m+1)^2 + d(y)^2} - \sqrt{1 + d(y)^2} \geq \sqrt{(m+1)^2 + d(x)^2} - \sqrt{1 + d(x)^2},$$

since $d(x) \geq d(y)$ and hence $g(d(y)) \geq g(d(x))$. Thus, combining the above inequalities we have $SO(T^*) - SO(T) > 0$, which is a contradiction.
Thus, combining all the above cases, we have that if $T \in T(\mathbf{n}, \varphi)$ is a tree with maximal Sombor index, then $T \in T_1(\mathbf{n}, \varphi) \cup T_2(\mathbf{n}, \varphi) \cup T_3(\mathbf{n}, \varphi)$. □

Remark 2. Observe that, in the proof of Lemma 5 it is possible that the vertices x and y coincide or the vertices u and v are adjacent. In both situations, an analogous argument yields the desired result. Therefore, these special cases do not affect the conclusion of the lemma.

Lemma 6. *Let $T \in T(\mathbf{n},\varphi)$ be a tree with maximum Sombor index. Then $T \in T_1(\mathbf{n},\varphi)$.*

Proof. Suppose $T \in T(\mathbf{n},\varphi)$ is a tree with maximal Sombor index and $T \in T_2(\mathbf{n},\varphi)$. From the definition of the class $T_2(\mathbf{n},\varphi)$ we have v_0 is the central vertex of the induced star graph and $N(v_0) = \{u\} \cup \{v_1, v_2, \cdots, v_{\mathbf{n}-\varphi}\}$. Let $N(v_1) = \{v_0\} \cup \{w_1, w_2, \cdots, w_k\}$. Using Lemma 3, we can choose a maximal dissociation set $D(T)$ such that it contains all the pendant and degree 2 quasi-pendant vertices. Note that $\{v_1, v_2, \cdots, v_{\mathbf{n}-\varphi}\} \notin D(T)$. Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $v_1 \sim w_j$ for all $1 \leq j \leq k$.
- Add the edges $v_0 \sim w_j$ for all $1 \leq j \leq k$.

Note that after the transformation, we have $\varphi(T) = \varphi(T^*)$, since the transformation does not add or delete any edges between vertices in $D(T)$. Thus, we have

$$\begin{aligned} SO(T^*) - SO(T) = &\sum_{i=1}^{\mathbf{n}-\alpha} \left(\sqrt{d_{T^*}(v_0)^2 + d_{T^*}(v_i)^2} - \sqrt{d_T(v_0)^2 + d_T(v_i)^2}\right) \\ &+ \sum_{j=1}^{k} \left(\sqrt{d_{T^*}(v_0)^2 + d_{T^*}(w_j)^2} - \sqrt{d_T(v_1)^2 + d_T(w_j)^2}\right) \\ &+ \sqrt{d_{T^*}(v_0)^2 + d_{T^*}(u)^2} - \sqrt{d_T(v_0)^2 + d_T(u)^2}. \end{aligned}$$

Note that, after the transformation only the degree of vertices v_0 and v_1 are changed, where $d_{T^*}(v_0) = (\mathbf{n} - \varphi + 1) + k$ and $d_{T^*}(v_1) = 1$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned} SO(T^*) - SO(T) = &\sqrt{(\mathbf{n} - \varphi + k + 1)^2 + 1^2} - \sqrt{(\mathbf{n} - \varphi + 1)^2 + (k+1)^2} \\ &+ \sum_{i=2}^{\mathbf{n}-\varphi} \left(\sqrt{(\mathbf{n} - \varphi + k + 1)^2 + d(v_i)^2} - \sqrt{(\mathbf{n} - \varphi + 1)^2 + d(v_i)^2}\right) \\ &+ \sum_{j=1}^{k} \left(\sqrt{(\mathbf{n} - \varphi + k + 1)^2 + d(w_j)^2} - \sqrt{(k+1)^2 + d(w_j)^2}\right) \\ &+ \sqrt{(\mathbf{n} - \varphi + k + 1)^2 + 1^2} - \sqrt{(\mathbf{n} - \varphi + 1)^2 + 1^2} \end{aligned}$$

