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Research article

Sombor index of directed graphs

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ARTICLE INFO

Keywords:
Sombor index
Digraphs
Connected digraphs
Strongly connected digraphs
Orientations

ABSTRACT

Let D be a digraph with set of arcs A. The Sombor index of D is defined as

$$SO(D) = \frac{1}{2} \sum_{uv \in A} \sqrt{\left(d_u^+\right)^2 + \left(d_v^-\right)^2},$$

where d_u^+ and d_v^- are the out-degree and in-degree of the vertices u and v of D. When D is a graph, we recover the Sombor index of graphs, a molecular descriptor recently introduced with a good predictive potential and a great research activity this year. In this paper we initiate the study of the Sombor index of digraphs. Specifically, we find sharp upper and lower bounds for $S\mathcal{O}$ over the class D_n of digraphs with n non-isolated vertices, the classes C_n and S_n of connected and strongly connected digraphs on n vertices, respectively, the class of oriented trees $\mathcal{OT}(n)$ with n vertices, and the class $\mathcal{O}(G)$ of orientations of a fixed graph G.

1. Introduction

A digraph D is an ordered tuple (V,A), where V is a nonempty set, called the set of vertices of D, and A is a subset of the set of ordered pairs of different vertices of D. The elements of A are called arcs. If a=(u,v) is an arc of D then we simply write a=uv and say that u is adjacent to v or v is adjacent from u. The outdegree d_u^+ of a vertex u of D is the number of vertices of D that are adjacent from u. The indegree d_u^- of u is the number of vertices of D adjacent to u. If u is a vertex of D such that $d_u^+=0$, then u is called a sink vertex of D whereas if $d_u^-=0$, then u is called a source vertex of D. We denote by p=p(D) the number of sink vertices and q=q(D) the number of source vertices of D. If $d_u^+=d_u^-=0$, then u is an isolated vertex. The set of digraphs with u non-isolated vertices is denoted by u.

A digraph D is symmetric if $uv \in A$ implies $vu \in A$, where $u,v \in V$. There is a natural one-to-one correspondence between the symmetric digraphs and the set of graphs. Thus, the set G_n of graphs with n non-isolated vertices satisfies $G_n \subseteq D_n$. On the other side, a digraph D is called an asymmetric digraph or an oriented graph if whenever $uv \in A$ then $vu \notin A$. Consequently, an oriented graph D can be obtained from a graph G by assigning a direction to each edge of G; D is called an orientation of G. For instance, in Fig. 1 we show the directed path \overline{P}_n and the directed cycle \overline{C}_n , which are orientations of the path P_n and

Fig. 1. Orientations of P_n , C_n .

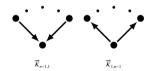


Fig. 2. Sink-source orientations of S_n .

the cycle C_n , respectively. If D is an orientation of G such that each vertex of D is a sink vertex or a source vertex, then D is called a sink-source orientation of G. The digraphs $\overline{K}_{1,n-1}$ and $\overline{K}_{n-1,1}$ in Fig. 2 are sink-source orientations of the star S_n .

Let $D \in \mathcal{D}_n$. Given $1 \le i, j \le n - 1$, consider the set

$$A_{ij} = \{uv \in A : d_u^+ = i \text{ and } d_v^- = j\}.$$

If $uv \in A_{ij}$ then we say uv is a (i,j)-arc. Let a_{ij} be the cardinality of A_{ij} and define

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https://doi.org/10.1016/j.heliyon.2022.e09035

Received 21 November 2021; Received in revised form 13 January 2022; Accepted 25 February 2022

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R. Cruz, J. Monsalve and J. Rada Heliyon 8 (2022) e09035

$$p_{ij} = a_{ij} + a_{ij},$$

for all $1 \le i, j \le n - 1$, and

 $p_{ii} = a_{ii}$,

for all i = 1, ..., n - 1. The Sombor index of D is defined as [12]

$$S\mathcal{O}(D) = \frac{1}{2} \sum_{(i,j) \in K} p_{ij} \sqrt{i^2 + j^2},\tag{1}$$

where

 $K = \{(i, j) \in \mathbb{N} \times \mathbb{N} : 1 \le i \le j \le n - 1\}.$

Equivalently,

$$SO(D) = \frac{1}{2} \sum_{uv \in A} \sqrt{\left(d_u^+\right)^2 + \left(d_v^-\right)^2}.$$
 (2)

The formulas (1) and (2) are particular cases of the general theory of vertex-degree-based topological indices over digraphs [12, 13]. When D is a graph, we recover the recently introduced Sombor index of graphs [7], a molecular descriptor with a good predictive potential [16] and with a great research activity this year [1, 2, 3, 5, 8, 9, 10, 11, 15, 17].

