General Randić matrix and general Randić energy*

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Abstract

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and d_i the degree of its vertex v_i, $i = 1, 2, \cdots, n$. Inspired by the Randić matrix and the general Randić index of a graph, we introduce the concept of general Randić matrix $\mathbf{R}_\alpha$ of G, which is defined by $(\mathbf{R}_\alpha)_{i,j} = (d_i d_j)^\alpha$ if v_i and v_j are adjacent, and zero otherwise. Similarly, the general Randić eigenvalues are the eigenvalues of the general Randić matrix, the greatest general Randić eigenvalue is the general Randić spectral radius of G, and the general Randić energy is the sum of the absolute values of the general Randić eigenvalues. In this paper, we prove some properties of the general Randić matrix and obtain lower and upper bounds for general Randić energy, also, we get some lower bounds for general Randić spectral radius of a connected graph. Moreover, we give a new sharp upper bound for the general Randić energy when $\alpha = -1/2$.

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1 Introduction

In this paper we are concerned with simple finite graphs. Let G be such a graph, with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For $i = 1, 2, \ldots, n$, let d_i be the degree of the vertex $v_i \in V(G)$.

A convenient parameter of G is the general Randić index $R_\alpha(G)$, which is defined as

$$R_\alpha = R_\alpha(G) = \sum_{i \sim j} (d_i d_j)^\alpha,$$

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where the summation is over all edges v_iv_j in G, and $\alpha \neq 0$ is a fixed real number. This topological index with $\alpha = -\frac{1}{2}$ was first proposed by Randić [11] in 1975 under the name "branching index". In 1998, Bollobás and Erdős [1] generalized this index by replacing $\alpha = -\frac{1}{2}$ with any real number α (as defined above). The Randić index has found a lot of chemical applications and becomes a popular topic of research in mathematics and mathematical chemistry.

The general Randić index suggests that it is purposeful to associate to the graph G a symmetric square matrix $\mathbf{R}_\alpha = \mathbf{R}_\alpha(G)$ of order n, whose (i,j)-entry is defined as

$$(\mathbf{R}_\alpha)_{i,j} = \begin{cases} 0 & \text{if i = j,} \\ (d_id_j)^\alpha & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent.} \end{cases}$$

The matrix defined above is called the *general Randić matrix*. Denote the eigenvalues of the general Randić matrix $\mathbf{R}_\alpha = \mathbf{R}_\alpha(G)$ by $\rho_1^{(\alpha)}, \rho_2^{(\alpha)}, \ldots, \rho_n^{(\alpha)}$ and label them in non-increasing order. The greatest eigenvalue $\rho_1^{(\alpha)}$ is called the *Randić spectral radius* of the graph G. The multiset $Sp_{R_\alpha} = Sp_{R_\alpha(G)} = \{\rho_1^{(\alpha)}, \rho_2^{(\alpha)}, \ldots, \rho_n^{(\alpha)}\}$ will be called the R_α-spectrum of the graph G. In addition, $\phi_{R_\alpha}(G,\lambda) = \det(\lambda\mathbf{I}_n - \mathbf{R}_\alpha)$ will be referred to as the R_α-characteristic polynomial of G. Here and later, I_n is denoted the unit matrix of order n.

The above notation and terminology are chosen so as to fully parallel with those used in ordinary graph spectral theory [5]. The adjacency matrix $\mathbf{A} = \mathbf{A}(G)$ of the graph G is defined so that its (i,j)-element is equal to 1 if the vertices v_i and v_j are adjacent, and is equal to 0 otherwise. The eigenvalues of $\mathbf{A}$ are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$ and said to form the A-spectrum of G. In addition, $\phi_A(G,\lambda) = \det(\lambda\mathbf{I}_n - \mathbf{A})$ is called the A-characteristic polynomial of G. The energy of the general Randić matrix is defined as $RE_\alpha = RE_\alpha(G) = \sum_{i=1}^n |\rho_i^{(\alpha)}|$ and is called the *general Randić energy*.

General Randić matrix and general Randić energy are generalizations of Randić matrix $\mathbf{R}$ and Randić energy RE [4] (with $\alpha = -\frac{1}{2}$). The properties about $\mathbf{R}$ and RE can be found in [4, 7, 9]. Almost all the results in the following are parallel to those in [4, 7, 9], and can be deduced similarly. We hope that after introducing the new concept of general Randić matrix, some new and nontrivial results could be obtained later, like the general Randić index [1].

At first, we give some obvious observations. If a graph G consists of components $G_1, G_2, \ldots, G_p$, i.e., $G = G_1 \cup G_2 \cup \ldots \cup G_p$, then

$$Sp_{R_\alpha}(G) = Sp_{R_\alpha}(G_1) \cup Sp_{R_\alpha}(G_2) \cup \ldots \cup Sp_{R_\alpha}(G_2). \tag{1}$$

Lemma 1.1 *Let $G = G_1 \cup G_2 \cup \ldots \cup G_p$, then $RE_\alpha(G) = RE_\alpha(G_1) + RE_\alpha(G_2) + \ldots + RE_\alpha(G_p)$.*

By K_n we denote the complete graph on n vertices, and by $\overline{K_n}$ its complement, i.e., the graph consisting of n isolated vertices. Then

$$Sp_{R_\alpha}(G) = \{0, n \text{ times}\} \tag{2}$$

if and only if $G \cong \overline{K_n}$.

