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Maximum and Second Maximum of Randić Index in the Class of Tricyclic Graphs

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Abstract

Let G be a graph. The Randić index of G is defined as the summation of $\left(\sqrt{d_G(u)d_G(v)}\right)^{-1}$ over all edges uv of G, where $d_G(x)$ denotes the vertex degree of x in G. The aim of this paper is to compute the first and second maximum of Randić index in the class of all $n-$vertex tricyclic graphs.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The quantity $d_G(v)$ denotes the vertex degree of $v \in V(G)$. A vertex u in G is called pendant if $\deg(u) = 1$ and the set of all of neighbors of u is denoted by $N_G(u)$. Other notation and terminology not defined here will conform to those in [3].

Topological indices are numerical graph invariants applicable in chemistry. The Randić index [12], is one of the most important topological indices in chemical graph theory having a lot of applications in chemistry. Since the appearance of this graph invariant, too many researchers has been focused on the problems of computing upper and lower bounds for

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this index in some classes of graphs [5, 9, 10]. To define, we assume that G is a graph. Then the Randić index of G is defined as:

$$R(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}} .$$

An $n-$vertex graph G is called tree, unicyclic, bicyclic or tricyclic, if it has $n + c$ edges such that $c = -1, 0, 1, 2$, respectively. Du and Zhou [8], investigated the Randić index of trees, unicyclic and bicyclic graphs. In this paper we report a new class of $n-$vertex tricyclic graphs with maximum Randić index. This class is not appeared in the classification of tricyclic graphs with maximum Randić index given in [9]. We also compute the second maximum of Randić index in the class of all $n-$vertex tricyclic graph. For simplify our argument, we denote the class of all $n-$vertex tricyclic graphs by Tr_n.

In what follows, we present two important lemmas which are crucial in our main result.

Lemma 1. *[8, Corollary 3] Suppose G is an $n-$vertex graph. Then $R(G) \leq \frac{n}{2}$. Equality holds if and only if G is regular.*

Lemma 2. *[5] For a simple $n-$vertex graph G, we have:*

$$R(G) = \frac{n}{2} - \frac{1}{2} f(G) ,$$

where $f(G) = \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \right)^2$.

Suppose $g(x, y) = \frac{1}{\sqrt{xy}}$, where $x, y \geq 1$. For fixed y, the function $g(x, y)$ is decreasing for x, since if $y \geq 1$ then

$$\frac{\partial g(x, y)}{\partial x} = \frac{-y}{2(xy)^{\frac{3}{2}}} < 0 .$$

We encourage the interested readers to consult papers [1, 2] for relationship between Randić index and some important problems in graph theory and [6, 7, 11] for more information on Randić index. The reference [4] is refer for computational techniques and softwares on Randić index.

2 Maximum and Second Maximum of Randić Index in Tr_n

In this section the maximum and second maximum of Randić index for tricyclic graphs are presented. Our main goal is to present a missing class which attains maximum Randić index of tricyclic graphs. The type of an arbitrary edge that one of its end vertices has degree i and another has degree j is denoted by d_{ij}. The class of all tricyclic graphs containing five edges of type e_{33}, two edges of type e_{23} and $n-5$ edges of type e_{22} is denoted by Φ_3, see Figure 1.

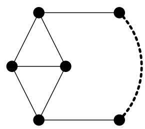


Figure 1: The Graph $G \in \Phi_3$.

Lemma 3. *If $G \in \Phi_3$ then*

$$R(G) = \frac{n}{2} + \frac{2\sqrt{6}-5}{6}.$$

We now introduce another class of tricyclic graphs. Suppose B_3 is the set of all tricyclic graphs with maximum degree 3, $|e_{23}| = |e_{33}| = 4$ and $|e_{22}| = n-6$, see Figure 2.

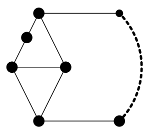


Figure 2: A Graph in the Class B_3.

Lemma 4. *Suppose $G \in B_3$. Then*

$$R(G) = \frac{n}{2} + \frac{2\sqrt{6}-5}{3} .$$

Lemma 5. *If $G \in B_3$ and $H \in \Phi_3$ are arbitrary then,*

$$R(G) < R(H) . \tag{2.1}$$

Proof. The proof follows from Lemmas 3 and 4. ■

We are now ready to prove that the graphs in classes Φ_3 and B_3 are having the maximum and second maximum Randić index, respectively. Notice that there is one tricyclic regular graph of order four, Figure 3.

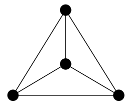
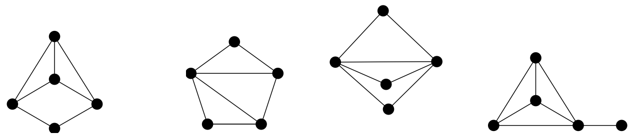


Figure 3: The Unique Regular Tricyclic Graph of Order 4.

