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Sharp Upper and Lower Bounds of VDB Topological Indices of Digraphs

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Abstract: A vertex-degree-based (VDB, for short) topological index φ induced by the numbers $\{\varphi_{ij}\}$ was recently defined for a digraph D, as $\varphi(D) = \frac{1}{2}\sum_{uv}\varphi_{d_u^+ d_v^-}$, where d_u^+ denotes the out-degree of the vertex u, d_v^- denotes the in-degree of the vertex v, and the sum runs over the set of arcs uv of D. This definition generalizes the concept of a VDB topological index of a graph. In a general setting, we find sharp lower and upper bounds of a symmetric VDB topological index over $\mathcal{D}_n$, the set of all digraphs with n non-isolated vertices. Applications to well-known topological indices are deduced. We also determine extremal values of symmetric VDB topological indices over $\mathcal{OT}(n)$ and $\mathcal{O}(G)$, the set of oriented trees with n vertices, and the set of all orientations of a fixed graph G, respectively.

Keywords: vertex-degree-based topological index; digraph; orientation of a graph; extremal value

MSC: 05C92; 05C09; 05C35

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1. Introduction

A digraph D is a finite nonempty set V called vertices, together with a set A of ordered pairs of distinct vertices of D, called arcs. If $a = (u, v)$ is an arc of D, then we write uv and say that the two vertices are adjacent. Given a vertex u of G, the out-degree of u is denoted by d_u^+ and defined as the number of arcs of the form uv, where $v \in V$. The in-degree of u is denoted by d_u^- and defined as the number of arcs of the form wu, where $w \in V$. A vertex u in D is called a sink vertex (resp. source vertex) if $d_u^+ = 0$ (resp. $d_u^- = 0$). We denote by $q = q(D)$ the number of vertices of D which are sink vertices or source vertices. If $d_u^+ = d_u^- = 0$, then u is an isolated vertex. The set of digraphs with n non-isolated vertices is denoted by $\mathcal{D}_n$.

One special class of digraphs is the oriented graphs. A pair of arcs of a digraph D of the form uv and vu are called symmetric arcs. If D has no symmetric arcs, then D is an oriented graph. We note that D can be obtained from a graph G by substituting each edge uv by an arc uv or vu, but not both. In this case, we say that D is an orientation of G. For example, in Figure 1 we show the directed path $\overrightarrow{P}_n$ and the directed cycle $\overrightarrow{C}_n$, orientations of the path P_n and cycle C_n, respectively. A sink-source orientation of a graph G is an orientation in which every vertex is a sink vertex or a source vertex. Clearly, when we reverse the orientations of all arcs in a sink-source orientation, we obtain a sink-source orientation again. For instance, the digraphs $\overrightarrow{K}_{1,n-1}$ and $\overrightarrow{K}_{n-1,1}$ in Figure 1 are sink-source orientations of the star S_n. Note that $\overrightarrow{K}_{n-1,1}$ is obtained by reversing all arcs of $\overrightarrow{K}_{1,n-1}$.

Let $D_1 = (V_1, A_1)$ and $D_2 = (V_2, A_2)$ be digraphs with no common vertices. The direct sum of digraphs D_1 and D_2, denoted by $D_1 \oplus D_2$, is the digraph with vertex and arc sets $V_1 \cup V_2$ and $A_1 \cup A_2$, respectively. In general, $\oplus_{i=1}^k D_i$ denote the direct sum of the digraphs $D_1 = (V_1, A_1), \ldots, D_k = (V_k, A_k)$. If $D_i = D$ for all i, then we simply write $\oplus_{i=1}^k D_i = kD$.

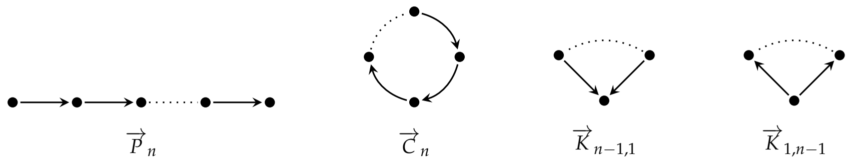

Figure 1. Orientations of P_n, C_n, and S_n.

The following notation and concepts were introduced in [1]. Let $D \in \mathcal{D}_n$. Let us denote by n_i^+ (resp. n_i^-) the number of vertices in D with out-degree (resp. in-degree) i, for all $0 \leq i \leq n-1$. For every $1 \leq i, j \leq n-1$, define the set

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

The cardinality of A_{ij} is denoted by a_{ij}. Clearly,

$$\sum_{1\leq i,j\leq n-1} a_{ij} = a \quad ; \quad \sum_{j=1}^{n-1} a_{ij} = in_i^+ \quad ; \quad \text{and} \quad \sum_{i=1}^{n-1} a_{ij} = jn_j^-, \tag{1}$$

where a is the number of arcs D has.

