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SKEW RANDIĆ MATRIX AND SKEW RANDIĆ ENERGY

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ABSTRACT. Let G be a simple graph with an orientation σ, which assigns to each edge a direction so that G^σ becomes a directed graph. G is said to be the underlying graph of the directed graph G^σ. In this paper, we define a weighted skew adjacency matrix with Randć weight, the skew Randić matrix $\mathbf{R_S}(G^\sigma)$, of G^σ as the real skew symmetric matrix $[(r_s)_{ij}]$ where $(r_s)_{ij} = (d_i d_j)^{-\frac{1}{2}}$ and $(r_s)_{ji} = -(d_i d_j)^{-\frac{1}{2}}$ if $v_i \to v_j$ is an arc of G^σ, otherwise $(r_s)_{ij} = (r_s)_{ji} = 0$. We derive some properties of the skew Randić energy of an oriented graph. Most properties are similar to those for the skew energy of oriented graphs. But, surprisingly, the extremal oriented graphs with maximum or minimum skew Randić energy are completely different, no longer being some kinds of oriented regular graphs.

1. Introduction

In this paper we are concerned with simple finite graphs. Undefined notation and terminology can be found in [5]. Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, and let d_i be the degree of vertex v_i, $i = 1, 2, \ldots, n$. We use P_k to denote the path on k vertices, and the *length* of a path is the number of edges that the path uses.

The Randić index [25] of G is defined as the sum of $\frac{1}{\sqrt{d_i d_j}}$ over all edges $v_i v_j$ of G. This topological index was first proposed by Randić [25] in 1975 under the name "branching index". In 1998, Bollobás and Erdős [4] generalized this index as $R_\alpha = R_\alpha(G) = \sum_{i\sim j}(d_i d_j)^\alpha$, called general Randić index.

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Let $\mathbf{A}(G)$ be the $(0,1)$-adjacency matrix of G. The *spectrum* $Sp(G)$ of G is defined as the spectrum of $\mathbf{A}(G)$. The Randić matrix [19] $\mathbf{R} = \mathbf{R}(G)$ of order n can be viewed as a weighted adjacency matrix, whose (i,j)-entry is defined as

$$r_{ij} = \begin{cases} 0 & \text{if } i = j, \\ (d_i d_j)^{-\frac{1}{2}} & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent}, \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent}. \end{cases}$$

The polynomial $\varphi_R(G,\lambda) = det(\lambda \mathbf{I}_n - \mathbf{R})$ will be referred to as the R-characteristic polynomial of G. Here and later by $\mathbf{I}_n$ is denoted the unit matrix of order n.

The spectrum $Sp_{\mathbf{R}}(G^\sigma)$ of G is defined as the spectrum of $\mathbf{R}(G)$. Denote the spectrum $Sp_{\mathbf{R}}(G^\sigma)$ of G by $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and label them in non-increasing order. The energy of the Randić matrix is defined as $RE = RE(G) = \sum_{i=1}^n |\lambda_i|$ and is called Randić energy. There have been a lot of results on the Randić matrix and Randić energy; see [6, 7, 8, 9, 10, 13, 14, 18, 19, 21]. There are other kinds of Randić type matrices and energies, for details see [16, 17]. The Randić matrix has an interesting relation with the normalized Lapacian matrix $\mathcal{L}(G)$ of a graph, i.e., $\mathcal{L}(G) = \mathbf{I}_n - \mathbf{R}(G)$; see any one of the above mentioned papers.

Let G be a simple graph with an orientation σ, which assigns to each edge a direction so that G^σ becomes a directed graph. G is said to be the underlying graph of the directed graph G^σ. With respect to a labeling, the skew-adjacency matrix $\mathbf{S}(G^\sigma)$ is the real skew symmetric matrix $[s_{ij}]$ where $s_{ij} = 1$ and $s_{ji} = -1$ if $v_i \to v_j$ is an arc of G^σ, otherwise $s_{ij} = s_{ji} = 0$.

Now we define the *skew Randić matrix* $\mathbf{R}_s = \mathbf{R}_s(G^\sigma)$ of order n, whose (i,j)-entry is

$$(r_s)_{ij} = \begin{cases} (d_i d_j)^{-\frac{1}{2}} & \text{if } v_i \to v_j, \\ -(d_i d_j)^{-\frac{1}{2}} & \text{if } v_j \to v_i, \\ 0 & \text{Otherwise}. \end{cases}$$

If G does not possess isolated vertices, and σ is an orientation of G, then it is easy to check that

$$\mathbf{R}_s(G^\sigma) = \mathbf{D}^{-\frac{1}{2}} \mathbf{S}(G^\sigma) \mathbf{D}^{-\frac{1}{2}},$$

where $\mathbf{D}$ is the diagonal matrix of vertex degrees. Note that the skew Randić matrix $\mathbf{R}_{\mathbf{S}}(G^\sigma)$ is a weighted skew-adjacency matrix of G^σ with the Randć weight.

Remark: In [2, 3], Adiga et al. defined the *skew Laplacian matrix* $\mathbf{L}(G^\sigma) = \mathbf{D} - \mathbf{S}(G^\sigma)$ of an oriented graph G^σ and two kinds of shew Laplacian energies. Combining this with the concept of normalized Laplacian matrix, we can use $\mathbf{R}_s(G^\sigma)$ to define a so-called *normalized skew Laplacian matrix* as $\mathcal{L}_s(G^\sigma) = \mathbf{I}_n - \mathbf{R}_s(G^\sigma)$.

The polynomial $\varphi_{R_s}(G,\lambda) = \det(\lambda \mathbf{I}_n - \mathbf{R}_s)$ will be referred to as the R_s-characteristic polynomial of G^σ. It is obvious that $\mathbf{R}_s(G^\sigma)$ is a real skew symmetric matrix. Hence the eigenvalues $\{\rho_1, \rho_2, \ldots, \rho_n\}$ of $\mathbf{R}_s(G^\sigma)$ are all purely imaginary numbers. The skew Randić spectrum $Sp_{\mathbf{R}_s}(G^\sigma)$ of G^σ is defined as the spectrum of $\mathbf{R}_s(G^\sigma)$.