Lemma 1.2 *Let G be a graph on n vertices, $n \geq 1$. Then $RE_\alpha(G) = 0$ if and only if $G \cong \overline{K_n}$.*

2 Basic properties of general Randić matrix

There is a close connection between the general Randić matrix $\mathbf{R}_\alpha$ and the adjacency matrix A. If G does not possess isolated vertices, then it is easy to check that

$$\mathbf{R}_\alpha = \mathbf{D}^\alpha\ \mathbf{A}\mathbf{D}^\alpha,$$

where $\mathbf{D}$ is the diagonal matrix of vertex degrees. If G has isolated vertices, we also have the above equality when $\alpha \geq 0$.

Theorem 2.1 *Let G be a graph on n vertices, and let $\boldsymbol{A}$ and $\boldsymbol{R}_\alpha$ be its adjacency and general Randić matrices. If $\boldsymbol{A}$ has n_+, n_0, and n_- positive, zero, and negative eigenvalues, respectively ($n_+ + n_0 + n_- = n$), then $\boldsymbol{R}_\alpha$ has n_+, n_0, and n_- positive, zero, and negative eigenvalues, respectively.*

Proof. If G has no isolated vertices, then $\mathbf{R}_\alpha = \mathbf{D}^\alpha \mathbf{A} \mathbf{D}^\alpha$. That is to say $\mathbf{R}_\alpha$ and $\mathbf{A}$ are congruent matrices. The result follows by Sylvester's inertia law [8].

Let $G \cong G' \cup \overline{K_l}$ and G' has no isolated vertices. Then $Sp_{R_\alpha}(G) = Sp_{R_\alpha}(G') \cup \{0, l \text{ times}\}$ and $Sp_A(G) = Sp_A(G') \cup \{0, l \text{ times}\}$. Consequently, both $\mathbf{R}_\alpha$ and $\mathbf{A}$ have $n_+(G')$ positive and $n_-(G')$ negative eigenvalues, whereas the number of their zero eigenvalues is $n_0(G') + l$. Theorem 2.1 holds also in this case. ■

As is known that complete multipartite graphs are precisely those connected graphs with a single positive eigenvalue [5], then from equation (1) and Theorem 2.1, we have the following results.

Theorem 2.2 *Let G be a graph on n vertices. Then $\rho_1^{(\alpha)}$ is the only positive general Randić eigenvalue of G if and only if one component of G is a complete multipartite graph, and all other components (if any) are isolated vertices.*

Theorem 2.3 *A simple connected graph G has exactly two distinct general Randić eigenvalues if and only if G is complete.*

Proof. The idea of proof is similar to [3]. Let G be a simple connected graph with the general Randić matrix $\mathbf{R}_\alpha$. We suppose that G has exactly two distinct general Randić eigenvalues. Let these be $\rho_1^{(\alpha)} > \rho_2^{(\alpha)}$. Since G is connected, $\mathbf{R}_\alpha$ is irreducible and by the Perron-Frobenius theorem, $\rho_1^{(\alpha)}$ is the greatest and simple eigenvalue of $\mathbf{R}_\alpha$. Thus all other eigenvalues of $\mathbf{R}_\alpha$ are equal to $\rho_2^{(\alpha)}$. In order to prove that $G \cong K_n$ we show that its diameter is one. For this reason, we prove that G does not contain an induced shortest path P_m, $m \geq 3$. Suppose that G contains an induced shortest path P_m, $m \geq 3$. Let $\mathbf{B}$ be the principal submatrix of $\mathbf{R}_\alpha$ indexed by the vertices of P_m and let $\mu_i(\mathbf{B})$ denote the i-th greatest eigenvalue of $\mathbf{B}$. Then by the interlacing theorem we obtain

$$\rho_2^{(\alpha)} \geq \mu_i(\mathbf{B}) \geq \rho_{n-m+i}^{(\alpha)},$$

for $i = 1, \cdots, m$. Thus, we have

$$\rho_2^{(\alpha)} \geq \mu_2(\mathbf{B}) \geq \mu_3(\mathbf{B}) \geq \cdots \geq \rho_n^{(\alpha)} = \rho_2^{(\alpha)}.$$

This implies that P_m has at most two distinct general Randić eigenvalues for $m \geq 3$, which is impossible. Therefore G does not contain two vertices at distance two or more, and hence it is a complete graph. Conversely, if $G \cong K_n$, then all non-zero terms in $\mathbf{R}_\alpha$ are equal to $1/(n-1)^{2\alpha}$ which implies that $\mathbf{R}_\alpha = 1/(n-1)^{2\alpha}\mathbf{A}$. Therefore, $\rho_i^{(\alpha)} = 1/(n-1)^{2\alpha}\lambda_i$, for $i = 1, \cdots, n$. Then from [5], G has exactly two distinct general Randić eigenvalues $1/(n-1)^{(2\alpha-1)}$ and $-1/(n-1)^{2\alpha}$. ■

Theorem 2.4 *Let the notation be the same as in Theorem 2.1. If G possesses isolated vertices, then $\det\boldsymbol{R}_\alpha = \det\boldsymbol{A} = 0$. If G does not possess isolated vertices, then*

$$\det\boldsymbol{R}_\alpha = (d_1 d_2 \ldots d_n)^\alpha \det\boldsymbol{A}.$$

Proof. If G has isolated vertices, then according to Theorem 2.1, both matrices $\mathbf{A}$ and $\mathbf{R}_\alpha$ have zero eigenvalues, and therefore their determinants are equal to zero.

