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Research Article

On the vertex-degree based invariants of digraphs

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Abstract

Let $D = (V, A)$ be a digraph without isolated vertices. A vertex-degree based invariant $I(D)$ related to a real function φ of D is defined as $I(D) = \frac{1}{2}\sum_{uv\in A}\varphi(d_u^+, d_v^-)$, where d_u^+ (respectively, d_u^-) denotes the out-degree (respectively, in-degree) of a vertex u. In this paper, we give the extremal values and extremal digraphs of $I(D)$ over all digraphs with n non-isolated vertices. By applying the obtained results, we determine the extremal values of some well-known vertex-degree based topological indices of digraphs, such as the Randić index, the Zagreb indices, the sum-connectivity index, the geometric-arithmetic index, the atom-bond connectivity index and the harmonic index, and characterize the corresponding extremal digraphs.

Keywords: graph invariant; digraph; Randić index; Zagreb indices; sum-connectivity index; geometric-arithmetic index; atom-bond connectivity index; harmonic index.

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1. Introduction

A digraph $D = (V, A)$ is an ordered pair (V, A) consisting of a non-empty finite set V of vertices and a finite set A of ordered pairs of distinct vertices called arcs (in particular, D has no loops). If $a \in A$ is an arc from vertex u to vertex v, then we indicate this by writing $a = uv$. The vertex u is the tail of a and the vertex v is its head. The out-degree (respectively, in-degree) of a vertex u, denoted by d_u^+ (respectively, d_u^-) is the number of arcs with tail u (respectively, with head u). A vertex u for which $d_u^+ = d_u^- = 0$ is called an isolated vertex. We denote by $\mathcal{D}_n$ the set of all digraphs with n non-isolated vertices.

Recently, J. Monsalve and J. Rada [7] extended the concept of vertex-degree based topological indices of graphs to digraphs. They obtained the extremal values of the Randić index of digraphs over $\mathcal{D}_n$, and found the extremal values of the Randić index over the set of all oriented trees with n vertices. Also, they found the extremal values of the Randić index over the set of all orientations of the path, the cycle with n vertices and the hypercube H_d of dimension d, respectively.

All the digraphs considered in this paper are strict, i.e., no loops and no two arcs with the same ends have the same orientation.

A vertex-degree-based (VDB, for short) VDB invariant (or VDB topological index) $I(D)$ related to a real function φ of a digraph D with n non-isolated vertices is defined as

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

where $\varphi_{ij} = \varphi(i, j)$ and a_{ij} is the number of arcs in D of the form uv such that $d_u^+ = i$ and $d_v^- = j$, i.e., (i, j)-arcs in D.

Recall that if G is a graph, we can identify G with the symmetric digraph $\overrightarrow{G}$ by replacing every edge of G with a pair of symmetric arcs. Under this correspondence,

$$I(G) = \sum_{1\le i\le j\le n-1} m_{ij}\varphi_{ij} = I(\overrightarrow{G})$$

for any VDB topological index φ with $\varphi_{ij} = \varphi_{ji}$ (symmetric) and m_{ij} the number of edges in G joining vertices of degree i and j. In other words, The VDB topological index of digraphs is a generalization of the concept of VDB topological index of graphs.

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In fact, a VDB topological index $I(D)$ of a digraph is an invariant based on the weights of all arcs depending on the out degrees of their tails and the in-degrees of their heads, i.e.,

$$I(G) = \sum_{uv \in A} \varphi(d_u^+, d_v^-)$$

where $\varphi(x, y)$ is a real function of x and y with $\varphi(x, y) \geq 0$ and $\varphi(x, y) = \varphi(y, x)$.

(i). If $\varphi(x, y) = (xy)^\alpha$, where $\alpha \neq 0$ is a real number, then $I(D)$ is the general Randić index of a digraph D. Furthermore, $I(D)$ is the Randić index, the second Zagreb index and the second modified Zagreb index for $\alpha = -\frac{1}{2}$, $\alpha = 1$ and $\alpha = -1$, respectively. For these indices of graphs, see [1,6,8,9].

(ii). If $\varphi(x, y) = (x + y)^\alpha$, then $I(D)$ is the general sum-connectivity index of a digraph D. Further, $I(G)$ is the sum-connectivity index and the first Zagreb index for $\alpha = -\frac{1}{2}$ and $\alpha = 1$, respectively. See [5,8,11,12] for graphs.

(iii). If $\varphi(x, y) = \frac{\sqrt{xy}}{\frac{1}{2}(x+y)}$, then $I(D)$ is the first geometric-arithmetic index GA of a digraph D. See [10] for the first geometric-arithmetic index of a graph.

(iv). If $\varphi(x, y) = \sqrt{\frac{x+y-2}{xy}}$, then $I(G)$ is the atom-bond connectivity (ABC) index of a digraph D. See [3] for the atom-bond connectivity index of a graph.

(v). If $\varphi(x, y) = \frac{2}{x+y}$, then $I(D)$ is the harmonic index of a digraph D. See [4] for the harmonic index of a graph.

In this paper, we give the extremal values and extremal graphs of the VDB topological indices over all digraphs with n non-isolated vertices by a unified linear-programming modeling, and provide a unified approach to determining some extremal values and characterizing extremal digraphs of Randić index, Zagreb indices, sum-connectivity index, GA index, ABC index and harmonic index by using the linear programming methods.