A VDB topological index is a function φ induced by real numbers $\{\varphi_{ij}\}$, where $1 \leq i, j \leq n-1$, defined as [1]

$$\varphi(D) = \frac{1}{2} \sum_{1\leq i,j\leq n-1} a_{ij}\varphi_{ij}. \tag{2}$$

Equivalently,

$$\varphi(D) = \frac{1}{2} \sum_{uv\in A} \varphi_{d_u^+ d_v^-}. \tag{3}$$

When $\varphi_{ij} = \varphi_{ji}$ for all $1 \leq i, j \leq n-1$, we say that φ is a symmetric VDB topological index. In this case, the expression given in (2) can be simplified. In fact, let

$$p_{ij} = a_{ij} + a_{ji}, \tag{4}$$

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

$$p_{ii} = a_{ii}, \tag{5}$$

for all $i = 1, \ldots, n-1$. Then

$$\varphi(D) = \frac{1}{2} \sum_{(i,j)\in K} p_{ij}\varphi_{ij}, \tag{6}$$

where

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

In particular, when $D = G$ is a graph, it was shown in [1] that Formula (6) reduces to

$$\varphi(G) = \sum_{(i,j)\in K} m_{ij}\varphi_{ij},$$

where m_{ij} is the number of edges in G which join vertices of degree i and j. So we recover the degree-based-topological indices of graphs, a concept which has been, and currently is, extensively investigated in the mathematical and chemical literature [2–4]. For recent results, we refer to [5–12].

This paper is organized as follows. In Section 2, in a general setting (Theorem 1), we find sharp lower and upper bounds of a symmetric VDB topological index over the set $\mathcal{D}_n$. As a byproduct, we obtain over $\mathcal{D}_n$, sharp upper and lower bounds of well-known VDB topological indices, which include the First Zagreb index $\mathcal{M}_1$ ($\varphi_{ij} = i + j$) [13], the Second Zagreb index $\mathcal{M}_2$ ($\varphi_{ij} = ij$) [13], the Randić index χ ($\varphi_{ij} = 1/\sqrt{ij}$) [14], the Harmonic index $\mathcal{H}$ ($\varphi_{ij} = 2/(i+j)$) [15], the Geometric-Arithmetic $\mathcal{GA}$ ($\varphi_{ij} = 2\sqrt{ij}/(i+j)$) [16], the Sum-Connectivity $\mathcal{SC}$ ($\varphi_{ij} = 1/\sqrt{i+j}$) [17], the Atom-Bond-Connectivity $\mathcal{ABC}$ ($\varphi_{ij} = \sqrt{(i+j-2)/ij}$) [18], and the Augmented Zagreb $\mathcal{AZ}$ ($\varphi_{ij} = (ij/(i+j-2))^3$) [19].

In Section 3, based on Theorem 2, we give sharp upper and lower bounds of symmetric VDB topological indices over the set $\mathcal{OT}(n)$, the set of oriented trees with n vertices. In particular, we deduce sharp upper and lower bounds for the well-known indices mentioned above over $\mathcal{OT}(n)$. Finally, in Section 4, we consider the problem of finding the extremal values of a symmetric VDB topological index among all orientations in $\mathcal{O}(G)$, the set of all orientations of a fixed graph G. In order to do this, we define strictly nondecreasing (resp. nonincreasing) symmetric VDB topological indices and show that for these indices, the value of any orientation at G is not greater (resp. smaller) than half the value at G. Moreover, equality occurs, and only if the orientation is a sink-source orientation of G. In particular, when G is a bipartite graph, we show that the sink-source orientations of G attain extremal values.

2. Bounds of VDB Topological Indices of Digraphs

From now on, when we say that φ is a symmetric VDB topological index, we mean that φ is induced by the numbers $\{\varphi_{ij}\}$, where $(i,j) \in K$, and it is defined as in the equivalent definitions (2), (3), or (6). In the first part of this section, we generalize several results of [20] to digraphs.

Let φ be a symmetric VDB topological index. Consider the function $f_{ij} = \frac{ij\varphi_{ij}}{i+j}$ defined over the set K. For each $(r,s) \in K$, consider the subset of K

$$K_{rs} = \{(i,j) \in K : (i,j) \neq (r,s)\}.$$

Recall that q is the number of vertices which are sink or source vertices of a digraph D.

Lemma 1. *Let φ be a symmetric VDB topological index and $D \in \mathcal{D}_n$. Let $(r,s) \in K$. Then*

$$2\varphi(D) = (2n-q)f_{rs} + \sum_{(i,j)\in K_{rs}} (f_{ij} - f_{rs}) \frac{i+j}{ij} p_{ij}.$$

Proof. The numbers $\{p_{ij}\}$ defined in (4) in (5) satisfy the relation (see (10) in [1])

$$\sum_{(i,j)\in K} \left(\frac{1}{i} + \frac{1}{j}\right) p_{ij} = 2n - \left(n_0^+ + n_0^-\right). \tag{7}$$

Note that $q = n_0^+ + n_0^-$. By (7),

$$\frac{r+s}{rs} p_{rs} + \sum_{(i,j)\in K_{rs}} \left(\frac{1}{i} + \frac{1}{j}\right) p_{ij} = 2n - q,$$

which implies

$$p_{rs} = \frac{rs}{r+s} \left(2n - q - \sum_{(i,j)\in K_{rs}} \left(\frac{1}{i} + \frac{1}{j}\right) p_{ij}\right). \tag{8}$$

On the other hand,

$$\varphi(D) = \frac{1}{2} p_{rs}\varphi_{rs} + \frac{1}{2} \sum_{(i,j)\in K_{rs}} p_{ij}\varphi_{ij}. \tag{9}$$

