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Vertex-degree based topological indices of digraphs

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ABSTRACT

Let $\mathcal{D}_n$ be the set of digraphs with n non-isolated vertices. Let $D \in \mathcal{D}_n$ and denote by d_u^+ and d_u^- the outer degree and inner degree, respectively, of the vertex u of D. We define the vertex-degree-based (VDB, for short) topological index φ induced by the real numbers $\{\varphi_{ij}\}$, as

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

where a_{ij} is the number of arcs in D of the form uv, where $d_u^+ = i$ and $d_v^- = j$. We show in this paper that this is a generalization of the concept of VDB topological indices of graphs. In the case $\varphi_{ij} = \frac{1}{\sqrt{ij}}$, we obtain the Randić index of digraphs, which we denote by χ. We find the extremal values of χ over $\mathcal{D}_n$. We also find the extremal values of χ over $\mathcal{OT}(n)$, the set of all oriented trees with n vertices. On the other hand, given a graph G, we consider the set $\mathcal{O}(G)$ of all orientations of G, and show that when G is a bipartite graph, the sink–source orientations of G uniquely attain the minimal value of χ over $\mathcal{O}(G)$. We find the extremal values of χ over $\mathcal{O}(P_n)$ and $\mathcal{O}(C_n)$, where P_n and C_n are the path and the cycle with n vertices, respectively. Finally, we find the extremal values of χ over $\mathcal{O}(H_d)$, the set of all orientations of the hypercube H_d of dimension d.

1. Introduction

Let $G = (V, E)$ be a graph with non-empty set of vertices V and set of edges E. If there is an edge from vertex u to vertex v we indicate this by writing uv (or vu). The degree of the vertex v of G is denoted by d_v. A vertex v is isolated if $d_v = 0$. We denote by $n_i = n_i(G)$ the number of vertices of G with degree i and $m_{ij} = m_{ij}(G)$ the number of edges in G joining vertices of degree i and j.

Let $\mathcal{G}_n$ be the set of graphs with n non-isolated vertices. A vertex-degree based (VDB, for short) topological index defined over $\mathcal{G}_n$, is a function φ induced by real numbers $\{\varphi_{ij}\}$, where $1 \le i \le j \le n-1$, and defined for a graph $G \in \mathcal{G}_n$

$$\varphi(G) = \sum_{1 \le i \le j \le n-1} m_{ij}\varphi_{ij}. \tag{1}$$

For recent results on VDB topological indices we refer to [1,2,4,5,10,11,13,19,20]. If $\varphi_{i,j} = \frac{1}{\sqrt{ij}}$, then we recover the Randić index χ [14]

$$\chi(G) = \sum_{1 \le i \le j \le n-1} \frac{m_{ij}}{\sqrt{ij}} = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}},$$

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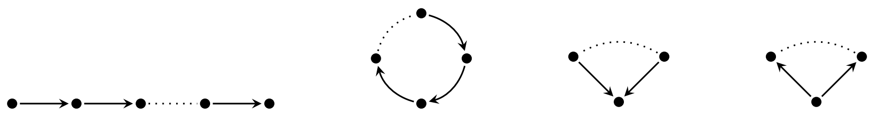

Fig. 1. Orientations of P_n, C_n, and S_n.

one of the most important topological indices for studying correlations between the structure of a molecular compound and its physico-chemical properties or biological activity (QSPR/QSAR) [6,16,17].

It is our interest to extend the concept of VDB topological indices to digraphs. A directed graph (or just digraph) $D = (V, A)$ consists 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 there is an arc from vertex u to vertex v we indicate this by writing uv. The in-degree (resp. out-degree) of a vertex v, denoted by d_v^- (resp. d_v^+) is the number of arcs of the form uv (resp. vu), where $u \in V$. A vertex v in D is called a sink vertex if $d_v^+ = 0$ and is called a source vertex if $d_v^- = 0$. A vertex v for which $d_v^+ = d_v^- = 0$ is called an isolated vertex. We denote by $\mathcal{D}_n$ the set of digraphs with n non-isolated vertices.

A digraph D is symmetric if $uv \in A$ then $vu \in A$, where $u, v \in V$. A one to one correspondence between graphs and symmetric digraphs is given by $G \rightsquigarrow \widehat{G}$, where $\widehat{G}$ has the same vertex set as the graph G, and each edge uv of G is replaced by a pair of symmetric arcs uv and vu. Under this correspondence, a graph can be identified with a symmetric digraph. In particular, $\mathcal{G}_n \subseteq \mathcal{D}_n$. On the other hand, a digraph containing no symmetric pair of arcs is called an oriented graph. Thus an oriented graph D is obtained from a graph G by replacing each edge uv of G by an arc uv or vu, but not both, in this case D also will be called an orientation of G. An orientation of G in which every vertex is a sink vertex or a source vertex will be called a sink–source orientation of G. If D is a sink–source orientation of a graph G, then the digraph obtained from D by reversing the orientation of its arcs is a sink–source orientation of G. The directed path $\overrightarrow{P}_n$ and the directed cycle $\overrightarrow{C}_n$ are shown in Fig. 1. The digraphs $\overrightarrow{K}_{1,n-1}$ and $\overrightarrow{K}_{n-1,1}$ in Fig. 1 are sink–source orientations of the star S_n.

The subjacent graph of a digraph $D = (V, A)$ is the graph with vertex set V and uv is an edge if uv or vu is an arc.

Let $D_1(V_1, A_1)$ and $D_2 = (V_2, A_2)$ 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 $D_1 = (V_1, A_1), \ldots, D_k = (V_k, A_k)$.