If G does not possess isolated vertices, then $\mathbf{R}_\alpha = \mathbf{D}^\alpha\mathbf{A}\mathbf{D}^\alpha$, and so

$$\mathbf{D}^\alpha\mathbf{R}_\alpha\mathbf{D}^{-\alpha} = \mathbf{D}^\alpha(\mathbf{D}^\alpha\mathbf{A}\mathbf{D}^\alpha)\mathbf{D}^{-\alpha} = \mathbf{D}^{2\alpha}\mathbf{A}.$$

Since $\mathbf{R}_\alpha$ and $\mathbf{D}^\alpha\mathbf{R}_\alpha\mathbf{D}^{-\alpha}$ are similar, they have equal eigenvalues. Therefore

$$\det\mathbf{R}_\alpha = \det(\mathbf{D}^\alpha\mathbf{R}_\alpha\mathbf{D}^{-\alpha}) = \det(\mathbf{D}^{2\alpha}\mathbf{A}).$$

The result follows. ■

3 Bounds for general Randić energy

In this section we first calculate $tr(\mathbf{R}_\alpha^2)$, $tr(\mathbf{R}_\alpha^3)$, and $tr(\mathbf{R}_\alpha^4)$, where tr denotes the trace of a matrix. Moreover, using these equalities we obtain an upper and a lower bound for the general Randić energy.

In order to obtain our main results we give the following result.

Lemma 3.1 *Let G be a graph with n vertices and general Randić matrix $\boldsymbol{R}_\alpha$. Then*

$$\begin{aligned} tr(\boldsymbol{R}_\alpha) &= 0, \\ tr(\boldsymbol{R}_\alpha^2) &= 2\sum_{i\sim j}(d_i d_j)^{2\alpha}, \\ tr(\boldsymbol{R}_\alpha^3) &= 2\sum_{i\sim j}(d_i d_j)^{2\alpha}\sum_{k\sim i,k\sim j} d_k^{2\alpha}, \\ tr(\boldsymbol{R}_\alpha^4) &= \sum_{i=1}^{n}(\sum_{i\sim j}(d_i d_j)^{2\alpha})^2 + \sum_{i\neq j}(d_i d_j)^{2\alpha}(\sum_{k\sim i,k\sim j} d_k^{2\alpha})^2. \end{aligned}$$

Proof. By definition, the diagonal elements of $\mathbf{R}_\alpha$ are equal to zero. Therefore the trace of $\mathbf{R}_\alpha$ is zero.

Next, we calculate the matrix $\mathbf{R}_\alpha^2$. For $i = j$,

$$(\mathbf{R}_\alpha^2)_{ii} = \sum_{j=1}^{n}(\mathbf{R}_\alpha)_{ij}(\mathbf{R}_\alpha)_{ji} = \sum_{j=1}^{n}(\mathbf{R}_\alpha)_{ij}^2 = \sum_{i\sim j}(\mathbf{R}_\alpha)_{ij}^2 = \sum_{i\sim j}(d_i d_j)^{2\alpha},$$

whereas for $i \neq j$,

$$(\mathbf{R}_\alpha^2)_{ij} = \sum_{k=1}^{n}(\mathbf{R}_\alpha)_{ik}(\mathbf{R}_\alpha)_{kj} = \sum_{k\sim i,k\sim j}(\mathbf{R}_\alpha)_{ik}(\mathbf{R}_\alpha)_{kj} = (d_i d_j)^\alpha \sum_{k\sim i,k\sim j} d_k^{2\alpha}.$$

Therefore

$$tr(\mathbf{R}_\alpha^2) = \sum_{i=1}^{n}(\mathbf{R}_\alpha^2)_{ii} = \sum_{i=1}^{n}\sum_{i\sim j}(d_i d_j)^\alpha = 2\sum_{i\sim j}(d_i d_j)^{2\alpha}.$$

The diagonal elements of $\mathbf{R}_\alpha^3$ are

$$(\mathbf{R}_\alpha^3)_{ii} = \sum_{j=1}^{n}(\mathbf{R}_\alpha)_{ij}(\mathbf{R}_\alpha^2)_{ji} = \sum_{j\sim i}(d_i d_j)^\alpha(\mathbf{R}_\alpha^2)_{ij} = \sum_{i\sim j}(d_i d_j)^{2\alpha}\sum_{k\sim i,k\sim j} d_k^{2\alpha},$$

so we obtain

$$tr(\mathbf{R}_\alpha^3) = \sum_{i=1}^{n} (\mathbf{R}_\alpha^3)_{ii} = \sum_{i=1}^{n} (\sum_{i\sim j} (d_i d_j)^{2\alpha} \sum_{k\sim i, k\sim j} d_k^{2\alpha}) = 2\sum_{i\sim j} (d_i d_j)^{2\alpha} \sum_{k\sim i, k\sim j} d_k^{2\alpha}.$$