Now, substituting (8) in (9), we deduce

$$\varphi(D) = \frac{1}{2} f_{rs}(2n-q) + \frac{1}{2} \sum_{(i,j)\in K_{rs}} p_{ij} \frac{i+j}{ij} (f_{ij} - f_{rs}).$$

□

Let φ be a symmetric VDB topological index with associated function $f_{ij} = \frac{ij\varphi_{ij}}{i+j}$. Define the sets

$$K_{\min}(f) = \left\{ (r,s) \in K : \ f_{rs} = \min_{(i,j)\in K} f_{ij} \right\},$$

and

$$K_{\max}(f) = \left\{ (r,s) \in K : \ f_{rs} = \max_{(i,j)\in K} f_{ij} \right\}.$$

We will denote by $K^c_{\min}(f)$ and $K^c_{\max}(f)$ the complements of $K_{\min}(f)$ and $K_{\max}(f)$ in K, respectively. We now generalize ([20], Theorem 2.3) to digraphs.

Theorem 1. *Let φ be a symmetric VDB topological index and $D \in \mathcal{D}_n$. Then*

$$\frac{1}{2}(2n-q) \min_{(i,j)\in K} f_{ij} \le \varphi(D) \le \frac{1}{2}(2n-q) \max_{(i,j)\in K} f_{ij}.$$

Moreover, equality on the left occurs, and only if $p_{xy} = 0$ for all $(x,y) \in K^c_{min}(f)$. Equality on the right occurs, and only if $p_{xy} = 0$ for all $(x,y) \in K^c_{max}(f)$.

Proof. Assume that $f_{rs} = \max_{(i,j)\in K} f_{ij}$, where $(r,s) \in K$. By Lemma 1 and the fact that $f_{ij} \le f_{rs}$ for all $(i,j) \in K$, we deduce

$$\begin{aligned} \varphi(D) &= \frac{1}{2}\left((2n-q) f_{rs} + \sum_{(i,j)\in K_{rs}} (f_{ij} - f_{rs}) \frac{i+j}{ij} p_{ij} \right) \\ &\le \frac{1}{2}(2n-q) f_{rs}. \end{aligned} \tag{10}$$

On the other hand, since $(f_{ij} - f_{rs}) \frac{i+j}{ij} p_{ij} = 0$ for all $(i,j) \in K_{\max}(f)$, it is clear that

$$\sum_{(i,j)\in K_{rs}} (f_{ij} - f_{rs}) \frac{i+j}{ij} p_{ij} = 0$$

if, and only if $p_{xy} = 0$ for all $(x,y) \in K^c_{\max}(f)$. By inequality (10), this is equivalent to $\varphi(D) = \frac{1}{2}\left(2n - n_0^+ - n_0^-\right) \max_{(i,j)\in K} f_{ij}$. The proof of the left inequality (and the equality condition) is similar. □

So by Theorem 1, in order to find extremal values of a VDB topological index φ over $\mathcal{D}_n$, we must find $K_{\min}(f)$ and $K_{\max}(f)$, where $f = \frac{ij\varphi_{ij}}{i+j}$. Fortunately, these were computed for the main VDB topological indices in [21] (see Table 1).

Table 1. $K_{\min}(f)$ and $K_{\max}(f)$ for some VDB topological indices.

VDB Index	Notation	φ_{ij}	$K_{\min}(f)$	$K_{\max}(f)$
First Zagreb [13]	$\mathcal{M}_1$	$i+j$	$(1,1)$	$(n-1,n-1)$
Second Zagreb [13]	$\mathcal{M}_2$	ij	$(1,1)$	$(n-1,n-1)$
Randić [14]	χ	$\frac{1}{\sqrt{ij}}$	$(1,n-1)$	$\{(i,j)\in K : i=j\}$
Harmonic [15]	$\mathcal{H}$	$\frac{2}{i+j}$	$(1,n-1)$	$\{(i,j)\in K : i=j\}$
Geometric-Arithmetic [16]	$\mathcal{GA}$	$\frac{2\sqrt{ij}}{i+j}$	$(1,n-1)$	$(n-1,n-1)$
Sum-Connectivity [17]	$\mathcal{SC}$	$\frac{1}{\sqrt{i+j}}$	$(1,n-1)$	$(n-1,n-1)$
Atom-Bond-Connectivity [18]	$\mathcal{ABC}$	$\sqrt{\frac{i+j-2}{ij}}$	$(1,1)$	$(n-1,n-1)$
Augmented Zagreb [19]	$\mathcal{AZ}$	$\left(\frac{ij}{i+j-2}\right)^3$	$(1,n-1)$	$(n-1,n-1)$

An important class of digraphs which occur frequently as extremal values of VDB topological indices are the arc-balanced digraphs, which we define as follows.

Definition 1. *A digraph D is arc-balanced if $d_u^+ = d_v^-$, for every arc uv of D, and $q = 0$.*

A regular digraph is a digraph D such that $d_u^+ = d_u^- = r$, for all vertices u in D, where r is a positive integer. Clearly, every regular digraph is arc-balanced.

Example 1. *The digraphs in Figure 2 are arc-balanced but not regular digraphs.*

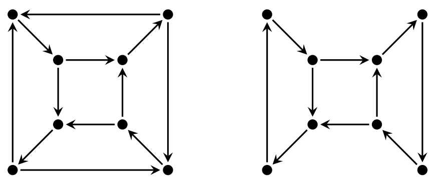

Figure 2. Arc-balanced digraphs.