In this paper we initiate the study of the Sombor index of digraphs. Specifically, we find sharp upper and lower bounds for $S\mathcal{O}$ over the class \mathcal{D}_n of digraphs with n non-isolated vertices, the classes \mathcal{C}_n and \mathcal{S}_n of connected and strongly connected digraphs on n vertices, respectively, the class of oriented trees $\mathcal{OT}(n)$ with n vertices, and the class $\mathcal{O}(G)$ of orientations of a fixed graph G with non-isolated vertices.

2. Upper and lower bounds of the Sombor index over significant classes of digraphs

We begin with the study of $S\mathcal{O}$ over the set \mathcal{D}_n of digraphs with n non-isolated vertices. Let $D_1=(V_1,A_1)$ and $D_2=(V_2,A_2)$ be digraphs with no common vertices. The digraph $D=\left(V_1\cup V_2,A_1\cup A_2\right)$ is called the direct sum of D_1 and D_2 and denoted by $D_1\oplus D_2$. In general, $\bigoplus_{i=1}^k D_i$ denotes the direct sum of the digraphs $D_1=(V_1,A_1),\ldots,D_k=(V_k,A_k)$ and kD denotes the direct sum of k copies of digraph D.

Theorem 2.1. Let $D \in \mathcal{D}_n$ with p sink vertices and q source vertices. Then

$$\frac{\sqrt{2}}{4} (2n - p - q) \le \mathcal{SO}(D) \le \frac{\sqrt{2}}{4} (n - 1)^2 (2n - p - q).$$

Equality on the left occurs if and only if

$$D = \bigoplus_{i=1}^{k_1} \overrightarrow{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overrightarrow{C}_{n_j},$$

for some nonnegative integers k_1 and k_2 . Equality on the right occurs if and only if $D = K_n$, the complete graph on n vertices.

Proof. Consider the function $f(x, y) = \frac{xy\sqrt{x^2+y^2}}{x+y}$ defined over the compact set

$$\widehat{K} = \{(x, y) \in \mathbb{R} \times \mathbb{R} : 1 \le x \le y \le n - 1\}.$$

Since

$$\frac{\partial f(x, y)}{\partial x} = \frac{y(x^3 + 2x^2y + y^3)}{\sqrt{x^2 + y^2}(x + y)^2} > 0$$

and

$$\frac{\partial f(x,y)}{\partial y} = \frac{x(x^3 + 2xy^2 + y^3)}{\sqrt{x^2 + y^2}(x + y)^2} > 0$$

for all $(x, y) \in \hat{K}$, we conclude that

$$\max_{(x,y)\in K} f(x,y) = f(n-1,n-1) = \frac{\sqrt{2}}{2} (n-1)^2,$$

and

$$\min_{(x,y)\in K} f(x,y) = f(1,1) = \frac{\sqrt{2}}{2}.$$

It follows from [13, Theorem 1] that

$$\frac{2n - p - q}{2\sqrt{2}} \le S\mathcal{O}(D) \le \frac{(n - 1)^2 (2n - p - q)}{2\sqrt{2}}.$$
 (3)

Moreover, equality on the left of (3) occurs if and only if $p_{ij}=0$ for all $(1,1)\neq (i,j)\in K$. Since the only connected digraphs such that every arc is a (1,1)-arc are the directed paths and the directed cycles, this is equivalent to

$$D = \bigoplus_{i=1}^{k_1} \overrightarrow{P}_{n_i} \oplus \bigoplus_{i=1}^{k_2} \overrightarrow{C}_{n_j},$$

for some nonnegative integers k_1 and k_2 . The equality on the right of (3) occurs if and only if $p_{ij} = 0$ for all $(n-1, n-1) \neq (i, j) \in K$, or equivalently, $D = K_n$. \square

Corollary 2.2. Let $D \in \mathcal{D}_n$. Then

$$\frac{\sqrt{2}}{4}n \le \mathcal{SO}(D) \le \frac{\sqrt{2}}{2}(n-1)^2 n.$$

Equality on the left occurs if and only if n is even and $D = \frac{n}{2} \overrightarrow{P}_2$. Equality on the right occurs if and only if $D = K_n$.

