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RANDIĆ INDEX OF A GRAPH WITH SELF-LOOPS

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Abstract. Let $G(n,m)$ be a simple graph with vertex set V and $S \subseteq V$ with $|S| = \sigma$. The graph G_S is obtained by adding a self-loop to each vertex of the graph G in the set S. The Randić index of a graph is one of the important topological indices which has its application in chemistry. In this manuscript, the Randić index of a graph with self-loops is defined and are obtained some bounds for the same.

1. Introduction

Let $G_S(n, m+\sigma)$ be a graph obtained by attaching a self-loop to each vertices in the set $S \subseteq V(G)$ of a simple graph $G(n,m)$, where $|S| = \sigma$. Degree of a vertex in a graph G is the number of edges incident on a vertex. The notation $\deg_G(v)$ represents the degree of a vertex v in the graph G. A self-loop contributes 2 to the number of edges incident on a vertex. The Randić index is one of the most studied degree-based topological index in the literature which has various applications in chemistry and pharmacology. Randić index was introduced by M. Randić [1] in 1976 and it is defined as

$$R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{\deg_G(v_i)\deg_G(v_j)}}.$$

For more studies on Randić index, one can refer the papers [2–6]. All the results with regards to Randić index are obtained for a simple graphs. In this paper, the authors define Randić index of a graph with self-loops. Let G_S be a graph obtained by attaching a self-loop to each vertices in the set $S \subseteq V$ of vertices of the graph

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$G(V,E)$, where $|S| = \sigma$. The Randić index of G_S is defined as

$$
\begin{aligned}
R(G_S) &= \sum_{v_iv_j \in E(G_S)} \frac{1}{\sqrt{\deg_{G_S}(v_i)\deg_{G_S}(v_j)}} \\
&= \sum_{\substack{v_iv_j \in E(G) \\ \wedge\ v_i,v_j \in V-S}} \frac{1}{\sqrt{\deg_G(v_i)\deg_G(v_j)}} + \sum_{\substack{v_iv_j \in E(G) \\ \wedge\ v_i \in S, v_j \in V-S}} \frac{1}{\sqrt{(\deg_G(v_i)+2)\deg_{G_S}(v_j)}} \\
&\quad + \sum_{\substack{v_iv_j \in E(G) \\ \wedge\ v_i,v_j \in S}} \frac{1}{\sqrt{(\deg_G(v_i)+2)(\deg_G(v_j)+2)}} + \sum_{v_i \in S} \frac{1}{\deg_G(v_i)+2}.
\end{aligned}
$$

A graph is a tree if it is connected and acyclic. In a tree, the vertex with degree 1 is called a pendant vertex and the vertex with degree 2 or more is called an internal vertex. The notation $\langle S \rangle$ represents the graph induced by the vertices of the set S.

For all notations and terminology, the reader is directed to the references [7,8].

2. Main Results

The Randić index of a graph G_S may increase, decrease or equal to the Randić index of the graph G. For instance, consider a path graph P_4 with path $v_1v_2v_3v_4$. Let $S = \{v_1\}$. Then, $R((P_4)_S) = 1.9486$, which is more than $R(P_4) = 1.9142$. For the same graph P_4, if $S = \{v_2\}$, then $R((P_4)_S) = 1.8106$ which is less than Randić index of P_4. For the path graph $P_2 = \{v_1, v_2\}$ with $S = \{v_1, v_2\}$, $R(P_2) = R((P_2)_S) = 1$.

Theorem 2.1. *Let $G(V,E)$ be a r-regular graph and $S \subseteq V$ with $|S| = \sigma$. For the graph G_S, obtained by attaching a self-loops to each vertices of S,*

$$R(G_S) = \frac{m_S + \sigma}{r+2} + \frac{m_{V-S}}{r} + \frac{m - m_S - m_{V-S}}{\sqrt{r(r+2)}},$$

where $m = |E(G)|$, $m_S = |E(\langle S \rangle)|$ and $m_{V-S} = |E(\langle V - S \rangle)|$.

