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 \( \varphi \) induced by the numbers \( \{ \varphi_{ij} \} \) was recently defined for a digraph \( D \), as \( \varphi(D) = \frac{1}{2} \sum_{u,v} \varphi_{uv} d_u^+ d_v^- \), 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 \( D_n \), 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 \( OT(n) \) and \( O(G) \), 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

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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 \( D \), 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 \( vu \), 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 \( D_n \).

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 \( P_n \) and the directed cycle \( C_n \), 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 \( K_{1,n−1} \) and \( K_{n−1,1} \) in Figure 1 are sink-source orientations of the star \( S_n \). Note that \( K_{n−1,1} \) is obtained by reversing all arcs of \( K_{1,n−1} \).

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, \( \odot_{i=1}^k D_i \) 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 \( \odot_{i=1}^k D_i = kD \).
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 $\mathcal{D}^+_n$ (resp. $\mathcal{D}^+_n$) 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,

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

where $a$ is the number of arcs $D$ has.

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

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

Equivalently,

$$\varphi(D) = \frac{1}{2} \sum_{uv \in A} \varphi_{d^+_u d^-_v}. \quad (3)$$

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

$$p_{ij} = a_{ij} + a_{ji}, \quad (4)$$

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

$$p_{ii} = a_{ii}, \quad (5)$$

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

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

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

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

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 $M_1 (\varphi_{ij} = i + j)$ [13], the Second Zagreb index $M_2 (\varphi_{ij} = ij)$ [13], the Randić index $\chi (\varphi_{ij} = 1/\sqrt{ij})$ [14], the Harmonic
index \( H (\phi_{ij} = 2/(i + j)) \) [15], the Geometric-Arithmetic \( GA \) \( (\phi_{ij} = 2\sqrt{i/j}/(i + j)) \) [16],
the Sum-Connectivity \( SC \) \( (\phi_{ij} = 1/\sqrt{i + j}) \) [17], the Atom-Bond-Connectivity \( ABC \) \( (\phi_{ij} = \sqrt{(i + j - 2)/ij}) \) [18], and the Augmented Zagreb \( AZ \) \( (\phi_{ij} = (ij/(i + j - 2))^3) \) [19].

In Section 3, based on Theorem 2, we give sharp upper and lower bounds of symmetric VDB topological indices over the set \( OT(n) \), 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 \( OT(n) \). Finally, in Section 4, we consider the problem of finding the extremal values of a symmetric VDB topological index among all orientations in \( O(G) \), 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, we say that \( \phi \) is a symmetric VDB topological index, we mean that \( \phi \) is induced by the numbers \( \{\phi_{ij}\} \), 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 \( \phi \) be a symmetric VDB topological index. Consider the function \( f_{ij} = i j \phi_{ij} / i + j \) 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 \( \phi \) be a symmetric VDB topological index and \( D \in D_n \). Let \((r, s) \in K\). Then

\[
2\phi(D) = (2n - q)frs + \sum_{(ij) \in Krs} (f_{ij} - frs) \frac{i + j}{ij} p_{ij}.
\]

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

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

(7)

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

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

which implies

\[
p_{rs} = \frac{rs}{r + s} \left( 2n - q - \sum_{(ij) \in Krs} \left( \frac{1}{i} + \frac{1}{j} \right) p_{ij} \right).
\]

(8)

On the other hand,

\[
\phi(D) = \frac{1}{2} p_{rs} \phi_{rs} + \frac{1}{2} \sum_{(ij) \in Krs} p_{ij} \phi_{ij}.
\]

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

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

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

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

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

and

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

We will denote by \( K_{\min}^c(f) \) and \( K_{\max}^c(f) \) 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 \( \varphi \) be a symmetric VDB topological index and \( D \in D_n \). Then

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

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

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

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

\[ \leq \frac{1}{2} (2n - q)f_{rs}. \] (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 \( (x,y) \in K_{\max}^c(f) \). By inequality (10), this is equivalent to \( \varphi(D) = \frac{1}{2} (2n - n_0^+ - n_0^-) \max_{(i,j) \in K} f_{ij} \). The proof of the left inequality (and the equality condition) is similar. \( \square \)