Now we can give sharp upper and lower bounds for all VDB topological indices listed in Table 1. The following result is clear.

Lemma 2. *Let $D \in \mathcal{D}_n$.*

1. $p_{ij} = 0$ *for all* $(i,j) \neq (1,1)$ *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.
2. $p_{ij} = 0$ *for all* $(i,j) \in K$ *such that* $i < j$ *and* $q = 0 \Leftrightarrow D$ *is an arc-balanced digraph;*
3. $p_{ij} = 0$ *for all* $(i,j) \in K$ *such that* $(i,j) \neq (n-1,n-1) \Leftrightarrow D = K_n$*;*
4. $p_{ij} = 0$ *for all* $(i,j) \neq (1,n-1)$ *and* $q = n \Leftrightarrow D = \overrightarrow{K}_{1,n-1}$ *or* $D = \overrightarrow{K}_{n-1,1}$*;*
5. $p_{ij} = 0$ *for all* $(i,j) \neq (1,1)$ *and* $q = n \Leftrightarrow n$ *is even and* $D = \frac{n}{2}\overrightarrow{P}_2$.
6. $p_{ij} = 0$ *for all* $(i,j) \neq (1,1)$ *and* $q = n-1 \Leftrightarrow n$ *is odd and* $D = \frac{n-3}{2}\overrightarrow{P}_2 \oplus \overrightarrow{P}_3$.

Lemma 3. *Assume that n is odd. Let $D \in \mathcal{D}_n$. If $q = n$, then $p_{11} \leq \frac{n-3}{2}$.*

Proof. Every vertex of D is a sink vertex or a source vertex. Consequently,

$$D = E \oplus p_{11} \overrightarrow{P}_2,$$

where $p_{11}(E) = 0$. In particular,

$$n = n(E) + 2p_{11}.$$

Since n is odd, then $n(E)$ is also odd. Moreover, $n(E) \geq 3$, since D has no isolated vertices. Hence,

$$2p_{11} = n - n(E) \leq n - 3.$$

□

Corollary 1. *Let $D \in \mathcal{D}_n$. Then*

1.
$$\left\lceil \frac{n}{2} \right\rceil \leq \mathcal{M}_1(D) \leq n(n-1)^2.$$

   (a) *Equality on the left occurs* $\Leftrightarrow$ *n is even and* $D = \frac{n}{2}\overrightarrow{P}_2$ *or n is odd, and* $D = \frac{n-3}{2}\overrightarrow{P}_2 \oplus \overrightarrow{P}_3$*;*
   (b) *Equality on the right occurs* $\Leftrightarrow D = K_n$*.*

2.
$$\left.\begin{array}{ll} \frac{n}{4} & \text{if } n \text{ even} \\ \frac{n+1}{4} & \text{if } n \text{ odd} \end{array}\right\} \leq \mathcal{M}_2(D) \leq \frac{1}{2}n(n-1)^3.$$

   (a) *Equality on the left occurs* $\Leftrightarrow$ *n is even and* $D = \frac{n}{2}\overrightarrow{P}_2$ *or n is odd and* $D = \frac{n-3}{2}\overrightarrow{P}_2 \oplus \overrightarrow{P}_3$*;*
   (b) *Equality on the right occurs* $\Leftrightarrow D = K_n$*.*

3.
$$\frac{1}{2}\sqrt{n-1} \leq \chi(D) \leq \frac{n}{2}.$$

   (a) *Equality on the left occurs* $\Leftrightarrow D = \overrightarrow{K}_{1,n-1}$ *or* $D = \overrightarrow{K}_{n-1,1}$*;*
   (b) *Equality on the right occurs* $\Leftrightarrow$ *D is an arc-balanced digraph.*

4.
$$\frac{n-1}{n} \leq \mathcal{H}(D) \leq \frac{n}{2}.$$

   (a) *Equality on the left occurs* $\Leftrightarrow D = \overrightarrow{K}_{1,n-1}$ *or* $D = \overrightarrow{K}_{n-1,1}$*;*
   (b) *Equality on the right occurs* $\Leftrightarrow$ *D is an arc-balanced digraph.*

5.
$$\frac{(n-1)^{\frac{3}{2}}}{n} \leq \mathcal{GA}(D) \leq \frac{n}{2\sqrt[3]{(n-1)^4}}.$$

   (a) *Equality on the left occurs* $\Leftrightarrow D = \overrightarrow{K}_{1,n-1}$ *or* $D = \overrightarrow{K}_{n-1,1}$*;*
   (b) *Equality on the right occurs* $\Leftrightarrow D = K_n$*.*

6.
$$\frac{n-1}{2\sqrt{n}} \leq \mathcal{SC}(D) \leq \frac{1}{4}n\sqrt{2(n-1)}.$$

   (a) *Equality on the left occurs* $\Leftrightarrow D = \overrightarrow{K}_{1,n-1}$ *or* $D = \overrightarrow{K}_{n-1,1}$*;*
   (b) *Equality on the right occurs* $\Leftrightarrow D = K_n$*.*

7.
$$0 \le \mathcal{ABC}(D) \le \frac{n}{2}\sqrt{2(n-2)}.$$

(a) *Equality on the left occurs* $\Leftrightarrow D = \bigoplus_{i=1}^{k_1} \overrightarrow{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overrightarrow{C}_{n_j}$, *for some nonnegative integers* k_1, k_2.