The energy of $\mathbf{R}_s(G^\sigma)$, called *skew Randić energy* which is defined as the sum of its singular values, is the sum of the absolute values of its eigenvalues. If we denote the skew Randić energy of G^σ

by $RE_s(G^\sigma)$, then $RE_s(G^\sigma) = \sum_{i=1}^{n} |\rho_i|$. In this paper, we will derive some properties of the skew Randić energy of an oriented graph. Most properties are similar to those for the skew energy of an unweighted oriented graph. But, surprisingly, the extremal oriented graphs with maximum or minimum skew Randić energy are completely different, no longer being some kinds of oriented regular graphs.

2. Basic properties

The following proposition on the skew Randić spectra of oriented graphs is obvious.

Proposition 2.1. *Let $\{i\mu_1, i\mu_2, \ldots, i\mu_n\}$ be the skew Randić spectrum of G^σ, where $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n$. Then (1) $\mu_j = -\mu_{n+1-j}$ for all $1 \leq j \leq n$; (2) when n is odd, $\mu_{(n+1)/2} = 0$ and when n is even, $\mu_{n/2} \geq 0$; and (3) $\sum_{i=1}^{n} \mu_i^2 = 2R_{-1}(G)$, where $R_{-1}(G)$ is the general Randić index of G with $\alpha = -1$.*

Let G be a graph. A *linear subgraph* L of G is a disjoint union of some edges and some cycles in G. Let $\mathcal{L}_i(G)$ be the set of all linear subgraphs L of G with i vertices. For a linear subgraphs $L \in \mathcal{L}_i(G)$, denote by $p_1(L)$ the number of components of size 2 in L and $p_2(L)$ the number of cycles in L.

Let

$$\varphi_R(G, \lambda) = a_0\lambda^n + a_1\lambda^{n-1} + \cdots + a_{n-1}\lambda + a_n \tag{1}$$

be the $R-$characteristic polynomial of G. From [12], we know that

$$a_i = \sum_{L \in \mathcal{L}_i} (-1)^{p_1(L)}(-2)^{p_2(L)} W(L), \tag{2}$$

where $W(L) = \prod_{v \in V(L)} \frac{1}{d(v)}$. If G is bipartite, then $a_i = 0$ for all odd i.

Now considering the oriented graph G^σ, let C be an even cycle of G. We say C is *evenly oriented relative to* G^σ if it has an even number of edges oriented in the direction of the routing. Otherwise C is oddly oriented.

We call a linear subgraph L of G *evenly linear* if L contains no cycle with odd length and denote by $\mathcal{EL}_i(G)$ (or $\mathcal{EL}_i$ for short) the set of all evenly linear subgraphs of G with i vertices. For an evenly linear subgraph $L \in \mathcal{EL}_i(G)$, we use $p_e(L)$ (resp., $p_o(L)$) to denote the number of evenly (resp., oddly) oriented cycles in L relative to G^σ.

Consider G^σ as a weighted oriented graph with each edge v_iv_j assigned the weight $\frac{1}{d(v_i)d(v_j)}$. Then the skew Randić characteristic polynomial of G^σ equals to the skew characteristic polynomial of weighted oriented graph G^σ. In [15], the authors studied the skew characteristic polynomial of weighted oriented graph. From their results, we can derive the skew Randić characteristic polynomial of an oriented graph G^σ as follows.

Theorem 2.1. *Let*

$$\varphi_{R_s}(G^\sigma, \lambda) = \det(\lambda \boldsymbol{I}_n - \boldsymbol{R}_s) = c_0\lambda^n + c_1\lambda^{n-1} + \ldots + c_{n-1}\lambda + c_n \tag{3}$$

be the R_s-characteristic polynomial of G^σ. Then

$$c_i = \sum_{L \in \mathcal{EL}_i} (-2)^{p_e(L)} 2^{p_o(L)} W(L). \tag{4}$$

In particular, we have (i) $c_0 = 1$, (ii) $c_2 = R_{-1}(G)$, the general Randić index with $\alpha = -1$ and (iii) $c_i = 0$ for all odd i.

3. The upper and lower bounds

Like in the existing literature for skew energy, we can establish the following lower and upper bounds for the skew Randić energy.

Theorem 3.1. $\sqrt{4R_{-1}(G) + n(n-2)p^{\frac{2}{n}}} \leq RE_s(G^\sigma) \leq 2\sqrt{\lfloor \frac{n}{2} \rfloor R_{-1}(G)}$, *where* $p = |det \boldsymbol{R}_s| = \prod_{i=1}^{n} |\rho_i|$.

Proof. Let $\{i\mu_1, i\mu_2, \ldots, i\mu_n\}$ be the skew Randić spectrum of G^σ, where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. Since $\sum_{j=1}^{n} (i\mu_j)^2 = tr(\mathbf{R}_s^2) = \sum_{j=1}^{n} \sum_{k=1}^{n} (r_s)_{jk} (r_s)_{kj} = -\sum_{j=1}^{n} \sum_{k=1}^{n} (r_s)_{jk}^2 = -2R_{-1}(G)$, we have $\sum_{j=1}^{n} |\mu_j|^2 = 2R_{-1}(G)$.