So by Theorem 1, in order to find extremal values of a VDB topological index \( \varphi \) over \( D_n \), 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 | $\varphi_{ij}$ | $K_{\min}(f)$ | $K_{\max}(f)$ |
|--------------------|----------|----------------|---------------|---------------|
| 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]        | $\chi$   | $\frac{1}{\sqrt{ij}}$ | $(1, n - 1)$  | $\{(i, j) \in K : i = j\}$ |
| Harmonic [15]      | $\mathcal{H}$ | $\frac{2}{\sqrt{ij}}$ | $(1, n - 1)$  | $\{(i, j) \in K : i = j\}$ |
| Geometric-Arithmetic [16] | $\mathcal{G}_A$ | $\frac{2\sqrt{\sqrt{ij}^2}}{1 + ij}$ | $(1, n - 1)$  | $(n - 1, n - 1)$ |
| Sum-Connectivity [17] | $\mathcal{S}_C$ | $\frac{1}{\sqrt{ij} + \sqrt{ij}^2}$ | $(1, n - 1)$  | $(n - 1, n - 1)$ |
| Atom-Bond-Connectivity [18] | $\mathcal{A}_B$ | $\sqrt{\sum_{ij}^n - 2}$ | $(1, 1)$       | $(n - 1, n - 1)$ |
| Augmented Zagreb [19] | $\mathcal{A}_Z$ | $\sqrt{\sum_{ij}^n - 2}$ | $(1, 1)$       | $(n - 1, n - 1)$ |

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.](image)

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 $q = 0$ if and only if $D$ is an arc-balanced digraph;

3. $p_{ij} = 0$ for all $(i, j) \in K$ such that $(i, j) \neq (n - 1, n - 1)$ if $D = K_n$;

4. $p_{ij} = 0$ for all $(i, j) \neq (1, n - 1)$ and $q = n$ if $D = \overrightarrow{K}_{1,n-1}^1$ or $D = \overrightarrow{K}_{n-1,1}^1$;

5. $p_{ij} = 0$ for all $(i, j) \neq (1, 1)$ and $q = n$ if $n$ is even and $D = \frac{n}{2} \overrightarrow{P}_2^2$.

6. $p_{ij} = 0$ for all $(i, j) \neq (1, 1)$ and $q = n - 1$ if $n$ is odd and $D = \frac{n-3}{2} \overrightarrow{P}_2^2 \oplus \overrightarrow{P}_3^3$.

**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,

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

\square

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

1. \[ \left\lfloor \frac{n}{2} \right\rfloor \leq \mathcal{M}_1(D) \leq n(n-1)^2. \]
   (a) Equality on the left occurs \iff $n$ 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 \iff $D = K_n$.

2. \[ \frac{n}{4} \quad \text{if } n \text{ even} \quad \frac{n+1}{4} \quad \text{if } n \text{ odd} \] \leq \mathcal{M}_2(D) \leq \frac{1}{2} n(n-1)^3.
   (a) Equality on the left occurs \iff $n$ 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 \iff $D = K_n$.

3. \[ \frac{1}{2} \sqrt{n-1} \leq \chi(D) \leq \frac{n}{2}. \]
   (a) Equality on the left occurs \iff $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$;
   (b) Equality on the right occurs \iff $D$ is an arc-balanced digraph.

4. \[ \frac{n-1}{n} \leq H(D) \leq \frac{n}{2}. \]
   (a) Equality on the left occurs \iff $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$;
   (b) Equality on the right occurs \iff $D$ is an arc-balanced digraph.

5. \[ \frac{(n-1)^2}{n} \leq GA(D) \leq \frac{n}{2\sqrt{(n-1)^2}}. \]
   (a) Equality on the left occurs \iff $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$;
   (b) Equality on the right occurs \iff $D = K_n$.

6. \[ \frac{n-1}{2\sqrt{n}} \leq SC(D) \leq \frac{1}{4} n \sqrt{2(n-1)}. \]
   (a) Equality on the left occurs \iff $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$;
   (b) Equality on the right occurs \iff $D = K_n$. 
7. \[ 0 \leq ABC(D) \leq \frac{n}{2} \sqrt{2(n - 2)}. \]

(a) Equality on the left occurs \( \iff D = \bigoplus_{i=1}^{k_1} p_i \oplus \bigoplus_{j=1}^{k_2} c_j \), for some nonnegative integers \( k_1, k_2 \).