We calculate $tr(\mathbf{R}_\alpha^4)$ by using Frobenius norm $(||.||_F)$. Since $tr(\mathbf{R}_\alpha^4) = ||\mathbf{R}_\alpha^2||_F$, we have that

$$\begin{aligned} tr(\mathbf{R}_\alpha^4) &= \sum_{i,j=1}^{n} |(\mathbf{R}_\alpha^2)_{ij}|^2 \\ &= \sum_{i=j} |(\mathbf{R}_\alpha^2)_{ij}|^2 + \sum_{i\neq j} |(\mathbf{R}_\alpha^2)_{ij}|^2 \\ &= \sum_{i=1}^{n} (\sum_{i\sim j} (d_i d_j)^{2\alpha})^2 + \sum_{i\neq j} (d_i d_j)^{2\alpha} (\sum_{k\sim i, k\sim j} d_k^{2\alpha})^2. \end{aligned}$$

The proof is complete. ■

Theorem 3.2 *Let G be a graph with n vertices. Then*

$$RE_\alpha(G) \leq \sqrt{2n \sum_{i\sim j} (d_i d_j)^\alpha}. \tag{3}$$

Equality is attained if and only if G is the graph without edges, or if all its vertices have degree one.

Proof. The variance of the numbers $|\rho_i^{(\alpha)}|$, $i = 1, 2, \ldots, n$, denoted by $Var(\rho)$, is equal to

$$\frac{1}{n} \sum_{i=1}^{n} |\rho_i^{(\alpha)}|^2 - (\frac{1}{n} \sum_{i=1}^{n} |\rho_i^{(\alpha)}|)^2.$$

It is well-known that $Var(\rho) \geq 0$, and equality is attained if and only if $|\rho_1^{(\alpha)}| = |\rho_2^{(\alpha)}| = \ldots = |\rho_n^{(\alpha)}|$. By the definition of general Randić energy, we have that

$$\frac{1}{n} tr(\mathbf{R}_\alpha^2) - (\frac{1}{n} RE_\alpha)^2 \geq 0,$$

and so

$$RE_\alpha \leq \sqrt{n tr(\mathbf{R}_\alpha^2)}.$$

Therefore

$$RE_\alpha(G) \leq \sqrt{2n \sum_{i\sim j} (d_i d_j)^\alpha}$$

by using Lemma 3.1.

If G is the graph without edges, or if all its vertices have degree one, the equality in (3) is clearly attained.

Conversely, suppose that $RE_\alpha(G) = \sqrt{2n\sum_{i\sim j}(d_id_j)^\alpha}$. Then we have that $|\rho_1^{(\alpha)}| = |\rho_2^{(\alpha)}| = \ldots = |\rho_n^{(\alpha)}| = k$, for some k. If $k = 0$, then $G \cong \overline{K_n}$ by Lemma 1.2. If $k > 0$, then $Sp_{R_\alpha}(G) = \{k(\frac{n}{2}\text{ times}), -k(\frac{n}{2}\text{ times})\}$. The R_α-spectrum for each component of G is $\{k, -k\}$, and therefore each component of G is isomorphic to K_2.

The proof is complete. ■

Theorem 3.3 *Let G be a graph with n vertices and at least one edge. Then*

$$RE_\alpha(G) \geq 2\sum_{i\sim j}(d_id_j)^{2\alpha}\sqrt{\frac{2\sum_{i\sim j}(d_id_j)^{2\alpha}}{\sum_{i=1}^n(\sum_{i\sim j}(d_id_j)^{2\alpha})^2 + \sum_{i\neq j}(d_id_j)^{2\alpha}(\sum_{k\sim i,k\sim j} d_k^{2\alpha})^2}}.$$

Proof. Our starting point is the Hölder inequality

$$\sum_{i=1}^n a_ib_i \leq (\sum_{i=1}^n a_i^p)^{1/p}(\sum_{i=1}^n b_i^q)^{1/q},$$

which holds for any non-negative real numbers a_i, b_i, $i = 1, 2, \ldots, n$. Setting $a_i = |\rho_i^{(\alpha)}|^{2/3}$, $b_i = |\rho_i^{(\alpha)}|^{4/3}$, $p = 3/2$, and $q = 3$, we obtain

$$\sum_{i=1}^n |\rho_i^{(\alpha)}|^2 = \sum_{i=1}^n |\rho_i^{(\alpha)}|^{2/3}|\rho_i^{(\alpha)}|^{4/3} \leq (\sum_{i=1}^n |\rho_i^{(\alpha)}|)^{2/3}(\sum_{i=1}^n |\rho_i^{(\alpha)}|^4)^{1/3}.$$