(b) *Equality on the right occurs* $\Leftrightarrow D = K_n$.

8.
$$\frac{1}{2}\frac{(n-1)^4}{(n-2)^3} \le \mathcal{AZ}(D) \le \frac{1}{16}n\frac{(n-1)^7}{(n-2)^3}.$$

(a) *Equality on the left occurs* $\Leftrightarrow D = \overrightarrow{K}_{1,n-1}$ *or* $D = \overrightarrow{K}_{n-1,1}$;

(b) *Equality on the right occurs* $\Leftrightarrow D = K_n$.

Proof. Recall that $f_{ij} = \frac{ij\varphi_{ij}}{i+j}$ is the associated function of the symmetric VDB topological index φ. The expressions for f_{ij} are shown in Table 2.

Table 2. f_{ij} for some VDB topological Indices.

VDB Index	$\mathcal{M}_1$	$\mathcal{M}_2$	χ	$\mathcal{H}$	$\mathcal{GA}$	$\mathcal{SC}$	$\mathcal{ABC}$	$\mathcal{AZ}$
f_{ij}	ij	$\frac{(ij)^2}{i+j}$	$\frac{\sqrt{ij}}{i+j}$	$\frac{2ij}{(i+j)^2}$	$\frac{2(ij)^{\frac{3}{2}}}{(i+j)^2}$	$\frac{ij}{(i+j)^{\frac{3}{2}}}$	$\frac{\sqrt{ij(i+j-2)}}{i+j}$	$\frac{(ij)^4}{(i+j)(i+j-2)^3}$

Since $0 \le q \le n$, we easily deduce the result from Theorem 1 and Lemma 2.
We only have to separately consider $\mathcal{M}_1$ and $\mathcal{M}_2$ when n is odd. By Theorem 1,

$$2\mathcal{M}_1(D) \ge 2n - q \ge n. \tag{11}$$

Since n is odd, $2\mathcal{M}_1(D) > n$, and so $2\mathcal{M}_1(D) \ge n+1$. Equivalently,

$$\mathcal{M}_1(D) \ge (n+1)/2 = \lceil n/2 \rceil.$$

For the equality condition, it is clear that $\mathcal{M}_1\left(\frac{n-3}{2}\overrightarrow{P}_2 \oplus \overrightarrow{P}_3\right) = \frac{n+1}{2}$. Conversely, suppose that $\mathcal{M}_1(D) = \frac{n+1}{2}$. Then by (11),

$$n+1 \ge 2n - q,$$

which implies $q \ge n-1$. So there are only two possibilities: $q = n-1$ and $q = n$. If $q = n$, then by Lemma 3, $p_{11} \le \frac{n-3}{2}$. On the other hand, by Lemma 1 applied to $(r,s) = (1,2)$,

$$\begin{aligned} n+1 &= 2\mathcal{M}_1(D) = 2n + \sum_{(i,j)\neq(1,2)} (ij-2)\frac{i+j}{ij}p_{ij} \\ &= 2n + (-1)2p_{11} + \sum_{\substack{(i,j)\neq(1,2)\\(i,j)\neq(1,1)}} (ij-2)\frac{i+j}{ij}p_{ij}. \end{aligned}$$

Thus,

$$0 \le \sum_{\substack{(i,j)\neq(1,2)\\(i,j)\neq(1,1)}} (ij-2)\frac{i+j}{ij}p_{ij} = 2p_{11} - n + 1,$$

which implies $p_{11} \geq \frac{n-1}{2}$, a contradiction. Hence, $q = n-1$. Consequently,

$$\mathcal{M}_1(D) = \frac{n+1}{2} = \frac{1}{2}(2n-q).$$

It follows from Theorem 1 that $p_{ij} = 0$ for all $(i,j) \neq (1,1)$. Finally, by Lemma 2,

$$D = \frac{n-3}{2}\overrightarrow{P}_2 \oplus \overrightarrow{P}_3.$$

The case of $\mathcal{M}_2$ when n is odd is similar.

In the case of the $\mathcal{ABC}$ index, note that $\varphi_{ij} = 0$ if, and only if $(i,j) = (1,1)$. Then it is clear that

$$\mathcal{ABC}\left(\bigoplus_{i=1}^{k_1} \overrightarrow{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overrightarrow{C}_{n_j}\right) = 0.$$

Conversely, if D is a digraph such that $0 = \mathcal{ABC}(D)$, then

$$0 = \mathcal{ABC}(D) = \frac{1}{2}\sum_{(i,j)\in K} p_{ij}\varphi_{ij} = \frac{1}{2}\sum_{\substack{(i,j)\in K\\(i,j)\neq(1,1)}} p_{ij}\varphi_{ij},$$

which implies $p_{ij} = 0$ for all $(i,j) \neq (1,1)$. Hence, by part 1 of Lemma 2, $D = \bigoplus_{i=1}^{k_1} \overrightarrow{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overrightarrow{C}_{n_j}$. □

Remark 1. *Using a linear programming modeling technique, the authors in [22] find some of the extremal values given in Corollary 1.*

Now we give bounds of VDB topological indices in terms of the number of arcs. Let φ be a symmetric VDB topological index. Let us define

$$L_{\max} = L_{\max}(\varphi) = \left\{(i,j) \in K : \varphi_{ij} = \max_K \varphi_{ij}\right\},$$

and

$$L_{\min} = L_{\min}(\varphi) = \left\{(i,j) \in K : \varphi_{ij} = \min_K \varphi_{ij}\right\}.$$

The complements in K are denoted by $L^c_{\max}$ and $L^c_{\min}$, respectively.