By Proposition 2.1, we know that $\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_j|^2 = R_{-1}(G)$ and $RE_s(G^\sigma) = 2\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_i|$. Applying the Cauchy-Schwartz inequality we have that

$$RE_s(G^\sigma) = 2\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_j| \leq 2\sqrt{\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_j|^2} \sqrt{\lfloor \frac{n}{2} \rfloor} = 2\sqrt{\lfloor \frac{n}{2} \rfloor R_{-1}(G)}. \tag{5}$$

By Proposition 2.1, we know that

$$[RE_s(G^\sigma)]^2 = \left(2\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_j| \right)^2 = 4\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_i|^2 + 4\sum_{1 \leq i \neq j \leq \lfloor \frac{n}{2} \rfloor} |\mu_i||\mu_j|.$$

If n is odd, $p = 0$ and $[RE_s(G^\sigma)]^2 \geq 4\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_j|^2 = 4R_{-1}(G)$. If n is even, by using arithmetic geometric average inequality, one can get that

$$[RE_s(G^\sigma)]^2 = 4\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_j|^2 + 4\sum_{1 \leq i \neq j \leq \lfloor \frac{n}{2} \rfloor} |\mu_i||\mu_j| \geq 4R_{-1}(G) + n(n-2)p^{\frac{2}{n}}.$$

Therefore we can obtain the lower bound on skew Randić energy,

$$RE_s(G^\sigma) \geq \sqrt{4R_{-1}(G) + n(n-2)p^{\frac{2}{n}}}. \tag{6}$$

□

Note that there are plenty results on the upper and lower bounds on $R_{-1}(G)$. Combining with Theorem 3.1, we can get upper and lower bounds for the skew Randić energy by replacing $R_{-1}(G)$ with other parameters. Li and Yang [22] provided the following bounds on $R_{-1}(G)$ given strictly in terms of the order of G.

Theorem 3.2. *Let G be a graph of order n with no isolated vertices. Then*

$$\frac{n}{2(n-1)} \leq R_{-1}(G) \leq \lfloor \frac{n}{2} \rfloor$$

with equality in the lower bound if and only if G is a complete graph and equality in the upper bound if and only if either (i) n is even and G is the disjoint union of $n = 2$ paths of length 1, or (ii) n is odd and G is the disjoint union of $\frac{n-3}{2}$ paths of length 1 and one path of length 2.

To depict the extremal oriented graphs attaining the bounds on skew Randić energy, we need another result proved by Li and Wang [21]. Note that it has been proved that $\lambda_1 = 1$ is the largest Randić eigenvalues with the Perron-Frobenius vector $\alpha^T = (\sqrt{d_1}, \ldots, \sqrt{d_n})$; see [19].

Theorem 3.3. *Let G be a connected graph with order $n \geq 3$ and size m. Let $\alpha^T = (\sqrt{d_1}, \ldots, \sqrt{d_n})$. Then G has exactly k $(2 \leq k \leq n)$ and distinct Randić eigenvalues if and only if there are $k-1$ distinct none-one real numbers $\lambda_2, \ldots, \lambda_k$ satisfying (i) $\boldsymbol{R}(G) - \lambda_k \boldsymbol{I}_n$ is a singular matrix for $2 \leq i \leq k$. (ii) $\prod_{i=2}^{k} (\boldsymbol{R}(G) - \lambda_i \boldsymbol{I}_n) = \frac{\prod_{i=2}^{k} (1-\lambda_i)}{2m} \alpha\alpha^T$. Moreover, 1, $\lambda_2, \ldots, \lambda_k$ are exactly the k distinct Randić eigenvalues of G.*

From the above theorem, the authors gave the following corollary in [21].

Corollary 3.4. *A connected graph G has exactly two and distinct Randić eigenvalues if and only if G is a complete graph with order at least two.*

Hence, we can obtain the following result.

Theorem 3.5. *Let G^σ be an oriented graph of order n with no isolated vertices. Then*

$$\sqrt{\frac{2n}{n-1} + n(n-2)p^{\frac{2}{n}}} \leq RE_s(G^\sigma) \leq 2\lfloor \frac{n}{2} \rfloor,$$

where $p = |det \boldsymbol{R}_s(G^\sigma)|$. The equality in the lower bound holds if and only if G is a complete graph with exactly two nonzero skew Randić eigenvalues when n is odd, and $\boldsymbol{R}_s(G^\sigma)^T \boldsymbol{R}_s(G^\sigma) = \frac{1}{n-1}\mathbf{I_n}$ when n is even. The equality in the upper bound holds if and only if either n is even and G is the disjoint union of paths of length 1, or, n is odd and G is the disjoint union of $\frac{n-3}{2}$ paths of length 1 and one path of length 2 and σ is an arbitrary orientation of G.

Proof. The bounds on $RE_s(G^\sigma)$ comes directly from Theorem 3.1 and Theorem 3.2. We focus on the equality. From Theorem 3.2 and Theorem 3.1, we know that, if n is odd, the equality in the lower bound holds if and only if G is a complete graph and $[RE_s(G^\sigma)]^2 = 4\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} |\mu_i|^2$, that is, $\mu_i = 0$ for all $i = 2, \cdots, \lfloor \frac{n}{2} \rfloor$. If n is even, the equality in the lower bound holds if and only if G is a complete graph and $|\mu_i| = |\mu_j|$ for all $i \neq j$. Thus, a complete oriented graph with odd number of vertices reaches the lower bound if and only if it has exactly two nonzero skew Randić eigenvalues or all the skew Randić eigenvalues are zero. Since we assume that G has no isolated vertices, the latter case can not happen. For an even n, the equality in the lower bound holds if and only if G is a complete graph and there exists a constant k such that $|\rho_i|^2 = k$ for all i, which holds if and only if $\mathbf{R}_s(G^\sigma)^T \mathbf{R}_s(G^\sigma) = \frac{1}{n-1}\mathbf{I_n}$.

From Theorem 3.2 and Theorem 3.1, the equality in the upper bound holds if and only if G is the graph described in Theorem 3.2 and $|\rho_i| = |\rho_j|$ for all $1 \leq i \neq j \leq \lfloor \frac{n}{2} \rfloor$, that is, either n is even and G is the disjoint union of paths of length 1, or n is odd and G is the disjoint union of $\frac{n-3}{2}$ paths of length 1 and one path of length 2. In both cases, let σ be an arbitrary orientation of G. By Corollary 5.6 and Corollary 3.4, G^σ attains the upper bound and the converse also holds. $\square$

Now let us consider the bounds on skew Randić energies of trees. On the index $R_{-1}(T)$ when T is a tree, Clark and Moon [11] gave the following result.