(b) Equality on the right occurs \( \iff D = K_n \).

8. \[ \frac{1}{2} \left( \frac{2n}{n - 2} \right)^3 \leq \mathcal{A} \mathcal{Z}(D) \leq \frac{1}{16} \left( \frac{n - 1}{n - 2} \right)^3. \]

(a) Equality on the left occurs \( \iff D = \mathcal{K}_1(n - 1) \) or \( D = \mathcal{K}_2(n - 1) \).

(b) Equality on the right occurs \( \iff D = K_n \).

**Proof.** Recall that \( f_{ij} = \frac{ij}{ij} \) is the associated function of the symmetric VDB topological index \( \varphi \). The expressions for \( f_{ij} \) are shown in Table 2.

**Table 2.** \( f_{ij} \) for some VDB topological Indices.

| VDB Index | \( \mathcal{M}_1 \) | \( \mathcal{M}_2 \) | \( \chi \) | \( \mathcal{H} \) | \( \mathcal{G} \mathcal{A} \) | \( \mathcal{SC} \) | \( ABC \) | \( \mathcal{A} \mathcal{Z} \) |
|-----------|----------------|----------------|------|-------------|-------------|----------------|--------|----------------|
| \( f_{ij} \) | \( ij \) | \( \frac{(ij)^2}{i+j} \) | \( \sqrt{\frac{i}{i+j}} \) | \( \sqrt{\frac{2ij}{(i+j)^2}} \) | \( \sqrt{\frac{2(ii)}{(i+j)^2}} \) | \( \sqrt{\frac{ij}{i+j}} \) | \( \sqrt{\frac{(ii)(i+j)}{(i+j)^2}} \) | \( \frac{(ij)^4}{(i+j)(i+j-2)^2} \) |

Since \( 0 \leq q \leq n \), 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,

\[ 2\mathcal{M}_1(D) \geq 2n - q \geq n. \]  

(11)

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

\[ \mathcal{M}_1(D) \geq (n + 1)/2 = \lceil n/2 \rceil. \]

For the equality condition, it is clear that \( \mathcal{M}_1 \left( \frac{n-3}{2} p_2 \oplus \frac{p_3}{2} \right) = \frac{n+1}{2} \). Conversely, suppose that \( \mathcal{M}_1(D) = \frac{n+1}{2} \). Then by (11),

\[ n + 1 \geq 2n - q, \]

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

\[ n + 1 = 2\mathcal{M}_1(D) = 2n + \sum_{(ij) \neq (1,2)} (ij - 2) \frac{i+j}{ij} p_{ij} \]

\[ = 2n + \sum_{(ij) \neq (1,2)} (ij - 2) \frac{i+j}{ij} p_{ij}. \]

Thus,

\[ 0 \leq \sum_{(ij) \neq (1,2)} (ij - 2) \frac{i+j}{ij} p_{ij} = 2p_{11} - n + 1, \]
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,
\[
D = \frac{n-3}{2} \overset{\rightarrow}{P}_2 \oplus \overset{\rightarrow}{P}_3.
\]
The case of \( \mathcal{M}_2 \) when \( n \) is odd is similar.

In the case of the \( ABC \) index, note that \( \varphi_{ij} = 0 \) if, and only if \((i, j) = (1, 1)\). Then it is clear that
\[
ABC \left( \bigoplus_{i=1}^{k_1} \overset{\rightarrow}{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overset{\rightarrow}{C}_{n_j} \right) = 0.
\]
Conversely, if \( D \) is a digraph such that \( 0 = ABC(D) \), then
\[
0 = ABC(D) = \frac{1}{2} \sum_{(i,j) \in K} p_{ij} \varphi_{ij} = \frac{1}{2} \sum_{(i,j) \in K} p_{ij} \varphi_{ij},
\]
which implies \( p_{ij} = 0 \) for all \((i, j) \neq (1, 1)\). Hence, by part 1 of Lemma 2, \( D = \bigoplus_{i=1}^{k_1} \overset{\rightarrow}{P}_{n_i} \oplus \bigoplus_{j=1}^{k_2} \overset{\rightarrow}{C}_{n_j} \). \( \Box \)

**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 \( \varphi \) be a symmetric VDB topological index. Let us define
\[
L_{\text{max}} = L_{\text{max}}(\varphi) = \left\{(i,j) \in K : \varphi_{ij} = \max_{K} \varphi_{ij} \right\},
\]
and
\[
L_{\text{min}} = L_{\text{min}}(\varphi) = \left\{(i,j) \in K : \varphi_{ij} = \min_{K} \varphi_{ij} \right\}.
\]
The complements in \( K \) are denoted by \( L_{\text{c} \text{max}} \) and \( L_{\text{c} \text{min}} \), respectively.