This paper is organized as follows. In Section 2 we give a definition of VDB topological index for digraphs. After giving some examples, we show that it is an extension of the concept of VDB topological index for graphs. In Section 3, we consider the Randić index χ of digraphs and find the extremal values of χ over $\mathcal{D}_n$. We show that in addition to regular digraphs, unlike graphs [8], there are also non-regular digraphs which attain the maximal Randi ć index among all digraphs in $\mathcal{D}_n$. On the other extreme, we show that the two sink–source orientations of S_n are the unique digraphs with minimal Randić index over $\mathcal{D}_n$.

In Section 4, we consider the extremal value problem of χ over $\mathcal{OT}(n)$, the set of all oriented trees with n vertices. We show that $\overrightarrow{K}_{1,n-1}$ and $\overrightarrow{K}_{n-1,1}$ are the oriented trees with minimal χ over $\mathcal{OT}(n)$ and $\overrightarrow{P}_n$ is the tree with maximal value of χ over $\mathcal{OT}(n)$. Also, we show that given a bipartite graph G, the sink–source orientations of G attain the minimal value of χ over $\mathcal{O}(G)$, the set of all orientations of the graph G. In particular, if T is a tree, then the two sink–source orientations of T have minimal χ over $\mathcal{O}(T)$.

In Section 5 we study the extremal values of χ over $\mathcal{O}(P_n)$ and $\mathcal{O}(C_n)$, where P_n and C_n are the path and cycle with n vertices, respectively. Finally, in Section 6, we study the extremal values of χ over hypercube orientations. Note that hypercube orientations have attracted attention in many areas. For instance, G. X. Tian [15] studied the skew energy of orientations of hypercubes, M. Levit et al. [9] studied Eulerian orientations of hypercubes, J. Buhler et al. [3] studied hypercube orientations with only two in-degrees, and C. Domshlak [7] studied directed hypercubes, among others. We find the extremal values of χ over $\mathcal{O}(H_d)$, where H_d is the hypercube of dimension d.

2. VDB topological indices of digraphs

The theory of VDB topological indices of graphs is well-established. However, to our knowledge, this theory has not been extended to digraphs (in [18], the zeroth-order general Randić index for digraphs is defined). It is our interest in this section to define VDB topological indices of digraphs.

Let $D \in \mathcal{D}_n$. For each $0 \leq i \leq n-1$, n_i^+ denotes the number of vertices of D with outer degree i, and n_i^- the number of vertices of D with inner degree i. Given $1 \leq i, j \leq n-1$, consider the set

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

An arc uv in A_{ij} will be called an i-j arc. Let a_{ij} be the cardinality of A_{ij}. If a is the number of arcs of D, then

$$\sum_{1 \leq i,j \leq n-1} a_{ij} = a, \tag{2}$$

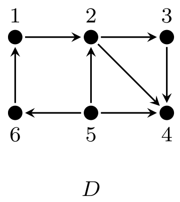

Fig. 2. The digraph D used in Examples 2.2 and 2.3.

$$\sum_{j=1}^{n-1} a_{ij} = in_i^+ \tag{3}$$

and

$$\sum_{i=1}^{n-1} a_{ij} = jn_j^- . \tag{4}$$

Definition 2.1. A VDB topological index over $\mathcal{D}_n$ is a function φ induced by real numbers $\{\varphi_{ij}\}$, where $1 \le i, j \le n-1$, defined for a digraph D with n vertices as

$$\varphi(D) = \frac{1}{2} \sum_{1 \le i,j \le n-1} a_{ij}\varphi_{ij}. \tag{5}$$

Example 2.2. Consider the VDB topological index φ induced by the numbers $\varphi_{ij} = i(j+1)$. Let D be the digraph of Fig. 2. Then

$$\begin{aligned} d_1^+ &= 1, d_2^+ = 2, d_3^+ = 1, d_4^+ = 0, d_5^+ = 3, d_6^+ = 1 \\ d_1^- &= 1, d_2^- = 2, d_3^- = 1, d_4^- = 3, d_5^- = 0, d_6^- = 1. \end{aligned}$$

Also,

$$\begin{array}{lll} a_{11} = 1, & a_{12} = 1, & a_{13} = 1, \\ a_{21} = 1, & a_{22} = 0, & a_{23} = 1, \\ a_{31} = 1, & a_{32} = 1, & a_{33} = 1. \end{array}$$

If $i > 3$ or $j > 3$ then $a_{ij} = 0$. Hence,

$$\begin{aligned} \varphi(D) &= \frac{1}{2}(\varphi_{11} + \varphi_{12} + \varphi_{13} + \varphi_{21} + \varphi_{23} + \varphi_{31} + \varphi_{32} + \varphi_{33}) \\ &= \frac{1}{2}(2 + 3 + 4 + 4 + 8 + 6 + 9 + 12) \\ &= 24. \end{aligned}$$

When φ is symmetric, i.e. $\varphi_{ij} = \varphi_{ji}$, for all $1 \le i < j \le n-1$, we can simplify the expression given in (5). In fact, for $i \ne j$ and $1 \le i, j \le n-1$, let

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

and

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

for all $i = 1, \ldots, n-1$. Note that $p_{ij} = p_{ji}$, for all $1 \le i, j \le n-1$. Then

$$\varphi(D) = \frac{1}{2} \sum_{1 \le i \le j \le n-1} p_{ij}\varphi_{ij}. \tag{6}$$

Example 2.3. Consider the VDB topological index ψ induced by the numbers $\psi_{ij} = ij$. Clearly, ψ is symmetric. Let D be the digraph of Fig. 2. Moreover,

$$\begin{array}{lll} p_{11} = 1, & p_{12} = 2, & p_{13} = 2, \\ & p_{22} = 0, & p_{23} = 2, \\ & & p_{33} = 1. \end{array}$$

Hence by (6),

$$\begin{aligned}\psi(D) &= \frac{1}{2}(\psi_{11}+2\psi_{12}+2\psi_{13}+2\psi_{23}+\psi_{33})\\ &= \frac{1}{2}(1+4+6+12+9)\\ &= 16.\end{aligned}$$

Recall that if G is a graph then G can be identified with the symmetric digraph $\widehat{G}$, where every edge of G is replaced with a pair of symmetric arcs. Under this correspondence, the set $\mathcal{D}_n$ contains the set $\mathcal{G}_n$ of graphs with n vertices.