Theorem 3.6. *For a tree T of order n, $1 \leq R_{-1}(T) \leq \frac{5n+8}{18}$. The equality in lower bound holds if and only if T is the star.*

Pavlović, Stojanvoić and Li [24] determined the sharp upper bound on the Randić index $R_{-1}(T)$ among all trees of order n for every $n \geq 720$.

Theorem 3.7. *Let T_t^n be a tree of order $n \geq 720$ and $n-1 \equiv t(mod\ 7)$. Denote by R_{-1}^* the maximum value of the Randić index $R_{-1}(T)$ among all trees T_t^n. Then,*

$$R_{-1}^* = \begin{cases} \frac{15n-1}{56} & t=0, \\ \frac{15n-1}{56} - \frac{1}{56} + \frac{7}{4(n+5)} & t=1, \\ \frac{15n-1}{56} - \frac{3}{5}\cdot\frac{1}{56} - \frac{7}{20(n-3)} & t=2, \\ \frac{15n-1}{56} - \frac{2}{3}\cdot\frac{1}{56} + \frac{7}{6(n+3)} & t=3, \\ \frac{15n-1}{56} - \frac{6}{5}\cdot\frac{1}{56} - \frac{7}{20(n-12)} & t=4, \\ \frac{15n-1}{56} - \frac{1}{3}\cdot\frac{1}{56} + \frac{7}{12(n+1)} & t=5, \\ \frac{15n-1}{56} - \frac{29}{27}\cdot\frac{1}{56} - \frac{35}{36(n-3)} & t=6. \end{cases}$$

Combining these bounds with Theorem 3.1, we can obtain the bounds on skew Randić energy of trees.

We point out that the lower bound is sharp and the equality in lower bound holds if and only if T is a star with odd vertices and an arbitrary orientation or $T = P_2$ with an arbitrary orientation. If n is odd, any oriented tree attains the lower bound if and only if it is a star and satisfies that its skew Randić spectrum is $\{i\mu_1, 0, \ldots, 0, -i\mu_1\}$, where $\mu_1 > 0$. With Theorem 5.5, we know that its Randić spectrum is $\{\mu_1, 0, \ldots, 0, -\mu_1\}$. Since 1 is the largest Randić eigenvalue of a connected graph, we have that $\mu_1 = 1$. Then apply Theorem 3.3 to the odd ordered star T with $\lambda_2 = 0$, $\lambda_3 = -1$, we can see that (i) and (ii) hold. So the skew Randić energy of a star with odd vertices and an arbitrary orientation equals to $\sqrt{4R_{-1}(T)} = 2$ which reaches the lower bound. If n is even, any oriented tree attains the lower bound must be a star and satisfy that $|\rho_i| = |\rho_j|$ for all $i \neq j$. By Theorem 5.5, that implies the extremal trees have exactly two distinct Randić eigenvalues. But it is impossible by Corollary 3.4 unless $T = P_2$. Thus, the equality in lower bound holds if and only if T is a star with odd vertices and an arbitrary orientation, or $T = P_2$.

Obviously, the upper bound on skew Randić energies of trees that obtained from Theorem 3.1 and Theorem 3.7 is not sharp. From the proof of Theorem 3.1, we know that the oriented trees attaining the upper bound in Theorem 3.1 must satisfy that $|\rho_i| = |\rho_j|$ for all $1 \le i \neq j \le \lfloor \frac{n}{2} \rfloor$. If n is even, by Theorem 5.5, the extremal trees have at most two distinct Randić eigenvalues, which is impossible by Corollary 3.4. If n is odd, the Randić spectrum of T is $\{1, \ldots, 1, 0, -1, \ldots, -1\}$. Since the Randić eigenvalue 1 has multiplicity one for connected graphs, we know that $T = P_3$, that is, $n = 3$. Hence the upper bound on skew Randić energies of trees that comes from Theorem 3.1 and Theorem 3.7 cannot be sharp.

A *chemical graph* is a graph in which no vertex has degree greater than four. Analogously, a *chemical tree* is a tree T for which $\Delta(T) \le 4$. Li and Yang [23] gave the sharp lower and upper bounds on $R_{-1}(T)$ among all chemical trees.

Theorem 3.8. *Let T be a chemical tree of order n. Then,*

$$R_{-1}(T) \ge \begin{cases} 1 & \text{if } n \le 5, \\ \frac{11}{8} & \text{if } n = 6, \\ \frac{3}{2} & \text{if } n = 7, \\ 2 & \text{if } n = 10, \\ \frac{3n+1}{16} & \text{for other values of } n. \end{cases}$$

Theorem 3.9. *Let T be a chemical tree of order n, $n > 6$. Then,*

$$R_{-1}(T) \le max\{F_1(n), F_2(n), F_3(n)\},$$

where

$$F_1(n) = \begin{cases} \frac{3n+1}{16} + \frac{1}{144}\frac{31n+53}{3} & \text{if } n = 1 \ mod\ 3, \\ \frac{3n+1}{16} + \frac{1}{144}\left(\frac{31n+22}{3} + 9\right) & \text{if } n = 2 \ mod\ 3, \\ \frac{3n+1}{16} + \frac{1}{144}\left(\frac{31n-9}{3} + 18\right) & \text{if } n = 0 \ mod\ 3. \end{cases}$$

$$F_2(n) = \frac{3n+1}{16} + \frac{1}{144} max\{11n - N_4 - 2k + 10, k = 0, 1, 2\}$$

with N_4 being the minimum integer solution of n_4 of the following system:

$$\begin{cases} n_3 + 2n_4 + 2 = n_1 \\ 2n_1 + n_3 + n_4 = n - k \\ n_3 \le 2n_4 + 2 \end{cases}$$

and

$$F_3(n) = \frac{3n+1}{16} + \frac{1}{144} max\{4n + 19N_1 + 5k + 4, k = 0, 1, 2\}$$

with N_1 being the minimum integer solution of n_1 of the following system:

$$\begin{cases} n_3 + 2n_4 + 2 = n_1 \\ 2n_1 + n_3 + n_4 = n - k \\ n_3 \ge 2n_4 + 2 \\ n_4 \ge 1. \end{cases}$$

Combining these bounds with Theorem 3.1, we can obtain the bounds on skew Randić energy of chemical trees. With the same argument as before, we can get that the lower bound is sharp and the equality in lower bound holds if and only if T is a star with 2, 3 or 5 vertices and an arbitrary orientation. Also, the equality in upper bound can not be attained by any chemical tree.