Proof. Let G_S be a graph obtained by attaching a self-loop to each vertex in the set $S \subseteq V$ of a r-regular graph $G(V,E)$. Consider,

$$
\begin{aligned}
R(G_S) = &\sum_{\substack{v_iv_j \in E(G) \\ \wedge\ v_i,v_j \in S}} \frac{1}{\sqrt{(r+2)^2}} + \sum_{\substack{v_iv_j \in E(G) \\ \wedge\ v_i \in S, v_j \notin S}} \frac{1}{\sqrt{r(r+2)}} + \sum_{\substack{v_iv_j \in E(G) \\ \wedge\ v_i,v_j \notin S}} \frac{1}{\sqrt{r^2}} \\
&+ \sum_{v_i \in S} \frac{1}{\sqrt{(r+2)^2}}.
\end{aligned}
$$

Let $|E| = m$, m_S be the number of edges of $\langle S \rangle$, and m_{V-S} be the number of edges of $\langle V - S \rangle$. Therefore,

$$R(G_S) = \frac{m_S + \sigma}{r+2} + \frac{m_{V-S}}{r} + \frac{m - m_S - m_{V-S}}{\sqrt{r(r+2)}}. \qquad \square$$

Theorem 2.2. *Let G be a r-regular graph of order n and size m and G_S be a graph obtained by attaching a self-loop to all the vertices of G. Then,*

$$R(G_S) = R(G) = \frac{n}{2}.$$

Proof. Let G_S be a graph obtained by attaching a self-loop to all the vertices of the graph G. Then,

$$R(G_S) = \frac{m+\sigma}{r+2}.$$

But $\sigma = n$ and $m = \frac{nr}{2}$ for r-regular graph. Therefore,

$$R(G_S) = \frac{nr+2n}{2(r+2)} = \frac{n}{2}.$$

Also,

$$R(G) = \frac{m}{r} = \frac{nr}{2r} = \frac{n}{2}.$$

Therefore, if $\sigma = n$,

$$R(G_S) = R(G) = \frac{n}{2}.$$ □

Theorem 2.3. *Let G_S be a graph obtained by attaching a self-loop to each vertices in the set $S \subseteq V$ of a graph $G(n,m)$. If $|S| = \sigma = n$, then*

$$\frac{m+n}{\Delta+2} \le R(G_S) \le \frac{m+n}{\delta+2}.$$

Upper and lower bound sharpness occur for the regular graph.

Proof. Let G be a graph and G_S be a graph obtained by attaching a self-loop to all the vertices of G. Then,

$$R(G_S) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{(\deg_G(v_i)+2)(\deg_G(v_j)+2)}} + \sum_{i=1}^{n} \frac{1}{\deg_G(v_i)+2}.$$

But,

$$\begin{aligned}\sqrt{(\deg_G(v_i)+2)(\deg_G(v_j)+2)} &= \sqrt{\deg_G(v_i)\deg_G(v_j) + 2(\deg_G(v_i)+\deg_G(v_j)) + 4} \\ &\le \sqrt{\Delta^2 + 4\Delta + 4} \\ &= \Delta + 2.\end{aligned}$$

This implies,

$$\frac{1}{\sqrt{(\deg_G(v_i)+2)(\deg_G(v_j)+2)}} \ge \frac{1}{\Delta+2}.$$

Also,

$$\frac{1}{\deg_G(v_i)+2} \ge \frac{1}{\Delta+2}.$$

Therefore,

$$R(G_S) \geq \frac{m}{\Delta+2} + \frac{n}{\Delta+2} \geq \frac{m+n}{\Delta+2}.$$

Similarly,

$$\frac{1}{\sqrt{(\deg_G(v_i)+2)(\deg_G(v_j)+2)}} \leq \frac{1}{\delta+2}$$

and

$$\frac{1}{\deg_G(v_i)+2} \leq \frac{1}{\delta+2}.$$

Therefore,

$$R(G_S) \leq \frac{m}{\delta+2} + \frac{n}{\delta+2} \leq \frac{m+n}{\delta+2}.$$

If G is a regular graph, then $\deg_G(v_i) = \Delta = \delta = r$, for each $i = 1, 2, \ldots, n$ and therefore,

$$R(G_S) = \frac{m+n}{r+2}.$$

□

Theorem 2.4. *Let T be a tree of order n having k-pendant vertices and T_S be a graph obtained by adding a self-loop to each pendant vertex. Then,*

$$\frac{n-1}{3} + \frac{n-1}{\sqrt{3(n-1)}} \leq R(T_S) \leq \frac{k}{3} + \frac{k}{\sqrt{6}} + \frac{n+k-1}{2}.$$

Lower bound sharpness occurs for a star graph and upper bound sharpness occurs for a path graph.

Proof. Let T_S be a graph obtained by adding a self-loop to all k-pendant vertices of a tree of order n. Now,

$$\begin{aligned} R(T_S) = & \sum_{\substack{v_iv_j \in E(T) \\ v_i, v_j \notin S}} \frac{1}{\sqrt{\deg_T(v_i)\deg_T(v_j)}} + \sum_{i=1}^{k} \frac{1}{\sqrt{\deg_T(v_i)(\deg_T(v_k)+2)}} \\ & + \sum_{i=1}^{k} \frac{1}{\sqrt{(\deg_T(v_k)+2)^2}} \\ \leq & \frac{n-k-1}{2} + \frac{k}{\sqrt{6}} + \frac{k}{3}. \end{aligned}$$

Equality holds for a path graph since each internal vertex of a path graph is of degree 2.