Theorem 2. *Let φ be a symmetric VDB topological index. If D is a digraph with a arcs, then*

$$\frac{1}{2}a\left(\min_K \varphi_{ij}\right) \leq \varphi(D) \leq \frac{1}{2}a\left(\max_K \varphi_{ij}\right).$$

Equality on the left occurs if, and only if $p_{ij} = 0$ for all $(i,j) \in L^c_{\min}$. Equality on the right occurs if, and only if $p_{ij} = 0$ for all $(i,j) \in L^c_{\max}$.

Proof. From (2) and (1),

$$\varphi(D) = \frac{1}{2}\sum_K p_{ij}\varphi_{ij} \leq \frac{1}{2}\sum_K p_{ij}\max_K \varphi_{ij} = \frac{1}{2}a\left(\max_K \varphi_{ij}\right). \tag{12}$$

If $\varphi(D) = \frac{1}{2}a\left(\max_K \varphi_{ij}\right)$, then by (12)

$$p_{ij}\left(\varphi_{ij} - \max_K \varphi_{ij}\right) = 0,$$

for all $(i,j) \in K$. Hence, if $(i,j) \in L_{\max}^c$, then $\varphi_{ij} - \max_K \varphi_{ij} \neq 0$ and so $p_{ij} = 0$.

Conversely, if $p_{ij} = 0$ for all $(i,j) \in L_{\max}^c$, then

$$\begin{aligned}\varphi(D) &= \frac{1}{2}\sum_K p_{ij}\varphi_{ij} = \frac{1}{2}\sum_{L_{\max}} p_{ij}\varphi_{ij} + \frac{1}{2}\sum_{L_{\max}^c} p_{ij}\varphi_{ij} \\ &= \frac{1}{2}\sum_{L_{\max}} p_{ij}\varphi_{ij} = \frac{1}{2}a\left(\max_K \varphi_{ij}\right).\end{aligned}$$

The proof of the left inequality (and equality) is similar. □

3. Bounds of VDB Topological Indices of Tree Orientations

The set of oriented trees with n vertices is denoted by $\mathcal{OT}(n)$. It is our interest in this section to determine the extremal values of a VDB topological index over $\mathcal{OT}(n)$. Clearly, $a = n - 1$ for every $T \in \mathcal{OT}(n)$. Hence, by Theorem 2 we deduce the following.

Corollary 2. *Let $T \in \mathcal{OT}(n)$. Then*

$$\frac{1}{2}(n-1)\min_K \varphi_{ij} \leq \varphi(T) \leq \frac{1}{2}(n-1)\max_K \varphi_{ij}.$$

Equality on the left occurs if, and only if $p_{ij} = 0$ for all $(i,j) \in L_{\min}^c$. Equality on the right occurs if, and only if $p_{ij} = 0$ for all $(i,j) \in L_{\max}^c$.

Now we can obtain a first list of sharp upper and lower bounds for some VDB topological indices over $\mathcal{OT}(n)$.

Theorem 3. *Let $T \in \mathcal{OT}(n)$. Then*

1. $\frac{1}{2}\sqrt{n-1} \leq \chi(T) \leq \frac{n-1}{2}$;
2. $\frac{n-1}{n} \leq \mathcal{H}(T) \leq \frac{n-1}{2}$;
3. $\frac{(n-1)^{\frac{3}{2}}}{n} \leq \mathcal{GA}(T) \leq \frac{n-1}{2}$;
4. $\frac{n-1}{2\sqrt{n}} \leq \mathcal{SC}(T) \leq \frac{\sqrt{2}}{4}(n-1)$;
5. $\frac{1}{2}\frac{(n-1)^4}{(n-2)^3} \leq \mathcal{AZ}(T)$.

Moreover, equality on the left of 1–5 *occurs* $\Leftrightarrow T = \overrightarrow{K}_{1,n-1}$ *or* $T = \overrightarrow{K}_{n-1,1}$. *Equality on the right of* 1–4 *occurs* $\Leftrightarrow T = \overrightarrow{P}_n$.

Proof. The inequalities on the left (and equality conditions) are immediate consequence of Corollary 1. The inequalities on the right of *1–4* are consequence of Corollary 2 having in mind Table 3.

Table 3. $L_{\max}$ and $\max_K \varphi_{ij}$ for χ, $\mathcal{H}$, $\mathcal{GA}$, and $\mathcal{SC}$.