4. Skew Randić energies of trees

It is well known that the skew energy of a directed tree is independent of its orientation [1]. In this section, we investigate the skew Randić energy of trees. Similarly, we present a basic lemma. The proof is also similar to the proof given in [1].

Lemma 4.1. *Let D be a digraph and let D' be the digraph obtained from D by reversing the orientations of all the arcs incident with a particular vertex of D. Then $RE_s(D) = RE_s(D')$.*

Proof. Let $\mathbf{R}_s(D)$ be the skew Randić matrix of D of order n with respect to a labeling of its vertex set. Suppose the orientations of all the arcs incident at vertex v_i of D are reversed. Let the resulting digraph be D'. Then $\mathbf{R}_s(D') = P_i\mathbf{R}_s(D)P_i$ where P_i is the diagonal matrix obtained from the identity matrix of order n by changing the $i-$th diagonal entry to -1. Hence $\mathbf{R}_s(D)$ and $\mathbf{R}_s(D')$ are orthogonally similar and so have the same eigenvalues and hence D and D' have the same skew Randić energy. □

Let σ be an orientation of a graph G. Let W be a subset of $V(G)$ and $\overline{W} = V(G) \setminus W$. The orientation τ of G obtained from σ by reversing the orientations of all arcs between W and $\overline{W}$ is said to be obtained from G^σ by a switching with respect to W. Moreover, two oriented graphs G^τ and G^σ of G are said to be *switching-equivalent* if G^τ can be obtained from G^σ by a switching. From lemma 4.1, we know that

Theorem 4.2. *If G^τ and G^σ are switching-equivalent, then $Sp_{\boldsymbol{R}_s}(G^\sigma) = Sp_{\boldsymbol{R}_s}(G^\tau)$.*

Lemma 4.3. [1] *Let T be a labeled directed tree rooted at vertex v. It is possible, through reversing the orientations of all arcs incident at some vertices other than v, to transform T to a directed tree T' in which the orientations of all the arcs go from low labels to high labels.*

We can also show that the skew energy of a directed tree is independent of its orientation by using Lemma 4.1 and Lemma 4.3.

Theorem 4.4. *The skew Randić energy of a directed tree is independent of its orientation.*

Corollary 4.5. *The skew Randić energy of a directed tree is the same as the Randić energy of its underlying tree.*

We omit the proofs of Theorem 4.4 and Corollary 4.5, since they are similar to the proofs of Theorem 3.3 and Corollary 3.4 in [1].

5. Graphs with $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$

The relationship between $Sp_s(G^\sigma)$ and $\mathbf{i}Sp(G)$ has been concerned in [26]. Similarly, we concentrate on the relationship between $Sp_{\mathbf{R}_s}(G^\sigma)$ and $\mathbf{i}Sp_{\mathbf{R}}(G)$, and we obtain some analogous results. The following two lemmas given in [26] will be used.

Lemma 5.1. [26] *Let* $\mathbf{A} = \begin{pmatrix} \mathbf{0} & X \\ X^T & \mathbf{0} \end{pmatrix}$ *and* $\mathbf{B} = \begin{pmatrix} \mathbf{0} & X \\ -X^T & \mathbf{0} \end{pmatrix}$ *be two real matrices. Then* $Sp(\mathbf{B}) = \mathbf{i}Sp(\mathbf{A})$.

Let $|\mathbf{X}|$ denote the matrix whose entries are the absolute values of the corresponding entries in $\mathbf{X}$. For real matrices $\mathbf{X}$ and $\mathbf{Y}$, $\mathbf{X} \leq \mathbf{Y}$ means that $\mathbf{Y} - \mathbf{X}$ has nonnegative entries. $\rho(\mathbf{X})$ denotes the spectral radius of a square matrix $\mathbf{X}$.

Lemma 5.2. [26] *Let* $\mathbf{A}$ *be an irreducible nonnegative matrix and* $\mathbf{B}$ *be a real positive semi-definite matrix such that* $|\mathbf{B}| \leq \mathbf{A}$ *(entry-wise) and* $\rho(\mathbf{A}) = \rho(\mathbf{B})$. *Then* $\mathbf{A} = \mathbf{DBD}$ *for some real matrix* $\mathbf{D}$ *such that* $|\mathbf{D}| = \mathbf{I}$, *the identity matrix.*

Theorem 5.3. *G is a bipartite graph if and only if there is an orientation σ such that* $Sp_{\boldsymbol{R}_s}(G^\sigma) = \mathbf{i}Sp_{\boldsymbol{R}}(G)$.

Proof. Necessity: If G is bipartite, then there is a labeling such that the Randić matrix of G is of the form

$$\mathbf{R}(G) = \begin{pmatrix} \mathbf{0} & \mathbf{X} \\ \mathbf{X}^T & \mathbf{0} \end{pmatrix}.$$

Let σ be the orientation such that the skew Randić matrix of G^σ is of the form

$$\mathbf{R}_s(G^\sigma) = \begin{pmatrix} \mathbf{0} & \mathbf{X} \\ -\mathbf{X}^T & \mathbf{0} \end{pmatrix}.$$

By Lemma 5.1, $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$.

