

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

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

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

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

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 $v_1 v_2 v_3 v_4$. 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,

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

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,

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

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 $\sigma = n$,

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

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*

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

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,

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

But,

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

This implies,

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

Also,

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

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 $i = 1, 2, \dots, n$ and therefore,

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

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,

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

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,

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

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

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

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

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

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

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

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,*

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

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,

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

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 $v_j \in S_2$. $\square$

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 $m+2 \neq n+2$. $\square$

3. FUTURE SCOPE

- 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.
- 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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