Since G has at least one edge, then not all $\rho_i^{(\alpha)}$'s are equal to zero, and so $\sum_{i=1}^n |\rho_i^{(\alpha)}|^4 \neq 0$. We then have that $RE_\alpha(G) = \sum_{i=1}^n |\rho_i^{(\alpha)}| \geq \sqrt{\frac{(\sum_{i=1}^n |\rho_i^{(\alpha)}|^2)^3}{\sum_{i=1}^n |\rho_i^{(\alpha)}|^4}} = \sqrt{\frac{(tr(\mathbf{R}_\alpha^2))^3}{tr(\mathbf{R}_\alpha^4)}}$. By using Lemma 3.1, we obtain

$$RE_\alpha(G) \geq 2\sum_{i\sim j}(d_id_j)^{2\alpha}\sqrt{\frac{2\sum_{i\sim j}(d_id_j)^{2\alpha}}{\sum_{i=1}^n(\sum_{i\sim j}(d_id_j)^{2\alpha})^2 + \sum_{i\neq j}(d_id_j)^{2\alpha}(\sum_{k\sim i,k\sim j} d_k^{2\alpha})^2}}.$$

■

Theorem 3.4 *If the graph G is regular of degree r, $r > 0$, then $RE_\alpha(G) = r^{2\alpha}E(G)$. If, in addition $r = 0$, then $RE_\alpha(G) = 0$.*

Proof. If $r = 0$, then $G \cong \overline{K_n}$. From Lemma 1.2, we know that $RE_\alpha(G) = 0$.

Suppose now that G is regular of degree $r > 0$, that is $d_1 = d_2 = \ldots = d_n = r$. Then all non-zero terms in $\mathbf{R}_\alpha(G)$ are equal to $r^{2\alpha}$. This implies that $\mathbf{R}_\alpha(G) = r^{2\alpha}\mathbf{A}(G)$. Then we have $\rho_i^{(\alpha)} = r^{2\alpha}\lambda_i$, and therefore $RE_\alpha(G) = r^{2\alpha}E(G)$. ■

4 Lower bounds for general Randić spectral radius of a connected graph

Before we give several lower bounds for the general Randić spectral radius of a connected graph, we need some auxiliary definitions.

Definition 4.1 *Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and general Randić matrix $\boldsymbol{R}_\alpha$. Then the Randić α-degree of v_i, denoted by $R_i^{(\alpha)}$, is defined as*

$$R_i^{(\alpha)} = \sum_{j=1}^{n} (\boldsymbol{R}_\alpha)_{ij}.$$

Definition 4.2 *Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and general Randić matrix $\boldsymbol{R}_\alpha$. Then the second Randić α-degree of v_i, denoted by $S_i^{(\alpha)}$, is defined as*

$$S_i^{(\alpha)} = \sum_{j=1}^{n} (\boldsymbol{R}_\alpha)_{ij} R_j^{(\alpha)}.$$

From the definition of $R_i^{(\alpha)}$, it is easy to get the following proposition.

Proposition 4.1 *Let G be a graph with n vertices. Let $\{R_1^{(\alpha)}, R_2^{(\alpha)}, \cdots, R_n^{(\alpha)}\}$ be its general Randić α-degree sequence, and $R_\alpha(G)$ be the general Randić index of G. Then*

$$\sum_{i=1}^{n} R_i^{(\alpha)} = 2R_\alpha(G).$$

The following lower bounds for $\rho_1^{(\alpha)}$ are analogous to results on lower bounds for $\rho_1^{(-\frac{1}{2})}$ given in [3].

Theorem 4.1 *Let G be a simple connected graph with n vertices and let $R_\alpha(G)$ be its general Randić index. Then*

$$\rho_1^{(\alpha)} \geq \frac{2R_\alpha(G)}{n}. \tag{4}$$

The equality holds in (4) if and only if

$$R_1^{(\alpha)} = R_2^{(\alpha)} = \cdots = R_n^{(\alpha)}.$$

Proof. Let $X = \frac{1}{\sqrt{n}}(1, \cdots, 1)^t$. Applying the Rayleigh principle to general Randić matrix $\mathbf{R}_\alpha$ of G, we obtain

$$\begin{aligned} \rho_1^{(\alpha)} &\geq \frac{X^t \mathbf{R}_\alpha X}{X^t X} = \frac{\frac{1}{\sqrt{n}}(R_1^{(\alpha)}, \cdots, R_n^{(\alpha)})\frac{1}{\sqrt{n}}(1, \cdots, 1)^t}{1} \\ &= \frac{1}{n}\sum_{i=1}^{n} R_n^{(\alpha)} = \frac{2R_\alpha(G)}{n}. \end{aligned}$$

Now we suppose that the equality holds. Then X is the eigenvector corresponding to $\rho_1^{(\alpha)}$, i.e., $\mathbf{R}_\alpha X = \rho_1^{(\alpha)} X$. This implies that $R_i^{(\alpha)} = \rho_1^{(\alpha)}$ for all i. Conversely, suppose that G satisfies that $R_1^{(\alpha)} = R_2^{(\alpha)} = \cdots = R_n^{(\alpha)} = k$, for some k. Then $\sum\limits_{i=1}^{n} R_i^{(\alpha)} = nk = 2R_\alpha(G)$. So $k = \frac{2R_\alpha(G)}{n}$. By the Perron-Frobenius theorem, k is the greatest and simple eigenvalue of $\mathbf{R}_\alpha$. Hence, $\rho_1^{(\alpha)} = k = \frac{2R_\alpha(G)}{n}$. This completes the proof. ■