**Theorem 2.** Let \( \varphi \) 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 \((i, j) \in L_{\text{c} \text{min}} \). Equality on the right occurs if, and only if \( p_{ij} = 0 \) for all \((i, j) \in L_{\text{c} \text{max}} \). \( \Box \)

**Proof.** From (2) and (1),
\[
\varphi(D) = \frac{1}{2} \sum_{K} p_{ij} \varphi_{ij} \leq \frac{1}{2} \sum_{K} p_{ij} \max_{K} \varphi_{ij} = \frac{1}{2} a \left( \max_{K} \varphi_{ij} \right).
\]
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 \((i, j) \in L_{\text{max}}^c\), then \(\varphi_{ij} - \max_k \varphi_{ij} \neq 0\) and so \(p_{ij} = 0\).

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

\[
\varphi(D) = \frac{1}{2} \sum_k p_{ij} \varphi_{ij} = \frac{1}{2} \sum_{\text{max}} p_{ij} \varphi_{ij} + \frac{1}{2} \sum_{\text{max}} p_{ij} \varphi_{ij} = \frac{1}{2} \sum_{\text{max}} p_{ij} \varphi_{ij} = \frac{1}{2} \left( \max_k \varphi_{ij} \right).
\]

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 \(OT(n)\). It is our interest in this section to determine the extremal values of a VDB topological index over \(OT(n)\). Clearly, \(a = n - 1\) for every \(T \in OT(n)\). Hence, by Theorem 2 we deduce the following.

**Corollary 2.** Let \(T \in OT(n)\). 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 \((i, j) \in L_{\text{min}}^c\). Equality on the right occurs if, and only if \(p_{ij} = 0\) for all \((i, j) \in L_{\text{max}}^c\).

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

**Theorem 3.** Let \(T \in OT(n)\). Then

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

Moreover, equality on the left of 1–5 occurs \(\Leftrightarrow T = K_{1,n-1}\) or \(T = K_{n-1,1}\). Equality on the right of 1–4 occurs \(\Leftrightarrow T = P_n\).

**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.** \(L_{\text{max}}^c\) and \(\max_k \varphi_{ij}\) for \(\chi, H, GA, \text{ and } SC\).

| VDB Index | \(\varphi_{ij}\) | \(L_{\text{max}}^c\) | \(\max_k \varphi_{ij}\) |
|-----------|-----------------|-----------------|-----------------|
| \(\chi\)  | \(\frac{1}{\sqrt{ij}}\) | (1, 1)          | 1               |
| \(H\)     | \(\frac{1}{i+j}\)  | (1, 1)          | 1               |
| \(GA\)    | \(\frac{1}{\sqrt{i+j}}\) | \((i, j) \in K : i = j\) | 1               |
| \(SC\)    | \(\frac{1}{\sqrt{i+j}}\) | (1, 1)          | \(\frac{1}{\sqrt{2}}\) |

We also use the fact that \(T \in OT(n)\) is such that \(p_{ij} = 0\) for all \((i, j) \neq (1, 1)\) if, and only if \(T = P_n\). Similarly, \(p_{ij} = 0\) for all \((i, j)\) such that \(i < j\) if, and only if \(T = P_n\).
Theorem 4. Let \( T \in OT(n) \). Then
1. \( 0 \leq ABC(T) \leq \frac{1}{2}(n-1)(n-2) \);
2. \( (n-1) \leq M_1(T) \);
3. \( \frac{1}{2}(n-1) \leq M_2(T) \).

