Bol. Soc. Paran. Mat.
©SPM –ISSN-2175-1188 on line
SPM: www.spm.uem.br/bspm

(3s.) **v. 2022 (40)** : 1–7.
ISSN-0037-8712 in press
doi:10.5269/bspm.47213

Some Notes on Randić Index

Şerife Büyükköse and Ismail Naci Cangul

ABSTRACT: In this paper we establish new inequalities involving Randić index, weigthed 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.

Contents

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 Randic 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

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

2010 *Mathematics Subject Classification:* 05C22, 05C50.
Submitted March 28, 2019. Published May 13, 2019

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 ρ_2^w 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*

$$(\sum_{j=1}^{k} a_j^2)^{\frac{1}{2}} (\sum_{j=1}^{k} b_j^2)^{\frac{1}{2}} \leq \frac{1}{2}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right) \sum_{j=1}^{k} a_j b_j$$

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:

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

where $w(u)$ is the sum of the weights on u and $w(v)$ is the sum of the weights on v, that is, $w(u) = \sum_{i\sim u} t_i$, t_i are the weights for $i = 1,\ 2,\ \cdots,\ n$ and $w(v) = \sum_{j\sim v} c_j$, 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 $[u_1 = v_1,\ u_2v_2 \in E(H)]$ or $[u_2 = v_2,\ u_1v_1 \in E(G)]$.

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

$$E(G \oplus H) = \{(u_1, u_2)(v_1, v_2) \mid u_1v_1 \in E(G) \ \text{ or } \ u_2v_2 \in E(H) \ \text{ but not both}\}.$$

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*

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

.

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,

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

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

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

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*

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

$$\begin{aligned} R(G[H]) &= \sum_{e_{ij}\in E(G)\cap E(H)} \frac{1}{\sqrt{(d(i)-t)(d(j)-t)}} \\ &+ \sum_{i,k\in V(G)\cap V(H), ik\notin E(G)\cap E(H)} \frac{1}{\sqrt{(d_G(i)+d_H(i))(d(k)-t)}} \\ &+ \sum_{ij\notin V(G)\cap V(H)} \frac{1}{\sqrt{d(i)d(j)}}, \end{aligned}$$

$$R(G\times H)=\sum_{(u_1,u_2)(v_1,v_2)\in V=V(G)\times V(H)}\frac{1}{\sqrt{(d(u_1)+d(u_2))(d(v_1)+d(v_2))}},$$

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,

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

Secondly, let $V=V(G)\cup V(H)$, $E=E(G)\cup E(H)-E(G)\cap E(H)$. Let $\mid E(G)\cap E(H)\mid= t$. 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,

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

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. □

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

$$R_\alpha=R_\alpha(G)=\sum_{i\sim j}(d_id_j)^\alpha$$

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,*

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

$$\text{with } k_{a,b}:=min\left\{\frac{2(\Delta\delta)^b}{\Delta^{2b}+\delta^{2b}},\frac{2(\Delta\delta)^a}{\Delta^{2a}+\delta^{2a}}\right\}=\begin{cases}\dfrac{2(\Delta\delta)^b}{\Delta^{2b}+\delta^{2b}} & ;\ \text{if } |a|\ge|b|\\ \dfrac{2(\Delta\delta)^a}{\Delta^{2a}+\delta^{2a}} & ;\ \text{if } |a|<|b|\end{cases}.$$

Proof. Cauchy-Schwarz inequality gives

$$\begin{aligned}\sum_{i\sim j}(d_id_j)^a &= \sum_{i\sim j}(d_id_j)^{\frac{(a+b)}{2}+\frac{(a-b)}{2}}\\ &\leq \sum_{i\sim j}((d_id_j)^{(a+b)})^{\frac{1}{2}}\sum_{i\sim j}((d_id_j)^{(a-b)})^{\frac{1}{2}}\\ &= \sqrt{R_{a+b}(G)R_{a-b}(G)},\end{aligned}$$