VDB Index	φ_{ij}	$L_{\max}$	$\max_K \varphi_{ij}$
χ	$\frac{1}{\sqrt{ij}}$	$(1,1)$	1
$\mathcal{H}$	$\frac{2}{i+j}$	$(1,1)$	1
$\mathcal{GA}$	$\frac{2\sqrt{ij}}{i+j}$	$\{(i,j) \in K : i = j\}$	1
$\mathcal{SC}$	$\frac{1}{\sqrt{i+j}}$	$(1,1)$	$\frac{1}{\sqrt{2}}$

We also use the fact that $T \in \mathcal{OT}(n)$ is such that $p_{ij} = 0$ for all $(i,j) \neq (1,1)$ if, and only if $T = \overrightarrow{P}_n$. Similarly, $p_{ij} = 0$ for all (i,j) such that $i < j$ if, and only if $T = \overrightarrow{P}_n$. □

Theorem 4. *Let $T \in \mathcal{OT}(n)$. Then*

1. $0 \leq \mathcal{ABC}(T) \leq \frac{1}{2}\sqrt{(n-1)(n-2)}$;
2. $(n-1) \leq \mathcal{M}_1(T)$;
3. $\frac{1}{2}(n-1) \leq \mathcal{M}_2(T)$.

Moreover, equality on the left of 1–3 *occurs* $\Leftrightarrow T = \overrightarrow{P}_n$. *Equality on the right of* 1 *occurs* $\Leftrightarrow T = \overrightarrow{K}_{1,n-1}$ *or* $T = \overrightarrow{K}_{n-1,1}$.

Proof. The inequalities on the left of *1–3* (and equality conditions) are a consequence of Corollary 2, having in mind Table 4.

Table 4. $L_{\min}$ and $\min_K \varphi_{ij}$ for $\mathcal{ABC}$, $\mathcal{M}_1$, and $\mathcal{M}_2$.

VDB Index	φ_{ij}	$L_{\min}$	$\min_K \varphi_{ij}$
$\mathcal{ABC}$	$\sqrt{\frac{i+j-2}{ij}}$	$(1,1)$	0
$\mathcal{M}_1$	$i+j$	$(1,1)$	2
$\mathcal{M}_2$	ij	$(1,1)$	1

And the fact that $T \in \mathcal{OT}(n)$ is such that $p_{ij} = 0$ for all $(i,j) \neq (1,1)$ if, and only if $T = \overrightarrow{P}_n$. On the other hand, the right inequality in *1* holds again by Corollary 2, bearing in mind Table 5.

Table 5. $L_{\max}$ and $\max_K \varphi_{ij}$ for $\mathcal{ABC}$.

VDB Index	φ_{ij}	$L_{\max}$	$\max_K \varphi_{ij}$
$\mathcal{ABC}$	$\sqrt{\frac{i+j-2}{ij}}$	$(1,n-1)$	$\sqrt{\frac{n-2}{n-1}}$

And the fact that $T \in \mathcal{OT}(n)$ is such that $p_{ij} = 0$ for all $(i,j) \neq (1,n-1)$ if, and only if $T = \overrightarrow{K}_{1,n-1}$ or $T = \overrightarrow{K}_{n-1,1}$. □

The only extremal values we have not determined yet are the maximal values of $\mathcal{M}_1, \mathcal{M}_2$, and $\mathcal{AZ}$ over $\mathcal{OT}(n)$. The problem in these indices is that $L_{\max} = (n-1, n-1)$, and there is no oriented tree such that $p_{ij} = 0$ for all $(i,j) \neq (n-1,n-1)$. In the next section we will show that the maximum value of $\mathcal{M}_1$ and $\mathcal{M}_2$ over $\mathcal{OT}(n)$ is attained in $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ (see Theorem 6). We propose the following problem.

Problem 1. *Find the maximum value of $\mathcal{AZ}$ over $\mathcal{OT}(n)$.*

4. Bounds of VDB Topological Indices over Orientations of a Fixed Graph

Let φ be a symmetric VDB topological index and G a graph. Let $\mathcal{O}(G)$ be the set of orientations of the graph G. Our main concern now is to determine the extremal values of a symmetric VDB topological index over $\mathcal{O}(G)$. In order to do this, let us define a partial order over K as follows: if $(i,j),(k,l) \in K$, then

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

Definition 2. *Let φ be a symmetric VDB topological index. We say that φ is nondecreasing (resp. nonincreasing) over K, if for every $(i,j),(k,l) \in K$:*

$$(i,j) \preceq (k,l) \Rightarrow \varphi_{ij} \leq \varphi_{kl} \text{ (resp. } \varphi_{ij} \geq \varphi_{kl}).$$

Furthermore, if for every $(i,j),(k,l) \in K$ *:*

$$(i,j) \preceq (k,l) \text{ and } \varphi_{ij} = \varphi_{kl} \Rightarrow (i,j) = (k,l),$$

we will say that φ *is strictly nondecreasing (resp. strictly nonincreasing).*

Example 2. *Consider the generalized Randić index* χ_α *induced by the numbers* $(ij)^\alpha$*, where* $\alpha \in \mathbb{R}$*,* $\alpha \neq 0$*. Clearly,* χ_α *is strictly nondecreasing when* $\alpha > 0$*, and strictly nonincreasing when* $\alpha < 0$*. In particular, the Randić index* χ *is strictly nonincreasing and the second Zagreb index* $\mathcal{M}_2$ *is strictly nondecreasing. Additionally, the harmonic index and the sum-connectivity index are strictly nonincreasing, and the first Zagreb* $\mathcal{M}_1$ *is strictly nondecreasing.*