Since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$, we have omitted the terms $\sqrt{(\mathbf{n} - \varphi + k + 1)^2 + 1^2} - \sqrt{(\mathbf{n} - \varphi + 1)^2 + (k+1)^2}$, $\sum_{i=2}^{\mathbf{n}-\varphi} \left(\sqrt{(\mathbf{n} - \varphi + k + 1)^2 + d(v_i)^2} - \sqrt{(\mathbf{n} - \varphi + 1)^2 + d(v_i)^2}\right)$ and $\sum_{j=1}^{k} \left(\sqrt{(\mathbf{n} - \varphi + k + 1)^2 + d(w_j)^2} - \sqrt{(k+1)^2 + d(w_j)^2}\right)$, while calculating the change in the Sombor index to get

$$SO(T^*) - SO(T) > \sqrt{(\mathbf{n} - \varphi + k + 1)^2 + 1} - \sqrt{(\mathbf{n} - \varphi + 1)^2 + (k+1)^2} \geq 0,$$

where the last inequality is true since $k(\mathbf{n} - \varphi) \geq 0$. Note that, $T^* \in T_1(\mathbf{n}, \alpha)$ and $SO(T^*) > SO(T)$, which is a contradiction.
Next, suppose $T \in T(\mathbf{n}, \varphi)$ is a tree with maximal Sombor index and $T \in T_3(\mathbf{n}, \varphi)$. From the definition of the class $T_3(\mathbf{n}, \varphi)$ we have v_0 is the central vertex of the induced star graph and $N(v_0) = \{v_1, v_2, \cdots, v_{\mathbf{n}-\varphi}\}$. Let $N(v_1) = \{v_0\} \cup \{w_1, w_2, \cdots, w_k\}$. Using Lemma 3, we can choose a maximal dissociation set $D(T)$ such that it contains all the pendant and degree 2 quasi-pendant vertices. Note that $\{v_1, v_2, \cdots, v_{\mathbf{n}-\varphi}\} \notin D(T)$. Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $v_1 \sim w_j$ for all $1 \leq j \leq k$.
- Add the edges $v_0 \sim w_j$ for all $1 \leq j \leq k$.

Note that after the transformation, we have $\varphi(T) = \varphi(T^*)$, since the transformation does not add or delete any edges between vertices in $D(T)$. Thus, we have

$$\begin{aligned} SO(T^*) - SO(T) = &\sum_{i=1}^{\mathbf{n}-\alpha} \left(\sqrt{d_{T^*}(v_0)^2 + d_{T^*}(v_i)^2} - \sqrt{d_T(v_0)^2 + d_T(v_i)^2} \right) \\ &+ \sum_{j=1}^{k} \left(\sqrt{d_{T^*}(v_0)^2 + d_{T^*}(w_j)^2} - \sqrt{d_T(v_1)^2 + d_T(w_j)^2} \right). \end{aligned}$$

Note that, after the transformation only the degree of vertices v_0 and v_1 are changed, where $d_{T^*}(v_0) = (\mathbf{n} - \varphi) + k$ and $d_{T^*}(v_1) = 1$. Thus, substituting the values of degree in the above expression we have

$$\begin{aligned} SO(T^*) - SO(T) = &\sqrt{(\mathbf{n} - \varphi + k)^2 + 1^2} - \sqrt{(\mathbf{n} - \varphi)^2 + (k+1)^2} \\ &+ \sum_{i=2}^{\mathbf{n}-\varphi} \left(\sqrt{(\mathbf{n} - \varphi + k)^2 + d(v_i)^2} - \sqrt{(\mathbf{n} - \varphi)^2 + d(v_i)^2} \right) \\ &+ \sum_{j=1}^{k} \left(\sqrt{(\mathbf{n} - \varphi + k)^2 + d(w_j)^2} - \sqrt{(k+1)^2 + d(w_j)^2} \right). \end{aligned}$$