2. General results on VDB invariants

Let D be a digraph on $n \geq 2$ vertices without isolated vertices and a_{ij} be the number of arcs of D from vertices of out-degree i to vertices of in-degree j. If φ is symmetric, i.e. $\varphi_{ij} = \varphi_{ji}$ for all $1 \leq i < j \leq n-1$, then we can simplify the expression in (1) in the following

$$I(D) = \frac{1}{2} \sum_{1 \leq i \leq j \leq n-1} p_{ij}\varphi_{ij} \tag{2}$$

where $p_{ij} = a_{ij} + a_{ji}$ for $i \neq j$ and $1 \leq i, j \leq n-1$, and $p_{ii} = a_{ii}$ for all $i = 1, 2, \cdots, n-1$.

Note that $p_{ij} = p_{ji}$ for all $1 \leq i, j \leq n-1$, and

$$\sum_{j=1}^{n-1} p_{ij} + p_{ii} = in_i, \quad 1 \leq i \leq n-1. \tag{3}$$

where n_i is the number of vertices of D with out-degree i or in-degree i. Also,

$$n_1 + n_2 + \cdots + n_{n-1} = 2n - n_0. \tag{4}$$

The digraphs with n non-isolated vertices which satisfy the following conditions are of great interest to us

(i).

$$\begin{cases} p_{ij} &= 0 \quad \text{for all } (i, j) \in \{(i, j) \mid 1 \leq i \leq j \leq n-1\} - \{(1, n-1)\}, \\ n_0 &= 0. \end{cases} \tag{5}$$

i.e., a digraph with only $(1, n-1)$- or $(n-1, 1)$-arcs and the out-degree or in-degree of each vertex greater than 0. The digraph obtained from the star on n vertices by replacing each of its edges with a pair of symmetric arcs satisfies (5). The converse of this example does not hold since $D_1 = (V, A)$ is also a digraph satisfied (5), where $V = \{v_1, v_2, \cdots, v_n\}$ and $A = \{v_1v_2, v_2v_1, v_iv_1, v_2v_i | 3 \leq i \leq n\}$.

(ii).

$$\begin{cases} p_{ij} &= 0 \quad \text{for all } (i, j) \in \{(i, j) \mid 1 \leq i < j \leq n-1\}, \\ n_0 &= n. \end{cases} \tag{6}$$

i.e., the digraphs with only (i, i)-arcs $(1 \leq i \leq n-1)$ and the out-degree or in-degree of each vertex equal to 0. $\overrightarrow{K}_2$ satisfies (6), and $D_2 = (V, A)$ is also a digraph satisfied (6), where $V = \{v_1, v_2, v_3, v_4\}$ and $A = \{v_1v_3, v_1v_4, v_2v_3, v_2v_4\}$. All digraphs in which each component is $\overrightarrow{K}_2$ or D_2 satisfy (6).

(iii).
$$\begin{cases} p_{ij} &= 0 \quad \text{for all } (i,j) \in \{(i,j) \mid 1 \le i < j \le n-1\}, \\ n_0 &= 0. \end{cases} \tag{7}$$
i.e., the digraphs with only (i,i)-arcs ($1 \le i \le n-1$) and the out-degree or in-degree of each vertex greater than 0. The directed cycle $\overrightarrow{C}_n$ on n vertices satisfies (7). All digraphs with n non-isolated vertices in which each component is regular satisfy (7). The converse of this example does not hold since $D_3 = (V, A)$ is also a digraph satisfied (7), where $V = \{v_1, v_2, v_3, v_4\}$ and $A = \{v_1v_3, v_1v_4, v_2v_3, v_2v_4, v_3v_1, v_4v_2\}$.

We try to find $\min(I(G))$ and $\max(I(G))$ under the constraints (3) and (4). The following results give the solutions of this problem for some VDB topological indices $I(D)$, i.e., determine the extremal values and the correspond extremal digraphs of $I(D)$ over all digraphs on n vertices without isolated vertices.

Theorem 2.1. *Let D be a digraph on n vertices without isolated vertices. Let*
$$L_{ij} = \frac{n-1}{n}\left(\frac{1}{i} + \frac{1}{j}\right)\varphi_{1,n-1} \quad \textit{and} \quad S_1 = \{(i,j) \mid 1 \le i \le j \le n-1\} - \{(1, n-1)\}.$$
Then

(i). *If $\varphi_{ij} > L_{ij}$ for all $(i,j) \in S_1$, then $I(D) \ge \frac{n-1}{2}\varphi_{1,n-1}$ with equality if and only if $n_0 = n$ and $p_{ij} = 0$ for all $(i,j) \in S_1$, i.e., D is the digraph $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$, a star on n vertices with its center of out-degree $n-1$ or 0.*

(ii). *If $\varphi_{ij} < L_{ij}$ for all $(i,j) \in S_1$, then $I(D) \le (n-1)\varphi_{1,n-1}$ with equality if and only if $n_0 = 0$ and $p_{ij} = 0$ for all $(i,j) \in S_1$, i.e., D satisfies the conditions (5).*

