Some Notes on Randić Index

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ABSTRACT: In this paper we establish new inequalities involving Randić index, weighted Randić index and general Randić index in terms of the eigenvalues, the number of edges, the number of vertices, the energy and vertex degrees.

Key Words: Randić index, Weighted graph, Eigenvalues.

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1. Introduction

Randić index is one of the most important tools of graph theory with applications in Mathematics, Physics and Chemistry. This graph theoretical index is invented by Milan Randić in [10]. He defined a molecular structure descriptor and composed a new summation using degrees of vertices. By $d_i$, we denote the degree of the vertex $v_i$ in $G$. Randić index of a graph $G$ is defined by

$$ R = R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}} $$

where summation goes over all pairs of adjacent vertices of the underlying (molecular) graph.

Some bounds are reported for Randić index in [10]. These bounds are obtained in a triangle-free graph. In [7], Randić index is investigated for molecular graphs and it is calculated for some graph classes in [8]. Considering the fact that these studies can be extended to the weighted graphs, new inequalities for weighted Randić index of a graph are obtained in this work. In [1], additively weighted Harary index of some composite graphs is formulated. We establish the weighted Randić index of some composite graphs in this study. Also, some special bounds are found for the energy of graphs in [3] and [4]. Using these results, some definitions and results for Randić index of weighted graphs are obtained. In addition, general Randić index is defined and some bounds for this index are given.

2. Preliminaries

Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The symmetric square matrix $R = R(G)$ of order $n$ defined by

$$ R_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_i \sim v_j \\ 0 & \text{otherwise} \end{cases} $$

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is called the Randić matrix of the graph $G$. Graph operations enable us to calculate some property of a large graph in terms of some smaller graphs. Some fundamental information about the graph operations and their properties can be found in [6], [2], [11] and [12]. In the third section, we introduce new inequalities about the weighted Randić index of some graph operations. We also generalize Randić index and we give some bounds related to this new generalized index. We define the weighted Randić matrix and weighted Randić energy and obtain an upper bound for the second greatest eigenvalue $\rho_2^G$ of the weighted Randić matrix.

The Randić energy of a graph $G$ is defined by

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i|,$$

where $\rho_1, \rho_2, \cdots, \rho_n$ are the eigenvalues of its Randić matrix. We recall the following result:

Lemma 2.1. [5] If $0 < n_1 \leq a_j \leq N_1$ and $0 < n_2 \leq b_j \leq N_2$, then

$$\left(\sum_{j=1}^{k} a_j^2 \right)^{1/2} \left(\sum_{j=1}^{k} b_j^2 \right)^{1/2} \leq \frac{1}{2} \left( \sqrt{\frac{N_1 N_2}{n_1 n_2}} + \sqrt{\frac{n_1 n_2}{N_1 N_2}} \right) \sum_{j=1}^{k} a_j b_j$$

for $1 \leq j \leq k$.

3. Main Results

3.1. Randić Index of Graph Operations

A weighted Randić index is obtained by adding a weight to each edge that is defined in [6] as follows:

Let $G$ be a simple, connected and weighted graph having $n$ vertices. Let each edge of $G$ be weighted with positive real numbers. The weighted Randić index $R^w = R^w(G)$ of $G$ is defined as follows:

$$R^w = R^w(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{w(u)w(v)}}$$

where $w(u)$ is the sum of the weights on $u$ and $w(v)$ is the sum of the weights on $v$, that is, $w(u) = \sum_{i=1}^{n} t_i$, $t_i$ are the weights for $i = 1, 2, \cdots, n$ and $w(v) = \sum_{j=1}^{n} c_j$, $c_j$ are the weights for $j = 1, 2, \cdots, n$.

We now recall some graph operations we shall need in this paper. Such operations help us to Let $G$ and $H$ be two simple graphs. The sum $G+H$ of these two graphs is defined as the graph having the vertex set $V(G+H) = V(G) \cup V(H)$ and the edge set $E(G+H) = E(G) \cup E(H) \cup \{(u, v) \mid u \in V(G), v \in V(H)\}$.