Theorem 2.4. *Let φ be a symmetric VDB topological index and G a graph. Then $\varphi(G) = \varphi\left(\widehat{G}\right)$. In other words, Definition 2.1 extends the concept of VDB topological index of a graph to digraphs.*

Proof. Clearly,

$$p_{ij}\left(\widehat{G}\right) = 2m_{ij}(G),$$

for all $1 \le i \le j \le n-1$. Consequently,

$$\varphi\left(\widehat{G}\right) = \frac{1}{2}\sum_{1\le i\le j\le n-1} p_{ij}\varphi_{ij} = \sum_{1\le i\le j\le n-1} m_{ij}\varphi_{ij} = \varphi(G). \quad \square$$

3. Randić index of digraphs

We begin this section with the definition of Randić index of a digraph, which is a symmetric VDB topological index.

Definition 3.1. The Randić index of a digraph $D \in \mathcal{D}_n$ is denoted by $\chi(D)$ and defined as (6), where $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ for all $1 \le i \le j \le n-1$. In other words,

$$\chi(D) = \frac{1}{2}\sum_{1\le i\le j\le n-1}\frac{p_{ij}}{\sqrt{ij}}. \tag{7}$$

Remark 3.2. Note that if $D = (V, A)$ is a digraph, then another expression for (7) is

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

In this section we find the extremal values of the Randić index χ over $\mathcal{D}_n$. Given $D \in \mathcal{D}_n$, we deduce from (3) and (4) the following relations:

$$\begin{aligned}2p_{11}+p_{12}+p_{13}+\cdots+p_{1,n-1} &= n_1^+ + n_1^-\\ p_{21}+2p_{22}+p_{23}+\cdots+p_{2,n-1} &= 2\left(n_2^+ + n_2^-\right)\\ p_{31}+p_{32}+2p_{33}+\cdots+p_{3,n-1} &= 3\left(n_3^+ + n_3^-\right)\\ \vdots &= \vdots\\ p_{n-1,1}+p_{n-1,2}+p_{n-1,3}+\cdots+2p_{n-1,n-1} &= (n-1)\left(n_{n-1}^+ + n_{n-1}^-\right).\end{aligned} \tag{8}$$

Also,

$$\begin{aligned}n_1^+ + n_2^+ + n_3^+ + \cdots + n_{n-1}^+ &= n - n_0^+\\ n_1^- + n_2^- + n_3^- + \cdots + n_{n-1}^- &= n - n_0^-.\end{aligned} \tag{9}$$

From relations (8) we express $n_i^+ + n_i^-$, $i = 1, \ldots, n-1$, and substitute in relations (9). After appropriate rearrangements this results in

$$\sum_{1\le i\le j\le n-1}\left(\frac{1}{i}+\frac{1}{j}\right)p_{ij} = 2n - \left(n_0^+ + n_0^-\right). \tag{10}$$

Theorem 3.3. *Let $D \in \mathcal{D}_n$. Then*

$$\chi(D) = \frac{n}{2} - \frac{1}{4}\left(n_0^+ + n_0^- + \sum_{1\le i<j\le n-1}\left(\frac{1}{\sqrt{j}}-\frac{1}{\sqrt{i}}\right)^2 p_{ij}.\right)$$

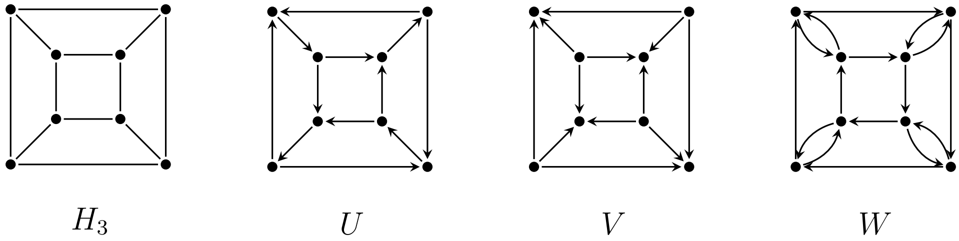

Fig. 3. The hypercube H_3 and some digraphs whose subjacent graph is H_3.

Proof. Let $n_0 = n_0^+ + n_0^-$. Using (10) we deduce:

$$\sum_{1\leq i<j\leq n-1}\left(\frac{1}{i}+\frac{1}{j}\right)p_{ij}+\sum_{i=1}^{n-1}\frac{2p_{ii}}{i}=2n-n_0.$$

Hence

$$\begin{aligned}
2\chi(D) &= \sum_{1\leq i\leq j\leq n-1}\frac{p_{ij}}{\sqrt{ij}} = \sum_{1\leq i<j\leq n-1}\frac{p_{ij}}{\sqrt{ij}}+\sum_{i=1}^{n-1}\frac{p_{ii}}{i}\\
&= \sum_{1\leq i<j\leq n-1}\frac{p_{ij}}{\sqrt{ij}}+\left(n-\frac{n_0}{2}\right)-\frac{1}{2}\sum_{1\leq i<j\leq n-1}\left(\frac{1}{i}+\frac{1}{j}\right)p_{ij}\\
&= n-\frac{n_0}{2}-\frac{1}{2}\sum_{1\leq i<j\leq n-1}\left(\frac{1}{i}+\frac{1}{j}-\frac{2}{\sqrt{ij}}\right)p_{ij}\\
&= n-\frac{n_0}{2}-\frac{1}{2}\sum_{1\leq i<j\leq n-1}\left(\frac{1}{\sqrt{j}}-\frac{1}{\sqrt{i}}\right)^2 p_{ij}.\\
&= n-\frac{1}{2}\left(n_0+\sum_{1\leq i<j\leq n-1}\left(\frac{1}{\sqrt{j}}-\frac{1}{\sqrt{i}}\right)^2 p_{ij}\right). \quad \square
\end{aligned}$$