Proof. From (3), we have
$$n_i = \frac{1}{i}\left(\sum_{j=1}^{n-1} p_{ij} + p_{ii}\right), \quad i = 2, 3, \cdots, n-2, \tag{8}$$
$$n_1 - p_{1,n-1} = \sum_{j=1}^{n-2} p_{1j} + p_{11}, \tag{9}$$
$$(n-1)n_{n-1} - p_{1,n-1} = \sum_{j=2}^{n-1} p_{j,n-1} + p_{n-1,n-1}. \tag{10}$$
By (4) and (8),
$$n_1 + n_{n-1} = 2n - n_0 - \sum_{i=2}^{n-2} \frac{1}{i}\left(\sum_{j=1}^{n-1} p_{ij} + p_{ii}\right). \tag{11}$$
Multiplying (9) by $(n-1)$ and adding (10), we obtain
$$(n-1)(n_1 + n_{n-1}) - np_{1,n-1} = (n-1)\sum_{j=1}^{n-2} p_{1j} + (n-1)p_{11} + \sum_{j=2}^{n-1} p_{j,n-1} + p_{n-1,n-1},$$
and by combining this equation with (11), we get
$$\begin{aligned} np_{1,n-1} = &\ (n-1)(n_1 + n_{n-1}) - (n-1)\left(\sum_{j=1}^{n-2} p_{1j} + p_{11}\right) - \left(\sum_{j=2}^{n-1} p_{j,n-1} + p_{n-1,n-1}\right) \\ = &\ (n-1)\left[2n - n_0 - \sum_{i=2}^{n-2}\frac{1}{i}\left(\sum_{j=1}^{n-1} p_{ij} + p_{ii}\right)\right] - (n-1)\left(\sum_{j=1}^{n-2} p_{1j} + p_{11}\right) - \left(\sum_{j=2}^{n-1} p_{j,n-1} + p_{n-1,n-1}\right). \end{aligned}$$
Hence,
$$\begin{aligned} p_{1,n-1} = &\ 2(n-1) - \tfrac{n-1}{n}n_0 - \tfrac{n-1}{n}\sum_{i=2}^{n-2}\tfrac{1}{i}\left(\sum_{j=1}^{n-1} p_{ij} + p_{ii}\right) - \tfrac{n-1}{n}\left(\sum_{j=1}^{n-2} p_{1j} + p_{11}\right) - \tfrac{1}{n}\sum_{j=2}^{n-1} p_{j,n-1} - \tfrac{1}{n}p_{n-1,n-1} \\ = &\ 2(n-1) - \tfrac{n-1}{n}n_0 - \tfrac{n-1}{n}\left[\sum_{i=1}^{n-1}\tfrac{1}{i}\left(\sum_{j=1}^{n-1} p_{ij} + p_{ii}\right) - \tfrac{n}{n-1}p_{1,n-1}\right] \\ = &\ 2(n-1) - \tfrac{n-1}{n}n_0 - \tfrac{n-1}{n}\left[\sum_{i=1}^{n-1}\tfrac{1}{i}\left(\sum_{j=1}^{n-1} p_{ij} + p_{ii}\right)\right] + p_{1,n-1} \\ = &\ 2(n-1) - \tfrac{n-1}{n}n_0 - \tfrac{n-1}{n}\left[\sum_{1 \le i \le j \le n-1}\left(\tfrac{1}{i} + \tfrac{1}{j}\right)p_{ij}\right] + p_{1,n-1} \\ = &\ 2(n-1) - \tfrac{n-1}{n}n_0 - \tfrac{n-1}{n}\sum{}'\left(\tfrac{1}{i} + \tfrac{1}{j}\right)p_{ij} \end{aligned}$$

where $\sum'$ indicates summation over all $(i,j) \in S_1$. Substituting it into (2), we obtain

$$\begin{aligned} 2\,I(D) = &\ \varphi_{1,n-1}p_{1,n-1} + \sum{}' \varphi_{ij}p_{ij} \\ = &\ \varphi_{1,n-1}[2(n-1) - \tfrac{n-1}{n}n_0 - \tfrac{n-1}{n}\sum{}'(\tfrac{1}{i}+\tfrac{1}{j})p_{ij}] + \sum{}'\varphi_{ij}p_{ij} \\ = &\ [2(n-1) - \tfrac{n-1}{n}n_0]\varphi_{1,n-1} + \sum{}'[\varphi_{ij} - \tfrac{n-1}{n}(\tfrac{1}{i}+\tfrac{1}{j})\varphi_{1,n-1}]p_{ij}. \end{aligned} \tag{12}$$

(i) If $\varphi_{ij} > L_{ij} = \frac{n-1}{n}(\frac{1}{i}+\frac{1}{j})\varphi_{1,n-1}$ for all $(i,j) \in S_1$, then (12) shows that $I(D) \geq \frac{1}{2}[2(n-1) - \frac{n-1}{n}n_0]\varphi_{1,n-1}$. Moreover,

$$I(D) \geq \frac{n-1}{2}\varphi_{1,n-1}$$

since $n_0 \leq n$, with equality if and only if $n_0 = n$ and $p_{ij} = 0$ for all $(i,j) \in S_1$, i.e., D is the digraph $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$.