Proof. By Theorem 2.1, bearing in mind that $0 \le p + q \le n$,

$$\frac{\sqrt{2}}{4}n \le \frac{\sqrt{2}}{4}(2n - (p+q)) \le S\mathcal{O}(D) \tag{4}$$

and

$$SO(D) \le \frac{\sqrt{2}}{4} (n-1)^2 (2n - (p+q))$$

$$\le \frac{\sqrt{2}}{2} (n-1)^2 n.$$
(5)

If $SO(D) = \frac{\sqrt{2}}{2}(n-1)^2 n$ then, by (5), p+q=0 and again, by Theorem 2.1, $D=K_n$. Conversely,

$$\begin{split} \mathcal{SO}\left(K_{n}\right) &= \frac{1}{2}n(n-1)\sqrt{(n-1)^{2} + (n-1)^{2}} \\ &= \frac{\sqrt{2}}{2}n(n-1)^{2}. \end{split}$$

On the other side, assume that $SO(D) = \frac{\sqrt{2}}{4}n$. Then p + q = n by (4) and by Theorem 2.1, n is even and $D = \frac{n}{2}\vec{P}_2$, since every vertex of D is a sink vertex or a source vertex. Conversely, if n is even then

$$SO\left(\frac{n}{2}\vec{P}_2\right) = \frac{n}{2}SO\left(\vec{P}_2\right) = \frac{n}{4}\sqrt{2}.$$

Corollary 2.3. Let n be odd and $D \in \mathcal{D}_n$. Then

$$\frac{\sqrt{2}}{4}(n+1) \le \mathcal{SO}(D).$$

Equality holds if and only if $D = \frac{n-3}{2} \overrightarrow{P}_2 \oplus \overrightarrow{P}_3$.

Proof. Let p and q be the number of sink and source vertices of D, respectively and assume first that $p + q \le n - 1$. Then, by Theorem 2.1,

$$SO(D) \ge \frac{\sqrt{2}}{4} (2n - p - q) \ge \frac{\sqrt{2}}{4} (n + 1).$$
 (6)

R. Cruz, J. Monsalve and J. Rada Heliyon 8 (2022) e09035

Now assume that p+q=n. Let P be the set of sink vertices of D and Q the set of source vertices of D. Then $V=P\cup Q$ and

$$2a = \sum_{u \in P} d_u^- + \sum_{v \in O} d_v^+ \ge p + q = n.$$

Hence $a \ge \frac{n+1}{2}$ since n is odd. Now, clearly $\left(d_u^+\right)^2 + \left(d_v^-\right)^2 \ge 2$ for all $uv \in A$, consequently,

$$SO(D) = \frac{1}{2} \sum_{uv \in A} \sqrt{\left(d_u^+\right)^2 + \left(d_v^-\right)^2}$$

$$\geq \frac{1}{2} \sqrt{2} a \geq \frac{\sqrt{2}}{4} (n+1). \tag{7}$$

For the second part, assume that $\frac{\sqrt{2}}{4}(n+1) = S\mathcal{O}(D)$. If $p+q \le n-1$ then, by (6) and Theorem 2.1, $p_{ij} = 0$ for all $(1,1) \ne (i,j) \in K$ and p+q = n-1. It follows from [13, Lemma 2 (6)] that $D = \frac{n-3}{2} \overrightarrow{P}_2 \oplus \overrightarrow{P}_3$.

n-1. It follows from [13, Lemma 2 (6)] that $D=\frac{n-3}{2} \overrightarrow{P}_2 \oplus \overrightarrow{P}_3$. If p+q=n then, by (7), $d_u^+=d_v^-=1$ for all $uv \in A$. It follows that $D=\bigoplus_{i=1}^{k_1} \overrightarrow{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overrightarrow{C}_{n_j}$. But then $D=\frac{n}{2} \overrightarrow{P}_2$, since every vertex of D is sink or source, and this is a contradiction because n is odd.