Since the function $h(x) = \sqrt{x^2 + a^2}$ is monotonically increasing for $x > 0$, we have omitted the terms $\sum_{i=2}^{\mathbf{n}-\varphi} \left(\sqrt{(\mathbf{n} - \varphi + k)^2 + d(v_i)^2} - \sqrt{(\mathbf{n} - \varphi)^2 + d(v_i)^2} \right)$ and $\sum_{j=1}^{k} \left(\sqrt{(\mathbf{n} - \varphi + k)^2 + d(w_j)^2} - \sqrt{(k+1)^2 + d(w_j)^2} \right)$, while calculating the change in the Sombor index to get $SO(T^*) - SO(T) > \sqrt{(\mathbf{n}-\varphi+k)^2+1} - \sqrt{(\mathbf{n}-\varphi)^2+(k+1)^2} \geq 0$, where the last inequality is true since $\mathbf{n}-\varphi \geq 1$. Note that, $T^* \in T_1(\mathbf{n},\alpha)$ and $SO(T^*) > SO(T)$, which is a contradiction. □

Now we state and prove the main result of the article.

Theorem 1. *Let $T \in T(\mathbf{n},\varphi)$. If $\varphi \leq \mathbf{n}-2$, then*

$$SO(T) \leq (3\varphi-2(\mathbf{n}-1))\sqrt{(2\varphi-\mathbf{n}+1)^2+1}+(\mathbf{n}-(\varphi+1))[\sqrt{(2\varphi-\mathbf{n}+1)^2+3^2}+2\sqrt{3^2+1}]$$

and equality is attained if and only if $T \cong T^*(\mathbf{n},\varphi)$. If $\varphi = \mathbf{n}-1$, then $T(\mathbf{n},\mathbf{n}-1) = \{S_\mathbf{n}\}$ and $SO(S_\mathbf{n}) = (\mathbf{n}-1)\sqrt{(\mathbf{n}-1)^2+1} = \varphi\sqrt{\varphi^2+1}$.

Proof. Let $\varphi \leq \mathbf{n}-2$ and $T \in T(\mathbf{n},\varphi) \neq T^*(\mathbf{n},\varphi)$ be a tree with maximal Sombor index, then using Lemmas 5 and 6, we have that $T \in T_1(\mathbf{n},\varphi)$. Since $T \in T(\mathbf{n},\varphi) \neq T^*(\mathbf{n},\varphi)$, there exists a vertex $v_1 \in N(v_0)$ which is not a pendant vertex and $d(v_1) \geq 4$. Let $N(v_1) = \{v_0\} \cup \{w_1, w_2, \cdots, w_k\}$, where $d(w_p) = 1$ for $1 \leq p \leq k$ and hence $d(v_1) = k+1$. Let $N(v_0) = \{v_1, v_2, \cdots, v_{\mathbf{n}-(\varphi+1)}\} \cup \{u_1, u_2, \cdots, u_m\}$, where $d(u_j) = 1$ for $1 \leq j \leq m$ and hence $d(v_0) = \mathbf{n}-(\varphi+1)+m \geq 2$. For simplicity of further calculations, we assume that $d(v_0) = l+2$. Let T^* be the graph obtained from T by applying the following transformations:

- Delete the edges $v_1 \sim w_p$ for all $3 \leq p \leq k$.
- Add the edges $v_0 \sim w_p$ for all $3 \leq p \leq k$.

Note that, after the transformation, we have $\varphi(T) = \varphi(T^*)$, since the transformation does not add or delete any edges between vertices in $D(T)$. Thus, we have

$$\begin{aligned}
SO(T^*) - SO(T) = &\sum_{i=1}^{\mathbf{n}-(\varphi+1)} \left(\sqrt{d_{T^*}(v_0)^2+d_{T^*}(v_i)^2} - \sqrt{d_T(v_0)^2+d_T(v_i)^2}\right) \\
&+ \sum_{j=1}^{m} \left(\sqrt{d_{T^*}(v_0)^2+d_{T^*}(u_j)^2} - \sqrt{d_T(v_0)^2+d_T(u_j)^2}\right) \\
&+ \sqrt{d_{T^*}(v_1)^2+d_{T^*}(w_1)^2} - \sqrt{d_T(v_1)^2+d_T(w_1)^2} \\
&+ \sqrt{d_{T^*}(v_1)^2+d_{T^*}(w_2)^2} - \sqrt{d_T(v_1)^2+d_T(w_2)^2} \\
&+ \sum_{p=3}^{k} \left(\sqrt{d_{T^*}(v_0)^2+d_{T^*}(w_p)^2} - \sqrt{d_T(v_1)^2+d_T(w_p)^2}\right).
\end{aligned}$$