Theorem 4.2 *Let G be a simple connected graph on the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and let $R_i^{(\alpha)}$ be the general Randić α-degree of v_i. Then*

$$\rho_1^{(\alpha)} \geq \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(R_i^{(\alpha)}\right)^2}. \tag{5}$$

The equality holds in (5) if and only if

$$R_1^{(\alpha)} = R_2^{(\alpha)} = \cdots = R_n^{(\alpha)}.$$

Proof. Let $\mathbf{R}_\alpha$ be the general Randić matrix of G and $X = (x_1, \cdots, x_n)^t$ be the unit positive Perron eigenvector of $\mathbf{R}_\alpha$ corresponding to $\rho_1^{(\alpha)}$. We take $C = \frac{1}{\sqrt{n}}(1, \cdots, 1)^t$. Since C is a unit positive vector, we have

$$\rho_1^{(\alpha)} = \sqrt{\rho_1(\mathbf{R}_\alpha^2)} = \sqrt{X^t \mathbf{R}_\alpha^2 X} \geq \sqrt{C^t \mathbf{R}_\alpha^2 C},$$

where $\rho_1(\mathbf{R}_\alpha^2)$ denotes the greatest eigenvalue of $\mathbf{R}_\alpha^2$. Since

$$\mathbf{R}_\alpha C = \frac{1}{\sqrt{n}}((R_1^{(\alpha)}, \cdots, R_n^{(\alpha)}))^t,$$

we get that

$$\rho_1^{(\alpha)} \geq \sqrt{C^t \mathbf{R}_\alpha^2 C} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(R_i^{(\alpha)}\right)^2}.$$

Now we suppose that the equality holds. Then C is the eigenvector corresponding to $\rho_1^{(\alpha)}$, i.e., $\mathbf{R}_\alpha X = \rho_1^{(\alpha)} X$. This implies that $R_i^{(\alpha)} = \rho_1^{(\alpha)}$ for all i. Conversely, suppose that G satisfies that $R_1^{(\alpha)} = R_2^{(\alpha)} = \cdots = R_n^{(\alpha)} = k$, for some k. Then $k = \sqrt{\frac{nk^2}{n}} = \sqrt{\frac{1}{n} \sum\limits_{i=1}^{n} \left(R_i^{(\alpha)}\right)^2}$. From the Perron-Frobenius theorem, k is the greatest and simple eigenvalue of $\mathbf{R}_\alpha$. Then we have $\rho_1^{(\alpha)} = k$. ■

Before we obtain another lower bound for $\rho_1^{(\alpha)}$, we define a sequence ${L_i}^{(\alpha,1)}, {L_i}^{(\alpha,2)}, \cdots, {L_i}^{(\alpha,p)}, \cdots$ for every vertex v_i, where $p \in \mathbb{N}$. Let ${L_i}^{(\alpha,1)} = \left(R_i^{(\alpha)}\right)^a$, where $a \in \mathbb{R}$, and for $p \geq 2$,

$${L_i}^{(\alpha,p)} = \sum_{i \sim j} (d_i d_j)^\alpha {L_j}^{(\alpha,p-1)}.$$

Theorem 4.3 *Let G be a simple connected graph, a be a real number, and p be an integer. Then*

$$\rho_1^{(\alpha)} \geq \sqrt{\frac{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p+1)} \right)^2}{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p)} \right)^2}}. \tag{6}$$

The equality holds in (6) if and only if

$$\frac{{L_1}^{(\alpha,p+1)}}{{L_1}^{(\alpha,p)}} = \frac{{L_2}^{(\alpha,p+1)}}{{L_2}^{(\alpha,p)}} = \cdots = \frac{{L_n}^{(\alpha,p+1)}}{{L_n}^{(\alpha,p)}}.$$

Proof. Let $\mathbf{R}_\alpha$ be the general Randić matrix of G and $X = (x_1, \cdots, x_n)^t$ be the unit positive Perron eigenvector of $\mathbf{R}_\alpha$ corresponding to $\rho_1^{(\alpha)}$. We take $C = \frac{1}{\sqrt{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p)} \right)^2}} (1, \cdots, 1)^t$.

Since C is a unit positive vector, we have

$$\rho_1^{(\alpha)} = \sqrt{\rho_1(\mathbf{R}_\alpha^2)} = \sqrt{X^t \mathbf{R}_\alpha^2 X} \geq \sqrt{C^t \mathbf{R}_\alpha^2 C}.$$

Since

$$\mathbf{R}_\alpha C = \frac{1}{\sqrt{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p)} \right)^2}} ((L_1^{(\alpha,p+1)}, \cdots, L_n^{(\alpha,p+1)}))^t,$$

$$\rho_1^{(\alpha)} \geq \sqrt{C^t \mathbf{R}_\alpha^2 C} = \sqrt{\frac{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p+1)} \right)^2}{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p)} \right)^2}}.$$

Now we suppose that the equality holds. Then we get that C is the eigenvector corresponding to $\rho_1^{(\alpha)}$, i.e., $\mathbf{R}_\alpha X = \rho_1^{(\alpha)} X$. This implies that $\frac{{L_i}^{(\alpha,p+1)}}{{L_i}^{(\alpha,p)}} = \rho_1^{(\alpha)}$ for all i. Conversely, suppose that G satisfies that $\frac{{L_1}^{(\alpha,p+1)}}{{L_1}^{(\alpha,p)}} = \frac{{L_2}^{(\alpha,p+1)}}{{L_2}^{(\alpha,p)}} = \cdots = \frac{{L_n}^{(\alpha,p+1)}}{{L_n}^{(\alpha,p)}} = k$, for some k. Then $k = \sqrt{\frac{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p+1)} \right)^2}{\sum\limits_{i=1}^{n} \left({L_i}^{(\alpha,p)} \right)^2}}$. From the Perron-Frobenius theorem, k is the greatest and simple eigenvalue of $\mathbf{R}_\alpha$. Then we have $\rho_1^{(\alpha)} = k$. ■

By setting $a = 1$ and $p = 1$ in (6), Corollary 4.4 directly follows.