Theorem 5. *Let* φ *be a strictly nondecreasing (resp. nonincreasing) symmetric VDB topological index and G a graph. Let D be any orientation of G. Then*

$$\varphi(D) \leq \frac{1}{2}\varphi(G) \text{ (resp. } \varphi(D) \geq \frac{1}{2}\varphi(G)\text{)}.$$

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

Proof. We will assume that φ is strictly nondecreasing, and the other case is similar. Note that

$$d_u = d_u^+ + d_u^- \tag{13}$$

for every vertex u of G. Hence, for any arc uv of D, $(d_u^+, d_v^-) \preceq (d_u, d_v)$. It follows by the nondecreasing property of φ and (3),

$$\varphi(D) = \frac{1}{2}\sum_{uv\in A} \varphi_{d_u^+ d_v^-} \leq \frac{1}{2}\sum_{uv\in G} \varphi_{d_u d_v} = \frac{1}{2}\varphi(G). \tag{14}$$

If D is a sink-source orientation of G, then $d_u^+ = 0$ or $d_u^- = 0$, for all vertices u of V. If vw is an arc of D then $d_v^+ \neq 0$ and $d_w^- \neq 0$. Hence, $d_v^- = 0$ and $d_w^+ = 0$, which implies by (13) that $d_v = d_v^+$ and $d_w = d_w^-$. Hence,

$$\varphi(D) = \frac{1}{2}\sum_{uv\in A} \varphi_{d_u^+ d_v^-} = \frac{1}{2}\sum_{uv\in G} \varphi_{d_u d_v} = \frac{1}{2}\varphi(G).$$

Conversely, assume that $\varphi(D) = \frac{1}{2}\varphi(G)$. Then by (14), for every $uv \in A$

$$(d_u^+, d_v^-) \preceq (d_u, d_v) \text{ and } \varphi_{d_u^+ d_v^-} = \varphi_{d_u d_v}.$$

Now since φ is strictly nondecreasing, $(d_u^+, d_v^-) = (d_u, d_v)$ for every $uv \in A$. Finally, by (13), $d_u^- = 0$ and $d_v^+ = 0$. This clearly implies that D is a sink-source orientation of G. □

Corollary 3. *Let* φ *be a strictly nondecreasing (resp. nonincreasing) symmetric VDB topological index and G a bipartite graph. Then the maximal (resp. minimal) value of* φ *over* $\mathcal{O}(G)$ *is attained in a sink-source orientation of G.*

Proof. We assume that φ is strictly nondecreasing, and the other case is similar. Since G is a bipartite graph, G has a sink-source orientation which we call E [23]. Let D be any orientation of G. Then by Theorem 5,

$$\varphi(E) = \frac{1}{2}\varphi(G) \geq \varphi(D).$$

□

Example 3. *Consider the path tree P_n. By Example 2 and Corollary 3, the sink-source orientation $E \in \mathcal{O}(P_n)$ depicted in Figure 3 attains the maximal value for $\mathcal{M}_1$, $\mathcal{M}_2$ and χ_α when $\alpha > 0$, over $\mathcal{O}(P_n)$. On the other hand, E attains the minimal value of $\mathcal{H}, \mathcal{SC}$ and χ_α when $\alpha < 0$, over $\mathcal{O}(P_n)$.*

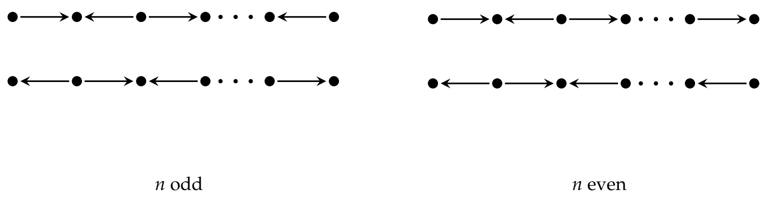

Figure 3. Sink-source orientations of P_n.

Example 4. *In [24] the authors studied the extreme values of χ on the set of all the orientations of hexagonal chains with k hexagons.*

Theorem 6. *Let $T \in \mathcal{OT}(n)$. Then*

1. $\mathcal{M}_1(T) \leqslant \frac{1}{2}n(n-1)$;
2. $\mathcal{M}_2(T) \leqslant \frac{1}{2}(n-1)^2$.

Moreover, equalities 1–2 *occur* $\Leftrightarrow T = \overrightarrow{K}_{1,n-1}$ *or* $T = \overrightarrow{K}_{n-1,1}$.

Proof. Let G be a tree of order n. If G is different from S_n, then [25]

$$\mathcal{M}_1(G) < \mathcal{M}_1(S_n) = n(n-1)$$
$$\mathcal{M}_2(G) < \mathcal{M}_2(S_n) = (n-1)^2.$$

Let $T \in \mathcal{OT}(n)$ and suppose that T is an orientation of a tree G. By Theorem 5 and the above equation,

$$\mathcal{M}_1(T) \leqslant \frac{1}{2}\mathcal{M}_1(G) \leqslant \frac{1}{2}n(n-1)$$
$$\mathcal{M}_2(T) \leqslant \frac{1}{2}\mathcal{M}_2(G) \leqslant \frac{1}{2}(n-1)^2.$$

Equality occurs if, and only if T is a sink-source orientation of S_n, in other words, $T = \overrightarrow{K}_{1,n-1}$ or $T = \overrightarrow{K}_{n-1,1}$. □

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