Remark 3.4. If G is a symmetric digraph (i.e. a graph) with n vertices, it was shown in [8, Eq. (7)] that

$$\chi(G)=\frac{n}{2}-\frac{1}{2}\sum_{1\leq i<j\leq n-1}\left(\frac{1}{\sqrt{j}}-\frac{1}{\sqrt{i}}\right)^2 m_{ij}.$$

Note that this expression can be deduced from Theorem 3.3, since $n_0^+ + n_0^- = 0$ and $p_{ij} = 2m_{ij}$.

The digraphs which satisfy the following conditions are of great interest to us:

$$\begin{aligned}
&p_{ij}=0 \qquad \text{for all } 1\leq i<j\leq n-1,\\
&n_0^+=n_0^-=0.
\end{aligned} \tag{11}$$

Recall that a digraph D is r-regular ($r>0$) if $d_u^+ = d_u^- = r$ for all $u\in V$.

Example 3.5. Every direct sum of regular digraphs satisfies conditions (11).

The converse of Example 3.5 does not hold. Recall that a digraph is strongly connected if for every pair u, v of vertices, there is a directed path from u to v and one from v to u.

Example 3.6. The digraph U in Fig. 3 is strongly connected and satisfies both conditions in (11), but U is not a regular digraph.

So the situation in digraphs is different from the situation in graphs. Recall that if G is a graph such that $m_{ij}=0$ for all $1\leq i<j\leq n-1$, then G is a direct sum of regular graphs. In fact, this is the argument used to find the graphs with maximal Randić index [8] . In $\mathcal{D}_n$, we will see that the digraphs which satisfy conditions (11) are the digraphs with maximal Randić index in $\mathcal{D}_n$. In particular, there are non-regular digraphs which attain maximal χ in $\mathcal{D}_n$.

Theorem 3.7. *If $D \in \mathcal{D}_n$, then $\chi(D) \leq \frac{n}{2}$. Equality occurs if and only if D satisfies conditions (11).*

Proof. Let D be a digraph with n vertices. By Theorem 3.3, $\chi(D) \leq \frac{n}{2}$, since $n_0^+ + n_0^- \geq 0$, $\left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{i}}\right)^2 > 0$ and $p_{ij} \geq 0$ for all $0 \leq i < j \leq n-1$. Moreover, by Theorem 3.3, $\chi(D) = \frac{n}{2}$ if and only if $n_0^+ + n_0^- = 0$, and $p_{ij} = 0$ for all $0 \leq i < j \leq n-1$. In other words, $\chi(D) = \frac{n}{2}$ if and only if D satisfies conditions (11). □

Corollary 3.8. *Every direct sum of regular digraphs in $\mathcal{D}_n$ attain the maximal value of χ over $\mathcal{D}_n$.*

Proof. This is a consequence of Theorem 3.7 and Example 3.5. □

Example 3.9. See the digraphs in Fig. 3. The digraph W is 2 -regular, H_3 is 3-regular and U is not regular but satisfies (11). The digraph $\overrightarrow{C}_8$ is 1-regular and satisfies (11). Hence, by Theorem 3.7, W, U, H_3 and $\overrightarrow{C}_8$ attain maximal Randić index in $\mathcal{D}_8$. Note that

$$\chi(W) = \chi(U) = \chi(H_3) = \chi\left(\overrightarrow{C}_8\right) = 4.$$

Next we find digraphs with minimal Randić index. Let

$$L = \{(i,j) : 1 \leq i \leq j \leq n-1, (i,j) \neq (1, n-1)\}.$$

Lemma 3.10. *Let D be a digraph with n vertices such that $p_{ij} = 0$ for all $(i,j) \in L$ and $n_0^+ + n_0^- = n$. Then $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$.*

Proof. $p_{ij} = 0$ for all $(i,j) \in L$ implies by (8)

$$\begin{aligned} n_1^+ + n_1^- &= p_{1,n-1} = p_{n-1,1} = (n-1)\left(n_{n-1}^+ + n_{n-1}^-\right), \\ n_i^+ &= n_i^- = 0 \text{ for all } i = 2, \ldots, n-2. \end{aligned} \tag{12}$$

By relations (9) and the fact that $n_0^+ + n_0^- = n$,

$$\left(n_1^+ + n_1^-\right) + \left(n_{n-1}^+ + n_{n-1}^-\right) = n. \tag{13}$$

It follows from (12) and (13) that

$$(n-1)\left(n_{n-1}^+ + n_{n-1}^-\right) = n - \left(n_{n-1}^+ + n_{n-1}^-\right)$$

and so

$$n_{n-1}^+ + n_{n-1}^- = 1, \tag{14}$$

One possibility in (14) is

$$n_{n-1}^+ = 0 \text{ and } n_{n-1}^- = 1.$$

But $n_{n-1}^- = 1$ implies $n_1^+ = n-1$, and so $D = \overrightarrow{K}_{n-1,1}$. The other possibility in (14) is

$$n_{n-1}^+ = 1 \text{ and } n_{n-1}^- = 0.$$

But $n_{n-1}^+ = 1$ implies $n_1^- = n-1$, and in this case $D = \overrightarrow{K}_{1,n-1}$. □

Theorem 3.11. *If $D \in \mathcal{D}_n$, then $\chi(D) \geq \frac{\sqrt{n-1}}{2}$. Equality occurs if and only if $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$.*