(ii) If $\varphi_{ij} < L_{ij}$ for all $(i,j) \in S_1$, then (12) shows that $I(D) \leq \frac{1}{2}[2(n-1) - \frac{n-1}{n}n_0]\varphi_{1,n-1}$. Moreover, $I(D) \leq (n-1)\varphi_{1,n-1}$ since $n_0 \geq 0$, with equality if and only if $n_0 = 0$ and $p_{ij} = 0$ for all $(i,j) \in S_1$, i.e., D is a digraph satisfied (5). □

Theorem 2.2. *Let* $M_{ij} = \frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})\varphi_{n-1,n-1}$ *and* $S_2 = \{(i,j) \mid 1 \leq i \leq j \leq n-1\} - \{(n-1,n-1)\}$. *Then*

(i). *If* $\varphi_{ij} > M_{ij}$ *for all* $(i,j) \in S_2$, *then* $I(D) \geq \frac{1}{4}n(n-1)\varphi_{n-1,n-1}$ *with equality if and only if* $n_0 = n$ *and* $p_{ij} = 0$ *for all* $(i,j) \in S_2$, *i.e.,* $D = \overrightarrow{K}_2$.

(ii). *If* $\varphi_{ij} < M_{ij}$ *for all* $(i,j) \in S_2$, *then* $I(D) \leq \frac{1}{2}n(n-1)\varphi_{n-1,n-1}$ *with equality if and only if* $n_0 = 0$ *and* $p_{ij} = 0$ *for all* $(i,j) \in S_2$, *i.e.,* D *is the digraph obtained from* K_n *by replacing each edge with a pair of symmetric arcs.*

Proof. From (3) and (4), we obtain

$$\begin{aligned} n_{n-1} &= (2n - n_0) - \sum_{i=1}^{n-2}\frac{1}{i}\left(\sum_{j=1}^{n-1}p_{ij} + p_{ii}\right) \\ &= (2n - n_0) - \left(\sum_{j=1}^{n-1}\sum_{i=1}^{n-2}\tfrac{1}{i}p_{ij} + \sum_{i=1}^{n-2}\tfrac{1}{i}p_{ii}\right) \\ &= (2n - n_0) - \sum_{1\leq i\leq j\leq n-1}(\tfrac{1}{i}+\tfrac{1}{j})p_{ij} + \tfrac{1}{n-1}\sum_{j=1}^{n-2}p_{j,n-1} + \tfrac{2}{n-1}p_{n-1,n-1}. \end{aligned}$$

By (3), it holds that

$$\sum_{j=1}^{n-2}p_{n-1,j} + 2p_{n-1,n-1} = (n-1)n_{n-1}$$

and

$$\begin{aligned} 2p_{n-1,n-1} = &\ (n-1)n_{n-1} - \sum_{j=1}^{n-2}p_{n-1,j} \\ = &\ (n-1)\left[(2n-n_0) - \sum_{1\leq i\leq j\leq n-1}(\tfrac{1}{i}+\tfrac{1}{j})p_{ij} + \tfrac{1}{n-1}\sum_{j=1}^{n-2}p_{j,n-1} + \tfrac{2}{n-1}p_{n-1,n-1}\right] - \sum_{j=1}^{n-2}p_{n-1,j} \\ = &\ (2n-n_0)(n-1) - (n-1)\sum{}''(\tfrac{1}{i}+\tfrac{1}{j})p_{ij} \end{aligned}$$

where $\sum''$ indicates summation over all $(i,j) \in S_2$. By substituting it into (2), we obtain

$$\begin{aligned} 2\,I(D) = &\ \varphi_{n-1,n-1}p_{n-1,n-1} + \sum{}''\varphi_{ij}p_{ij} \\ = &\ \varphi_{n-1,n-1}[\tfrac{1}{2}(2n-n_0)(n-1) - \tfrac{1}{2}(n-1)\sum{}''(\tfrac{1}{i}+\tfrac{1}{j})p_{ij}] + \sum{}''\varphi_{ij}p_{ij} \\ = &\ \tfrac{1}{2}(2n-n_0)(n-1)\varphi_{n-1,n-1} + \sum{}''[\varphi_{ij} - \tfrac{n-1}{2}(\tfrac{1}{i}+\tfrac{1}{j})\varphi_{n-1,n-1}]p_{ij}. \end{aligned} \tag{13}$$

(i) If $\varphi_{ij} > M_{ij}$ for all $(i,j) \in S_2$, then (13) shows that $I(D) \geq \frac{1}{4}(2n-n_0)(n-1)\varphi_{n-1,n-1}$. Moreover, $I(D) \geq \frac{1}{4}n(n-1)\varphi_{n-1,n-1}$ since $n_0 \leq n$, with equality if and only if $n_0 = n$ and $p_{ij} = 0$ for all $(i,j) \in S_2$, i.e., D is a digraph with only $(n-1,n-1)$-arcs and the out-degree or in-degree of each vertex equal to 0. So, $D = \overrightarrow{K}_2$.

(ii) If $\varphi_{ij} < M_{ij}$ for all $(i,j) \in S_2$, then (13) shows that $I(D) \leq \frac{1}{4}(2n-n_0)(n-1)\varphi_{n-1,n-1}$. Moreover, $I(D) \leq \frac{1}{2}n(n-1)\varphi_{n-1,n-1}$ since $n_0 \geq 0$, with equality if and only if $n_0 = 0$ and $p_{ij} = 0$ for all $(i,j) \in S_2$, i.e., D is the digraph obtained from the complete graph K_n by replacing each edge with a pair of symmetric arcs. □