Note that, after the transformation only the degree of vertices v_0 and v_1 are changed, where $d_{T^*}(v_0) = l+k$ and $d_{T^*}(v_1) = 3$. Thus, substituting the values of degree in the above expression we have

$$
\begin{aligned}
SO(T^*) - SO(T) = & \sqrt{(l+k)^2+3^2} - \sqrt{(l+2)^2+(k+1)^2} \\
& + \sum_{i=2}^{\mathbf{n}-(\varphi+1)} \left(\sqrt{(l+k)^2+d(v_i)^2} - \sqrt{(l+2)^2+d(v_i)^2} \right) \\
& + \sum_{j=1}^{m} \left(\sqrt{(l+k)^2+1^2} - \sqrt{(l+2)^2+1^2} \right) \\
& + 2(\sqrt{3^2+1^2} - \sqrt{(k+1)^2+1^2}) \\
& + \sum_{p=3}^{k} \left(\sqrt{(l+k)^2+1^2} - \sqrt{(k+1)^2+1^2} \right).
\end{aligned}
$$

Since there are at least two pendant vertex attached to v_0, we have $m > 1$. Let u_1 and u_2 be two pendant vertices adjacent to v_0. In the next step, while calculating the difference between the Sombor index, we omit the sums $\sum_{i=2}^{\mathbf{n}-(\varphi+1)} \left(\sqrt{(l+k)^2+d(v_i)^2} - \sqrt{(l+2)^2+d(v_i)^2} \right)$, $\sum_{j=1}^{m} \left(\sqrt{(l+k)^2+1^2} - \sqrt{(l+2)^2+1^2} \right)$ and $\sum_{p=3}^{k} \left(\sqrt{(l+k)^2+1^2} - \sqrt{(k+1)^2+1^2} \right)$, except the terms corresponding to the edge $v_0 \sim u_1$ and $v_0 \sim u_2$, since the function $h(x) = \sqrt{x^2+a^2}$ is monotonically increasing for $x > 0$. Thus, we have

$$
\begin{aligned}
SO(T^*) - SO(T) > & \sqrt{(l+k)^2+3^2} - \sqrt{(l+1)^2+(k+1)^2} \\
& + 2(\sqrt{(l+k)^2+1} - \sqrt{(l+2)^2+1}) \\
& + 2(\sqrt{3^2+1} - \sqrt{(k+1)^2+1}).
\end{aligned}
$$

Using Lemma 1 and substituting $c = k-2$ and $d = 1$, we have

$$
\sqrt{(l+k)^2+1} - \sqrt{(l+2)^2+1} \geq \sqrt{(k+1)^2+1} - \sqrt{3^2+1},
$$

since $f(l+2) \geq f(3)$, which holds true since $l \geq 1$. Also, it follows from the inequality $(l+k)^2 + 9 - \left((l+2)^2+(k+1)^2\right) = 2(k-2)(l-1) \geq 0$, which holds for $l \geq 1$ and $k \geq 3$, that $\sqrt{(l+k)^2+3^2} \geq \sqrt{(l+2)^2+(k+1)^2}$ for all $l \geq 1$ and $k \geq 3$. Hence, combining the inequalities we have $SO(T^*) > SO(T)$, which is a contradiction. Thus, $T \cong T^*(\mathbf{n}, \varphi)$ and the result follows.

If $\varphi = \mathbf{n} - 1$, then we have already shown in the beginning of the section that $T(\mathbf{n}, \mathbf{n}-1) = \{S_{\mathbf{n}}\}$ and $SO(S_{\mathbf{n}}) = (\mathbf{n}-1)\sqrt{(\mathbf{n}-1)^2+1} = \varphi\sqrt{\varphi^2+1}$. □

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