Now, for upper bound, $\deg_T(v_i) \leq n-1$ and therefore $\frac{1}{\sqrt{\deg_T(v_i)}} \geq \frac{1}{n-1}$. Consider,

$$
\begin{aligned}
R(T_S) = &\sum_{\substack{v_iv_j \in E(T) \\ v_i, v_j \notin S}} \frac{1}{\sqrt{\deg_T(v_i)\deg_T(v_j)}} + \sum_{i=1}^{k} \frac{1}{\sqrt{\deg_T(v_i)(\deg_T(v_k)+2)}} \\
&+ \sum_{i=1}^{k} \frac{1}{\sqrt{(\deg_T(v_k)+2)^2}} \\
\geq &\frac{n-1}{\sqrt{3(n-1)}} + \frac{n-1}{3}.
\end{aligned}
$$

Equality holds for a star graph since maximum degree of an internal vertex of a star graph is $n-1$. □

Theorem 2.5. *Let T be a tree of order n having k-pendant vertices and T_S be a graph obtained by adding a self-loop to each internal vertex. Then,*

$$
\frac{\sqrt{n+1}+(n-1)}{n+1} \leq R(T_S) \leq \frac{2n-1}{4}.
$$

Lower bound sharpness occurs for a star graph and upper bound sharpness occurs for a path graph.

Proof. Let T be a tree of order n having k-pendant vertices and T_S be a graph obtained by adding a self-loop to each internal vertex. Let v_k and v_i represent pendant vertex and internal vertex, respectively. Now, consider

$$
\begin{aligned}
R(T_S) = &\sum_{v_iv_j \in E(T)} \frac{1}{\sqrt{(\deg_T(v_i)+2)(\deg_T(v_j)+2)}} + \sum_{i=1}^{n-k} \frac{1}{\sqrt{(\deg_T(v_i)+2)\deg_T(v_k)}} \\
&+ \sum_{i=1}^{n-k} \frac{1}{\sqrt{(\deg_T(v_i)+2)^2}} \\
\leq &\frac{n-k-1}{4} + \frac{k}{2} + \frac{n-k}{4} \\
= &\frac{2n-1}{4}.
\end{aligned}
$$

Equality holds for a path graph since each internal vertex of a path graph is of degree 2.

For upper bound, $\deg_T(v_i) \leq n-1$ and therefore $\frac{1}{\sqrt{\deg_T(v_i)+2}} \geq \frac{1}{n+1}$. Consider

$$\begin{aligned}
R(T_S) = & \sum_{v_iv_j \in E(T)} \frac{1}{\sqrt{(\deg_T(v_i)+2)(\deg_T(v_j)+2)}} + \sum_{i=1}^{n-k} \frac{1}{\sqrt{(\deg_T(v_i)+2)\deg_T(v_k)}} \\
& + \sum_{i=1}^{n-k} \frac{1}{\sqrt{(\deg_T(v_i)+2)^2}} \\
\geq & \frac{1}{n+1} + \frac{n-1}{\sqrt{n+1}}.
\end{aligned}$$

Equality holds for a star graph since maximum degree of an internal vertex of a star graph is $n-1$. ☐

Theorem 2.6. *Let G be a bipartite graph with partition $V = \{V_1, V_2\}$ and G_S be a graph obtained by adding a self-loop to each vertex of S in G. Let $S_1, S_2 \subseteq S$ with $S_1 \cup S_2 = S$, $S_1 \cap V_2 = \emptyset$, $S_2 \cap V_1 = \emptyset$, $|S_1| = \sigma_1$ and $|S_2| = \sigma_2$. Then,*

$$\begin{aligned}
R(G_S) \geq & \frac{m\langle S_1 \cup S_2 \rangle}{\sqrt{(m+2)(n+2)}} + \frac{m\langle V - (S_1 \cup S_2) \rangle}{\sqrt{mn}} \\
& + \frac{m\langle S_1 \cup (V_2 - S_2) \rangle}{\sqrt{m(n+2)}} + \frac{m\langle S_2 \cup (V_1 - S_1) \rangle}{\sqrt{n(m+2)}} + \frac{\sigma_1}{n+2} + \frac{\sigma_2}{m+2}.
\end{aligned}$$

The bound sharpness occurs for the complete bipartite graph.