Theorem 2.3. *Let* $S_3 = \{(i,j) \mid 1 \leq i \neq j \leq n-1\}$. *Then*

(i). *If* $\varphi_{ij} > M_{ij}$ *for all* $(i,j) \in S_3$, *and* $i\varphi_{ii} = (n-1)\varphi_{n-1,n-1}$ *for* $1 \leq i \leq n-2$, *then* $I(D) \geq \frac{1}{4}n(n-1)\varphi_{n-1,n-1}$ *with equality if and only if* $n_0 = n$ *and* $p_{ij} = 0$ *for all* $(i,j) \in S_3$, *i.e.,* D *is a digraph satisfied (6).*

(ii). *If $\varphi_{ij} < M_{ij}$ for all $(i,j) \in S_3$, and $i\varphi_{ii} = (n-1)\varphi_{n-1,n-1}$ for $1 \le i \le n-2$, then $I(D) \le \frac{1}{2}n(n-1)\varphi_{n-1,n-1}$ with equality if and only if $n_0 = 0$ and $p_{ij} = 0$ for all $(i,j) \in S_3$, i.e., D is a digraph satisfied (7).*

Proof. From (13), we have

$$2I(G) = \frac{1}{2}(2n-n_0)(n-1)\varphi_{n-1,n-1} + \sum_{1\le i<j\le n-1}[\varphi_{ij} - \tfrac{n-1}{2}(\tfrac{1}{i}+\tfrac{1}{j})\varphi_{n-1,n-1}]p_{ij} + \sum_{i=1}^{n-2}[\varphi_{ii} - \tfrac{n-1}{i}\varphi_{n-1,n-1}]p_{ii}. \quad (14)$$

(i) If $\varphi_{ij} > M_{ij}$ for all $(i,j) \in S_3$, and $i\varphi_{ii} = (n-1)\varphi_{n-1,n-1}$ for $1 \le i \le n-2$, then (14) shows that

$$I(D) \ge \frac{1}{4}(2n-n_0)(n-1)\varphi_{n-1,n-1}.$$

Moreover, $I(D) \ge \frac{1}{4}n(n-1)\varphi_{n-1,n-1}$ since $n_0 \le n$, with equality if and only if $n_0 = n$ and $p_{ij} = 0$ for all $(i,j) \in S_3$, i.e., D is the digraph satisfied (6).

(ii) If $\varphi_{ij} < M_{ij}$ for all $(i,j) \in S_3$, and $i\varphi_{ii} = (n-1)\varphi_{n-1,n-1}$ for $1 \le i \le n-2$, then (14) shows that

$$I(D) \le \frac{1}{4}(2n-n_0)(n-1)\varphi_{n-1,n-1}.$$

Moreover, $I(D) \le \frac{1}{2}n(n-1)\varphi_{n-1,n-1}$ since $n_0 \ge 0$, with equality if and only if $n_0 = 0$ and $p_{ij} = 0$ for all $(i,j) \in S_3$, i.e., D is a digraph satisfied (7). □

Theorems 2.1-2.3 show that the results on digraphs are different from the results on graphs in [2].

3. Applications

In this section, we give some results on Randić index, Zagreb indices, sum-connectivity index, GA index and ABC index of digraphs by using Theorems 2.1-2.3.

3.1. The general Randić index of digraphs

Let $\varphi_{ij} = (ij)^\alpha$. Then $I(D) = R_\alpha(D) = \frac{1}{2}\sum_{1\le i\le j\le n-1} p_{ij}(ij)^\alpha$ is the general Randić index of a digraph D with n non-isolated vertices. In particular, $R_\alpha(D)$ is the Randić index, the second Zagreb index and the modified Zagreb index of a digraph for $\alpha = -\frac{1}{2}$, $\alpha = 1$ and $\alpha = -1$, respectively.

(i) Let $-\frac{1}{2} \le \alpha < +\infty$. Then $2\alpha + 1 \ge 0$.
Note that $ij \le (\frac{i+j}{2})^2$ and $i, j \le n-1$, we have

$$\begin{aligned}(ij)^{\alpha+1} \le \left(\frac{i+j}{2}\right)^{2\alpha+2} &= \frac{1}{2^{2\alpha+2}}(i+j)^{2\alpha+1}(i+j)\\ &\le \frac{1}{2^{2\alpha+2}}[2(n-1)]^{2\alpha+1}(i+j) = \frac{1}{2}(n-1)^{2\alpha+1}(i+j),\end{aligned}$$

and $\varphi_{ij} \le \frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})\varphi_{n-1,n-1}$ with equality if and only if (a) $i = j = n-1$ for $-\frac{1}{2} < \alpha < +\infty$, or (b) $i = j$ for $\alpha = -\frac{1}{2}$. By Theorems 2.2(ii) and 2.3(ii), we have

$$R_\alpha(D) \le \frac{1}{2}n(n-1)\varphi_{n-1,n-1} = \frac{1}{2}n(n-1)^{2\alpha+1}$$

with equality if and only if (a) D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs for $-\frac{1}{2} < \alpha < +\infty$, or (b) D is a digraph satisfied (7). So, (a) the digraph with the maximal general Randić index (including the second Zagreb index) for $-\frac{1}{2} < \alpha < +\infty$ is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs; (b) the digraphs with the maximal Randić index are those satisfied (7), see Theorem 3.7 in [7].