Corollary 4.4 *Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, general Randić α-degree sequence $\{R_1^{(\alpha)}, R_2^{(\alpha)}, \cdots, R_n^{(\alpha)}\}$, and second general Randić α-degree sequence $\{S_1^{(\alpha)}, S_2^{(\alpha)}, \cdots, S_n^{(\alpha)}\}$. Then*

$$\rho_1^{(\alpha)} \geq \sqrt{\frac{\sum\limits_{i=1}^{n} (S_i^{(\alpha)})^2}{\sum\limits_{i=1}^{n} (R_i^{(\alpha)})^2}}. \tag{7}$$

The equality holds in (7) if and only if

$$\frac{S_1^{(\alpha)}}{R_1^{(\alpha)}} = \cdots = \frac{S_n^{(\alpha)}}{R_n^{(\alpha)}}.$$

The next lemma will help us to find the best lower bounds among lower bounds given in (4), (5), (7).

Lemma 4.5 *Let G be a graph on n vertices. Then*

$$\sum_{i=1}^{n} S_i^{(\alpha)} = \sum_{i=1}^{n} (R_i^{(\alpha)})^2.$$

Proof. By the definitions given previously, along with the associative law of matrix multiplication, we obtain

$$\begin{aligned} S_1^{(\alpha)} + \cdots + S_n^{(\alpha)} &= (1, \cdots, 1)(\mathbf{R}_\alpha (R_1^{(\alpha)}, R_2^{(\alpha)}, \cdots, R_n^{(\alpha)})^t) \\ &= ((1, \cdots, 1)\mathbf{R}_\alpha)(R_1^{(\alpha)}, R_2^{(\alpha)}, \cdots, R_n^{(\alpha)})^t \\ &= (R_1^{(\alpha)})^2 + \cdots + (R_n^{(\alpha)})^2. \end{aligned}$$

■

Theorem 4.6 *The lower bound for $\rho_1^{(\alpha)}$ given in (7) improves the lower bounds given in (4), (5).*

Proof. By the Cauchy-Schwarz inequality and Lemma 4.5, we have

$$\begin{aligned} \sqrt{\frac{\sum_{i=1}^{n} (S_i^{(\alpha)})^2}{\sum_{i=1}^{n} (R_i^{(\alpha)})^2}} &\geq \sqrt{\frac{(\sum_{i=1}^{n} S_i^{(\alpha)})^2}{n \sum_{i=1}^{n} (R_i^{(\alpha)})^2}} = \sqrt{\frac{(\sum_{i=1}^{n} (R_i^{(\alpha)})^2)^2}{n \sum_{i=1}^{n} (R_i^{(\alpha)})^2}} \\ &= \sqrt{\frac{\sum_{i=1}^{n} (R_i^{(\alpha)})^2}{n}} \geq \sqrt{\frac{(\sum_{i=1}^{n} R_i^{(\alpha)})^2}{n^2}} = \frac{2R_\alpha(G)}{n}. \end{aligned}$$

Thus completes the proof. ■

5 Upper bound for Randić energy

In this section, we present an upper bound for Randić energy, i.e., we give an upper bound for general Randić energy when $\alpha = -1/2$. And we characterize those graphs for which this bound is sharp. For convenience, in this section, we omit α in corresponding notation.

The following theorem will help us obtain an upper bound for Randić energy. The proof is similar to the proof of Theorem 2.2 given in [12].

Theorem 5.1 *Let G be a connected graph of order n. Suppose G has minimum vertex degree δ. Then*

$$R_{-1}(G) \leq \frac{n}{2\delta}.$$

Equality occurs if and only if G is a regular graph.

Proof. This follows directly from the Cauchy-Schwarz inequality.

$$R_{-1}(G) = \sum_{u\sim v} [d(u)d(v)]^{-1} \leq \sum_{u\sim v} [d(u)^{-2} + d(v)^{-2}]/2 = \sum_{v\in V} d(v)^{-1}/2 \leq n\delta^{-1}/2,$$

with equality if and only if G is regular. ■

To characterize the extremal graphs achieving our upper bound, let us recall the concept of strong regular graphs. Let x and y be any two distinct vertices of a graph and let $n(x, y)$ denote the number of vertices adjacent to both x and y. A regular graph G with n vertices and positive degree r, not the complete graph, is called *strongly regular* with parameters (n, r, e, f) if there exist non-negative integers e and f such that $n(x, y) = e$ for each pair of adjacent vertices x, y and $n(x, y) = f$ for each pair of (distinct) non-adjacent vertices x, y of G. It is easy to see that a strong regular graph is connected if $f > 0$.