The composition of two graphs $G$ and $H$ is denoted by $G[H]$ and it is the graph with vertex set $V(G[H]) = V(G) \times V(H)$ and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ are adjacent in $G[H]$ if $(u_1$ is adjacent to $v_1)$ or $(u_1 = v_1$ and $u_2$ and $v_2$ are adjacent in $H$). It is obtained by connecting every vertex of $G$ into a copy of $H$ and replace every edge of $G$ by all possible edges between the copies of $H$ that arose from its end-vertices.

The cartesian product $G \times H$ is the graph with vertex set $V(G \times H) = V(G) \times V(H)$; the vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G \times H$ are adjacent if and only if $[u_1 = v_1, u_2 v_2 \in E(H)]$ or $[u_2 = v_2, u_1 v_1 \in E(G)]$.

The symmetric difference $G \oplus H$ of $G$ and $H$ is the graph having vertex set $V(G) \times V(H)$ and edge set

$$E(G \oplus H) = \{(u_1, u_2)(v_1, v_2) \mid u_1 v_1 \in E(G) \text{ or } u_2 v_2 \in E(H) \text{ but not both}\}.$$
The union $G = G \cup H$ of graphs $G$ and $H$ with vertex sets $V(G)$, $V(H)$ and edge sets $E(G)$, $E(H)$ is the graph such that $V(G \cup H) = V(G) \cup V(H)$ and $E(G \cup H) = E(G) \cup E(H)$.

We can now calculate some indices:

**Theorem 3.1.** Let $G$ and $H$ be two simple weighted graphs. Then the weighted Randić index of the sum of $G$ and $H$ is

$$R^w(G + H) = \sum_{i,j \in V(G), i \in E(G)} \frac{1}{\sqrt{(w(i) + \sum_{k \in V(G)} w(k)) \times (w(j) + \sum_{k \in V(G)} w(k))}} \sum_{i,j \in E(H)} \frac{1}{\sqrt{(w(i) + \sum_{t \in V(H)} w(t)) \times (w(j) + \sum_{t \in V(H)} w(t))}} \sum_{i \in V(G), j \in V(H)} \frac{1}{\sqrt{(w(i) + \sum_{k \in V(G)} w(k)) \times (w(j) + \sum_{t \in V(H)} w(t))}}.$$

**Proof.** Let $V = V(G) \cup V(H)$, $E = E(G) \cup E(H) \cup \{(u_1, u_2) \mid u_1 \in V(G), u_2 \in V(H)\}$. We partition the set of pairs of vertices of $G + H$ to obtain the following three sums denoted by $S_1$, $S_2$, $S_3$, respectively. Firstly, for each sum, we consider $w_i$ as the sum of the weights in each vertex $i$. In $S_1$, we collect all pairs of vertices $i$ and $j$ so that $i, j$ are in $V(G)$ and $ij$ is in $E(G)$. Hence, $i$ and $j$ are adjacent vertices in $E(G)$. For $S_1$, we obtain,

$$S_1 = \sum_{i,j \in V(G), i \in E(G)} \frac{1}{\sqrt{(w(i) + \sum_{k \in V(G)} w(k)) \times (w(j) + \sum_{k \in V(G)} w(k))}}.$$

For the second sum $S_2$, we take the vertices $i$ and $j$ in $V(H)$ so that $ij$ is in $E(H)$. Hence,

$$S_2 = \sum_{i,j \in V(H), i \in E(H)} \frac{1}{\sqrt{(w(i) + \sum_{t \in V(H)} w(t)) \times (w(j) + \sum_{t \in V(H)} w(t))}}.$$

In the third sum $S_3$, $i$ is taken in $V(G)$ and $j$ is in $V(H)$. So,

$$S_3 = \sum_{i \in V(G), j \in V(H)} \frac{1}{\sqrt{(w(i) + \sum_{k \in V(G)} w(k)) \times (w(j) + \sum_{t \in V(H)} w(t))}}.$$

The result now follows by adding the three contributions and simplifying the resulting expression. □

Similarly, the weighted Randić indices of some other operations are obtained as follows:

**Theorem 3.2.** Let $G$ and $H$ be two simple weighted graphs with edge sets $E(G)$ and $E(H)$ and vertex sets $V(G)$ and $V(H)$, respectively. The weighted Randić indices of the composition, symmetric difference, cartesian product and union of graphs $G$ and $H$ are respectively given by

$$R^w(G[H]) = \sum_{i \in G, j \in H} \frac{1}{\sqrt{2w(i) + 2w(j) - w(ij)}},$$

$$R(G[H]) = \sum_{e \in E(G) \cap E(H)} \frac{1}{\sqrt{(d(i) - t)(d(j) - t)}} + \sum_{i, k \in V(G) \cap V(H), i, k \notin E(G) \cap E(H)} \frac{1}{\sqrt{(d_G(i) + d_H(i))(d(k) - t)}} + \sum_{ij \notin V(G) \cap V(H)} \frac{1}{\sqrt{d(i)d(j)}},$$
\[ R(G \times H) = \sum_{(u_1, u_2)(v_1, v_2) \in V(G) \times V(H)} \frac{1}{\sqrt{(d(u_1) + d(u_2))(d(v_1) + d(v_2))}} \]

and

\[ R(G \cup H) = \sum_{(i, j) \in V} \frac{1}{\sqrt{d(i) + d(j) + 2}} \]

Proof. We denote by \( w(i) \) the sum of the weights in each vertex \( i \). For each vertex \( i \) of \( G \), we name the corresponding copy of \( H \) by \( H_i \). If two vertices \( i, j \) of \( G \) are adjacent, then every pair of vertices of \( H_i \) and \( H_j \) are adjacent, too. Hence,

\[ R^w(G \circ H) = \sum_{i, j \in H} \frac{1}{\sqrt{2w(i) + 2w(j) - w(ij)}} \]

Secondly, let \( V = V(G) \cup V(H) \), \( E = E(G) \cup E(H) - E(G) \cap E(H) \). Let \( |E(G) \cap E(H)| = t \). We partition this sum into three sums \( S_1 \), \( S_2 \) and \( S_3 \) as follows: The first one \( S_1 \) runs over all pairs of \( e_{ij} \) in \( E(G) \cap E(H) \) for each vertex pair \( i, j \) in \( V(G) \cap V(H) \). Hence,

\[ S_1 = \sum_{e_{ij} \in E(G) \cap E(H)} \frac{1}{\sqrt{(d(i) - t)(d(j) - t)}} \]

The second one \( S_2 \) is over all pairs \( ik \) such that \( ik \) is not in \( E(G) \cap E(H) \) for \( i, k \) in \( V(G) \cap V(H) \). Hence,

\[ S_2 = \sum_{i, k \in V(G) \cap V(H), i, k \notin E(G) \cap E(H)} \frac{1}{\sqrt{(d_G(i) + d_H(i))(d(k) - t)}} \]

The third one \( S_3 \) is over all pairs \( ij \) such that \( ij \) is not in \( V(G) \cap V(H) \) for each vertex \( i, j \) in \( V(G) \cup V(H) \). Hence,

\[ S_3 = \sum_{ij \notin V(G) \cap V(H)} \frac{1}{\sqrt{d(i)d(j)}} \]

Now the result follows. The third and fourth indices follow by the definitions of the operations. \( \square \)

### 3.2. On The General Randić Index

In this section, we obtain inequalities giving upper and lower bounds for general Randić index of a graph \( G \) which is defined by

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

for \( \alpha \in \mathbb{R} \). We first have

**Theorem 3.3.** Let \( G \) be a nontrivial connected graph and let \( a, b \in \mathbb{R} \). Then,

\[ k_{a, b} \sqrt{R_{a+b}(G)R_{a-b}(G)} \leq R_a(G) \leq \sqrt{R_{a+b}(G)R_{a-b}(G)} \]

with \( k_{a, b} := \min \left\{ \frac{2(\Delta \delta)^b}{\Delta^2 b + \delta^2 b}, \frac{2(\Delta \delta)^a}{\Delta^2 a + \delta^2 a} \right\} = \begin{cases} \frac{2(\Delta \delta)^b}{\Delta^2 b + \delta^2 b} & \text{if } |a| \geq |b| \\ \frac{2(\Delta \delta)^a}{\Delta^2 a + \delta^2 a} & \text{if } |a| < |b| \end{cases} \)
3.3. The Eigenvalues of Randić Matrix

In this section we will define and study the weighted Randić matrix and correspondingly, the weighted Randić energy of a graph. Also, we will establish a bound in terms of the weighted Randić energy and the eigenvalues of the weighted Randić matrix.