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 \( ABC, M_1 \), and \( M_2 \).

| VDB Index | \( \varphi_{ij} \) | \( L_{\min} \) | \( \min_{k} \varphi_{ij} \) |
|------------|-----------------|-------------|-----------------|
| \( ABC \)  | \( \sqrt{\frac{i+j-2}{ij}} \) | (1, 1)       | 0               |
| \( M_1 \)  | \( i + j \)      | (1, 1)       | 2               |
| \( M_2 \)  | \( ij \)         | (1, 1)       | 1               |

And the fact that \( T \in OT(n) \) 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 \( ABC \).

| VDB Index | \( \varphi_{ij} \) | \( L_{\max} \) | \( \max_{k} \varphi_{ij} \) |
|------------|-----------------|-------------|-----------------|
| \( ABC \)  | \( \sqrt{\frac{i+j-2}{ij}} \) | (1, n − 1)  | \( \sqrt{\frac{n-2}{n-1}} \) |

And the fact that \( T \in OT(n) \) 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 \( M_1, M_2 \), and \( AZ \) over \( OT(n) \). 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 \( M_1 \) and \( M_2 \) over \( OT(n) \) 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 \( AZ \) over \( OT(n) \).

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

Let \( \varphi \) be a symmetric VDB topological index and \( G \) a graph. Let \( O(G) \) 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 \( O(G) \). 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 \( \varphi \) be a symmetric VDB topological index. We say that \( \varphi \) 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 \((i,j),(k,l) \in K:\)
\[(i,j) \leq (k,l)\text{ and } \varphi_{ij} = \varphi_{kl} \Rightarrow (i,j) = (k,l),\]
we will say that \(\varphi\) is strictly nondecreasing (resp. strictly nonincreasing).

**Example 2.** Consider the generalized Randić index \(\chi_\alpha\) induced by the numbers \((ij)^\alpha\), where \(\alpha \in \mathbb{R},\ \alpha \neq 0\). Clearly, \(\chi_\alpha\) is strictly nondecreasing when \(\alpha > 0\), and strictly nonincreasing when \(\alpha < 0\). In particular, the Randić index \(\chi\) is strictly nonincreasing and the second Zagreb index \(M_2\) is strictly nondecreasing. Additionally, the harmonic index and the sum-connectivity index are strictly nonincreasing, and the first Zagreb \(M_1\) is strictly nondecreasing.

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

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

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

**Proof.** We will assume that \(\varphi\) is strictly nondecreasing, and the other case is similar. Note that

\[
d_u = d_u^+ + d_u^-
\]
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 \(\varphi\) and (3),

\[
\varphi(D) = \frac{1}{2} \sum_{uv \in A} \varphi(d_u^+, d_v^-) \leq \frac{1}{2} \sum_{uv \in G} \varphi(d_u, d_v) = \frac{1}{2} \varphi(G).
\]

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 \(uv \in A\)

\[
(d_u^+, d_v^-) \preceq (d_u, d_v) \quad \text{and} \quad \varphi(d_u^+, d_v^-) = \varphi(d_u, d_v).
\]

Now since \(\varphi\) 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 \(G\). \(\square\)

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

**Proof.** We assume that \(\varphi\) 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,

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

\(\square\)
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 $M_1$, $M_2$ and $\chi_\alpha$ when $\alpha > 0$, over $\mathcal{O}(P_n)$. On the other hand, $E$ attains the minimal value of $H$, $\mathcal{S}C$ and $\chi_\alpha$ when $\alpha < 0$, over $\mathcal{O}(P_n)$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{path_tree.png}
\caption{Sink-source orientations of $P_n$.}
\end{figure}

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

Theorem 6. Let $T \in \mathcal{OT}(n)$. Then
1. $M_1(T) \leq \frac{1}{2}n(n - 1)$;
2. $M_2(T) \leq \frac{1}{2}(n - 1)^2$.

Moreover, equalities 1–2 occur $\iff T = K_{1,n-1}$ or $T = K_{n-1,1}$.

Proof. Let $G$ be a tree of order $n$. If $G$ is different from $S_n$, then [25]
$$M_1(G) < M_1(S_n) = n(n - 1)$$
$$M_2(G) < M_2(S_n) = (n - 1)^2.$$

Let $T \in \mathcal{OT}(n)$ and suppose that $T$ is an orientation of a tree $G$. By Theorem 5 and the above equation,
$$M_1(T) \leq \frac{1}{2}M_1(G) \leq \frac{1}{2}n(n - 1)$$
$$M_2(T) \leq \frac{1}{2}M_2(G) \leq \frac{1}{2}(n - 1)^2.$$

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

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