Conversely.

$$SO\left(\frac{n-3}{2}\overrightarrow{P}_2 \oplus \overrightarrow{P}_3\right) = \frac{1}{2}\left(\frac{n-3}{2}\sqrt{2} + 2\sqrt{2}\right)$$
$$= \frac{\sqrt{2}}{4}(n+1). \quad \Box$$

Let us consider other interesting classes of digraphs. Recall that a digraph is *connected* if its underlying graph is connected. Moreover, a digraph is *strongly connected* if there is a directed path between any pair of vertices. We denote by C_n the set of connected digraphs with n vertices and S_n the set of strongly connected digraphs with n vertices. Clearly, $S_n \subseteq C_n \subseteq \mathcal{D}_n$.

Theorem 2.4. Let $D \in C_n$. Then

$$\frac{\sqrt{2}}{2}(n-1) \le S\mathcal{O}(D) \le \frac{\sqrt{2}}{2}(n-1)^2 n.$$
 (8)

Equality in the left occurs if and only if $D = \overrightarrow{P}_n$. Equality on the right occurs if and only if $D = K_n$.

Proof. The right part of (8) is a direct application of Corollary 2.2, because $C_n \subseteq D_n$ and the complete graph $K_n \in C_n$.

Consider the function $g(x, y) = \sqrt{x^2 + y^2}$ defined over the compact set

$$\widehat{K} = \{(x, y) \in \mathbb{R} \times \mathbb{R} : 1 \le x \le y \le n - 1\}.$$

Since

$$\frac{\partial g(x,y)}{\partial x} = \frac{x}{\sqrt{x^2 + y^2}} > 0$$

and

$$\frac{\partial g(x,y)}{\partial y} = \frac{y}{\sqrt{x^2 + y^2}} > 0$$

for all $(x, y) \in \hat{K}$, we conclude that

$$\min_{(x,y)\in K} g(x,y) = g(1,1) = \sqrt{2}.$$

Let a be the number of arcs of D. Since D is connected, $a \ge n-1$. It follows from [13, Theorem 2] that

$$S\mathcal{O}(D) \ge \frac{1}{2} a \min_{(x,y) \in K} g(x,y)$$

$$= \frac{\sqrt{2}}{2} a \ge \frac{\sqrt{2}}{2} (n-1). \tag{9}$$

By (9) and [13, Theorem 2], $\mathcal{SO}(D) = \frac{\sqrt{2}}{2}(n-1)$ if and only if a = n-1 and $a_{ij} = 0$ for all $(i,j) \in K$ such that $(i,j) \neq (1,1)$. This is equivalent to $D = \overrightarrow{P}_n$. \square

Theorem 2.5. Let $D \in S_n$. Then

$$\frac{\sqrt{2}}{2}n \le SO(D) \le \frac{\sqrt{2}}{2}(n-1)^2 n.$$
 (10)

Equality in the left occurs if and only if $D = \overline{C}_n$. Equality on the right occurs if and only if $D = K_n$.

Proof. The right part of (10) is a direct application of Corollary 2.2, because $S_n \subseteq D_n$ and the complete graph $K_n \in S_n$.

Since D is strongly connected, $d_u^+ \ge 1$ for all vertex u of D. Consequently,

$$a = \sum_{u \in V} d_u^+ \ge n. \tag{11}$$

Now by [13, Theorem 2] and (11),

$$SO(D) \ge \frac{1}{2} a \min_{(x,y) \in K} g(x,y) = \frac{\sqrt{2}}{2} a \ge \frac{\sqrt{2}}{2} n.$$
 (12)

Moreover, by (12) and [13, Theorem 2], $SO(D) = \frac{\sqrt{2}}{2}n$ if and only if a = n and $a_{ij} = 0$ for all $(i, j) \in K$ such that $(i, j) \neq (1, 1)$. This is equivalent to $D = \overrightarrow{C}_n$.

Let us denote by $\mathcal{O}(G)$ the set of all orientations of the graph G. One natural problem is to determine the extremal values of the Sombor index in $\mathcal{O}(G)$. Let us consider the partial order over K defined as follows: if $(i, j), (k, l) \in K$, then

 $(i,j) \leq (k,l) \Leftrightarrow i \leq k \text{ and } j \leq l.$

Note that if $(i, j) \leq (k, l)$, then

$$\sqrt{i^2+i^2} < \sqrt{k^2+l^2}$$

Moreover, if $(i, j) \le (k, l)$ and $\sqrt{i^2 + j^2} = \sqrt{k^2 + l^2}$, then (i, j) = (k, l). In other words, SO is a strictly nondecreasing VDB topological index as defined in [13, Definition 2].