Proof. Let $n_0 = n_0^+ + n_0^-$. From (10) we deduce

$$\frac{np_{1,n-1}}{n-1} + \sum_L \left(\frac{1}{i} + \frac{1}{j}\right) p_{ij} = 2n - \left(n_0^+ + n_0^-\right). \tag{15}$$

From (15) we express $p_{1,n-1}$ and substitute in (7) to obtain

$$\begin{aligned} 2\chi(D) &= \frac{p_{1,n-1}}{\sqrt{n-1}} + \sum_L \frac{p_{ij}}{\sqrt{ij}} \\ &= \frac{\sqrt{n-1}}{n}\left(2n - n_0 - \sum_L \left(\frac{1}{i} + \frac{1}{j}\right) p_{ij}\right) + \sum_L \frac{p_{ij}}{\sqrt{ij}} \end{aligned}$$

$$= \frac{\sqrt{n-1}\,(2n-n_0)}{n} + \sum_{L}\left(\frac{1}{\sqrt{ij}} - \frac{\sqrt{n-1}}{n}\left(\frac{1}{i}+\frac{1}{j}\right)\right)p_{ij}$$

$$\geq \sqrt{n-1} + \sum_{L}\left(\frac{1}{\sqrt{ij}} - \frac{\sqrt{n-1}}{n}\left(\frac{1}{i}+\frac{1}{j}\right)\right)p_{ij}. \tag{16}$$

The last inequality occurs because $n_0 \leq n$, since there are no isolated vertices. On the other hand, $p_{ij} \geq 0$ and

$$\frac{1}{\sqrt{ij}} - \frac{\sqrt{n-1}}{n}\left(\frac{1}{i}+\frac{1}{j}\right) > 0$$

for all $(i,j) \in L$. Consequently by (16),

$$2\chi(D) \geq \sqrt{n-1}.$$

Moreover, equality occurs if and only if $p_{ij} = 0$ for all $(i,j) \in L$ and $n_0 = n$. By Lemma 3.10, equality occurs if and only if $D = \overrightarrow{K}_{1,n-1}$ or $D = \overrightarrow{K}_{n-1,1}$. □

Remark 3.12. If G is a symmetric digraph (with no isolated vertices), then $n_0 = 0$ and so as in the proof of Theorem 3.11 we deduce

$$2\chi(G) = 2\sqrt{n-1} + 2\sum_{L}\left(\frac{1}{\sqrt{ij}} - \frac{\sqrt{n-1}}{n}\left(\frac{1}{i}+\frac{1}{j}\right)\right)m_{ij}.$$

Consequently,

$$\chi(G) \geq \sqrt{n-1}.$$

Moreover, equality occurs if and only if $m_{ij} = 0$ for all $(i,j) \in L$. The only graph with this property is $G = S_n$. This result was obtained in [8, Theorem 3].

We end this section with a sharp upper bound of the Randić index of digraphs which depend on the number of arcs.

Theorem 3.13. *If D is a digraph with a arcs, then $\chi(D) \leqslant \frac{a}{2}$. Equality occurs if and only if*

$$D = \bigoplus_{i=1}^{r} \overrightarrow{P}_{r_i} \oplus \bigoplus_{j=1}^{s} \overrightarrow{C}_{s_j}, \tag{17}$$

where $\sum_{i=1}^{r}(r_i - 1) + \sum_{j=1}^{s} s_j = a$.

Proof. By (5), (2) and the fact that $\frac{1}{\sqrt{ij}} \leq 1$ for all $1 \leq i,j \leq n-1$,

$$\chi(D) = \frac{1}{2}\sum_{1\leq i,j\leq n-1}\frac{a_{ij}}{\sqrt{ij}} \leqslant \frac{1}{2}\sum_{1\leq i,j\leq n-1} a_{ij} = \frac{a}{2}. \tag{18}$$

If D is of the form (17), then

$$\chi(D) = \frac{1}{2}\left[\sum_{i=1}^{r}(r_i - 1) + \sum_{j=1}^{s} s_j\right] = \frac{a}{2}.$$

Conversely, if $\chi(D) = \frac{a}{2}$ then by (18), $a_{11} = a$. This clearly implies that D is of the form (17). □

Remark 3.14. Note that $\overrightarrow{P}_{a+1}$ and $\overrightarrow{C}_a$ are the unique connected digraphs with maximal Randić value $\frac{a}{2}$ in Theorem 3.13.

4. Randić index of graph orientations

In this section we solve extremal value problems of the Randić index over graph orientations. Let us begin with $\mathcal{OT}(n)$, the set of oriented trees with n vertices.

Theorem 4.1. *Let $T \in \mathcal{OT}(n)$. Then*

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

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

Proof. The inequality on the left (and equality condition) is a direct consequence of Theorem 3.11.

Let $T \in \mathcal{OT}(n)$. Then $a = n-1$ and by Theorem 3.13,

$$\chi(T) \leq \frac{a}{2} = \frac{n-1}{2}. \tag{19}$$

Clearly, $\chi\left(\overrightarrow{P}_n\right) = \frac{n-1}{2}$. Conversely, assume that $\chi(T) = \frac{n-1}{2}$. Then by inequality (19)$\chi(T) = \frac{a}{2}$, and by Remark 3.14, $T = \overrightarrow{P}_{a+1} = \overrightarrow{P}_n$. □

Let G be a graph and $\mathcal{O}(G)$ the set of all orientations of G. The following problem arises naturally: which of the orientations in $\mathcal{O}(G)$ attain extremal values of the Randić index. When G is a bipartite graph, we show that the sink–source orientations of G attain the minimal Randić value. Recall that an orientation of G is a sink–source orientation if every vertex of G is a sink vertex or a source vertex.