Corollary 3.1. *If $D \in \mathcal{D}_n$, then (a) $R_\alpha(D) \le \frac{1}{2}n(n-1)^{2\alpha+1}$ for $-\frac{1}{2} < \alpha < +\infty$ with equality if and only if D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs; (b) (Theorem 3.7 in [7]) $R_{-\frac{1}{2}}(D) \le \frac{n}{2}$ with equality if and only if D satisfies (7).*

(ii) Let $-\infty < \alpha \le -1$.
Because $ij \le (\frac{i+j}{2})^2$ and $\alpha \le -1$, we have

$$(ij)^{\alpha+1} \ge \left(\frac{i+j}{2}\right)^{2\alpha+2} = \frac{1}{2^{2\alpha+2}}(i+j)^{2\alpha+1}(i+j)$$

$$\geq \frac{1}{2^{2\alpha+2}}[2(n-1)]^{2\alpha+1}(i+j) = \frac{1}{2}(n-1)^{2\alpha+1}(i+j),$$

and $\varphi_{ij} \geq \frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})\varphi_{n-1,n-1}$ with equality if and only if $i=j=n-1$. By Theorem 2.2(i), we have

$$R_\alpha(D) \geq \frac{1}{4}n(n-1)\varphi_{n-1,n-1} = \frac{1}{4}n(n-1)^{2\alpha+1}$$

with equality if and only if $D=\overrightarrow{K}_2$. So, the digraph with the minimal general Randić index (including the modified Zagreb index) for $-\infty<\alpha\leq -1$ is $\overrightarrow{K}_2$.

Corollary 3.2. *If $D\in\mathcal{D}_n$, then $R_\alpha(D)\leq \frac{1}{4}n(n-1)^{2\alpha+1}$ for $-\infty<\alpha\leq-1$ with equality if and only if $D=\overrightarrow{K}_2$.*

(iii) Let $-\frac{1}{2}\leq\alpha<0$.
In the following, we show that $\varphi_{ij} > \frac{n-1}{n}(\frac{1}{i}+\frac{1}{j})\varphi_{1,n-1}$ for all $(i,j)\in\{(i,j)\mid 1\leq i\leq j\leq n-1\}-\{(1,n-1)\}$. Let $g(x,y)=\frac{(xy)^{\alpha+1}}{x+y}$, where $1\leq x\leq y\leq n-1$. Note that $\alpha x+y+\alpha y\geq(2\alpha+1)x\geq 0$, $\frac{\partial g}{\partial x}=\frac{y(xy)^\alpha(\alpha x+y+\alpha y)}{(x+y)^2}=0$ and $\frac{\partial g}{\partial y}=\frac{x(xy)^\alpha(\alpha x+x+\alpha y)}{(x+y)^2}=0$ if and only if $\alpha=-\frac{1}{2}$ and $x=y$. So, the minimal point of $g(x,y)$ in the region $\{(x,y)\mid 1\leq x\leq y\leq n-1\}$ is on the boundary of this region, and the minimal value of $g(x,y)$ in the region $\{(x,y)\mid 1\leq x\leq y\leq n-1\}$ is $\min\{g(1,1),g(1,n-1)\}=\min\{\frac{1}{2},\frac{(n-1)^{\alpha+1}}{n}\}$. If $\alpha\in(-\frac{1}{2},0)$, then $\frac{(n-1)^{\alpha+1}}{n}<\frac{1}{2}$ for sufficiently large n; and if $\alpha=-\frac{1}{2}$, then $\frac{(n-1)^{\alpha+1}}{n}<\frac{1}{2}$ for $n\geq 3$. Hence, $g(i,j)\geq g(1,n-1)$, and

$$(ij)^\alpha \geq \frac{(n-1)^{\alpha+1}}{n}(\frac{1}{i}+\frac{1}{j}),\ \text{ i.e. }\quad \varphi_{ij}\geq\frac{n-1}{n}(\frac{1}{i}+\frac{1}{j})\varphi_{1,n-1}$$

with equality if and only if $(i,j)=(1,n-1)$. By Theorem 2.1(i), we have

$$R_\alpha(D)\geq\frac{n-1}{2}\varphi_{1,n-1}=\frac{1}{2}(n-1)^{\alpha+1}$$

with equality if and only if D is the digraph $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ for sufficiently large n. So, the digraph with the minimal Randić index is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ over $\mathcal{D}_n$ for $n\geq 3$; and the digraph with the minimal general Randić index for $\alpha\in(-\frac{1}{2},0)$ is also $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ over $\mathcal{D}_n$ for sufficiently large n.

Corollary 3.3. *(a) (Theorem 3.11 in [7]) If $D\in\mathcal{D}_n$, $n\geq 3$, then $R_{-\frac{1}{2}}(D)\geq\frac{1}{2}\sqrt{n-1}$ with equality if and only if $D=\overrightarrow{K}_{1,n-1}$ or $D=\overrightarrow{K}_{n-1,1}$;*
(b) Let $-\frac{1}{2}\leq\alpha<0$. If $D\in\mathcal{D}_n$, then $R_\alpha(D)\geq\frac{1}{2}(n-1)^{\alpha+1}$ for sufficiently large n, with equality if and only if $D=\overrightarrow{K}_{1,n-1}$ or $D=\overrightarrow{K}_{n-1,1}$.

3.2. The general sum-connectivity index of digraphs

Let $\varphi_{ij}=(i+j)^\alpha$. Then $I(D)=\chi_\alpha(D)=\frac{1}{2}\sum_{1\leq i\leq j\leq n-1}p_{ij}(i+j)^\alpha$ is the general sum-connectivity index of a digraph D, and $\chi_\alpha(D)$ is the sum-connectivity index and the first Zagreb index of D for $\alpha=-\frac{1}{2}$ and $\alpha=1$, respectively.