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 $\delta^{a+b}\leq (d_id_j)^{\frac{a+b}{2}}\leq \Delta^{a+b}$. If $a+b\leq 0$, then $\Delta^{a+b}\leq (d_id_j)^{\frac{a+b}{2}}\leq \delta^{a+b}$. If $a-b\geq 0$, then $\delta^{a-b}\leq (d_id_j)^{\frac{a-b}{2}}\leq \Delta^{a-b}$. Finally if $a-b\leq 0$, then $\Delta^{a-b}\leq (d_id_j)^{\frac{a-b}{2}}\leq \delta^{a-b}$. By Lemma 2.1, $(a+b)(a-b)\geq 0$ implying

$$\begin{aligned}\sum_{i\sim j}(((d_id_j)^{\frac{a+b}{2}})^2)^{\frac{1}{2}}(((d_id_j)^{\frac{a-b}{2}})^2)^{\frac{1}{2}} &\leq \frac{1}{2}(\sqrt{\frac{\Delta^{a+b}\Delta^{a-b}}{\delta^{a+b}\delta^{a-b}}}+\sqrt{\frac{\delta^{a+b}\delta^{a-b}}{\Delta^{a+b}\Delta^{a-b}}})\times\\ &\quad (\sum_{i\sim j}(d_id_j)^{\frac{a+b}{2}}(d_id_j)^{\frac{a-b}{2}})\end{aligned}$$

and so

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

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,

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

Hence,

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

□

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*

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

and the weighted Randić eigenvalues ρ_1^w, ρ_2^w, $\cdots$, ρ_n^w are defined as the eigenvalues of the Randić matrix WR.

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 ρ_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 ρ_2^w is the second greatest eigenvalue of WR.

Proof. Let ρ_1^w, ρ_2^w, $\cdots$, ρ_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,

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

Hence, if we make necessary calculations, we have

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

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*

$$\rho_2^w \leq \sqrt{\frac{d_1 RE^w(G) + m}{3}}$$

where ρ_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,

$$\rho_2^w \leq \sqrt{\frac{d_1 RE^w(G) + m}{3}}.$$

□

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 ρ_2^w of the weighted Randić matrix.

References

1. Y. Alizadeh, A. Iranmanesh and T. Doslic, *Additively Weighted Harary Index of Some Composite Graphs*, Discrete Mathematics 313, 26-34 (2013).
2. R. B. Bapat, *Graphs and Matrices*, Indian Statistical Institute, New Delhi (2014).
3. K. C. Das, I. Gutman, *Bounds for the Energy of Graphs*, Hacettepe Journal of Mathematics and Statistics 45 (3), 695-703 (2016).
4. I. Gutman and B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac (2008).
5. G. Kaya Gok, *Some Bounds on the Distance-Sum-Connectivity Matrix*, Journal of Inequalities and Applications 171 (2018).
6. G. Kaya Gok and S. Buyukkose, *Graph Operations of Randić Index*, AIP Conference Proceedings 1926 (2018).
7. X. Li and I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Univ. Kragujevac (2006).
8. X. Li and Y. Shi, *A survey on the Randić index*, MATCH Commun. Math. Comput. Chem. 59, 127-156 (2008).
9. H. Liu, M. Lu and F. Tian, *On the Randić index*, Journal of Mathematical Chemistry 38 (3) (2005).
10. M. Randić, *On characterization of molecular branching*, J. Amer. Chem. Soc. 97, 6609-6615 (1975).
11. C. Vasudev, *Graph Theory With Applications*, New Delhi-India: New Age International Publishers 4-5, 21, 56-57 (2006).
12. D. B. Werst, *Introduction to Graph Theory*, Prentice-Hall, Upper Saddle River, NJ (1996).

Şerife Büyükköse,
Gazi University,
Faculty of Science,
Department of Mathematics,
Ankara 06500 Turkey.
E-mail address: `sbuyukkose@gazi.edu.tr`

and

Ismail Naci Cangul,
Bursa Uludag University,
Faculty of Arts and Science,
Department of Mathematics,
Bursa 16059 Turkey.
E-mail address: `cangul@uludag.edu.tr`