Proposition 4.2 (*[12, Proposition 2.2]*). *Let G be a graph. The following conditions are equivalent:*

1. *G is a bipartite graph;*
2. *G has a sink–source orientation.*

If G is a connected bipartite graph, then there exist exactly two sink- source orientations of G (see [12, Proposition 2.3]).

Now we can show one of our main results.

Theorem 4.3. *Let $D \in \mathcal{O}(G)$. Then*

$$\chi(D) \geqslant \frac{\chi(G)}{2}.$$

Equality occurs if and only if D is a sink–source orientation of G.

Proof. Suppose that $G = (V, E)$ and $D = (V, A)$. Note that for each $u \in V$,

$$d_u = d_u^+ + d_u^-. \tag{20}$$

In particular, $d_u \geq d_u^+$ and $d_u \geq d_u^-$, for all vertices $u \in V$. Consequently,

$$\chi(D) = \frac{1}{2}\sum_{uv\in A}\frac{1}{\sqrt{d_u^+ d_v^-}} \geq \frac{1}{2}\sum_{uv\in E}\frac{1}{\sqrt{d_u d_v}} = \frac{\chi(G)}{2}. \tag{21}$$

If D is a sink–source orientation of G, then, for each $u \in V$, one has either $d_u^+ = 0$ or $d_u^- = 0$. Moreover, if $uv \in A$, then $d_u^+ \neq 0$ and so $d_u^- = 0$, which implies by (20) that $d_u = d_u^+$. Similarly, $d_v^- \neq 0$ implies $d_v^+ = 0$ and by (20), $d_v = d_v^-$. Hence

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

Conversely, if $\chi(D) = \frac{\chi(G)}{2}$, then by inequality (21), $d_u = d_u^+$ and $d_v = d_v^-$, for all $uv \in A$. This clearly implies by (20) that for each vertex $w \in V$, either $d_w^+ = 0$ or $d_w^- = 0$. □

As an immediate consequence of Theorem 4.3 we get the following results.

Corollary 4.4. *If G is a bipartite graph, then the sink–source orientations of G are the unique orientations with minimal Randić index over $\mathcal{O}(G)$.*

Corollary 4.5. *Let T be a tree with n vertices. Then sink–source orientations of T are the unique orientations with minimal χ over $\mathcal{O}(T)$.*

Proof. This is a consequence of Corollary 4.4, since trees are bipartite graphs. □

Example 4.6. Consider the tree T in Fig. 4. The two sink–source orientations T_1 and T_2 of T given in Fig. 4 have minimal χ over $\mathcal{O}(T)$.

So we have solved the problem of minimal Randić index over $\mathcal{O}(T)$, when T is a tree. What about the maximal value of χ over $\mathcal{O}(T)$? For the tree T of Fig. 4, T_3 attains the maximal value. But for general trees it is an open problem:

Problem 4.7. Let T be a tree. Find the maximal value of χ over $\mathcal{O}(T)$.

Or more generally,

Problem 4.8. Let G be a bipartite graph. Find the maximal value of χ over $\mathcal{O}(G)$.

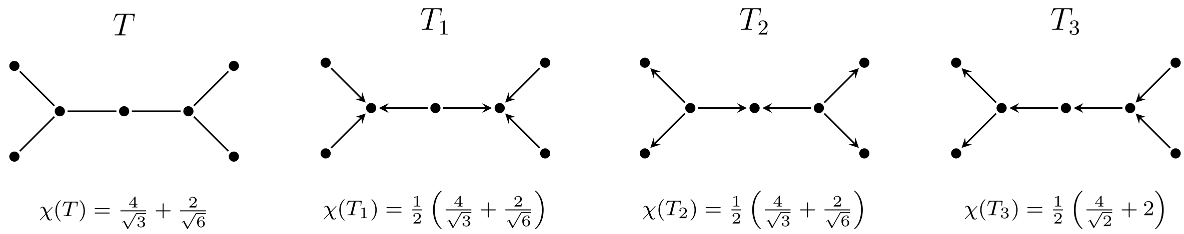

Fig. 4. Some orientations of the tree T.

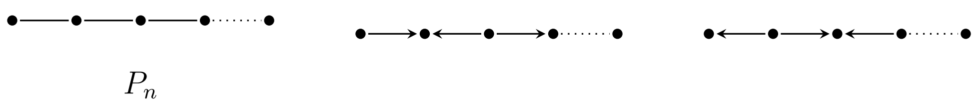

Fig. 5. The sink–source orientations of P_n.

5. Extremal values of χ over $\mathcal{O}(P_n)$ and $\mathcal{O}(C_n)$

In this section we solve the extremal value problem of χ over $\mathcal{O}(G)$, when G is the path P_n, and when G is the cycle C_n.

Theorem 5.1. *Let P_n be the path tree with n vertices. Then for every $T \in \mathcal{O}(P_n)$,*

$$\frac{1}{2}\left(\frac{n-3}{2} + \frac{2}{\sqrt{2}}\right) \leq \chi(T) \leq \frac{n-1}{2}.$$

Equality on the left occurs if and only if T is a sink–source orientation of P_n (see Fig. 5). Equality on the right occurs if and only if $T = \overrightarrow{P}_n$.

Proof. This is a consequence of Theorem 4.1 and Corollary 4.5. □

Next we discuss the extremal values of χ over $\mathcal{O}(C_n)$. Note that if $C \in \mathcal{O}(C_n)$, then for all vertex u of C

$$d_u^+ + d_u^- = 2,$$

and by (2),

$$p_{11} + p_{12} + p_{22} = a = n. \tag{22}$$

Lemma 5.2. *Let $C \in \mathcal{O}(C_n)$.*

1. $(p_{11}, p_{12}, p_{22}) = (0, 0, n)$ *if and only if C is a sink–source orientation of C_n, see Fig. 6;*
2. $(p_{11}, p_{12}, p_{22}) = (0, 2, n-2)$ *if and only if C is one of the orientations in Fig. 7;*
3. *There are no orientations of C_n such that* $(p_{11}, p_{12}, p_{22}) = (0, 1, n-1)$.