Sufficiency: Suppose that $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$, for some orientation σ. Since $\mathbf{R}_s(G^\sigma)$ is a real skew symmetric matrix, $Sp_{\mathbf{R}_s}(G^\sigma)$ has only pure imaginary eigenvalues and so is symmetric about the real axis. Then $Sp_{\mathbf{R}}(G) = -\mathbf{i}Sp_{\mathbf{R}_s}(G^\sigma)$ is symmetric about the imaginary axis. Hence G is bipartite. □

Trees are special bipartite graphs, actually, we will prove that G is a tree if and only if for any orientation σ, $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$. The next lemma plays an important role in the proof of the above statement.

Lemma 5.4. *Let* $\mathbf{X} = \begin{pmatrix} \mathbf{C} & * \\ * & * \end{pmatrix}$ *be a nonnegative matrix, where* $\mathbf{C} = (c_{ij})$ *is a* $k \times k$ $(k > 2)$ *matrix whose nonzero entries are* $c_{i,i-1}$ *and* $c_{i,i}$ *with the subscripts modulo* k, *for* $1 \leq i \leq k$. *Let* $\mathbf{Y}$ *be obtained from* $\mathbf{X}$ *by changing the* $(1,1)$ *entry to* $-c_{1,1}$. *If* $\mathbf{X}^T\mathbf{X}$ *is irreducible then* $\rho(\mathbf{X}^T\mathbf{X}) > \rho(\mathbf{Y}^T\mathbf{Y})$.

Proof. Note that $|\mathbf{Y}^T\mathbf{Y}| \leq \mathbf{X}^T\mathbf{X}$ (entry-wise) and so $\rho(\mathbf{X}^T\mathbf{X}) \geq \rho(\mathbf{Y}^T\mathbf{Y})$ by Perron- Frobenius theory [20]. Now suppose that $\rho(\mathbf{X}^T\mathbf{X}) = \rho(\mathbf{Y}^T\mathbf{Y})$. Since $\mathbf{X}^T\mathbf{X}$ is irreducible, by Lemma 5.2, there exists a signature matrix $\mathbf{D} = Diag(d_1, d_2, \ldots, d_n)$ such that $\mathbf{X}^T\mathbf{X} = \mathbf{D}\mathbf{Y}^T\mathbf{Y}\mathbf{D}$. Therefore $[\mathbf{X}^T\mathbf{X}]_{ij} = d_i d_j [\mathbf{Y}^T\mathbf{Y}]_{ij}$ for all i, j. Now, for $i = 1, \ldots, k-1$, $[\mathbf{X}^T\mathbf{X}]_{i,i+1} = [\mathbf{Y}^T\mathbf{Y}]_{i,i+1} \neq 0$. Using $[\mathbf{X}^T\mathbf{X}]_{ij} = d_i d_j [\mathbf{Y}^T\mathbf{Y}]_{ij}$, we have $d_i d_{i+1} = 1$ for $i = 1, \ldots, k-1$. Hence $d_1 d_k = 1$. On the other hand, let $[\mathbf{X}^T\mathbf{X}]_{1k} = c_{1,1}c_{1,k} + M$ and so we have $-c_{1,1}c_{1,k} + M = d_1 d_k [\mathbf{Y}^T\mathbf{Y}]_{1k} = [\mathbf{X}^T\mathbf{X}]_{1k} = c_{1,1}c_{1,k} + M$, which is impossible. □

Theorem 5.5. *G is a tree if and only if for any orientation σ, $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$.*

Proof. Necessity: The necessity follows directly from Theorem 4.4 and Theorem 5.3.

Sufficiency: Suppose that $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$, for any orientation σ. By Theorem 5.3, G is a bipartite graph. So there is a labeling such that the Randić matrix of G is of the form

$$\mathbf{R}(G) = \begin{pmatrix} \mathbf{0} & \mathbf{X} \\ \mathbf{X}^T & \mathbf{0} \end{pmatrix},$$

where $\mathbf{X}$ is a nonnegative matrix. Since G is connected, $\mathbf{X}^T\mathbf{X}$ is indeed a positive matrix and so irreducible. Now assume that G is not a tree. Then G has at least an even cycle because G is bipartite. W. L. O. G. $\mathbf{X}$ has the form $\begin{pmatrix} \mathbf{C} & * \\ * & * \end{pmatrix}$ where $\mathbf{C} = (c_{ij})$ is a $k \times k$ $(k > 2)$ matrix whose nonzero entries are $c_{i,i-1}$ and $c_{i,i}$ with the subscripts modulo k, for $1 \leq i \leq k$. Let $\mathbf{Y}$ be obtained from $\mathbf{X}$ by changing the $(1,1)$ entry to $-c_{1,1}$. Consider the orientation σ of G such that

$$\mathbf{R}_s(G^\sigma) = \begin{pmatrix} \mathbf{0} & \mathbf{Y} \\ -\mathbf{Y}^T & \mathbf{0} \end{pmatrix}.$$

By hypothesis, $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ and hence $\mathbf{X}$ and $\mathbf{Y}$ have the same singular values. It follows that $\rho(\mathbf{X}^T\mathbf{X}) = \rho(\mathbf{Y}^T\mathbf{Y})$, which contradicts Lemma 5.4. □

Corollary 5.6. *G is a forest if and only if for any orientation σ, $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$.*

Proof. Necessity: Let $G = G_1 \cup \ldots \cup G_r$ where G_j's are trees. Then $G^\sigma = G_1^{\sigma_1} \cup \ldots \cup G_r^{\sigma_r}$. By Theorem 5.5, $Sp_{\mathbf{R}_s}(G_j^{\sigma_j}) = \mathbf{i}Sp_{\mathbf{R}}(G_j)$ for all $j = 1, 2, \ldots, r$. Hence $Sp_{\mathbf{R}_s}(G^\sigma) = Sp_{\mathbf{R}_s}(G_1^{\sigma_1}) \cup \cdots \cup Sp_{\mathbf{R}_s}(G_r^{\sigma_r}) = \mathbf{i}Sp_{\mathbf{R}}(G_1) \cup \cdots \cup \mathbf{i}Sp_{\mathbf{R}}(G_r) = \mathbf{i}Sp_{\mathbf{R}}(G_1 \cup \ldots \cup G_r) = \mathbf{i}Sp_{\mathbf{R}}(G)$.