**Definition 3.1.** Let $G$ be a simple, connected and weighted graph. The weighted Randić matrix $WR = WR(G)$ of $G$ is defined by

$$WR_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_i \sim v_j \\ 0 & \text{otherwise} \end{cases}$$

and the weighted Randić eigenvalues $\rho^w_1, \rho^w_2, \cdots, \rho^w_n$ are defined as the eigenvalues of the Randić matrix $WR$. 

**Proof.** Cauchy-Schwarz inequality gives

$$\sum_{i \sim j} (d_i d_j)^a = \sum_{i \sim j} (d_i d_j)^{\left(\frac{a+b}{2}\right)} \leq \sum_{i \sim j} \left((d_i d_j)^{a+b}\right)^{\frac{1}{2}} \sum_{i \sim j} \left((d_i d_j)^{(a-b)}\right)^{\frac{1}{2}}$$

$$= \sqrt{R_{a+b}(G)R_{a-b}(G)},$$

which proves the second inequality. For the first expression, we have four cases: $a + b \geq 0$, $a + b \leq 0$, $a - b \geq 0$ and $a - b \leq 0$. If $a + b \geq 0$, then $\delta^{a+b} \leq \left((d_i d_j)^{\frac{a+b}{2}}\right) \leq \Delta^{a+b}$. If $a + b \leq 0$, then $\Delta^{a+b} \leq \left((d_i d_j)^{\frac{a+b}{2}}\right) \leq \delta^{a+b}$. If $a - b \geq 0$, then $\delta^{a-b} \leq \left((d_i d_j)^{\frac{a-b}{2}}\right) \leq \Delta^{a-b}$. Finally if $a - b \leq 0$, then $\Delta^{a-b} \leq \left((d_i d_j)^{\frac{a-b}{2}}\right) \leq \delta^{a-b}$. By Lemma 2.1, $(a + b)(a - b) \geq 0$ implying

$$\sum_{i \sim j} \left((d_i d_j)^{\frac{a+b}{2}}\right)^2 \leq \frac{1}{2} \sqrt{\frac{\Delta^{a+b} \Delta^{a-b}}{\delta^{a+b} \delta^{a-b}}} \times \left(\sum_{i \sim j} (d_i d_j)^{\frac{a+b}{2}} \sum_{i \sim j} (d_i d_j)^{\frac{a-b}{2}}\right)$$

and so

$$\sum_{i \sim j} \left((d_i d_j)^{a+b}\right)^{\frac{1}{2}} \left((d_i d_j)^{a-b}\right)^{\frac{1}{2}} \leq \frac{1}{2} \left(\frac{\Delta}{\delta}\right)^a + \left(\frac{\delta}{\Delta}\right)^a \sum_{i \sim j} (d_i d_j)^a.$$

Hence

$$(R_{a+b}(G))^{\frac{1}{2}} (R_{a-b}(G))^{\frac{1}{2}} \leq k_{a,b}(R_a(G)),$$

$$R_a(G) \geq k_{a,b} \sqrt{R_{a+b}(G)R_{a-b}(G)}.$$

If $(a + b)(a - b) < 0$, then,

$$\sum_{i \sim j} \left((d_i d_j)^{a+b}\right)^{\frac{1}{2}} \left((d_i d_j)^{a-b}\right)^{\frac{1}{2}} \leq \frac{1}{2} \left(\frac{\Delta}{\delta}\right)^b + \left(\frac{\delta}{\Delta}\right)^b \sum_{i \sim j} (d_i d_j)^a.$$

Hence,

$$R_a(G) \geq k_{a,b} \sqrt{R_{a+b}(G)R_{a-b}(G)}.$$

□
**Definition 3.2.** Let $G$ be a simple, connected and weighted graph. The weighted Randić energy $RE^w = RE^w(G)$ of $G$ is defined as follows:

$$RE^w = RE^w(G) = \sum_{i=1}^{n} |\rho_i^w|$$

where $\rho_i^w$ are the eigenvalues of the weighted Randić matrix $WR$.