Theorem 1. *Suppose* $G \in Tr_n \setminus (B_3 \cup \Phi_3)$, $n \geq 5$. *Then*

$$R(G) < \frac{n-6}{2} + \frac{4+2\sqrt{6}}{3} < \frac{n}{2} + \frac{2\sqrt{6}-5}{6} . \tag{2.2}$$

Proof. In Figure 4, all non-isomorphic tricyclic graphs of order 5 together with their Randić indices are depicted. So, it is enough to assume that $n \geq 6$. Two cases are considered as follows:



(a) 2.4826 (b) 2.4338 (c) 2.3713 (d) 2.3660

Figure 4: Non-Isomorphic Tricyclic Graphs of Order 5 and Their Randić Indices.

a) Tricyclic graphs containing at least one pendant vertex.

b) Tricyclic graphs without pendant vertex.

Case (a): Assume that G is a tricyclic graph containing at least one pendant vertex u adjacent to the vertex v of degree $r \geq 2$. Thus,

$$f(G) \geq (1 - \frac{1}{\sqrt{r}})^2 \geq \left(1 - \frac{1}{\sqrt{2}}\right)^2 = 2\left(\frac{3}{4} - \frac{\sqrt{2}}{2}\right) .$$

Apply Lemma 2 to deduce that,

$$\begin{aligned} R(G) &= \frac{n}{2} - \frac{1}{2}f(G) \leq \frac{n}{2} - \frac{3}{4} + \frac{\sqrt{2}}{2} \\ &\leq \frac{n}{2} - \frac{6}{2} + \frac{4}{\sqrt{6}} + \frac{4}{3} = \frac{n}{2} + \frac{2\sqrt{6}-5}{3} . \end{aligned}$$

Now the theorem follows from Lemma 5.

Case (b): Assume that G is a tricyclic graph without pendant vertex. We proceed by induction on n. From Figure 5, the result is clear for $n = 6$. Define $k(n) = \frac{n}{2} + \frac{2\sqrt{6}-5}{3}$. Suppose that the result is correct for each graph of order $< n$ and G is an $n-$vertex tricyclic graph without pendant vertex.

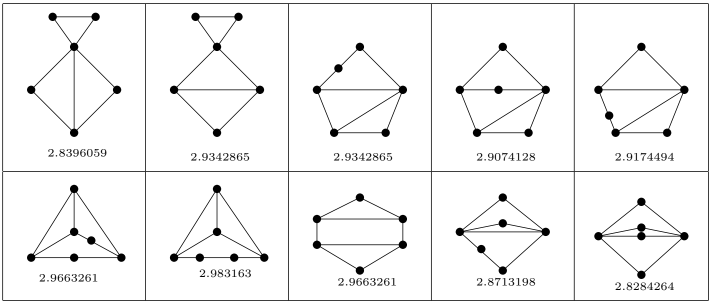


Figure 5: Non-Isomorphic Tricyclic Graphs of Order 6 Without Pendant Vertex.

If $\delta(G) \geq 3$ then $e = |E(G)| \geq 3n/2$. On the other hand, every $n-$vertex tricyclic graph has exactly $n + 2$ edges. So, $n + 2 \geq 3n/2$ which implies that $n = 4$, contradict by $n \geq 6$. This shows that there exists a vertex u of degree two adjacent to two vertices v and w of degrees $r, s \geq 2$, respectively. We have two sub-cases that $vw \notin E(G)$ and $vw \in E(G)$.

Sub-Case 1. $vw \notin E(G)$. Define $G' = G \setminus \{u\} + vw$. Then $d_{G'}(v) = d_G(v)$ and $d_{G'}(w) = d_G(w)$ and by induction hypothesis $R(G') < k(n-1)$. On the other hand,

$$\begin{aligned} R(G) - R(G') &= \frac{1}{\sqrt{2s}} + \frac{1}{\sqrt{2r}} - \frac{1}{\sqrt{rs}} \\ &= \frac{1}{\sqrt{r}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{s}}\right) + \frac{1}{\sqrt{2s}} \\ &\leq \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{s}}\right) + \frac{1}{\sqrt{2s}} = \frac{1}{2}\,. \end{aligned}$$

Therefore,

$$R(G) < R(G') + \frac{1}{2} = \frac{n}{2} + \frac{2\sqrt{6}-5}{3}\ .$$

Apply again Lemma 5 to deduce our result.