Sufficiency: Suppose that G is not a forest. Then $G = G_1 \cup, \ldots, \cup G_r$ where $G_1, \ldots, G_t$ are connected, but not trees and $G_{t+1}, \ldots, G_r$ are trees. By Theorem 5.3, G is a bipartite graph. So there is a labeling such that the Randić matrix of G is of the form

$$\mathbf{R}(G) = \begin{pmatrix} \mathbf{0} & \mathbf{X} \\ \mathbf{X}^T & \mathbf{0} \end{pmatrix},$$

where $\mathbf{X} = \mathbf{X_1} \bigoplus \cdots \bigoplus \mathbf{X_r}$. Let $\mathbf{Y_j}$ be obtained from $\mathbf{X_j}$ by changing the $(1,1)$ entry to its negative. Consider the orientation σ of G such that

$$\mathbf{R}_s(G^\sigma) = \begin{pmatrix} \mathbf{0} & \mathbf{Y} \\ -\mathbf{Y}^T & \mathbf{0} \end{pmatrix}.$$

where $\mathbf{Y} = \mathbf{Y_1} \bigoplus \cdots \bigoplus \mathbf{Y_r}$. By Lemma 5.1, $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ implies that the singular values of $\mathbf{X}$ coincide with the singular values of $\mathbf{Y}$. Since $G_{t+1}, \ldots, G_r$ are trees, the singular values of $\mathbf{X_j}$ coincide with the singular values of $\mathbf{Y_j}$ for $j = t+1, \ldots, r$. Hence the singular values of $\mathbf{X_1} \bigoplus \cdots \bigoplus \mathbf{X_t}$ coincide with the singular values of $\mathbf{Y_1} \bigoplus \cdots \bigoplus \mathbf{Y_t}$. Since $G_1, \ldots, G_t$ are not trees, we have $\rho(\mathbf{X_j}^T\mathbf{X_j}) > \rho(\mathbf{Y_j}^T\mathbf{Y_j})$ for $j = 1, \ldots, t$. Consequently, for some j_0,

$$\max_{1\le j\le t} \rho(\mathbf{X_j}^T\mathbf{X_j}) = \max_{1\le j\le t} \rho(\mathbf{Y_j}^T\mathbf{Y_j}) = \rho(\mathbf{Y_{j_0}}^T\mathbf{Y_{j_0}}) < \rho(\mathbf{X_{j_0}}^T\mathbf{X_{j_0}}) \le \max_{1\le j\le t} \rho(\mathbf{X_j}^T\mathbf{X_j}),$$

a contradiction. □

Let σ be an orientation of G. From Theorem 5.3, we know that $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ only if G is bipartite. We concentrate on the orientation σ of bipartite graph G so that $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ in the sequel. Let the characteristic polynomials of $\mathbf{R}(G)$ and $\mathbf{R}_s(G^\sigma)$ be expressed as in (1) and (3), respectively. $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ if and only if $\varphi_R(G,\lambda) = \sum_{i=0}^n a_i\lambda^{n-i} = \lambda^{n-2r}\prod_{i=1}^r(\lambda^2 - \lambda_i^2)$ and $\varphi_{R_s}(G^\sigma,\lambda) = \sum_{i=0}^n c_i\lambda^{n-i} = \lambda^{n-2r}\prod_{i=1}^r(\lambda^2 + \lambda_i^2)$ for some non-zero real numbers $\lambda_1, \lambda_2, \ldots, \lambda_r$. Hence, we have that $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ if and only if

$$a_{2i} = (-1)^i c_{2i},\ a_{2i+1} = c_{2i+1} = 0, \tag{7}$$

for $i = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$.

An even cycle C_{2l} is said to be *oriented uniformly* if C_{2l} is oddly (resp., evenly) oriented relative to G^σ when l is odd (resp., even). If every even cycle in G^σ is oriented uniformly, then the orientation σ is defined to be a *parity-linked* orientation of G.

Theorem 5.7. *Let G be a bipartite graph and σ be an orientation of G. Then $Sp_{\boldsymbol{R}_s}(G^\sigma) = \mathbf{i}Sp_{\boldsymbol{R}}(G)$ if and only if σ is a parity-linked orientation of G.*

Proof. Since G is bipartite, all cycles in G are even and all linear subgraphs are even. Then $a_{2i+1} = 0$ for all i.

Sufficiency: Since every even cycle is oriented uniformly, for every cycle C_{2l} with length $2l$, C_{2l} is evenly oriented relative to G^σ if and only if l is even. Thus $(-1)^{p_e(C_{2l})} = (-1)^{l+1}$.

By Eqs (2) and (4), we have

$$\begin{aligned} (-1)^i a_{2i} &= \sum_{L\in\mathcal{M}_{2i}} W(L) + \sum_{L\in\mathcal{CL}_{2i}} (-1)^{p_1(L)+i}(-2)^{p_2(L)}W(L), \\ c_{2i} &= \sum_{L\in\mathcal{M}_{2i}} W(L) + \sum_{L\in\mathcal{CL}_{2i}} (-2)^{p_e(L)}2^{p_o(L)}W(L), \end{aligned}$$

where $\mathcal{M}_{2i}$ is the set of matchings with i edges and $\mathcal{CL}_{2i}$ is the set of all linear subgraphs with $2i$ vertices of G and containing at least one cycle.

For a linear subgraph $L \in \mathcal{CL}_{2i}$ of G, assume that L contains the cycles $C_{2l_1}, C_{2l_2}, \ldots, C_{2l_{p_2}}$, then the number of components of L that are single edges is $p_1(L) = i - \sum_{j=1}^{p_2(L)} l_j$. Hence $(-1)^{p_1(L)+i} = (-1)^{\sum_{j=1}^{p_2(L)} l_j}$.