**Theorem 3.4.** Let $G$ be a simple, connected and weighted graph with $n$ vertices. Let $\rho_1^w \geq \rho_2^w \geq \cdots \geq \rho_n^w$ be the eigenvalues of the weighted Randić matrix and $RE^w(G)$ be the weighted Randić energy of $G$. Then,

$$\rho_2^w \leq \sqrt{\frac{2|\rho_1^w|RE^w(G) + 2m}{6}}$$

where $\rho_2^w$ is the second greatest eigenvalue of $WR$.

**Proof.** Let $\rho_1^w, \rho_2^w, \cdots, \rho_n^w$ be the $n$ eigenvalues of $WR$. It is well-known that $\sum_{i=1}^{n} \rho_i^w = 0$ and $\sum_{i=1}^{n}(\rho_i^w)^2 = 2m$ where $m$ is the average of the degrees of the vertices adjacent to $v$. Therefore, $\rho_1^w + \rho_2^w = -\sum_{i=3}^{n} \rho_i^w$. Hence,

$$\rho_2^w \leq |\rho_1^w| + \sum_{i=3}^{n} |\rho_i^w|.$$

If we take the square of both sides, we obtain

$$(\rho_2^w)^2 \leq (\rho_1^w)^2 + 2|\rho_1^w|\sum_{i=3}^{n} \rho_i^w + \sum_{i=3}^{n} (\rho_i^w)^2.$$

By the Cauchy-Schwarz inequality,

$$(\rho_2^w)^2 \leq (\rho_1^w)^2 + 2|\rho_1^w|\sum_{i=3}^{n} |\rho_i^w| + \sum_{i=3}^{n} (\rho_i^w)^2 \leq (\rho_1^w)^2 + 2|\rho_1^w|(|RE^w(G)| - |\rho_2^w|) + 2m - (\rho_2^w)^2.$$

Hence, if we make necessary calculations, we have

$$(\rho_2^w)^2 \leq |\rho_1^w|RE^w(G) - |\rho_2^w|^2 - |\rho_1^w||\rho_2^w| + m.$$

Since $\rho_1^w \geq \rho_2^w$, taking $\rho_1^w = \rho_2^w$ does not effect the inequality:

$$(\rho_2^w)^2 \leq |\rho_1^w|RE^w(G) - |\rho_2^w|^2 - |\rho_2^w||\rho_2^w| + m.$$

Hence,

$$\rho_2^w \leq \sqrt{\frac{|\rho_1^w|RE^w(G) + m}{3}}.$$

**Corollary 3.5.** Let $G$ be a simple, connected, weighted regular graph with $n$ vertices. Let $RE^w(G)$ be the weighted Randić energy of $G$, then

$$\rho_2^w \leq \sqrt{\frac{d_1RE^w(G) + m}{3}}$$

where $\rho_2^w$ is the second greatest eigenvalue of $WR$.

**Proof.** If we apply the Perron-Frobenius Theorem, [2], we obtain $\rho_1^w \leq d_1$. By Theorem 3.4,

$$\rho_2^w \leq \sqrt{\frac{d_1RE^w(G) + m}{3}}.$$

\[\square\]
4. Conclusions

Many studies on the Randić index have been made and many results about this subject have been obtained. However, no study on the weighted Randić index of any kind of graphs existed. We give new inequalities about the weighted Randić index and generalize it to find some bounds related to this index. We define the weighted Randić matrix and relatedly, the weighted Randić energy. Also, we obtain an upper bound for the second greatest eigenvalue $\rho_w$ of the weighted Randić matrix.

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