Theorem 2.6. Let G be a graph and D any orientation of G. Then

$$SO(D) \le \frac{1}{2}SO(G)$$
.

Equality holds if and only if D is a sink-source orientation of G.

Proof. This is a direct application of [13, Theorem 5] bearing in mind that SO is a strictly nondecreasing VDB topological index.

Note that a graph G has a sink-source orientation if and only if G is a bipartite graph [14, Proposition 2.2]. A consequence of Theorem 2.6 is that among all orientations of a fixed bipartite graph G, the orientation with maximal Sombor index is a sink-source orientation of G. Indeed, let E be a sink-source orientation of G and D any orientation of G. Then

$$S\mathcal{O}(D) \le \frac{1}{2}S\mathcal{O}(G) = S\mathcal{O}(E)$$
.

What can we say about the minimal value of SO in O(G)? For a general bipartite graph G this is apparently a difficult problem. However, in our next results we will analyze the case when G is the path P_n or the cycle C_n on n vertices.

Theorem 2.7. Let D be any orientation of P_n . Then

$$SO(\overrightarrow{P}_n) \leq SO(D) \leq SO(\widehat{P}_n),$$

where \hat{P}_n is any of the sink-source orientations of P_n shown in Fig. 3.

R. Cruz, J. Monsalve and J. Rada Heliyon 8 (2022) e09035

Fig. 3. Sink-source orientations of P_n .

Proof. This is a consequence of Theorem 2.6 and Theorem 2.4.

In order to study the orientations of the cycle C_n , we say that D is a quasi-sink-source orientation of C_n if all vertices are sink or source vertices, except for one. In this case, n is odd, $(p_{11}, p_{12}, p_{22}) = (0, 2, n-2)$, and

$$SO(D) = \frac{1}{2} \left(2\sqrt{5} + (n-2)\sqrt{8} \right) = \sqrt{5} + (n-2)\sqrt{2}.$$

Theorem 2.8. Let C_n be the cycle on n vertices. Let D be any orientation of C_n . Then

$$\frac{\sqrt{2}}{2}n \le \mathcal{SO}(D) \le \begin{cases} \sqrt{2}n & \text{if } n \text{ is even} \\ \sqrt{5} + (n-2)\sqrt{2} & \text{if } n \text{ is odd} \end{cases}.$$

Equality in the left occurs if and only if $D = \overline{C}_n$. Equality in the right occurs if and only if D is a sink-source (resp. quasi sink-source) orientation when n is even (resp. when n is odd).

Proof. Let $g(x, y) = \sqrt{x^2 + y^2}$ defined over K. Then $\min_{(x,y) \in K} g(x,y) = \sqrt{2}$ (see proof of Theorem 2.4). By [13, Theorem 2],

$$\frac{\sqrt{2}}{2}n \le S\mathcal{O}(D).$$

Moreover, $\frac{\sqrt{2}}{2}n = S\mathcal{O}(D)$ if and only if $a_{ij} = 0$ for all $(i, j) \in K$ such that $(i, j) \neq (1, 1)$. This is equivalent to $D = \overline{C}_n$.

On the other hand, assume first that n is even. Then C_n is a bipartite graph and so by Theorem 2.6, if E is a sink-source orientation of C_n (all arcs of E are (2,2)-arcs), then

$$SO(D) \le SO(E) = \frac{n}{2}\sqrt{8} = \sqrt{2}n.$$
 (13)

Moreover, by (13), $SO(D) = \frac{\sqrt{2}}{2}n$ if and only if *D* is a sink-source orientation of C_n .