(i) Let $-1\leq\alpha<+\infty$.
Because $1\leq i\leq j\leq n-1$ and $\alpha+1\geq 0$,

$$ij\leq(\frac{i+j}{2})^2=\left(\frac{i+j}{2}\right)^{1-\alpha}\left(\frac{i+j}{2}\right)^{1+\alpha}$$
$$\leq\left(\frac{i+j}{2}\right)^{1-\alpha}(n-1)^{1+\alpha},$$

and $\varphi_{ij}=(i+j)^\alpha\leq\frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})[2(n-1)]^\alpha=\frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})\varphi_{n-1,n-1}$ with equality if and only if (a) $i=j=n-1$ for $-1<\alpha<+\infty$, or (b) $i=j$ for $\alpha=-1$. By Theorems 2.2(ii) and 2.3(ii), we have

$$\chi_\alpha(D)\leq\frac{1}{2}n(n-1)\varphi_{n-1,n-1}=2^{\alpha-1}n(n-1)^{\alpha+1}$$

with equality if and only if (a) D is the digraph obtained from the complete graph K_n by replacing each edge with a pair of symmetric arcs, or (b) D satisfies (7). Especially, this shows that the graph with the maximal sum-connectivity index, or the maximal first Zagreb index is K_n among all graphs of order n.

Corollary 3.4. *If $D\in\mathcal{D}_n$, then (a) $\chi_\alpha(D)\leq 2^{\alpha-1}n(n-1)^{\alpha+1}$ for $-\frac{1}{2}<\alpha<+\infty$ with equality if and only if D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs; (b) $\chi_{-1}(D)\leq\frac{n}{4}$ with equality if and only if D satisfies (7).*

(ii) Let $-1 \le \alpha < 0$.
We consider the function $g(x,y) = (xy)(x+y)^{\alpha-1}$, where $1 \le x \le y \le n-1$. It is easy to know that the minimal value of $g(x,y) = (xy)(x+y)^{\alpha-1}$ in the region $\{(x,y) \mid 1 \le x \le y \le n-1\}$ is $\min\{g(1,1), g(1,n-1)\} = \min\{2^{\alpha-1}, (n-1)n^{\alpha-1}\}$. If $\alpha \in (-\frac{1}{2}, 0)$, then $(n-1)n^{\alpha-1} < 2^{\alpha-1}$ for sufficiently large n; and if $\alpha \in [-1, -\frac{1}{2}]$, then $(n-1)n^{\alpha-1} < 2^{\alpha-1}$ for $n \ge 6$. Hence, $g(i,j) \ge g(1,n-1)$, and

$$(i+j)^{\alpha} \ge (n-1)n^{\alpha-1}(\frac{1}{i}+\frac{1}{j}), \text{ i.e., } \quad \varphi_{ij} \ge \frac{n-1}{n}(\frac{1}{i}+\frac{1}{j})\varphi_{1,n-1}$$

with equality if and only if $(i,j) = (1, n-1)$. By Theorem 2.1(i), we have

$$\chi_{\alpha}(D) \ge \frac{1}{2}(n-1)\varphi_{1,n-1} = \frac{1}{2}(n-1)n^{\alpha}$$

with equality if and only if D is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ for $\alpha \in [-1, 0)$ and sufficiently large n, or for $\alpha \in [-1, -\frac{1}{2}]$ and $n \ge 6$. So that the graph with the minimal general sum-connectivity index for $\alpha \in [-1, -\frac{1}{2}]$ is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ over $\mathcal{D}_n$; and the digraph with the minimal general sum-connectivity index for $\alpha \in [-1, 0)$ is also $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$ over $\mathcal{D}_n$ when n is sufficiently large.

Corollary 3.5. *Let $D \in \mathcal{D}_n$. If $\alpha \in [-1, -\frac{1}{2}]$ and $n \ge 6$, or $\alpha \in [-1, 0)$ and n is sufficiently large, then $\chi_{\alpha}(D) \ge \frac{1}{2}(n-1)n^{\alpha}$ with equality if and only if D is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$.*

3.3. The geometric-arithmetic index of digraphs

Let $\varphi_{ij} = \frac{\sqrt{ij}}{\frac{1}{2}(i+j)}$. Then $I(D) = GA(D) = \frac{1}{2}\sum_{1 \le i \le j \le n-1} p_{ij}\frac{\sqrt{ij}}{\frac{1}{2}(i+j)}$ is the first geometric-arithmetic index GA of a digraph D.

(i) Note that $\varphi_{n-1,n-1} = 1$ and $(ij)^{\frac{3}{2}} \le (\frac{i+j}{2})^3 = \frac{i+j}{8}(i+j)^2 \le \frac{n-1}{4}(i+j)^2$, i.e. $\frac{\sqrt{ij}}{\frac{1}{2}(i+j)} \le \frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})$, we have $\varphi_{ij} \le \frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})\varphi_{n-1,n-1}$ with equality if and only if $i = j = n-1$. By Theorem 2.2(ii),

$$GA(D) \le \frac{1}{2}n(n-1)\varphi_{n-1,n-1} = \frac{1}{2}n(n-1)$$

with equality if and only if D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs.