Proof. 1. Clearly, if C is a sink–source orientation of C_n, then $(p_{11}, p_{12}, p_{22}) = (0, 0, n)$. Conversely, assume that C satisfies $(p_{11}, p_{12}, p_{22}) = (0, 0, n)$. If C is not a sink–source orientation of C_n, then C has arcs uv and vw, for some vertices u, v, w of C. Let x be the vertex of C adjacent to u. If xu is an arc of C then $d_u^+ = 1$ and $d_v^- = 1$, which implies that $a_{11} = p_{11} \neq 0$, a contradiction. If ux is an arc of C, then $d_u^+ = 2$ and $d_v^- = 1$, which implies $a_{21} \neq 0$ and so $p_{12} \neq 0$. Again a contradiction. Hence, C is a sink–source orientation of C_n.

2. If C is one of the orientations in Fig. 7, it is clear that $(p_{11}, p_{12}, p_{22}) = (0, 2, n-2)$. Conversely, assume that $(p_{11}, p_{12}, p_{22}) = (0, 2, n-2)$. By part 1, C is not a sink–source orientation. Then, there exist vertices u, v, w of C such that uv and vw are arcs of C. But then w is a sink vertex and u is a source vertex, otherwise $a_{11} = p_{11} \neq 0$. In particular, uv is a 2-1-arc and vw is a 1- 2-arc. Since $p_{12} = 2$, all other arcs different from uv and vw are 2-2-arcs. Consequently, C is of the form in Fig. 7.

3. Assume that C is an orientation of C_n such that $(p_{11}, p_{12}, p_{22}) = (0, 1, n-1)$. By part 1, C is not a sink–source orientation of C_n. In particular, there exist arcs of the form uv and vw, for some vertices u, v, w of C. As in part 2, w is a sink vertex and u is a source vertex, otherwise $a_{11} = p_{11} \neq 0$. But then uv is a 2-1-arc and vw are 1-2-arc, which implies $p_{12} \geq 2$, a contradiction. □

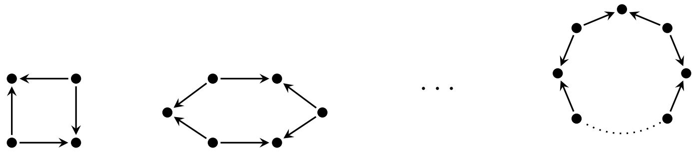

Fig. 6. Orientations in $\mathcal{O}(C_n)$ with minimal χ for n even.

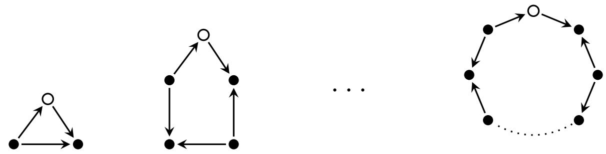

Fig. 7. Orientations in $\mathcal{O}(C_n)$ with minimal χ for n odd.

Theorem 5.3. *Let C_n be the cycle with n vertices. Then for every $C \in \mathcal{O}(C_n)$,*

$$\left.\begin{array}{ll} n \text{ even} & \frac{n}{4} \\ n \text{ odd} & \frac{n-2}{4}+\frac{1}{\sqrt{2}} \end{array}\right\} \leq \chi(C) \leq \frac{n}{2}.$$

Equality on the left occurs if and only if C is a sink–source orientation of C_n (n even) or C is one of the orientations in Fig. 7 (n odd). Equality on the right occurs if and only if $C = \overrightarrow{C}_n$.

Proof. By Theorem 3.7, for all $C \in \mathcal{O}(C_n)$,

$$\frac{n}{2} = \chi\left(\overrightarrow{C}_n\right) \geq \chi(C).$$

Moreover, if $C \in \mathcal{O}(C_n)$ and $\frac{n}{2} = \chi(C)$, then by Theorem 3.7, C satisfies condition (11). In particular, C has no sink vertices nor source vertices. Since C is an orientation of C_n, then $C = \overrightarrow{C}_n$.

Now we show the inequality (and equality condition) on the left. If n is even, then C_n is bipartite and the result follows from Corollary 4.4. So assume now that n is odd. We affirm that

$$\frac{1}{2}p_{11} + \left(\frac{\sqrt{2}-1}{2}\right)p_{12} \geq \sqrt{2}-1. \tag{23}$$

In fact, inequality (23) only fails when $p_{11} = 0 = p_{12}$ or when $p_{11} = 0$ and $p_{12} = 1$. In the first case, by (22) we deduce that $(p_{11}, p_{12}, p_{22}) = (0, 0, n)$, and by part 1 of Lemma 5.2, C is a sink–source orientation. This is a contradiction by Proposition 4.2, since n is odd. The latter case implies $(p_{11}, p_{12}, p_{22}) = (0, 1, n-1)$, which is also a contradiction by part 3 of Lemma 5.2. Hence, inequality (23) holds. This clearly implies by (22) and (23) that

$$\chi(C) = \frac{1}{2}\left(p_{11} + \frac{p_{12}}{\sqrt{2}} + \frac{p_{22}}{2}\right) \geq \frac{1}{2}\left(\frac{p_{11}+p_{12}+p_{22}-2}{2} + \frac{2}{\sqrt{2}}\right) = \frac{n-2}{4} + \frac{1}{\sqrt{2}}. \tag{24}$$

Finally, assume that $\chi(C) = \frac{n-2}{4} + \frac{1}{\sqrt{2}}$. Then by (24), there is an equality in (23), i.e.

$$\frac{1}{2}p_{11} + \left(\frac{\sqrt{2}-1}{2}\right)p_{12} = \sqrt{2}-1. \tag{25}$$

Equivalently,

$$\left(\frac{\sqrt{2}-1}{2}\right)(p_{12}-2) = -\frac{1}{2}p_{11}.$$

If $p_{12} - 2 \neq 0$, then $\sqrt{2}$ is a rational number, this is a contradiction. Hence $p_{12} = 2$. It follows from (25) that $p_{11} = 0$ and by (22), $(p_{11}, p_{12}, p_{22}) = (0, 2, n-2)$. Now by part 2 of Lemma 5.2, C is one of the orientations in Fig. 7. □

6. Extremal values of χ over hypercube orientations

We end this work with the study of the extremal values of χ over the hypercube orientations. We begin with the hypercube of dimension 3, which we denote by H_3.