Now assume that n is odd. We affirm that for every orientation D of C_n ,

$$\frac{\sqrt{2}}{2}p_{11} + \left(\sqrt{2} - \frac{\sqrt{5}}{2}\right)p_{12} \ge 2\sqrt{2} - \sqrt{5}.\tag{14}$$

In fact, (14) only fails when $p_{11} = p_{12} = 0$ or when $p_{11} = 0$ and $p_{12} = 1$. In the first case, since

$$p_{11} + p_{12} + p_{22} = a = n,$$

we deduce that $(p_{11}, p_{12}, p_{22}) = (0, 0, n)$ and so by [12, Lemma 5.2], D is a sink-source orientation of C_n . But this is not possible because n is odd. In the second case we have $(p_{11}, p_{12}, p_{22}) = (1, 0, n-1)$, which is not possible by [12, Lemma 5.2]. It follows from (14) that

$$SO(D) = \frac{1}{2} \left(p_{11} \sqrt{2} + p_{12} \sqrt{5} + 2\sqrt{2} p_{22} \right)$$

$$\leq \sqrt{5} + \left(p_{11} + p_{12} + p_{22} - 2 \right) \sqrt{2}$$

$$= \sqrt{5} + (n - 2) \sqrt{2}.$$
(15)

If $SO(D) = \sqrt{5} + (n-2)\sqrt{2}$, then by (15) and (14) we deduce

$$\frac{\sqrt{2}}{2}p_{11} + \left(\sqrt{2} - \frac{\sqrt{5}}{2}\right)p_{12} = 2\sqrt{2} - \sqrt{5}.$$

Equivalently,

$$\sqrt{2}(p_{11}+2p_{12}-4)=\sqrt{5}(p_{12}-2).$$

Hence $p_{12} - 2 = 0$ and $p_{11} + 2p_{12} - 4 = 0$ which implies $p_{12} = 2$ and $p_{11} = 0$. In other words, $(p_{11}, p_{12}, p_{22}) = (0, 2, n - 2)$. It follows from [12, Lemma 5.2] that D is a quasi-sink-source orientation. The converse is clear.

In Theorems 2.7 and 2.8 the extremal value problem of SO over the orientations of the path P_n and the cycle C_n were solved. Another interesting problem would be to find the extremal values of SO over the set of orientations of the complete graph K_n .

Problem 2.9. Find the extremal values of SO among all tournaments of n vertices.

Let $\mathcal{OT}(n)$ denote the set of all oriented trees with n vertices.

Theorem 2.10. Let $T \in \mathcal{OT}(n)$. Then

$$\frac{\sqrt{2}}{2}(n-1) \le S\mathcal{O}(T) \le \frac{1}{2}(n-1)\sqrt{n^2 - 2n + 2}.$$
 (16)

Equality on the left occurs if and only if $T = \overrightarrow{P}_n$. Equality on the right occurs if and only if $T = \overrightarrow{K}_{n-1,1}$ or $T = \overrightarrow{K}_{1,n-1}$.

Proof. The left part of (16) is a direct application of Theorem 2.4, because $\mathcal{OT}(n) \subseteq C_n$ and $\overrightarrow{P}_n \in \mathcal{OT}(n)$.

Let $T \in \mathcal{OT}(n)$. Assume that T is an orientation of a tree G order n. Then by [7, Theorem 3] and Theorem 2.6,

$$SO(T) \le \frac{1}{2}SO(G)$$

$$\le \frac{1}{2}SO(S_n)$$

$$= \frac{1}{2}(n-1)\sqrt{n^2 - 2n + 2}.$$
(17)

By [7, Theorem 3], Theorem 2.6, and (17), equality occurs if and only if $G = S_n$ and T is a sink-source orientation of G, and this is equivalent to $T = \overline{K}_{n-1,1}$ or $T = \overline{K}_{1,n-1}$. \square

3. Conclusion

In 2021, Ivan Gutman proposed a new topological index on graphs called the Sombor index [7], which gave rise to numerous publications on its mathematical properties and chemical applications [8], a clear indicator of the quality of the index. On the other hand, motivated by the important role of the directed graphs in real-world situations, for instance, chemical and biological networks, transportation networks, social networks, just to mention a few [4, 6], the concept of vertex-degree-based topological indices was recently introduced in [12]. Bearing in mind these ideas, we initiated the study of the Sombor index of directed graphs. Concretely, we determined extremal values of the Sombor index over significant classes of digraphs, and characterized the digraphs were these extremal values are attained.

Declarations

Author contribution statement

Roberto Cruz; Juan Monsalve; Juan Rada: Conceived and designed the analysis; Analyzed and interpreted the data; Contributed analysis tools or data; Wrote the paper.

Funding statement

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Data availability statement

No data was used for the research described in the article.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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