(ii) It is easy to know that the minimal value of $g(x,y) = \frac{(xy)^{\frac{3}{2}}}{(x+y)^2}$ in the region $\{(x,y) \mid 1 \le x \le y \le n-1\}$ is $g(1,n-1) = \frac{(n-1)^{\frac{3}{2}}}{n^2}$, $g(i,j) \ge g(1,n-1)$, i.e. $\frac{(ij)^{\frac{3}{2}}}{(i+j)^2} \ge \frac{(n-1)^{\frac{3}{2}}}{n^2}$. Hence,

$$\frac{\sqrt{ij}}{\frac{1}{2}(i+j)} \ge \frac{n-1}{n}(\frac{1}{i}+\frac{1}{j})\frac{\sqrt{n-1}}{\frac{1}{2}n} \quad \text{i.e.,} \quad \varphi_{ij} \ge \frac{n-1}{n}(\frac{1}{i}+\frac{1}{j})\varphi_{1,n-1}$$

with equality if and only if $(i,j) = (1,n-1)$. By Theorem 2.1(i), we have

$$GA(D) \ge \frac{1}{2}(n-1)\varphi_{1,n-1} = \frac{(n-1)^{\frac{3}{2}}}{n}$$

with equality if and only if D is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$.

So, we obtain the digraphs with the maximal and the minimal geometric-arithmetic index GA over $\mathcal{D}_n$.

Corollary 3.6. *If $D \in \mathcal{D}_n$, then $GA(D) \le \frac{1}{2}n(n-1)$ with equality if and only if D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs; $GA(D) \ge \frac{(n-1)^{\frac{3}{2}}}{n}$ with equality if and only if D is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$.*

3.4. The atom-bond connectivity index of digraphs

Let $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$, then $I(D) = ABC(D) = \frac{1}{2}\sum_{1 \le i \le j \le n-1} p_{ij}\sqrt{\frac{i+j-2}{ij}}$ is the ABC index of a digraph D. Since $1 \le i \le j \le n-1$,

$$\frac{i+j-2}{ij} \le \frac{2(n-2)}{ij} \le \frac{2(n-2)}{(ij)^2}\left(\frac{i+j}{2}\right)^2 \le \frac{n-2}{2}\left(\frac{i+j}{ij}\right)^2,$$

and $\sqrt{\frac{i+j-2}{ij}} \le \sqrt{\frac{n-2}{2}}(\frac{i+j}{ij})$, i.e., $\varphi_{ij} \le \frac{n-1}{2}(\frac{1}{i}+\frac{1}{j})\varphi_{n-1,n-1}$ with equality if and only if $i = j = n-1$. By Theorem 2.2(ii), we have

$$ABC(D) \le \frac{1}{2}n(n-1)\varphi_{n-1,n-1} = \frac{1}{2}n\sqrt{2n-4}$$

with equality if and only if D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs.

This shows that the digraphs with the maximal ABC index over $\mathcal{D}_n$ is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs.

Corollary 3.7. *If $D \in \mathcal{D}_n$, then $ABC(D) \le \frac{1}{2}n\sqrt{2n-4}$ with equality if and only if D is the digraph obtained from K_n by replacing each edge with a pair of symmetric arcs.*

3.5. The harmonic index of digraphs

Let $\varphi_{ij} = \frac{2}{i+j}$. Then $I(D) = h(D) = \frac{1}{2}\sum_{1\le i\le j\le n-1} p_{ij}\frac{2}{i+j}$ is the harmonic index of a digraph D.

(i) Note that

$$\varphi_{ij} = \frac{2}{i+j} \le \frac{i+j}{2ij} = \frac{n-1}{2}\left(\frac{1}{i}+\frac{1}{j}\right)\varphi_{n-1,n-1}$$

with equality if and only if $i = j$, and $i\varphi_{ii} = 1 = (n-1)\varphi_{n-1,n-1}$, from Theorem 2.3(ii), we have

$$h(D) \le \frac{1}{2}n(n-1)\varphi_{n-1,n-1} = \frac{n}{2}$$

with equality if and only if D is a digraph satisfied (7).

(ii) Also, the minimal value of $g(x,y) = \frac{(xy)}{(x+y)^2}$ in the region $\{(x,y) \mid 1 \le x \le y \le n-1\}$ is $g(1,n-1) = \frac{n-1}{n^2}$, we have $g(i,j) = \frac{ij}{(i+j)^2} \ge \frac{n-1}{n^2} = g(1,n-1)$ and

$$\varphi_{ij} = \frac{2}{i+j} \ge \frac{n-1}{n}\left(\frac{1}{i}+\frac{1}{j}\right)\frac{2}{n} = \frac{n-1}{n}\left(\frac{1}{i}+\frac{1}{j}\right)\varphi_{1,n-1}$$

with equality if and only if $(i,j) = (1,n-1)$. By Theorem 2.1(i), we have

$$h(D) \ge \frac{1}{2}(n-1)\varphi_{1,n-1} = \frac{n-1}{n}$$

with equality if and only if D is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$.

So, we obtain the digraphs with the minimal and maximal harmonic index over $\mathcal{D}_n$.

Corollary 3.8. *If $D \in \mathcal{D}_n$, then $h(D) \le \frac{n}{2}$ with equality if and only if D is a digraph satisfied (7); $h(D) \ge \frac{n-1}{n}$ with equality if and only if D is $\overrightarrow{K}_{1,n-1}$ or $\overrightarrow{K}_{n-1,1}$.*

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