Proof. Let G_S be a graph obtained by adding a self-loop to each vertex in the set $S \subseteq V$ of a bipartite graph G with partition $V = \{V_1, V_2\}$. Also, let $S = S_1 \cup S_2$, with $S_1 \cap V_2 = S_2 \cap V_1 = \emptyset$. Then,

$$\begin{aligned}
R(G_S) = & \sum_{\substack{v_iv_j \in E(G) \,\wedge \\ v_i, v_j \notin S}} \frac{1}{\sqrt{\deg_G(v_i)\deg_G(v_j)}} \\
& + \sum_{\substack{v_iv_j \in E(G) \,\wedge \\ v_i, v_j \in S}} \frac{1}{\sqrt{(\deg_G(v_i)+2)(\deg_G(v_j)+2)}} \\
& + \sum_{\substack{v_iv_j \in E(G) \,\wedge \\ v_i \in S, v_j \notin S}} \frac{1}{\sqrt{(\deg_G(v_i)+2)\deg_G(v_j)}} \\
& + \sum_{\substack{v_iv_j \in E(G) \,\wedge \\ v_i \notin S, v_j \in S}} \frac{1}{\sqrt{\deg_G(v_i)(\deg_G(v_j)+2)}} \\
& + \sum_{v_i \in S_1} \frac{1}{\sqrt{(\deg_G(v_i)+2)^2}} + \sum_{v_j \in S_2} \frac{1}{\sqrt{(\deg_G(v_j)+2)^2}}.
\end{aligned}$$

But, $\deg_G(v_i)\deg_G(v_j) \leq mn$, $\deg_G(v_i) \leq n$ if $v_i \in S_1$ and $\deg_G(v_j) \leq m$ if $v_j \in S_2$. Therefore,

$$\begin{aligned}R(G_S) \geq & \frac{m\langle S_1 \cup S_2\rangle}{\sqrt{(m+2)(n+2)}} + \frac{m\langle V-(S_1 \cup S_2)\rangle}{\sqrt{mn}} \\ & + \frac{m\langle S_1 \cup (V_2 - S_2)\rangle}{\sqrt{m(n+2)}} + \frac{m\langle S_2 \cup (V_1 - S_1)\rangle}{\sqrt{n(m+2)}} + \frac{\sigma_1}{n+2} + \frac{\sigma_2}{m+2}.\end{aligned}$$

Equality holds for a complete bipartite graph since $\deg_G(v_i)\deg_G(v_j) = mn$, $\deg_G(v_i) = n$ if $v_i \in S_1$ and $\deg_G(v_j) = m$ if $v_j \in S_2$. ☐

Theorem 2.7. *Let $K_{m,n}$, $m \leq n$, be a complete bipartite graph with partition $V = \{V_1, V_2\}$, $(K_{m,n})_S{}'$ be a graph obtained by attaching a self-loop to each vertex of V_1 and $(K_{m,n})_S{}''$ be a graph obtained by attaching a self-loop to each vertex of V_2. Then,*

$$R(K_{m,n})_S{}' \leq R((K_{m,n})_S{}'').$$

Equality holds if and only if $m = n$.

Proof. Let $(K_{m,n})_S{}'$ be a graph obtained by attaching a self-loop to each vertex of V_1 and $(K_{m,n})_S{}''$ be a graph obtained by attaching a self-loop to each vertex of V_2 of a complete bipartite graph $K_{m,n}$, $m \leq n$, with partition $V = \{V_1, V_2\}$. Now, $R((K_{m,n})_S{}') = \frac{mn}{\sqrt{m(n+2)}} + \frac{m}{n+2}$ and $R((K_{m,n})_S{}'') = \frac{mn}{\sqrt{n(m+2)}} + \frac{n}{m+2}$. From this, one can easily observe that

$$R(K_{m,n})_S{}' \leq R((K_{m,n})_S{}'').$$

If $m = n$, then $m(n+2) = n(m+2)$, $m+2 = n+2$ and therefore $R((K_{m,n})_S{}'') = R((K_{m,n})_S{}')$. Conversely, if $m \neq n$, then $R((K_{m,n})_S{}'') \neq R((K_{m,n})_S{}')$ since $m(n+2) \neq n(m+2)$ and $m+2 \neq n+2$. ☐

3. Future Scope

(a) Characterize the class of graphs for which Randić index of a graph with self-loops is more than the Randić index of a simple graph and vice versa.
(b) Obtain the minimum and maximum Randić index for the class of graphs of given order.

4. Conclusion

The Randić index of a graph with self-loop is defined and bounds for Randić index of regular graph, tree and complete bipartite graph with self-loops are obtained.

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