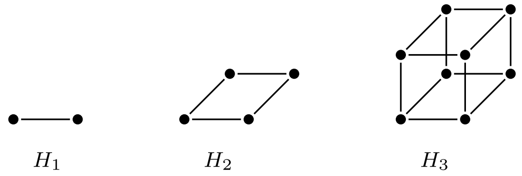

Fig. 8. Hypercubes of dimension 1,2,3.

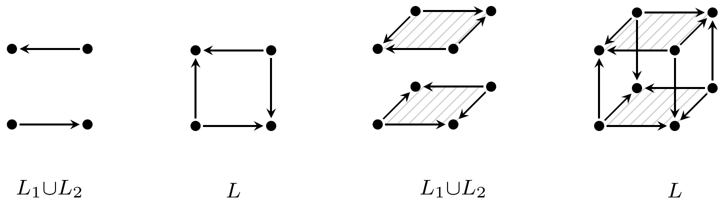

Fig. 9. The orientation L of H_2 and H_3.

Example 6.1. The digraph V in Fig. 3 is a sink–source orientation of H_3. By Corollary 4.4, V attains minimal χ over $\mathcal{O}(H_3)$, with value

$$\chi(V) = \frac{1}{2}\chi(H_3) = \frac{4}{2} = 2.$$

On the other hand, by Example 3.9, U has maximal χ over $\mathcal{O}(H_3)$ with value $\chi(U) = 4$.

More generally, recall that a hypercube H_d of dimension d is defined recursively in terms of the Cartesian product of graphs as follows:

$$H_d = \begin{cases} P_2 & \text{, if } d = 1, \\ H_{d-1} \times H_1 & \text{, if } d \geqslant 2. \end{cases}$$

In Fig. 8 we see the hypercubes of dimension 1, 2, and 3.

For every $d \geq 1$, H_d is a bipartite d-regular graph with 2^d vertices and $2^{d-1} \cdot d$ edges. So by Theorem 4.3, for every $D \in \mathcal{O}(H_d)$

$$\chi(D) \geq \frac{\chi(H_d)}{2} = \frac{\frac{2^{d-1}d}{d}}{2} = 2^{d-2}.$$

Moreover, the sink–source orientations of H_d have minimal χ over $\mathcal{O}(H_d)$ equal to 2^{d-2}. We now indicate how to construct a sink–source orientation L of H_d. If $d = 1$, then $L = \overrightarrow{P}_2$. For $d \geqslant 2$, let L_1 be a sink–source orientation of H_{d-1}, and let L_2 be the orientation obtained from L_1 by reversing all its arcs. Then, L is obtained from L_1 and L_2 by adding an arc from every source vertex of L_1 to its corresponding sink vertex in L_2, and adding an arc from every source vertex of L_2 to its corresponding sink vertex in L_1. Then L is a sink–source orientation of H_d. In Fig. 9 we illustrate the sink–source orientations L of H_2 and H_3. On the other hand, if $C \in \mathcal{O}(H_d)$, then by Theorem 3.7,

$$\chi(C) \leq \frac{2^d}{2} = 2^{d-1}.$$

We now show how to construct an $M \in \mathcal{O}(H_d)$ which satisfies conditions (11), so again by Theorem 3.7, M attains the maximal value of χ over $\mathcal{O}(H_d)$. If $d = 1$, then $M = \overrightarrow{P}_2$. For $d \geqslant 2$, let L_1 be a sink–source orientation of H_{d-1}, and let L_2 the orientation obtained from L_1 by reversing all its arcs. Then, M is obtained from L_1 and L_2 by adding an arc from every sink vertex of L_1 to its corresponding source vertex in L_2, and adding an arc from every sink vertex of L_2 to its corresponding source vertex in L_1. In Fig. 10 we can see the orientations M of H_2 and H_3. Note that every arc uv in $L_1 \cup L_2$ is a (d-1)-(d-1)-arc, and every arc wz not in $L_1 \cup L_2$ is a 1-1-arc. Consequently, $M \in \mathcal{O}(H_d)$ satisfies condition (11). In summary, we have proved the following result.

Theorem 6.2. *If $D \in \mathcal{O}(H_d)$, then*

$$2^{d-2} \leq \chi(D) \leq 2^{d-1}.$$

Equality on the left occurs in the sink–source orientation L of H_d. Equality on the right occurs in the orientation $M \in \mathcal{O}(H_d)$.

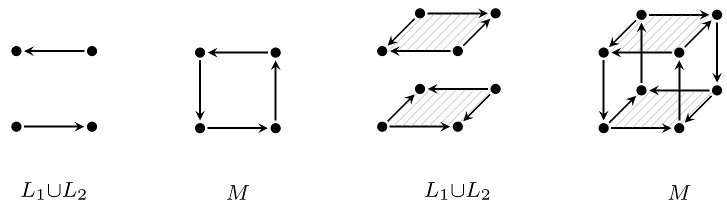

Fig. 10. The orientation M of H_2 and H_3.

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