Sub-Case 2. $vw \in E(G)$. In this case, it is enough to consider tricyclic graphs in which neighbors of any vertex of degree two are adjacent to each other. Suppose u is a vertex of degree two adjacent to v and w, where $d(w) = s \geq 3$ and $d(v) = r \geq 2$. One can easily seen that the maximum degree of graph among all tricyclic graphs without pendant vertices is between three and six. Therefore, we have the following four cases:

1) $\Delta = 3$. Suppose $\deg(w) = 3$ and w is adjacent to the vertex y of degree three. We also consider the vertex z of degree two that is adjacent to vertices x_1 and x_2. Clearly, the degree of one of x_1 and x_2 is three, say x_2. By removing vertex w and linking vertex v to the vertex z and vertex u to y, we obtain a new graph $G' = G \setminus \{w\} + uy + vz$, which is a tricyclic graph with $n-1$ vertices. By induction hypothesis, $R(G') < k(n-1)$. On the other hand

$$R(G) - R(G') = \frac{1}{\sqrt{3}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{d(x_1)}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right) + \frac{1}{3} \leq \frac{1}{2}\,.$$

Therefore,

$$R(G) < \frac{n}{2} + \frac{2\sqrt{6}-5}{3}\,.$$

and by Lemma 5 the result holds.

2) $\Delta = 4$. Suppose u is a vertex adjacent to two vertices v and w with $d(w) = 4$ and $d(v) = 3$ in which $N_G(w) = \{u, v, x, y\}$ and $N_G(v) = \{u, w, x\}$. We consider vertex z of degree two adjacent to vertices y and y_1. Now, we delete vertex v and linking vertex u to z and also linking vertex x to the vertex y. We get a new tricyclic graph $G' = G \setminus \{v\} + uz + xy$ on $n-1$ vertices. So by induction hypothesis, $R(G') < k(n-1)$. But

$$\begin{aligned} R(G) - R(G') &= \frac{1}{\sqrt{d(y_1)}}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{d(y_1)}}\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right) \\ &+ \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{3d(x)}} - \frac{1}{\sqrt{6}} \leq \frac{1}{2}\,, \end{aligned}$$

which implies that

$$R(G) < \frac{n}{2} + \frac{2\sqrt{6}-5}{3}\,,$$

and the result holds by Lemma 5.

Notice that if $d(v) = 4$ and v is adjacent to vertex w then we can easily seen that other vertices have degree two. On the other hand, $n > 6$ implies that there are some vertices with degree two with non-adjacent neighbors, contradict by our assumption. Also, it is impossible that our tricyclic graph has two vertices of degree four. Therefore, only one vertex has degree four in which one of neighbors has at least degree three.

3) $\Delta = 5$**.** According to our hypothesis the vertex u is adjacent to vertices v and w, in which $d(w) = 5$. Let y be a vertex of degree three adjacent to w. Consider vertex z of degree two adjacent to vertices x, y. Now delete vertex v and connect u to z and x to y. This constructs a new $n-1$ vertices graph $G' = G \setminus \{v\} + uz + xy$. By induction hypothesis, $R(G') < k(n-1)$. But

$$R(G) - R(G') \leq \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3d(x)}} + \frac{1}{\sqrt{15}} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{5d(x)}} \leq \frac{1}{2} .$$

Therefore,

$$R(G) < \frac{n}{2} + \frac{2\sqrt{6}-5}{3} .$$

Hence the result holds by Lemma 5.

4) $\Delta = 6$**.** It is easy to see that there exists a unique 7−vertex graph depicted in Figure 6. If $n \geq 8$ then by a simple calculation and applying Lemma 5, the result can be proved.

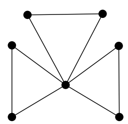


Figure 6: The Unique Tri_7 Graph.

This completes the proof. ■

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References

[1] P. Balister, B. Bollobás, S. Gerke, The generalised Randić index of trees, *J. Graph Theory* **56** (2007) 270–286.

[2] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Comb.* **50** (1998) 225–233.

[3] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan, London, 1976.

[4] G. Caporossi, P. Hansen, Variable neighborhood search for extremal graphs 1: The Autographix system, *Discr. Math.* **212** (2000) 29–44.

[5] G. Caporossi, I. Gutman, P. Hansen, L. Pavlović, Graphs with maximum connectivity index, *Comput. Biol. Chem.* **27** (2003) 85–90.

[6] T. Dehghan–Zadeh, H. Hua, A. R. Ashrafi, N. Habibi, Remarks on a conjecture about Randić index and graph radius, *Miskolc Math. Notes* **14** (2013) 845–850.

[7] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, *Discr. Math.* **257** (2002) 29–38.

[8] Z. Du, B. Zhou, On Randić indices of trees, unicyclic graphs, and bicyclic graphs, *Int. J. Quantum Chem.* **111** (2011) 2760–2770.

[9] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.

[10] X. Li, I. Gutman, *Mathematical Aspects of Randić–Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.

[11] B. Liu, I. Gutman, On a conjecture in Randić indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 143–154.

[12] M. Randić, Characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.