The following theorem describes the properties of eigenvalues of a strong regular graph.

Theorem 5.2 *[5] A regular connected graph G of degree r is strongly regular if and only if it has exactly three distinct eigenvalues $\lambda_1 = r$, λ_2, λ_3. If G is strongly regular, then $e = r + \lambda_2\lambda_3 + \lambda_2 + \lambda_3$ and $f = r + \lambda_2\lambda_3$.*

Now we give an upper bound for RE in terms of n and minimum degree δ.

Theorem 5.3 *Let G be a connected graph with n vertices, and $\delta > 1$ be its minimum degree. Then*

$$RE(G) \leq 1 + \sqrt{(n-1)\left(\frac{n}{\delta} - 1\right)}.$$

The equality holds if and only if $G \cong K_n$ or G is a strongly regular graph with parameters $(n, \delta, \delta - \frac{\delta(n-\delta)}{n-1}, \delta - \frac{\delta(n-\delta)}{n-1})$.

Proof. Let $\rho_1 \geq \rho_2 \geq \ldots \geq \rho_n$ be the Randić eigenvalues of G. We have $\sum\limits_{i=1}^{n} \rho_i = 0$, $\sum\limits_{i=1}^{n} |\rho_i| = RE(G)$, and $\sum\limits_{i=1}^{n} {\rho_i}^2 = 2\sum\limits_{i\sim j} \frac{1}{d_i d_j}$. By the Cauchy-Schwarz inequality we get that

$$\sum_{i=2}^{n} |\rho_i| \leq \sqrt{(n-1)\sum_{i=2}^{n} {\rho_i}^2} = \sqrt{(n-1)\left(2\sum_{i\sim j}\frac{1}{d_i d_j} - {\rho_1}^2\right)}. \tag{8}$$

Note that $\rho_1 \geq 0$, therefore,

$$RE(G) \leq \rho_1 + \sqrt{(n-1)\left(2\sum_{i\sim j}\frac{1}{d_i d_j} - {\rho_1}^2\right)}.$$

In [6], the authors proved that if G possesses at least one edge, then $\rho_1 = 1$. And since $R_{-1}(G) = \sum\limits_{i\sim j}\frac{1}{d_i d_j}$, we have

$$RE(G) \leq 1 + \sqrt{(n-1)\left(2R_{-1}(G) - 1\right)}.$$

Combining with Theorem 5.1, we obtain that

$$RE(G) \leq 1 + \sqrt{(n-1)\left(\frac{n}{\delta} - 1\right)}.$$

Now suppose that the equality holds. From (8), we have

$$|\rho_i| = \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_i d_j} - {\rho_1}^2}{n-1}} = \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_i d_j} - 1}{n-1}},$$

for $i = 2, 3, \cdots, n$. And by Theorem 5.1, G is a δ-regular graph. If $\rho_2, \cdots, \rho_n$ are equal to a same negative number, we have that $G \cong K_n$. Otherwise, we claim that G must be a strong regular graph. Let $\mathbf{R}$ denote the Randić matrix and $\mathbf{A}$ denote the adjacency matrix of G. Note that $\mathbf{R} = \frac{1}{\delta}\mathbf{A}$. Since

$$|\rho_i| = \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_i d_j} - 1}{n-1}} = \sqrt{\frac{2\frac{n\delta}{2}\frac{1}{\delta^2} - 1}{n-1}} = \sqrt{\frac{\frac{n}{\delta} - 1}{n-1}},$$

for $i = 2, 3, \cdots, n$. We have the eigenvalues λ_i of G satisfying

$$|\lambda_i| = \delta\sqrt{\frac{\frac{n}{\delta} - 1}{n-1}},$$

for $i = 2, 3, \cdots, n$. By Theorem 5.2, we know that G is a strong regular graph and the parameters e and f are as follows.

$$e = \delta - \delta^2\frac{\frac{n}{\delta} - 1}{n-1} + \sqrt{\frac{\frac{n}{\delta} - 1}{n-1}} - \sqrt{\frac{\frac{n}{\delta} - 1}{n-1}} = \delta - \frac{\delta(n-\delta)}{n-1},$$

$$f = \delta - \delta^2\frac{\frac{n}{\delta} - 1}{n-1} = \delta - \frac{\delta(n-\delta)}{n-1}.$$

We point out that such strong regular graphs with parameters $(n, \delta, \delta - \frac{\delta(n-\delta)}{n-1}, \delta - \frac{\delta(n-\delta)}{n-1})$ do exist. For example, see [10], the strong regular graph with parameters $(16, 6, 2, 2)$ is such a graph with $n = 16$, $\delta = 6$. Its eigenvalues are 6, 2 (6 times), -2 (9 times). So its Randić eigenvalues are 1, $\frac{1}{3}$ (6 times), $-\frac{1}{3}$ (9 times). Conversely, one can easily see that the equality in Theorem 5.3 holds for the strong regular graphs with parameters $(n, \delta, \delta - \frac{\delta(n-\delta)}{n-1}, \delta - \frac{\delta(n-\delta)}{n-1})$. ■

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