Therefore, for a linear subgraph $L \in \mathcal{CL}_{2i}$,

$$(-2)^{p_e(L)}2^{p_o(L)} = (-1)^{p_e(L)}2^{p_2(L)} = (-1)^{\sum_{j=1}^{p_2}(l_j+1)}2^{p_2(L)} = (-1)^{p_1(L)+i}(-2)^{p_2(L)}.$$

Thus $(-1)^i a_{2i} = c_{2i}$, and the sufficiency is proved.

Necessity: If there is an even cycle of G that is not oriented uniformly in G^σ, then choose a shortest cycle C_{2l} with length $2l$ such that C_{2l} is not oriented uniformly, that is, C_{2l} is oddly oriented in G^σ if l is even and evenly oriented if l is odd. Let $\mathcal{C}_{2l}$ be the set of cycles with length $2l$ such that they are not oriented uniformly and let $\mathcal{UCL}_{2l}$ denote the set of all even linear subgraphs with $2l$ vertices of G and all even cycles that are oriented uniformly. Thus, we have

$$\begin{aligned} (-1)^l a_{2l} &= \sum_{L\in\mathcal{M}_{2l}} W(L) + \sum_{L\in\mathcal{C}_{2l}} (-1)^l(-2)W(L) + \sum_{L\in\mathcal{UCL}_{2l}} (-1)^{p_1(L)+l}(-2)^{p_2(L)}W(L), \\ c_{2l} &= \sum_{L\in\mathcal{M}_{2l}} W(L) + \sum_{L\in\mathcal{C}_{2l}} (-1)^l 2W(L) + \sum_{L\in\mathcal{UCL}_{2l}} (-2)^{p_e(L)}2^{p_o(L)}W(L). \end{aligned}$$

By the choice of C_{2l} and the proof of the necessity, we have that

$$\sum_{L\in\mathcal{UCL}_{2l}} (-1)^{p_1(L)+l}(-2)^{p_2(L)}W(L) = \sum_{L\in\mathcal{UCL}_{2l}} (-2)^{p_e(L)}2^{p_o(L)}W(L).$$

However,

$$\sum_{L\in\mathcal{C}_{2l}} (-1)^l(-2)W(L) \neq \sum_{L\in\mathcal{C}_{2l}} (-1)^l 2W(L).$$

Thus $(-1)^l a_{2l} \neq c_{2l}$. This contradicts $Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G)$ by Eq. (7). □

Let G be a bipartite graph with the bipartition $V(G) = X \cup Y$. We call an orientation σ of G the *canonical* orientation if it assigns each edge of G the direction from X to Y. For the canonical orientation σ of $G(X,Y)$, from the proof of Theorem 5.3, we have that

$$Sp_{\mathbf{R}_s}(G^\sigma) = \mathbf{i}Sp_{\mathbf{R}}(G). \tag{8}$$

Theorem 5.8. *Suppose τ is an orientation of a bipartite graph $G = G(X,Y)$. Then $Sp_{\boldsymbol{R}_s}(G^\tau) = \mathbf{i}Sp_{\boldsymbol{R}}(G)$ if and only if G^τ is switching-equivalent to G^σ, where σ is the canonical orientation of G.*

Proof. The sufficiency can be easily obtained from Theorem 4.2 and Eq. (8).

We prove the necessity by induction on the number of edges m of the bipartite graph G in the following. The result is trivial for $m = 1$. Assume that the result is true for all bipartite graphs with at most $m-1$ ($m > 2$) arcs. Let G be a bipartite graph with m edges and (X,Y) be the bipartition of the vertex set of G. Suppose that τ is an orientation of G such that $Sp_{\mathbf{R}_s}(G^\tau) = \mathbf{i}Sp_{\mathbf{R}}(G)$. We have to prove that τ is switching-equivalent to σ. Let e be any edge of G. By Theorem 5.7 every even cycle is oriented uniformly in G^τ and hence in $(G-e)^\tau$. Consequently, τ_e is a parity-linked orientation of $G-e$, where τ_e is the restriction of τ to the graph $G-e$. So by Theorem 5.7, $Sp_{\mathbf{R}_s}((G-e)^{\tau_e}) = \mathbf{i}Sp_{\mathbf{R}}(G-e)$.

Consequently, by induction hypothesis, $(G-e)^{\tau_e}$ is switching-equivalent to $(G-e)^{\sigma_e}$, where σ_e is the restriction of σ to the graph $G-e$. Let α be the switch that takes $(G-e)^{\tau_e}$ to $(G-e)^{\sigma_e}$ effected by the subset U of $V(G-e) = V(G)$. We claim that α takes τ to σ in G. If not, then the resulting oriented graph $G^{\tau'}$ will be of the following type (see Fig.1): all the arcs of $G-e$ will be oriented from one partite set (say, X) to the other (namely, Y) while the arc e will be oriented in the reverse direction, that is, from Y to X.

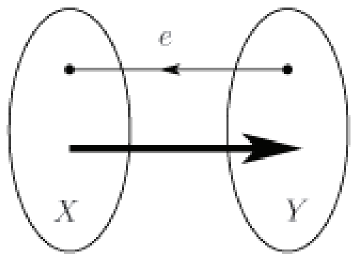

Figure 1. the oriented graph $G^{\tau'}$

Consider first the case when e is a cut edge of G. The subgraph $G-e$ will then consist of two components with vertex sets, say, S_1 and S_2. Now switch with respect to S_1. This will change the orientation of the only arc e and the resulting orientation is σ. Consequently, τ is switching-equivalent to σ.

Note that the above argument also takes care of the case when G is a tree since each edge of G will then be a cut edge. Hence we now assume that G contains an even cycle C_{2k} containing the arc e. But then any such C_{2k} has $k-1$ arcs in one direction and $k+1$ arcs in the opposite direction, thereby not oriented uniformly. Hence this case can not arise. Consequently, τ is switching-equivalent to σ in G. $\square$

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